# Package: nlme (via r-universe)

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```
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Contact see 'MailingList'
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     mixed-effects models.
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NeedsCompilation yes
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ACF

Autocorrelation Function

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: gls and lme.

# Usage

```
ACF(object, maxLag, ...)
```

# **Arguments**

object	any object from which an autocorrelation function can be obtained. Generally an object resulting from a model fit, from which residuals can be extracted.
maxLag	maximum lag for which the autocorrelation should be calculated.
	some methods for this generic require additional arguments.

### Value

will depend on the method function used; see the appropriate documentation.

# Author(s)

José Pinheiro and Douglas Bates <Bates@stat.wisc.edu>

#### References

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

# See Also

```
ACF.gls, ACF.lme, plot.ACF
```

# **Examples**

## see the method function documentation

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ACF.gls

Autocorrelation Function for gls Residuals

### **Description**

This method function calculates the empirical autocorrelation function for the residuals from a gls fit. If a grouping variable is specified in form, the autocorrelation values are calculated using pairs of residuals within the same group; otherwise all possible residual pairs are used. The autocorrelation function is useful for investigating serial correlation models for equally spaced data.

# Usage

```
## S3 method for class 'gls'
ACF(object, maxLag, resType, form, na.action, ...)
```

# **Arguments**

object	an object inheriting from class "gls", representing a generalized least squares fitted model.
maxLag	an optional integer giving the maximum lag for which the autocorrelation should be calculated. Defaults to maximum lag in the residuals.
resType	an optional character string specifying the type of residuals to be used. If "response", the "raw" residuals (observed - fitted) are used; else, if "pearson", the standardized residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals pre-multiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the first character needs to be provided. Defaults to "pearson".
form	an optional one sided formula of the form $^{\sim}$ t, or $^{\sim}$ t   g, specifying a time covariate t and, optionally, a grouping factor g. The time covariate must be integer valued. When a grouping factor is present in form, the autocorrelations are calculated using residual pairs within the same group. Defaults to $^{\sim}$ 1, which corresponds to using the order of the observations in the data as a covariate, and no groups.
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes ACF.gls to print an error message and terminate if there are any incomplete observations.
	some methods for this generic require additional arguments.

#### Value

a data frame with columns lag and ACF representing, respectively, the lag between residuals within a pair and the corresponding empirical autocorrelation. The returned value inherits from class ACF.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

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### References

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

### See Also

```
ACF.lme, plot.ACF
```

# **Examples**

ACF.lme

Autocorrelation Function for lme Residuals

### **Description**

This method function calculates the empirical autocorrelation function for the within-group residuals from an 1me fit. The autocorrelation values are calculated using pairs of residuals within the innermost group level. The autocorrelation function is useful for investigating serial correlation models for equally spaced data.

# Usage

```
## S3 method for class 'lme'
ACF(object, maxLag, resType, ...)
```

### **Arguments**

object an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

maxLag an optional integer giving the maximum lag for which the autocorrelation should

be calculated. Defaults to maximum lag in the within-group residuals.

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resType

an optional character string specifying the type of residuals to be used. If "response", the "raw" residuals (observed - fitted) are used; else, if "pearson", the standardized residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals pre-multiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the first character needs to be provided. Defaults to "pearson".

... some methods for this generic require additional arguments – not used.

### Value

a data frame with columns lag and ACF representing, respectively, the lag between residuals within a pair and the corresponding empirical autocorrelation. The returned value inherits from class ACF.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

### See Also

```
ACF.gls, plot.ACF
```

### **Examples**

Alfalfa

Split-Plot Experiment on Varieties of Alfalfa

# Description

The Alfalfa data frame has 72 rows and 4 columns.

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#### **Format**

This data frame contains the following columns:

Variety a factor with levels Cossack, Ladak, and Ranger

**Date** a factor with levels None S1 S20 07 **Block** a factor with levels 1 2 3 4 5 6

Yield a numeric vector

#### **Details**

These data are described in Snedecor and Cochran (1980) as an example of a split-plot design. The treatment structure used in the experiment was a 3x4 full factorial, with three varieties of alfalfa and four dates of third cutting in 1943. The experimental units were arranged into six blocks, each subdivided into four plots. The varieties of alfalfa (*Cossac*, *Ladak*, and *Ranger*) were assigned randomly to the blocks and the dates of third cutting (*None*, SI—September 1, S20—September 20, and O7—October 7) were randomly assigned to the plots. All four dates were used on each block.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.1)

Snedecor, G. W. and Cochran, W. G. (1980), *Statistical Methods (7th ed)*, Iowa State University Press, Ames, IA

allCoef

Extract Coefficients from a Set of Objects

### **Description**

The extractor function is applied to each object in ..., with the result being converted to a vector. A map attribute is included to indicate which pieces of the returned vector correspond to the original objects in dots.

#### **Usage**

```
allCoef(..., extract)
```

### Arguments

... objects to which extract will be applied. Generally these will be model components, such as corStruct and varFunc objects.

extract an optional extractor function. Defaults to coef.

### Value

a vector with all elements, generally coefficients, obtained by applying extract to the objects in ....

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#### Author(s)

José' Pinheiro and Douglas Bates

#### See Also

lmeStruct,nlmeStruct

### **Examples**

```
cs1 <- corAR1(0.1)
vf1 <- varPower(0.5)
allCoef(cs1, vf1)</pre>
```

anova.gls

Compare Likelihoods of Fitted Objects

### Description

When only one fitted model object is present, a data frame with the numerator degrees of freedom, F-values, and P-values for Wald tests for the terms in the model (when Terms and L are NULL), a combination of model terms (when Terms in not NULL), or linear combinations of the model coefficients (when L is not NULL). Otherwise, when multiple fitted objects are being compared, a data frame with the degrees of freedom, the (restricted) log-likelihood, the Akaike Information Criterion (AIC), and the Bayesian Information Criterion (BIC) of each object is returned. If test=TRUE, whenever two consecutive objects have different number of degrees of freedom, a likelihood ratio statistic with the associated p-value is included in the returned data frame.

### Usage

```
## S3 method for class 'gls'
anova(object, ..., test, type, adjustSigma, Terms, L, verbose)
```

### Arguments

obje	ect	an object inheriting from class "gls", representing a generalized least squares fit.
		other optional fitted model objects inheriting from classes "gls", "gnls", "lm", "lme", "lmList", "nlme", "nlsList", or "nls".
test	:	an optional logical value controlling whether likelihood ratio tests should be used to compare the fitted models represented by object and the objects in Defaults to TRUE.
type	2	an optional character string specifying the type of sum of squares to be used in F-tests for the terms in the model. If "sequential", the sequential sum of squares obtained by including the terms in the order they appear in the model is used; else, if "marginal", the marginal sum of squares obtained by deleting a term from the model at a time is used. This argument is only used when a single

fitted object is passed to the function. Partial matching of arguments is used, so only the first character needs to be provided. Defaults to "sequential".

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adjustSigma

an optional logical value. If TRUE and the estimation method used to obtain object was maximum likelihood, the residual standard error is multiplied by  $\sqrt{n_{obs}/(n_{obs}-n_{par})}$ , converting it to a REML-like estimate. This argument is only used when a single fitted object is passed to the function. Default is TRUE.

Terms

an optional integer or character vector specifying which terms in the model should be jointly tested to be zero using a Wald F-test. If given as a character vector, its elements must correspond to term names; else, if given as an integer vector, its elements must correspond to the order in which terms are included in the model. This argument is only used when a single fitted object is passed to the function. Default is NULL.

L

an optional numeric vector or array specifying linear combinations of the coefficients in the model that should be tested to be zero. If given as an array, its rows define the linear combinations to be tested. If names are assigned to the vector elements (array columns), they must correspond to coefficients names and will be used to map the linear combination(s) to the coefficients; else, if no names are available, the vector elements (array columns) are assumed in the same order as the coefficients appear in the model. This argument is only used when a single fitted object is passed to the function. Default is NULL.

verbose

an optional logical value. If TRUE, the calling sequences for each fitted model object are printed with the rest of the output, being omitted if verbose = FALSE. Defaults to FALSE.

#### Value

a data frame inheriting from class "anova.lme".

### Note

Likelihood comparisons are not meaningful for objects fit using restricted maximum likelihood and with different fixed effects.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

#### See Also

```
gls, gnls, nlme, lme, logLik.gls, AIC, BIC, print.anova.lme
```

# **Examples**

anova.lme

```
anova(fm1)
# variance changes with a power of the absolute fitted values?
fm2 <- update(fm1, weights = varPower())</pre>
anova(fm1, fm2)
# Pinheiro and Bates, p. 251-252
fm1Orth.gls <- gls(distance ~ Sex * I(age - 11), Orthodont,</pre>
                correlation = corSymm(form = ~ 1 | Subject),
                weights = varIdent(form = ~ 1 | age))
fm2Orth.gls <- update(fm1Orth.gls,</pre>
                corr = corCompSymm(form = ~ 1 | Subject))
anova(fm10rth.gls, fm20rth.gls)
# Pinheiro and Bates, pp. 215-215, 255-260
#p. 215
fm1Dial.lme <-
 lme(rate ~(pressure + I(pressure^2) + I(pressure^3) + I(pressure^4))*QB,
      Dialyzer, ~ pressure + I(pressure^2))
# p. 216
fm2Dial.lme <- update(fm1Dial.lme,</pre>
                  weights = varPower(form = ~ pressure))
# p. 255
fm1Dial.gls <- gls(rate ~ (pressure +
     I(pressure^2) + I(pressure^3) + I(pressure^4))*QB,
        Dialyzer)
fm2Dial.gls <- update(fm1Dial.gls,</pre>
                 weights = varPower(form = ~ pressure))
anova(fm1Dial.gls, fm2Dial.gls)
fm3Dial.gls <- update(fm2Dial.gls,</pre>
                    corr = corAR1(0.771, form = ~1 | Subject))
anova(fm2Dial.gls, fm3Dial.gls)
# anova.gls to compare a gls and an lme fit
anova(fm3Dial.gls, fm2Dial.lme, test = FALSE)
# Pinheiro and Bates, pp. 261-266
fm1Wheat2 <- gls(yield ~ variety - 1, Wheat2)</pre>
fm3Wheat2 <- update(fm1Wheat2,</pre>
      corr = corRatio(c(12.5, 0.2),
        form = ~ latitude + longitude, nugget = TRUE))
# Test a specific contrast
anova(fm3Wheat2, L = c(-1, 0, 1))
```

anova.lme

Compare Likelihoods of Fitted Objects

#### **Description**

When only one fitted model object is present, a data frame with the numerator degrees of freedom, denominator degrees of freedom, F-values, and P-values for Wald tests for the terms in the model

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(when Terms and L are NULL), a combination of model terms (when Terms in not NULL), or linear combinations of the model coefficients (when L is not NULL). Otherwise, when multiple fitted objects are being compared, a data frame with the degrees of freedom, the (restricted) log-likelihood, the Akaike Information Criterion (AIC), and the Bayesian Information Criterion (BIC) of each object is returned. If test=TRUE, whenever two consecutive objects have different number of degrees of freedom, a likelihood ratio statistic with the associated p-value is included in the returned data frame.

# Usage

```
## S3 method for class 'lme'
anova(object, ..., test, type, adjustSigma, Terms, L, verbose)
## S3 method for class 'anova.lme'
print(x, verbose, ...)
```

### **Arguments**

L

object an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

... other optional fitted model objects inheriting from classes "gls", "gnls", "lm",

"lme", "lmList", "nlme", "nlsList", or "nls".

test an optional logical value controlling whether likelihood ratio tests should be

used to compare the fitted models represented by object and the objects in  $\dots$ 

Defaults to TRUE.

type an optional character string specifying the type of sum of squares to be used

in F-tests for the terms in the model. If "sequential", the sequential sum of squares obtained by including the terms in the order they appear in the model is used; else, if "marginal", the marginal sum of squares obtained by deleting a term from the model at a time is used. This argument is only used when a single fitted object is passed to the function. Partial matching of arguments is used, so

only the first character needs to be provided. Defaults to "sequential".

 $\hbox{adjustSigma} \qquad \hbox{an optional logical value. If TRUE and the estimation method used to obtain} \\$ 

object was maximum likelihood, the residual standard error is multiplied by  $\sqrt{n_{obs}/(n_{obs}-n_{par})}$ , converting it to a REML-like estimate. This argument is

only used when a single fitted object is passed to the function. Default is TRUE.

Terms an optional integer or character vector specifying which terms in the model should be jointly tested to be zero using a Wald F-test. If given as a character

vector, its elements must correspond to term names; else, if given as an integer vector, its elements must correspond to the order in which terms are included in the model. This argument is only used when a single fitted object is passed to

the function. Default is NULL.

cients in the model that should be tested to be zero. If given as an array, its rows define the linear combinations to be tested. If names are assigned to the vector

elements (array columns), they must correspond to coefficients names and will be used to map the linear combination(s) to the coefficients; else, if no names are

an optional numeric vector or array specifying linear combinations of the coeffi-

available, the vector elements (array columns) are assumed in the same order as

anova.lme

the coefficients appear in the model. This argument is only used when a single fitted object is passed to the function. Default is NULL.

x an object inheriting from class "anova.lme"

verbose an optional logical value. If TRUE, the calling sequences for each fitted model

object are printed with the rest of the output, being omitted if verbose = FALSE.

Defaults to FALSE.

#### Value

a data frame inheriting from class "anova.lme".

#### Note

Likelihood comparisons are not meaningful for objects fit using restricted maximum likelihood and with different fixed effects.

### Author(s)

José Pinheiro and Douglas Bates <bate=@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
gls, gnls, nlme, lme, AIC, BIC, print.anova.lme, logLik.lme,
```

### **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)</pre>
anova(fm1)
fm2 <- update(fm1, random = pdDiag(~age))</pre>
anova(fm1, fm2)
## Pinheiro and Bates, pp. 251-254 ------
fm10rth.gls <- gls(distance ~ Sex * I(age - 11), Orthodont,
    correlation = corSymm(form = ~ 1 | Subject),
     weights = varIdent(form = ~ 1 | age))
fm2Orth.gls <- update(fm1Orth.gls,</pre>
       corr = corCompSymm(form = ~ 1 | Subject))
## anova.gls examples:
anova(fm10rth.gls, fm20rth.gls)
fm3Orth.gls <- update(fm2Orth.gls, weights = NULL)</pre>
anova(fm2Orth.gls, fm3Orth.gls)
fm4Orth.gls <- update(fm3Orth.gls, weights = varIdent(form = ~ 1 | Sex))</pre>
anova(fm30rth.gls, fm40rth.gls)
# not in book but needed for the following command
fm3Orth.lme <- lme(distance ~ Sex*I(age-11), data = Orthodont,</pre>
                   random = \sim I(age-11) | Subject,
                   weights = varIdent(form = ~ 1 | Sex))
```

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```
# Compare an "lme" object with a "gls" object (test would be non-sensical!)
anova(fm30rth.lme, fm40rth.gls, test = FALSE)
## Pinheiro and Bates, pp. 222-225 ------
op <- options(contrasts = c("contr.treatment", "contr.poly"))</pre>
fm1BW.lme <- lme(weight ~ Time * Diet, BodyWeight, random = ~ Time)</pre>
fm2BW.lme <- update(fm1BW.lme, weights = varPower())</pre>
# Test a specific contrast
anova(fm2BW.lme, L = c("Time:Diet2" = 1, "Time:Diet3" = -1))
## Pinheiro and Bates, pp. 352-365 ------
fm1Theo.lis <- nlsList(</pre>
     conc ~ SSfol(Dose, Time, 1Ke, 1Ka, 1Cl), data=Theoph)
fm1Theo.lis
fm1Theo.nlme <- nlme(fm1Theo.lis)</pre>
fm2Theo.nlme <- update(fm1Theo.nlme, random= pdDiag(lKe+lKa+lCl~1) )</pre>
fm3Theo.nlme <- update(fm2Theo.nlme, random= pdDiag(</pre>
                                                       lKa+lCl~1) )
# Comparing the 3 nlme models
anova(fm1Theo.nlme, fm3Theo.nlme, fm2Theo.nlme)
options(op) # (set back to previous state)
```

### **Description**

This method function extracts the correlation matrix, or list of correlation matrices, associated with object.

### Usage

```
## S3 method for class 'corStruct'
as.matrix(x, ...)
```

#### **Arguments**

x an object inheriting from class "corStruct", representing a correlation structure.

further arguments passed from other methods.

# Value

If the correlation structure includes a grouping factor, the returned value will be a list with components given by the correlation matrices for each group. Otherwise, the returned value will be a matrix representing the correlation structure associated with object.

as.matrix.pdMat

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

### See Also

```
corClasses, corMatrix
```

### **Examples**

```
cst1 <- corAR1(form = ~1|Subject)
cst1 <- Initialize(cst1, data = Orthodont)
as.matrix(cst1)</pre>
```

as.matrix.pdMat

Matrix of a pdMat Object

# **Description**

This method function extracts the positive-definite matrix represented by x.

### Usage

```
## S3 method for class 'pdMat'
as.matrix(x, ...)
```

### **Arguments**

x an object inheriting from class "pdMat", representing a positive-definite matrix.

... further arguments passed from other methods.

#### Value

a matrix corresponding to the positive-definite matrix represented by x.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

20 as.matrix.reStruct

### See Also

```
pdMat, corMatrix
```

### **Examples**

```
as.matrix(pdSymm(diag(4)))
```

as.matrix.reStruct

Matrices of an reStruct Object

# **Description**

This method function extracts the positive-definite matrices corresponding to the pdMat elements of object.

### Usage

```
## S3 method for class 'reStruct'
as.matrix(x, ...)
```

### **Arguments**

x an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.

... further arguments passed from other methods.

# Value

a list with components given by the positive-definite matrices corresponding to the elements of object.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

# See Also

```
as.matrix.pdMat, reStruct, pdMat
```

# **Examples**

```
rs1 <- reStruct(pdSymm(diag(3), ~age+Sex, data = Orthodont))
as.matrix(rs1)</pre>
```

asOneFormula 21

asOneFormula

Combine Formulas of a Set of Objects

### **Description**

The names of all variables used in the formulas extracted from the objects defined in . . . are converted into a single linear formula, with the variables names separated by +.

# Usage

```
asOneFormula(..., omit)
```

# Arguments

... objects, or lists of objects, from which a formula can be extracted.

omit an optional character vector with the names of variables to be omitted from the

returned formula. Defaults to c(".", "pi").

### Value

a one-sided linear formula with all variables named in the formulas extracted from the objects in  $\dots$ , except the ones listed in omit.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
formula, all.vars
```

# **Examples**

```
asOneFormula(y \sim x + z \mid g, list(\sim w, \sim t * sin(2 * pi)))
```

Assay

Bioassay on Cell Culture Plate

# **Description**

The Assay data frame has 60 rows and 4 columns.

22 as Table

#### **Format**

This data frame contains the following columns:

**Block** an ordered factor with levels 2 < 1 identifying the block where the wells are measured.

sample a factor with levels a to f identifying the sample corresponding to the well.

**dilut** a factor with levels 1 to 5 indicating the dilution applied to the well

logDens a numeric vector of the log-optical density

### **Details**

These data, courtesy of Rich Wolfe and David Lansky from Searle, Inc., come from a bioassay run on a 96-well cell culture plate. The assay is performed using a split-block design. The 8 rows on the plate are labeled A–H from top to bottom and the 12 columns on the plate are labeled 1–12 from left to right. Only the central 60 wells of the plate are used for the bioassay (the intersection of rows B–G and columns 2–11). There are two blocks in the design: Block 1 contains columns 2–6 and Block 2 contains columns 7–11. Within each block, six samples are assigned randomly to rows and five (serial) dilutions are assigned randomly to columns. The response variable is the logarithm of the optical density. The cells are treated with a compound that they metabolize to produce the stain. Only live cells can make the stain, so the optical density is a measure of the number of cells that are alive and healthy.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.2)

asTable

Convert groupedData to a matrix

#### Description

Create a tabular representation of the response in a balanced groupedData object.

#### Usage

asTable(object)

### **Arguments**

object

A balanced groupedData object

### **Details**

A balanced groupedData object can be represented as a matrix or table of response values corresponding to the values of a primary covariate for each level of a grouping factor. This function creates such a matrix representation of the data in object.

augPred 23

#### Value

A matrix. The data in the matrix are the values of the response. The columns correspond to the distinct values of the primary covariate and are labelled as such. The rows correspond to the distinct levels of the grouping factor and are labelled as such.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York

### See Also

groupedData, isBalanced, balancedGrouped

### **Examples**

```
asTable(Orthodont)
# Pinheiro and Bates, p. 109
ergoStool.mat <- asTable(ergoStool)</pre>
```

augPred

Augmented Predictions

# Description

Predicted values are obtained at the specified values of primary. If object has a grouping structure (i.e. getGroups(object) is not NULL), predicted values are obtained for each group. If level has more than one element, predictions are obtained for each level of the max(level) grouping factor. If other covariates besides primary are used in the prediction model, their average (numeric covariates) or most frequent value (categorical covariates) are used to obtain the predicted values. The original observations are also included in the returned object.

### Usage

24 augPred

### **Arguments**

object	a fitted model object from which predictions can be extracted, using a predict
	method.

primary an optional one-sided formula specifying the primary covariate to be used to

generate the augmented predictions. By default, if a covariate can be extracted from the data used to generate object (using getCovariate), it will be used as

primary.

minimum an optional lower limit for the primary covariate. Defaults to min(primary).

maximum an optional upper limit for the primary covariate. Defaults to max(primary).

length.out an optional integer with the number of primary covariate values at which to

evaluate the predictions. Defaults to 51.

level an optional integer vector specifying the desired prediction levels. Levels in-

crease from outermost to innermost grouping, with level 0 representing the pop-

ulation (fixed effects) predictions. Defaults to the innermost level.

... some methods for the generic may require additional arguments.

#### Value

a data frame with four columns representing, respectively, the values of the primary covariate, the groups (if object does not have a grouping structure, all elements will be 1), the predicted or observed values, and the type of value in the third column: original for the observed values and predicted (single or no grouping factor) or predict.groupVar (multiple levels of grouping), with groupVar replaced by the actual grouping variable name (fixed is used for population predictions). The returned object inherits from class "augPred".

#### Note

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: gls, lme, and lmList.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

#### See Also

```
plot.augPred, getGroups, predict
```

### **Examples**

```
fm1 <- lme(Orthodont, random = \sim1)
augPred(fm1, length.out = 2, level = c(0,1))
```

balancedGrouped 25

balancedGrouped Create a groupedData object from a matrix
---

# Description

Create a groupedData object from a data matrix. This function can be used only with balanced data. The opposite conversion, from a groupedData object to a matrix, is done with asTable.

# Usage

balancedGrouped(form, data, labels=NULL, units=NULL)

# Arguments

form	A formula of the form $y \sim x \mid g$ giving the name of the response, the primary covariate, and the grouping factor.
data	A matrix or data frame containing the values of the response grouped according to the levels of the grouping factor (rows) and the distinct levels of the primary covariate (columns). The dimnames of the matrix are used to construct the levels of the grouping factor and the primary covariate.
labels	an optional list of character strings giving labels for the response and the primary covariate. The label for the primary covariate is named x and that for the response is named y. Either label can be omitted.
units	an optional list of character strings giving the units for the response and the primary covariate. The units string for the primary covariate is named x and that for the response is named y. Either units string can be omitted.

# Value

A balanced groupedData object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

#### See Also

groupedData, isBalanced, asTable

26 bdf

### **Examples**

bdf

Language scores

# **Description**

The bdf data frame has 2287 rows and 25 columns of language scores from grade 8 pupils in elementary schools in The Netherlands.

### Usage

```
data(bdf)
```

### **Format**

```
schoolNR a factor denoting the school.
```

pupilNR a factor denoting the pupil.

**IQ.verb** a numeric vector of verbal IQ scores

IQ.perf a numeric vector of IQ scores.

sex Sex of the student.

Minority a factor indicating if the student is a member of a minority group.

repeatgr an ordered factor indicating if one or more grades have been repeated.

aritPRET a numeric vector

classNR a numeric vector

aritPOST a numeric vector

langPRET a numeric vector

langPOST a numeric vector

ses a numeric vector of socioeconomic status indicators.

**denomina** a factor indicating of the school is a public school, a Protestant private school, a Catholic private school, or a non-denominational private school.

schoolSES a numeric vector

BodyWeight 27

```
satiprin a numeric vector
natitest a factor with levels 0 and 1
meetings a numeric vector
currmeet a numeric vector
mixedgra a factor indicating if the class is a mixed-grade class.
percmino a numeric vector
aritdiff a numeric vector
homework a numeric vector
classsiz a numeric vector
groupsiz a numeric vector
```

#### **Source**

```
'http://stat.gamma.rug.nl/snijders/multilevel.htm', the first edition of http://www.stats.ox.ac.uk/~snijders/mlbook.htm.
```

#### References

Snijders, Tom and Bosker, Roel (1999), Multilevel Analysis: An Introduction to Basic and Advanced Multilevel Modeling, Sage.

### **Examples**

```
summary(bdf)
## More examples, including lme() fits reproducing parts in the above
## book, are available in the R script files
system.file("mlbook", "ch04.R", package ="nlme") # and
system.file("mlbook", "ch05.R", package ="nlme")
```

BodyWeight

Rat weight over time for different diets

# **Description**

The BodyWeight data frame has 176 rows and 4 columns.

### **Format**

This data frame contains the following columns:

weight a numeric vector giving the body weight of the rat (grams).

Time a numeric vector giving the time at which the measurement is made (days).

**Rat** an ordered factor with levels 2 < 3 < 4 < 1 < 8 < 5 < 6 < 7 < 11 < 9 < 10 < 12 < 13 < 15 < 14 < 16 identifying the rat whose weight is measured.

**Diet** a factor with levels 1 to 3 indicating the diet that the rat receives.

28 Cefamandole

#### **Details**

Hand and Crowder (1996) describe data on the body weights of rats measured over 64 days. These data also appear in Table 2.4 of Crowder and Hand (1990). The body weights of the rats (in grams) are measured on day 1 and every seven days thereafter until day 64, with an extra measurement on day 44. The experiment started several weeks before "day 1." There are three groups of rats, each on a different diet.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.3)

Crowder, M. and Hand, D. (1990), Analysis of Repeated Measures, Chapman and Hall, London.

Hand, D. and Crowder, M. (1996), *Practical Longitudinal Data Analysis*, Chapman and Hall, London.

Cefamandole

Pharmacokinetics of Cefamandole

### **Description**

The Cefamandole data frame has 84 rows and 3 columns.

#### **Format**

This data frame contains the following columns:

Subject a factor giving the subject from which the sample was drawn.

**Time** a numeric vector giving the time at which the sample was drawn (minutes post-injection).

**conc** a numeric vector giving the observed plasma concentration of cefamandole (mcg/ml).

#### **Details**

Davidian and Giltinan (1995, 1.1, p. 2) describe data obtained during a pilot study to investigate the pharmacokinetics of the drug cefamandole. Plasma concentrations of the drug were measured on six healthy volunteers at 14 time points following an intraveneous dose of 15 mg/kg body weight of cefamandole.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.4)

Davidian, M. and Giltinan, D. M. (1995), *Nonlinear Models for Repeated Measurement Data*, Chapman and Hall, London.

Coef 29

### **Examples**

```
plot(Cefamandole)
fm1 <- nlsList(SSbiexp, data = Cefamandole)
summary(fm1)</pre>
```

Coef

Assign Values to Coefficients

# Description

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include all "pdMat", "corStruct" and "varFunc" classes, "reStruct", and "modelStruct".

```
coefficients<- is an alias for coef<-.
```

# Usage

```
coef(object, ...) <- value
coefficients(object, ...) <- value</pre>
```

### **Arguments**

any object representing a fitted model, or, by default, any object with a coef component.
 some methods for this generic function may require additional arguments.
 a value to be assigned to the coefficients associated with object.

#### Value

will depend on the method function; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

coef

30 coef.corStruct

coef.corStruct

Coefficients of a corStruct Object

### **Description**

This method function extracts the coefficients associated with the correlation structure represented by object.

### Usage

```
## $3 method for class 'corStruct'
coef(object, unconstrained, ...)
## $3 replacement method for class 'corStruct'
coef(object, ...) <- value</pre>
```

### **Arguments**

object an object inheriting from class "corStruct", representing a correlation struc-

ture.

unconstrained a logical value. If TRUE the coefficients are returned in unconstrained form (the

same used in the optimization algorithm). If FALSE the coefficients are returned

in "natural", possibly constrained, form. Defaults to TRUE.

value a vector with the replacement values for the coefficients associated with object.

It must be a vector with the same length of coef{object} and must be given in

unconstrained form.

... some methods for this generic require additional arguments. None are used in

this method.

### Value

a vector with the coefficients corresponding to object.

# SIDE EFFECTS

On the left side of an assignment, sets the values of the coefficients of object to value. Object must be initialized (using Initialize) before new values can be assigned to its coefficients.

### Author(s)

José Pinheiro and Douglas Bates

### References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

coef.gnls 31

# See Also

```
corAR1, corARMA, corCAR1, corCompSymm, corExp, corGaus, corLin, corRatio, corSpatial, corSpher, corSymm,Initialize
```

### **Examples**

```
cst1 <- corARMA(p = 1, q = 1)
coef(cst1)</pre>
```

coef.gnls

Extract gnls Coefficients

# **Description**

The estimated coefficients for the nonlinear model represented by object are extracted.

# Usage

```
## S3 method for class 'gnls'
coef(object, ...)
```

# Arguments

object an object inheriting from class "gnls", representing a generalized nonlinear

least squares fitted model.

... some methods for this generic require additional arguments. None are used in

this method.

# Value

a vector with the estimated coefficients for the nonlinear model represented by object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

gnls

# **Examples**

32 coef.lme

coef.lme

Extract lme Coefficients

# Description

The estimated coefficients at level i are obtained by adding together the fixed effects estimates and the corresponding random effects estimates at grouping levels less or equal to i. The resulting estimates are returned as a data frame, with rows corresponding to groups and columns to coefficients. Optionally, the returned data frame may be augmented with covariates summarized over groups.

### Usage

#### Arguments

object an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

augFrame an optional logical value. If TRUE, the returned data frame is augmented with

variables defined in data; else, if FALSE, only the coefficients are returned. De-

faults to FALSE.

level an optional positive integer giving the level of grouping to be used in extracting

the coefficients from an object with multiple nested grouping levels. Defaults to

the highest or innermost level of grouping.

data an optional data frame with the variables to be used for augmenting the returned

data frame when augFrame = TRUE. Defaults to the data frame used to fit object.

which an optional positive integer or character vector specifying which columns of

data should be used in the augmentation of the returned data frame. Defaults to

all columns in data.

FUN an optional summary function or a list of summary functions to be applied to group-varying variables, when collapsing data by groups. Group-invariant vari-

ables are always summarized by the unique value that they assume within that group. If FUN is a single function it will be applied to each non-invariant variable by group to produce the summary for that variable. If FUN is a list of functions, the names in the list should designate classes of variables in the frame such as ordered, factor, or numeric. The indicated function will be applied to any group-varying variables of that class. The default functions to be used are mean for numeric factors, and Mode for both factor and ordered. The Mode function, defined internally in gsummary, returns the modal or most popular value of the variable. It is different from the mode function that returns the S-language mode

of the variable.

coef.lmList 33

omitGroupingFactor

an optional logical value. When TRUE the grouping factor itself will be omitted from the group-wise summary of data but the levels of the grouping factor will continue to be used as the row names for the returned data frame. Defaults to

FALSE.

subset an optional expression specifying a subset

... some methods for this generic require additional arguments. None are used in

this method.

#### Value

a data frame inheriting from class "coef.lme" with the estimated coefficients at level level and, optionally, other covariates summarized over groups. The returned object also inherits from classes "ranef.lme" and "data.frame".

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York, esp. pp. 455-457.

#### See Also

```
lme, ranef.lme, plot.ranef.lme, gsummary
```

### **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)
coef(fm1)
coef(fm1, augFrame = TRUE)</pre>
```

coef.lmList

Extract lmList Coefficients

### **Description**

The coefficients of each 1m object in the object list are extracted and organized into a data frame, with rows corresponding to the 1m components and columns corresponding to the coefficients. Optionally, the returned data frame may be augmented with covariates summarized over the groups associated with the 1m components.

### Usage

```
## S3 method for class 'lmList'
coef(object, augFrame, data, which, FUN,
   omitGroupingFactor, ...)
```

34 coef.lmList

#### **Arguments**

object an object inheriting from class "lmList", representing a list of lm objects with

a common model.

augFrame an optional logical value. If TRUE, the returned data frame is augmented with

variables defined in the data frame used to produce object; else, if FALSE, only

the coefficients are returned. Defaults to FALSE.

data an optional data frame with the variables to be used for augmenting the returned

data frame when augFrame = TRUE. Defaults to the data frame used to fit object.

which an optional positive integer or character vector specifying which columns of the

data frame used to produce object should be used in the augmentation of the

returned data frame. Defaults to all variables in the data.

FUN an optional summary function or a list of summary functions to be applied to

group-varying variables, when collapsing the data by groups. Group-invariant variables are always summarized by the unique value that they assume within that group. If FUN is a single function it will be applied to each non-invariant variable by group to produce the summary for that variable. If FUN is a list of functions, the names in the list should designate classes of variables in the frame such as ordered, factor, or numeric. The indicated function will be applied to any group-varying variables of that class. The default functions to be used are mean for numeric factors, and Mode for both factor and ordered. The Mode function, defined internally in gsummary, returns the modal or most popular value of the variable. It is different from the mode function that returns

the S-language mode of the variable.

omitGroupingFactor

an optional logical value. When TRUE the grouping factor itself will be omitted from the group-wise summary of data but the levels of the grouping factor will continue to be used as the row names for the returned data frame. Defaults to

FALSE.

... some methods for this generic require additional arguments. None are used in

this method.

#### Value

a data frame inheriting from class "coef.lmList" with the estimated coefficients for each "lm" component of object and, optionally, other covariates summarized over the groups corresponding to the "lm" components. The returned object also inherits from classes "ranef.lmList" and "data.frame".

#### Author(s)

José Pinheiro and Douglas Bates <bate=@stat.wisc.edu>

### References

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York, esp. pp. 457-458.

coef.modelStruct 35

# See Also

```
lmList, fixed.effects.lmList, ranef.lmList, plot.ranef.lmList, gsummary
```

### **Examples**

```
fm1 <- lmList(distance ~ age|Subject, data = Orthodont)
coef(fm1)
coef(fm1, augFrame = TRUE)</pre>
```

coef.modelStruct

Extract modelStruct Object Coefficients

# Description

This method function extracts the coefficients associated with each component of the modelStruct list.

# Usage

```
## $3 method for class 'modelStruct'
coef(object, unconstrained, ...)
## $3 replacement method for class 'modelStruct'
coef(object, ...) <- value</pre>
```

### **Arguments**

object an object inheriting from class "modelStruct", representing a list of model

components, such as "corStruct" and "varFunc" objects.

unconstrained a logical value. If TRUE the coefficients are returned in unconstrained form (the

same used in the optimization algorithm). If FALSE the coefficients are returned

in "natural", possibly constrained, form. Defaults to TRUE.

value a vector with the replacement values for the coefficients associated with object.

It must be a vector with the same length of coef{object} and must be given in

unconstrained form.

... some methods for this generic require additional arguments. None are used in

this method.

#### Value

a vector with all coefficients corresponding to the components of object.

# SIDE EFFECTS

On the left side of an assignment, sets the values of the coefficients of object to value. Object must be initialized (using Initialize) before new values can be assigned to its coefficients.

36 coef.pdMat

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
Initialize
```

# **Examples**

```
lms1 <- lmeStruct(reStruct = reStruct(pdDiag(diag(2), ~age)),
    corStruct = corAR1(0.3))
coef(lms1)</pre>
```

coef.pdMat

pdMat Object Coefficients

### **Description**

This method function extracts the coefficients associated with the positive-definite matrix represented by object.

### Usage

```
## S3 method for class 'pdMat'
coef(object, unconstrained, ...)
## S3 replacement method for class 'pdMat'
coef(object, ...) <- value</pre>
```

# Arguments

object an object inheriting from class "pdMat", representing a positive-definite matrix.

 $unconstrained \quad a \ logical \ value. \ If \ \mathsf{TRUE} \ the \ coefficients \ are \ returned \ in \ unconstrained \ form \ (the$ 

same used in the optimization algorithm). If FALSE the upper triangular elements of the positive-definite matrix represented by object are returned. Defaults to

TRUE.

value a vector with the replacement values for the coefficients associated with object.

It must be a vector with the same length of coef{object} and must be given in

unconstrained form.

... some methods for this generic require additional arguments. None are used in

this method.

#### Value

a vector with the coefficients corresponding to object.

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## SIDE EFFECTS

On the left side of an assignment, sets the values of the coefficients of object to value.

#### Author(s)

José Pinheiro and Douglas Bates

#### References

Pinheiro, J.C. and Bates., D.M. (1996) "Unconstrained Parametrizations for Variance-Covariance Matrices", Statistics and Computing, 6, 289-296.

## See Also

pdMat

## **Examples**

```
coef(pdSymm(diag(3)))
```

coef.reStruct

reStruct Object Coefficients

## **Description**

This method function extracts the coefficients associated with the positive-definite matrix represented by object.

#### Usage

```
## S3 method for class 'reStruct'
coef(object, unconstrained, ...)
## S3 replacement method for class 'reStruct'
coef(object, ...) <- value</pre>
```

## **Arguments**

object an object inheriting from class "reStruct", representing a random effects struc-

ture and consisting of a list of pdMat objects.

unconstrained a logical value. If TRUE the coefficients are returned in unconstrained form (the

same used in the optimization algorithm). If FALSE the coefficients are returned

in "natural", possibly constrained, form. Defaults to TRUE.

value a vector with the replacement values for the coefficients associated with object.

It must be a vector with the same length of coef(object) and must be given in

unconstrained form.

... some methods for this generic require additional arguments. None are used in

this method.

38 coef.varFunc

## Value

a vector with the coefficients corresponding to object.

### SIDE EFFECTS

On the left side of an assignment, sets the values of the coefficients of object to value.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
coef.pdMat, reStruct, pdMat
```

## **Examples**

```
rs1 <- reStruct(list(A = pdSymm(diag(1:3), form = ~Score),
   B = pdDiag(2 * diag(4), form = ~Educ)))
coef(rs1)</pre>
```

coef.varFunc

varFunc Object Coefficients

## **Description**

This method function extracts the coefficients associated with the variance function structure represented by object.

### Usage

```
## $3 method for class 'varFunc'
coef(object, unconstrained, allCoef, ...)
## $3 replacement method for class 'varIdent'
coef(object, ...) <- value</pre>
```

# **Arguments**

object an object inheriting from class "varFunc" representing a variance function struc-

ture.

unconstrained a logical value. If TRUE the coefficients are returned in unconstrained form (the

same used in the optimization algorithm). If FALSE the coefficients are returned

in "natural", generally constrained form. Defaults to TRUE.

allCoef a logical value. If FALSE only the coefficients which may vary during the opti-

mization are returned. If TRUE all coefficients are returned. Defaults to FALSE.

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value a vector with the replacement values for the coefficients associated with object.

It must be have the same length of coef{object} and must be given in unconstrained form. Object must be initialized before new values can be assigned to

its coefficients.

... some methods for this generic require additional arguments. None are used in

this method.

## Value

a vector with the coefficients corresponding to object.

## SIDE EFFECTS

On the left side of an assignment, sets the values of the coefficients of object to value.

#### Author(s)

José Pinheiro and Douglas Bates

## See Also

varFunc

## **Examples**

```
vf1 <- varPower(1)
coef(vf1)
coef(vf1) <- 2</pre>
```

collapse

Collapse According to Groups

# Description

This function is generic; method functions can be written to handle specific classes of objects. Currently, only a groupedData method is available.

## Usage

```
collapse(object, ...)
```

# **Arguments**

object an object to be collapsed, usually a data frame.

... some methods for the generic may require additional arguments.

## Value

will depend on the method function used; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
collapse.groupedData
```

### **Examples**

## see the method function documentation

collapse.groupedData Collapse a groupedData Object

# **Description**

If object has a single grouping factor, it is returned unchanged. Else, it is summarized by the values of the displayLevel grouping factor (or the combination of its values and the values of the covariate indicated in preserve, if any is present). The collapsed data is used to produce a new groupedData object, with grouping factor given by the displayLevel factor.

## Usage

## **Arguments**

object an object inheriting from class groupedData, generally with multiple grouping

factors.

collapseLevel an optional positive integer or character string indicating the grouping level to

use when collapsing the data. Level values increase from outermost to innermost

grouping. Default is the highest or innermost level of grouping.

displayLevel an optional positive integer or character string indicating the grouping level to

use as the grouping factor for the collapsed data. Default is collapseLevel.

outer an optional logical value or one-sided formula, indicating covariates that are

outer to the displayLevel grouping factor. If equal to TRUE, the displayLevel element attr(object, "outer") is used to indicate the outer covariates. An outer covariate is invariant within the sets of rows defined by the grouping factor. Ordering of the groups is done in such a way as to preserve adjacency of groups with the same value of the outer variables. Defaults to NULL, meaning that no

outer covariates are to be used.

collapse.groupedData 41

inner an optional logical value or one-sided formula, indicating a covariate that is

inner to the displayLevel grouping factor. If equal to TRUE, attr(object, "outer") is used to indicate the inner covariate. An inner covariate can change within the sets of rows defined by the grouping factor. Defaults to NULL, meaning

that no inner covariate is present.

preserve an optional one-sided formula indicating a covariate whose levels should be

preserved when collapsing the data according to the collapseLevel grouping factor. The collapsing factor is obtained by pasting together the levels of the collapseLevel grouping factor and the values of the covariate to be preserved.

Default is NULL, meaning that no covariates need to be preserved.

FUN an optional summary function or a list of summary functions to be used for

collapsing the data. The function or functions are applied only to variables in object that vary within the groups defined by collapseLevel. Invariant variables are always summarized by group using the unique value that they assume within that group. If FUN is a single function it will be applied to each non-invariant variable by group to produce the summary for that variable. If FUN is a list of functions, the names in the list should designate classes of variables in the data such as ordered, factor, or numeric. The indicated function will be applied to any non-invariant variables of that class. The default functions to be used are mean for numeric factors, and Mode for both factor and ordered. The Mode function, defined internally in gsummary, returns the modal or most popular value of the variable. It is different from the mode function that returns

the S-language mode of the variable.

subset an optional named list. Names can be either positive integers representing

grouping levels, or names of grouping factors. Each element in the list is a vector indicating the levels of the corresponding grouping factor to be preserved

in the collapsed data. Default is NULL, meaning that all levels are used.

.. some methods for this generic require additional arguments. None are used in

this method.

#### Value

a groupedData object with a single grouping factor given by the displayLevel grouping factor, resulting from collapsing object over the levels of the collapseLevel grouping factor.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
groupedData, plot.nmGroupedData
```

```
# collapsing by Dog
collapse(Pixel, collapseLevel = 1)
# same as collapse(Pixel, collapseLevel = "Dog")
```

42 compareFits

compareFits

Compare Fitted Objects

## **Description**

The columns in object1 and object2 are put together in matrices which allow direct comparison of the individual elements for each object. Missing columns in either object are replaced by NAs.

## Usage

```
compareFits(object1, object2, which)
```

## **Arguments**

object1, object2

data frames, or matrices, with the same row names, but possibly different column names. These will usually correspond to coefficients from fitted objects with a grouping structure (e.g. lme and lmList objects).

which

an optional integer or character vector indicating which columns in object1 and object2 are to be used in the returned object. Defaults to all columns.

### Value

a three-dimensional array, with the third dimension given by the number of unique column names in either object1 or object2. To each column name there corresponds a matrix with as many rows as the rows in object1 and two columns, corresponding to object1 and object2. The returned object inherits from class compareFits.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
plot.compareFits, pairs.compareFits, comparePred, coef, random.effects
```

```
fm1 <- lmList(Orthodont)</pre>
fm2 \leftarrow lme(fm1)
(cF12 <- compareFits(coef(fm1), coef(fm2)))</pre>
```

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comparePred Compare Predictions
---------------------------------

#### **Description**

Predicted values are obtained at the specified values of primary for each object. If either object1 or object2 have a grouping structure (i.e. getGroups(object) is not NULL), predicted values are obtained for each group. When both objects determine groups, the group levels must be the same. If other covariates besides primary are used in the prediction model, their group-wise averages (numeric covariates) or most frequent values (categorical covariates) are used to obtain the predicted values. The original observations are also included in the returned object.

## Usage

```
comparePred(object1, object2, primary, minimum, maximum,
    length.out, level, ...)
```

#### **Arguments**

object1,	object2
----------	---------

fitted model objects, from which predictions can be extracted using the predict

method.

primary an optional one-sided formula specifying the primary covariate to be used to

generate the augmented predictions. By default, if a covariate can be extracted from the data used to generate the objects (using getCovariate), it will be used

as primary.

minimum an optional lower limit for the primary covariate. Defaults to min(primary),

after primary is evaluated in the data used in fitting object1.

maximum an optional upper limit for the primary covariate. Defaults to max(primary),

after primary is evaluated in the data used in fitting object1.

length.out an optional integer with the number of primary covariate values at which to

evaluate the predictions. Defaults to 51.

level an optional integer specifying the desired prediction level. Levels increase from

outermost to innermost grouping, with level 0 representing the population (fixed effects) predictions. Only one level can be specified. Defaults to the innermost

level.

... some methods for the generic may require additional arguments.

#### Value

a data frame with four columns representing, respectively, the values of the primary covariate, the groups (if object does not have a grouping structure, all elements will be 1), the predicted or observed values, and the type of value in the third column: the objects' names are used to classify the predicted values and original is used for the observed values. The returned object inherits from classes comparePred and augPred.

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#### Note

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: gls, lme, and lmList.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
augPred, getGroups
```

### **Examples**

```
fm1 <- lme(distance ~ age * Sex, data = Orthodont, random = ~ age)
fm2 <- update(fm1, distance ~ age)
comparePred(fm1, fm2, length.out = 2)</pre>
```

corAR1

AR(1) Correlation Structure

# Description

This function is a constructor for the corAR1 class, representing an autocorrelation structure of order 1. Objects created using this constructor must later be initialized using the appropriate Initialize method.

## Usage

```
corAR1(value, form, fixed)
```

## **Arguments**

value the value of the lag 1 autocorrelation, which must be between -1 and 1. Defaults

to 0 (no autocorrelation).

form a one sided formula of the form ~ t, or ~ t | g, specifying a time covariate t and,

optionally, a grouping factor g. A covariate for this correlation structure must be integer valued. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to ~ 1, which corresponds to using the order of the observations in the data

as a covariate, and no groups.

fixed an optional logical value indicating whether the coefficients should be allowed

to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE,

in which case the coefficients are allowed to vary.

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#### Value

an object of class corAR1, representing an autocorrelation structure of order 1.

#### Author(s)

José Pinheiro and Douglas Bates <bate="englast: bates@stat.wisc.edu">

#### References

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 235, 397.

## See Also

ACF.lme, corARMA, corClasses, Dim. corSpatial, Initialize.corStruct, summary.corStruct

```
## covariate is observation order and grouping factor is Mare
cs1 <- corAR1(0.2, form = \sim 1 | Mare)
# Pinheiro and Bates, p. 236
cs1AR1 \leftarrow corAR1(0.8, form = ~1 | Subject)
cs1AR1. <- Initialize(cs1AR1, data = Orthodont)
corMatrix(cs1AR1.)
# Pinheiro and Bates, p. 240
fm1Ovar.lme <- lme(follicles ~ sin(2*pi*Time) + cos(2*pi*Time),</pre>
                    data = Ovary, random = pdDiag(~sin(2*pi*Time)))
fm20var.lme <- update(fm10var.lme, correlation = corAR1())</pre>
# Pinheiro and Bates, pp. 255-258: use in gls
fm1Dial.gls <-
  gls(rate ~(pressure + I(pressure^2) + I(pressure^3) + I(pressure^4))*QB,
      Dialyzer)
fm2Dial.gls <- update(fm1Dial.gls,</pre>
                  weights = varPower(form = ~ pressure))
fm3Dial.gls <- update(fm2Dial.gls,</pre>
                     corr = corAR1(0.771, form = ~1 | Subject))
# Pinheiro and Bates use in nlme:
# from p. 240 needed on p. 396
fm10var.lme <- lme(follicles ~ sin(2*pi*Time) + cos(2*pi*Time),</pre>
                    data = Ovary, random = pdDiag(~sin(2*pi*Time)))
fm50var.lme <- update(fm10var.lme,</pre>
                correlation = corARMA(p = 1, q = 1))
# p. 396
fm10var.nlme <- nlme(follicles~</pre>
     A+B*sin(2*pi*w*Time)+C*cos(2*pi*w*Time),
```

46 corARMA

corARMA

ARMA(p,q) Correlation Structure

# Description

This function is a constructor for the corARMA class, representing an autocorrelation-moving average correlation structure of order (p, q). Objects created using this constructor must later be initialized using the appropriate Initialize method.

# Usage

```
corARMA(value, form, p, q, fixed)
```

## **Arguments**

value	a vector with the values of the autoregressive and moving average parameters, which must have length p + q and all elements between -1 and 1. Defaults to a vector of zeros, corresponding to uncorrelated observations.
form	a one sided formula of the form $\sim$ t, or $\sim$ t   g, specifying a time covariate t and, optionally, a grouping factor g. A covariate for this correlation structure must be integer valued. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to $\sim$ 1, which corresponds to using the order of the observations in the data as a covariate, and no groups.
p, q	non-negative integers specifying respectively the autoregressive order and the moving average order of the ARMA structure. Both default to $0$ , but at least one should be $> 0$ .
fixed	an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE,

## Value

an object of class corARMA, representing an autocorrelation-moving average correlation structure.

in which case the coefficients are allowed to vary.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

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#### References

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 236, 397.

#### See Also

corAR1, corClasses Initialize.corStruct, summary.corStruct

## **Examples**

```
## ARMA(1,2) structure, with observation order as a covariate and
## Mare as grouping factor
cs1 <- corARMA(c(0.2, 0.3, -0.1), form = \sim 1 | Mare, p = 1, q = 2)
# Pinheiro and Bates, p. 237
cs1ARMA <- corARMA(0.4, form = \sim 1 | Subject, q = 1)
cs1ARMA <- Initialize(cs1ARMA, data = Orthodont)</pre>
corMatrix(cs1ARMA)
cs2ARMA <- corARMA(c(0.8, 0.4), form = \sim 1 | Subject, p=1, q=1)
cs2ARMA <- Initialize(cs2ARMA, data = Orthodont)
corMatrix(cs2ARMA)
# Pinheiro and Bates use in nlme:
# from p. 240 needed on p. 396
fm1Ovar.lme <- lme(follicles ~ sin(2*pi*Time) + cos(2*pi*Time),</pre>
                    data = Ovary, random = pdDiag(~sin(2*pi*Time)))
fm50var.lme <- update(fm10var.lme,</pre>
                correlation = corARMA(p = 1, q = 1))
# p. 396
fm10var.nlme <- nlme(follicles~
     A+B*sin(2*pi*w*Time)+C*cos(2*pi*w*Time),
   data=Ovary, fixed=A+B+C+w~1,
   random=pdDiag(A+B+w~1),
   start=c(fixef(fm50var.lme), 1) )
# p. 397
fm30var.nlme <- update(fm10var.nlme,</pre>
         correlation=corARMA(p=0, q=2) )
```

corCAR1

Continuous AR(1) Correlation Structure

## **Description**

This function is a constructor for the corCAR1 class, representing an autocorrelation structure of order 1, with a continuous time covariate. Objects created using this constructor must be later initialized using the appropriate Initialize method.

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#### **Usage**

```
corCAR1(value, form, fixed)
```

#### **Arguments**

value the correlation between two observations one unit of time apart. Must be be-

tween 0 and 1. Defaults to 0.2.

form a one sided formula of the form ~ t, or ~ t | g, specifying a time covariate t and,

optionally, a grouping factor g. Covariates for this correlation structure need not be integer valued. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to  $\sim$  1, which corresponds to using the order of the observations

in the data as a covariate, and no groups.

fixed an optional logical value indicating whether the coefficients should be allowed

to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE,

in which case the coefficients are allowed to vary.

#### Value

an object of class corCAR1, representing an autocorrelation structure of order 1, with a continuous time covariate.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Jones, R.H. (1993) "Longitudinal Data with Serial Correlation: A State-space Approach", Chapman and Hall.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 236, 243.

### See Also

```
corClasses, Initialize.corStruct, summary.corStruct
```

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corClasses	Correlation Structure Classes	
------------	-------------------------------	--

# Description

Standard classes of correlation structures (corStruct) available in the nlme package.

## Value

Available standard classes:

corAR1 autoregressive process of order 1.

corARMA autoregressive moving average process, with arbitrary orders for the autoregres-

sive and moving average components.

corCAR1 continuous autoregressive process (AR(1) process for a continuous time covari-

ate).

corCompSymm compound symmetry structure corresponding to a constant correlation.

corExp exponential spatial correlation.
corGaus Gaussian spatial correlation.
corLin linear spatial correlation.

corRatio Rational quadratics spatial correlation.

corSpher spherical spatial correlation.

corSymm general correlation matrix, with no additional structure.

### Note

Users may define their own corStruct classes by specifying a constructor function and, at a minimum, methods for the functions corMatrix and coef. For examples of these functions, see the methods for classes corSymm and corAR1.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

 $\verb|corARMA|, \verb|corCARMA|, \verb|corCompSymm|, \verb|corExp|, \verb|corGaus|, \verb|corLin|, \verb|corRatio|, \verb|corSpher|, \verb|corSymm|, \verb|summary|, \verb|corStruct||$ 

50 corCompSymm

corCompSymm	Compound Symmetry Correlation Structure	

## **Description**

This function is a constructor for the corCompSymm class, representing a compound symmetry structure corresponding to uniform correlation. Objects created using this constructor must later be initialized using the appropriate Initialize method.

## Usage

```
corCompSymm(value, form, fixed)
```

## **Arguments**

value	the correlation between any two correlated observations. Defaults to 0.
form	a one sided formula of the form $\sim$ t, or $\sim$ t   g, specifying a time covariate t and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the

the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to ~1, which corresponds to using the order of the

observations in the data as a covariate, and no groups.

fixed an optional logical value indicating whether the coefficients should be allowed

to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE,

in which case the coefficients are allowed to vary.

## Value

an object of class corCompSymm, representing a compound symmetry correlation structure.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Milliken, G. A. and Johnson, D. E. (1992) "Analysis of Messy Data, Volume I: Designed Experiments", Van Nostrand Reinhold.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 233-234.

#### See Also

corClasses, Initialize.corStruct, summary.corStruct

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## **Examples**

```
## covariate is observation order and grouping factor is Subject
cs1 <- corCompSymm(0.5, form = \sim 1 | Subject)
# Pinheiro and Bates, pp. 222-225
fm1BW.lme <- lme(weight ~ Time * Diet, BodyWeight,</pre>
                    random = \sim Time)
# p. 223
fm2BW.lme <- update(fm1BW.lme, weights = varPower())</pre>
# p. 225
cs1CompSymm <- corCompSymm(value = 0.3, form = ~ 1 | Subject)
cs2CompSymm <- corCompSymm(value = 0.3, form = ~ age | Subject)
cs1CompSymm <- Initialize(cs1CompSymm, data = Orthodont)</pre>
corMatrix(cs1CompSymm)
## Print/Summary methods for the empty case:
(cCS <- corCompSymm()) # Uninitialized correlation struc..</pre>
summary(cCS)
                              (ditto)
```

corExp

Exponential Correlation Structure

## **Description**

This function is a constructor for the "corExp" class, representing an exponential spatial correlation structure. Letting d denote the range and n denote the nugget effect, the correlation between two observations a distance r apart is  $\exp(-r/d)$  when no nugget effect is present and  $(1-n)\exp(-r/d)$  when a nugget effect is assumed. Objects created using this constructor must later be initialized using the appropriate Initialize method.

# Usage

```
corExp(value, form, nugget, metric, fixed)
```

## **Arguments**

value

an optional vector with the parameter values in constrained form. If nugget is FALSE, value can have only one element, corresponding to the "range" of the exponential correlation structure, which must be greater than zero. If nugget is TRUE, meaning that a nugget effect is present, value can contain one or two elements, the first being the "range" and the second the "nugget effect" (one minus the correlation between two observations taken arbitrarily close together); the first must be greater than zero and the second must be between zero and one. Defaults to numeric(0), which results in a range of 90% of the minimum distance and a nugget effect of 0.1 being assigned to the parameters when object is initialized.

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a one sided formula of the form ~ \$1+...+\$p, or ~ \$1+...+\$p | g, specifying spatial covariates \$1 through \$p\$ and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to ~ 1, which corresponds to using the order of the observations in the data as a covariate, and no

groups.

nugget an optional logical value indicating whether a nugget effect is present. Defaults

to FALSE.

metric an optional character string specifying the distance metric to be used. The cur-

rently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the

first three characters need to be provided. Defaults to "euclidean".

fixed an optional logical value indicating whether the coefficients should be allowed

to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE,

in which case the coefficients are allowed to vary.

#### Value

an object of class "corExp", also inheriting from class "corSpatial", representing an exponential spatial correlation structure.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

Littel, Milliken, Stroup, and Wolfinger (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. p. 238.

#### See Also

```
corClasses, Initialize.corStruct, summary.corStruct, dist
```

```
sp1 <- corExp(form = \sim x + y + z)

# Pinheiro and Bates, p. 238

spatDat <- data.frame(x = (0:4)/4, y = (0:4)/4)

cs1Exp <- corExp(1, form = \sim x + y)
```

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```
cs1Exp <- Initialize(cs1Exp, spatDat)
corMatrix(cs1Exp)
cs2Exp \leftarrow corExp(1, form = ~ x + y, metric = "man")
cs2Exp <- Initialize(cs2Exp, spatDat)</pre>
corMatrix(cs2Exp)
cs3Exp \leftarrow corExp(c(1, 0.2), form = ~ x + y,
                  nugget = TRUE)
cs3Exp <- Initialize(cs3Exp, spatDat)</pre>
corMatrix(cs3Exp)
# example lme(..., corExp ...)
# Pinheiro and Bates, pp. 222-247
# p. 222
options(contrasts = c("contr.treatment", "contr.poly"))
fm1BW.lme <- lme(weight ~ Time * Diet, BodyWeight,</pre>
                    random = ~ Time)
# p. 223
fm2BW.lme <- update(fm1BW.lme, weights = varPower())</pre>
# p. 246
fm3BW.lme <- update(fm2BW.lme,</pre>
           correlation = corExp(form = ~ Time))
# p. 247
fm4BW.lme <-
      update(fm3BW.lme, correlation = corExp(form = ~ Time,
                          nugget = TRUE))
anova(fm3BW.lme, fm4BW.lme)
```

corFactor

Factor of a Correlation Matrix

# Description

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include all corStruct classes.

## Usage

```
corFactor(object, ...)
```

## **Arguments**

object an object from which a correlation matrix can be extracted.
... some methods for this generic function require additional arguments.

## Value

will depend on the method function used; see the appropriate documentation.

54 corFactor.corStruct

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
corFactor.corStruct, recalc.corStruct
```

## **Examples**

## see the method function documentation

corFactor.corStruct

Factor of a corStruct Object Matrix

### **Description**

This method function extracts a transpose inverse square-root factor, or a series of transpose inverse square-root factors, of the correlation matrix, or list of correlation matrices, represented by object. Letting  $\Sigma$  denote a correlation matrix, a square-root factor of  $\Sigma$  is any square matrix L such that  $\Sigma = L'L$ . This method extracts  $L^{-t}$ .

#### **Usage**

```
## S3 method for class 'corStruct'
corFactor(object, ...)
```

## **Arguments**

object an object inheriting from class "corStruct" representing a correlation structure, which must have been initialized (using Initialize).

. . some methods for this generic require additional arguments. None are used in this method.

## Value

If the correlation structure does not include a grouping factor, the returned value will be a vector with a transpose inverse square-root factor of the correlation matrix associated with object stacked column-wise. If the correlation structure includes a grouping factor, the returned value will be a vector with transpose inverse square-root factors of the correlation matrices for each group, stacked by group and stacked column-wise within each group.

## Note

This method function is used intensively in optimization algorithms and its value is returned as a vector for efficiency reasons. The corMatrix method function can be used to obtain transpose inverse square-root factors in matrix form.

corGaus 55

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
corFactor, corMatrix.corStruct, recalc.corStruct, Initialize.corStruct
```

## **Examples**

```
cs1 <- corAR1(form = ~1 | Subject)
cs1 <- Initialize(cs1, data = Orthodont)
corFactor(cs1)</pre>
```

corGaus

Gaussian Correlation Structure

## **Description**

This function is a constructor for the corGaus class, representing a Gaussian spatial correlation structure. Letting d denote the range and n denote the nugget effect, the correlation between two observations a distance r apart is  $\exp(-(r/d)^2)$  when no nugget effect is present and  $(1-n)\exp(-(r/d)^2)$  when a nugget effect is assumed. Objects created using this constructor must later be initialized using the appropriate 'Initialize method.

## Usage

```
corGaus(value, form, nugget, metric, fixed)
```

# **Arguments**

value

an optional vector with the parameter values in constrained form. If nugget is FALSE, value can have only one element, corresponding to the "range" of the Gaussian correlation structure, which must be greater than zero. If nugget is TRUE, meaning that a nugget effect is present, value can contain one or two elements, the first being the "range" and the second the "nugget effect" (one minus the correlation between two observations taken arbitrarily close together); the first must be greater than zero and the second must be between zero and one. Defaults to numeric(0), which results in a range of 90% of the minimum distance and a nugget effect of 0.1 being assigned to the parameters when object is initialized.

form

a one sided formula of the form  $\sim S1+\ldots+Sp$ , or  $\sim S1+\ldots+Sp \mid g$ , specifying spatial covariates S1 through Sp and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to  $\sim 1$ , which corresponds to using the order of the observations in the data as a covariate, and no groups.

56 corGaus

nugget	an optional logical value indicating whether a nugget effect is present. Defaults to FALSE.
metric	an optional character string specifying the distance metric to be used. The currently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the first three characters need to be provided. Defaults to "euclidean".
fixed	an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE, in which case the coefficients are allowed to vary.

#### Value

an object of class corGaus, also inheriting from class corSpatial, representing a Gaussian spatial correlation structure.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

Littel, Milliken, Stroup, and Wolfinger (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

```
Initialize.corStruct, summary.corStruct, dist
```

corLin 57

corLin

Linear Correlation Structure

## **Description**

This function is a constructor for the corLin class, representing a linear spatial correlation structure. Letting d denote the range and n denote the nugget effect, the correlation between two observations a distance r < d apart is 1 - (r/d) when no nugget effect is present and (1 - n)(1 - (r/d)) when a nugget effect is assumed. If  $r \ge d$  the correlation is zero. Objects created using this constructor must later be initialized using the appropriate Initialize method.

## Usage

```
corLin(value, form, nugget, metric, fixed)
```

#### **Arguments**

value

an optional vector with the parameter values in constrained form. If nugget is FALSE, value can have only one element, corresponding to the "range" of the linear correlation structure, which must be greater than zero. If nugget is TRUE, meaning that a nugget effect is present, value can contain one or two elements, the first being the "range" and the second the "nugget effect" (one minus the correlation between two observations taken arbitrarily close together); the first must be greater than zero and the second must be between zero and one. Defaults to numeric(0), which results in a range of 90% of the minimum distance and a nugget effect of 0.1 being assigned to the parameters when object is initialized.

form

a one sided formula of the form ~ S1+...+Sp, or ~ S1+...+Sp | g, specifying spatial covariates S1 through Sp and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to ~ 1, which corresponds to using the order of the observations in the data as a covariate, and no groups.

nugget

an optional logical value indicating whether a nugget effect is present. Defaults to FALSE.

metric

an optional character string specifying the distance metric to be used. The currently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the first three characters need to be provided. Defaults to "euclidean".

fixed

an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE, in which case the coefficients are allowed to vary.

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## Value

an object of class corLin, also inheriting from class corSpatial, representing a linear spatial correlation structure.

#### Author(s)

José Pinheiro and Douglas Bates <bate="englast: bates@stat.wisc.edu">

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

Littel, Milliken, Stroup, and Wolfinger (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
Initialize.corStruct, summary.corStruct, dist
```

# **Examples**

corMatrix

Extract Correlation Matrix

### **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include all corStruct classes.

## Usage

```
corMatrix(object, ...)
```

corMatrix.corStruct 59

### **Arguments**

object an object for which a correlation matrix can be extracted.

... some methods for this generic function require additional arguments.

## Value

will depend on the method function used; see the appropriate documentation.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
corMatrix.corStruct, corMatrix.pdMat
```

## **Examples**

## see the method function documentation

#### **Description**

This method function extracts the correlation matrix (or its transpose inverse square-root factor), or list of correlation matrices (or their transpose inverse square-root factors) corresponding to covariate and object. Letting  $\Sigma$  denote a correlation matrix, a square-root factor of  $\Sigma$  is any square matrix L such that  $\Sigma = L'L$ . When corr = FALSE, this method extracts  $L^{-t}$ .

## Usage

```
## S3 method for class 'corStruct'
corMatrix(object, covariate, corr, ...)
```

## **Arguments**

object	an object inheriting from class	"corStruct"	representing a correlation struc-
--------	---------------------------------	-------------	-----------------------------------

ture.

covariate an optional covariate vector (matrix), or list of covariate vectors (matrices), at

which values the correlation matrix, or list of correlation matrices, are to be

evaluated. Defaults to getCovariate(object).

corr a logical value. If TRUE the function returns the correlation matrix, or list of

correlation matrices, represented by object. If FALSE the function returns a transpose inverse square-root of the correlation matrix, or a list of transpose

inverse square-root factors of the correlation matrices.

... some methods for this generic require additional arguments. None are used in

this method.

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#### Value

If covariate is a vector (matrix), the returned value will be an array with the corresponding correlation matrix (or its transpose inverse square-root factor). If the covariate is a list of vectors (matrices), the returned value will be a list with the correlation matrices (or their transpose inverse square-root factors) corresponding to each component of covariate.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
corFactor.corStruct, Initialize.corStruct
```

```
cs1 <- corAR1(0.3)
corMatrix(cs1, covariate = 1:4)
corMatrix(cs1, covariate = 1:4, corr = FALSE)
# Pinheiro and Bates, p. 225
cs1CompSymm <- corCompSymm(value = 0.3, form = ~ 1 | Subject)
cs1CompSymm <- Initialize(cs1CompSymm, data = Orthodont)</pre>
corMatrix(cs1CompSymm)
# Pinheiro and Bates, p. 226
cs1Symm <- corSymm(value = c(0.2, 0.1, -0.1, 0, 0.2, 0),
                    form = ~ 1 | Subject)
cs1Symm <- Initialize(cs1Symm, data = Orthodont)</pre>
corMatrix(cs1Symm)
# Pinheiro and Bates, p. 236
cs1AR1 \leftarrow corAR1(0.8, form = ~1 | Subject)
cs1AR1 <- Initialize(cs1AR1, data = Orthodont)</pre>
corMatrix(cs1AR1)
# Pinheiro and Bates, p. 237
cs1ARMA <- corARMA(0.4, form = \sim 1 | Subject, q = 1)
cs1ARMA <- Initialize(cs1ARMA, data = Orthodont)</pre>
corMatrix(cs1ARMA)
# Pinheiro and Bates, p. 238
spatDat <- data.frame(x = (0:4)/4, y = (0:4)/4)
cs1Exp \leftarrow corExp(1, form = ~ x + y)
cs1Exp <- Initialize(cs1Exp, spatDat)</pre>
corMatrix(cs1Exp)
```

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corMatrix.pdMat

Extract Correlation Matrix from a pdMat Object

# Description

The correlation matrix corresponding to the positive-definite matrix represented by object is obtained.

## Usage

```
## S3 method for class 'pdMat'
corMatrix(object, ...)
```

# Arguments

object an object inheriting from class "pdMat", representing a positive definite matrix.

some methods for this generic require additional arguments. None are used in

this method.

## Value

the correlation matrix corresponding to the positive-definite matrix represented by object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
as.matrix.pdMat, pdMatrix
```

```
pd1 <- pdSymm(diag(1:4))
corMatrix(pd1)</pre>
```

62 corMatrix.reStruct

corMatrix.reStruct

Extract Correlation Matrix from Components of an reStruct Object

## **Description**

This method function extracts the correlation matrices corresponding to the pdMat elements of object.

## Usage

```
## S3 method for class 'reStruct'
corMatrix(object, ...)
```

## **Arguments**

object an object inheriting from class "reStruct", representing a random effects struc-

ture and consisting of a list of pdMat objects.

... some methods for this generic require additional arguments. None are used in

this method.

## Value

a list with components given by the correlation matrices corresponding to the elements of object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
as.matrix.reStruct, corMatrix, reStruct, pdMat
```

```
rs1 <- reStruct(pdSymm(diag(3), ~age+Sex, data = Orthodont))
corMatrix(rs1)</pre>
```

corNatural 63

corNatural	General correlation in natural parameterization

## **Description**

This function is a constructor for the corNatural class, representing a general correlation structure in the "natural" parameterization, which is described under pdNatural. Objects created using this constructor must later be initialized using the appropriate Initialize method.

# Usage

```
corNatural(value, form, fixed)
```

## **Arguments**

-8	
value	an optional vector with the parameter values. Default is numeric(0), which results in a vector of zeros of appropriate dimension being assigned to the parameters when object is initialized (corresponding to an identity correlation structure).
form	a one sided formula of the form $\sim$ t, or $\sim$ t   g, specifying a time covariate t and, optionally, a grouping factor g. A covariate for this correlation structure must be integer valued. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to $\sim$ 1, which corresponds to using the order of the observations in the data as a covariate, and no groups.
fixed	an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE, in which case the coefficients are allowed to vary.

## Value

an object of class corNatural representing a general correlation structure.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
Initialize.corNatural, pdNatural, summary.corNatural
```

```
## covariate is observation order and grouping factor is Subject cs1 <- corNatural(form = ^{\sim} 1 | Subject)
```

64 corRatio

corRatio

Rational Quadratic Correlation Structure

#### **Description**

This function is a constructor for the corRatio class, representing a rational quadratic spatial correlation structure. Letting d denote the range and n denote the nugget effect, the correlation between two observations a distance r apart is  $1/(1+(r/d)^2)$  when no nugget effect is present and  $(1-n)/(1+(r/d)^2)$  when a nugget effect is assumed. Objects created using this constructor need to be later initialized using the appropriate Initialize method.

## Usage

```
corRatio(value, form, nugget, metric, fixed)
```

## **Arguments**

value

an optional vector with the parameter values in constrained form. If nugget is FALSE, value can have only one element, corresponding to the "range" of the rational quadratic correlation structure, which must be greater than zero. If nugget is TRUE, meaning that a nugget effect is present, value can contain one or two elements, the first being the "range" and the second the "nugget effect" (one minus the correlation between two observations taken arbitrarily close together); the first must be greater than zero and the second must be between zero and one. Defaults to numeric(0), which results in a range of 90% of the minimum distance and a nugget effect of 0.1 being assigned to the parameters when object is initialized.

form

a one sided formula of the form ~ S1+...+Sp, or ~ S1+...+Sp | g, specifying spatial covariates S1 through Sp and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to ~ 1, which corresponds to using the order of the observations in the data as a covariate, and no groups.

nugget

an optional logical value indicating whether a nugget effect is present. Defaults to FALSE.

metric

an optional character string specifying the distance metric to be used. The currently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the first three characters need to be provided. Defaults to "euclidean".

fixed

an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE, in which case the coefficients are allowed to vary.

corRatio 65

#### Value

an object of class corRatio, also inheriting from class corSpatial, representing a rational quadratic spatial correlation structure.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

Littel, Milliken, Stroup, and Wolfinger (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
Initialize.corStruct, summary.corStruct, dist
```

```
sp1 \leftarrow corRatio(form = x + y + z)
# example lme(..., corRatio ...)
# Pinheiro and Bates, pp. 222-249
fm1BW.lme <- lme(weight ~ Time * Diet, BodyWeight,</pre>
                   random = ~ Time)
# p. 223
fm2BW.lme <- update(fm1BW.lme, weights = varPower())</pre>
# p 246
fm3BW.lme <- update(fm2BW.lme,</pre>
            correlation = corExp(form = ~ Time))
fm5BW.lme <- update(fm3BW.lme, correlation =</pre>
                    corRatio(form = ~ Time))
# example gls(..., corRatio ...)
# Pinheiro and Bates, pp. 261, 263
fm1Wheat2 <- gls(yield ~ variety - 1, Wheat2)</pre>
# p. 263
fm3Wheat2 <- update(fm1Wheat2, corr =</pre>
    corRatio(c(12.5, 0.2),
       form = ~ latitude + longitude,
              nugget = TRUE))
```

66 corSpatial

corSpatial

Spatial Correlation Structure

## **Description**

This function is a constructor for the corSpatial class, representing a spatial correlation structure. This class is "virtual", having four "real" classes, corresponding to specific spatial correlation structures, associated with it: corExp, corGaus, corLin, corRatio, and corSpher. The returned object will inherit from one of these "real" classes, determined by the type argument, and from the "virtual" corSpatial class. Objects created using this constructor must later be initialized using the appropriate Initialize method.

## Usage

corSpatial(value, form, nugget, type, metric, fixed)

#### **Arguments**

value

an optional vector with the parameter values in constrained form. If nugget is FALSE, value can have only one element, corresponding to the "range" of the spatial correlation structure, which must be greater than zero. If nugget is TRUE, meaning that a nugget effect is present, value can contain one or two elements, the first being the "range" and the second the "nugget effect" (one minus the correlation between two observations taken arbitrarily close together); the first must be greater than zero and the second must be between zero and one. Defaults to numeric(0), which results in a range of 90% of the minimum distance and a nugget effect of 0.1 being assigned to the parameters when object is initialized.

form

a one sided formula of the form ~ S1+...+Sp, or ~ S1+...+Sp | g, specifying spatial covariates S1 through Sp and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to ~ 1, which corresponds to using the order of the observations in the data as a covariate, and no groups.

nugget

an optional logical value indicating whether a nugget effect is present. Defaults to FALSE.

type

an optional character string specifying the desired type of correlation structure. Available types include "spherical", "exponential", "gaussian", "linear", and "rational". See the documentation on the functions corSpher, corExp, corGaus, corLin, and corRatio for a description of these correlation structures. Partial matching of arguments is used, so only the first character needs to be provided.Defaults to "spherical".

metric

an optional character string specifying the distance metric to be used. The currently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the first three characters need to be provided. Defaults to "euclidean".

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fixed

an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE, in which case the coefficients are allowed to vary.

#### Value

an object of class determined by the type argument and also inheriting from class corSpatial, representing a spatial correlation structure.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

Littel, Milliken, Stroup, and Wolfinger (1996) "SAS Systems for Mixed Models", SAS Institute.

#### See Also

```
corExp, corGaus, corLin, corRatio, corSpher, Initialize.corStruct, summary.corStruct,
dist
```

# **Examples**

```
sp1 \leftarrow corSpatial(form = ~ x + y + z, type = "g", metric = "man")
```

corSpher

Spherical Correlation Structure

## **Description**

This function is a constructor for the corSpher class, representing a spherical spatial correlation structure. Letting d denote the range and n denote the nugget effect, the correlation between two observations a distance r < d apart is  $1-1.5(r/d)+0.5(r/d)^3$  when no nugget effect is present and  $(1-n)(1-1.5(r/d)+0.5(r/d)^3)$  when a nugget effect is assumed. If  $r \geq d$  the correlation is zero. Objects created using this constructor must later be initialized using the appropriate Initialize method.

## Usage

```
corSpher(value, form, nugget, metric, fixed)
```

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### **Arguments**

value

an optional vector with the parameter values in constrained form. If nugget is FALSE, value can have only one element, corresponding to the "range" of the spherical correlation structure, which must be greater than zero. If nugget is TRUE, meaning that a nugget effect is present, value can contain one or two elements, the first being the "range" and the second the "nugget effect" (one minus the correlation between two observations taken arbitrarily close together); the first must be greater than zero and the second must be between zero and one. Defaults to numeric(0), which results in a range of 90% of the minimum distance and a nugget effect of 0.1 being assigned to the parameters when object is initialized.

form

a one sided formula of the form ~ S1+...+Sp, or ~ S1+...+Sp | g, specifying spatial covariates S1 through Sp and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to ~ 1, which corresponds to using the order of the observations in the data as a covariate, and no groups.

nugget

an optional logical value indicating whether a nugget effect is present. Defaults to FALSE.

metric

an optional character string specifying the distance metric to be used. The currently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the first three characters need to be provided. Defaults to "euclidean".

fixed

an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE, in which case the coefficients are allowed to vary.

## Value

an object of class corSpher, also inheriting from class corSpatial, representing a spherical spatial correlation structure.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

Littel, Milliken, Stroup, and Wolfinger (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

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## See Also

```
Initialize.corStruct, summary.corStruct, dist
```

#### **Examples**

```
sp1 \leftarrow corSpher(form = ~ x + y)
# example lme(..., corSpher ...)
# Pinheiro and Bates, pp. 222-249
fm1BW.lme <- lme(weight ~ Time * Diet, BodyWeight,</pre>
                    random = \sim Time)
# p. 223
fm2BW.lme <- update(fm1BW.lme, weights = varPower())</pre>
# p 246
fm3BW.lme <- update(fm2BW.lme,</pre>
           correlation = corExp(form = ~ Time))
# p. 249
fm6BW.lme <- update(fm3BW.lme,</pre>
           correlation = corSpher(form = ~ Time))
# example gls(..., corSpher ...)
# Pinheiro and Bates, pp. 261, 263
fm1Wheat2 <- gls(yield ~ variety - 1, Wheat2)</pre>
# p. 262
fm2Wheat2 <- update(fm1Wheat2, corr =</pre>
   corSpher(c(28, 0.2),
     form = ~ latitude + longitude, nugget = TRUE))
```

corSymm

General Correlation Structure

### **Description**

This function is a constructor for the corSymm class, representing a general correlation structure. The internal representation of this structure, in terms of unconstrained parameters, uses the spherical parametrization defined in Pinheiro and Bates (1996). Objects created using this constructor must later be initialized using the appropriate Initialize method.

# Usage

```
corSymm(value, form, fixed)
```

## **Arguments**

value

an optional vector with the parameter values. Default is numeric(0), which results in a vector of zeros of appropriate dimension being assigned to the parameters when object is initialized (corresponding to an identity correlation structure).

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form a one sided formula of the form  $\sim t$ , or  $\sim t \mid g$ , specifying a time covariate t and,

optionally, a grouping factor g. A covariate for this correlation structure must be integer valued. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to  $\sim$  1, which corresponds to using the order of the observations in the data

as a covariate, and no groups.

fixed an optional logical value indicating whether the coefficients should be allowed to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE,

in which case the coefficients are allowed to vary.

#### Value

an object of class corSymm representing a general correlation structure.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C. and Bates., D.M. (1996) "Unconstrained Parametrizations for Variance-Covariance Matrices", Statistics and Computing, 6, 289-296.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
Initialize.corSymm, summary.corSymm
```

```
## covariate is observation order and grouping factor is Subject
cs1 <- corSymm(form = ~ 1 | Subject)
# Pinheiro and Bates, p. 225
cs1CompSymm <- corCompSymm(value = 0.3, form = ~ 1 | Subject)
cs1CompSymm <- Initialize(cs1CompSymm, data = Orthodont)</pre>
corMatrix(cs1CompSymm)
# Pinheiro and Bates, p. 226
cs1Symm <- corSymm(value =
        c(0.2, 0.1, -0.1, 0, 0.2, 0),
                   form = ~ 1 | Subject)
cs1Symm <- Initialize(cs1Symm, data = Orthodont)
corMatrix(cs1Symm)
# example gls(..., corSpher ...)
# Pinheiro and Bates, pp. 261, 263
fm1Wheat2 <- gls(yield ~ variety - 1, Wheat2)</pre>
# p. 262
fm2Wheat2 <- update(fm1Wheat2, corr =</pre>
```

Covariate 71

Covariate

Assign Covariate Values

## **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include all "varFunc" classes.

# Usage

```
covariate(object) <- value</pre>
```

# **Arguments**

object any object with a covariate component.

value a value to be assigned to the covariate associated with object.

## Value

will depend on the method function; see the appropriate documentation.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
getCovariate
```

```
## see the method function documentation
```

72 Covariate.varFunc

Covariate.varFunc

Assign varFunc Covariate

# Description

The covariate(s) used in the calculation of the weights of the variance function represented by object is (are) replaced by value. If object has been initialized, value must have the same dimensions as getCovariate(object).

## Usage

```
## S3 replacement method for class 'varFunc'
covariate(object) <- value</pre>
```

## **Arguments**

object an object inheriting from class "varFunc", representing a variance function

structure.

value a value to be assigned to the covariate associated with object.

## Value

a varFunc object similar to object, but with its covariate attribute replaced by value.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
getCovariate.varFunc
```

```
vf1 <- varPower(1.1, form = ~age)
covariate(vf1) <- Orthodont[["age"]]</pre>
```

Dialyzer 73

Dialyzer

High-Flux Hemodialyzer

### **Description**

The Dialyzer data frame has 140 rows and 5 columns.

#### **Format**

This data frame contains the following columns:

**Subject** an ordered factor with levels 10 < 8 < 2 < 6 < 3 < 5 < 9 < 7 < 1 < 4 < 17 < 20 < 11 < 12 < 16 < 13 < 14 < 18 < 15 < 19 giving the unique identifier for each subject

QB a factor with levels 200 and 300 giving the bovine blood flow rate (dL/min).

pressure a numeric vector giving the transmembrane pressure (dmHg).

rate the hemodialyzer ultrafiltration rate (mL/hr).

**index** index of observation within subject—1 through 7.

#### **Details**

Vonesh and Carter (1992) describe data measured on high-flux hemodialyzers to assess their *in vivo* ultrafiltration characteristics. The ultrafiltration rates (in mL/hr) of 20 high-flux dialyzers were measured at seven different transmembrane pressures (in dmHg). The *in vitro* evaluation of the dialyzers used bovine blood at flow rates of either 200~dl/min or 300~dl/min. The data, are also analyzed in Littell, Milliken, Stroup, and Wolfinger (1996).

# Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.6)

Vonesh, E. F. and Carter, R. L. (1992), Mixed-effects nonlinear regression for unbalanced repeated measures, *Biometrics*, **48**, 1-18.

Littell, R. C., Milliken, G. A., Stroup, W. W. and Wolfinger, R. D. (1996), SAS System for Mixed Models, SAS Institute, Cary, NC.

74 Dim

Dim

Extract Dimensions from an Object

## **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: "corSpatial", "corStruct", "pdCompSymm", "pdDiag", "pdIdent", "pdMat", and "pdSymm".

# Usage

```
Dim(object, ...)
```

# Arguments

object any object for which dimensions can be extracted.

... some methods for this generic function require additional arguments.

### Value

will depend on the method function used; see the appropriate documentation.

### Note

If dim allowed more than one argument, there would be no need for this generic function.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
Dim.pdMat, Dim.corStruct
```

# **Examples**

## see the method function documentation

Dim.corSpatial 75

Di	m.corSpatial	Dimensions of a corSpatial Object

# Description

if groups is missing, it returns the Dim attribute of object; otherwise, calculates the dimensions associated with the grouping factor.

### Usage

```
## S3 method for class 'corSpatial'
Dim(object, groups, ...)
```

## **Arguments**

object	an object inheriting from class "corSpatial", representing a spatial correlation
	structure

structure.

groups an optional factor defining the grouping of the observations; observations within

a group are correlated and observations in different groups are uncorrelated.

... further arguments to be passed to or from methods.

## Value

a list with components:

N	length of groups	
М	number of groups	

spClass an integer representing the spatial correlation class; 0 = user defined class, 1 = user defined class,  $1 = \text{use$ 

corSpher, 2 = corExp, 3 = corGaus, 4 = corLin

sumLenSq sum of the squares of the number of observations per group

len an integer vector with the number of observations per group

start an integer vector with the starting position for the distance vectors in each group,

beginning from zero

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
Dim, Dim.corStruct
```

76 Dim.corStruct

### **Examples**

```
Dim(corGaus(), getGroups(Orthodont))

cs1ARMA <- corARMA(0.4, form = ~ 1 | Subject, q = 1)
cs1ARMA <- Initialize(cs1ARMA, data = Orthodont)
Dim(cs1ARMA)</pre>
```

Dim.corStruct

Dimensions of a corStruct Object

### **Description**

if groups is missing, it returns the Dim attribute of object; otherwise, calculates the dimensions associated with the grouping factor.

# Usage

```
## S3 method for class 'corStruct'
Dim(object, groups, ...)
```

### Arguments

object an object inheriting from class "corStruct", representing a correlation structure.

groups an optional factor defining the grouping of the observations; observations within a group are correlated and observations in different groups are uncorrelated.

some methods for this generic require additional arguments. None are used in

this method.

### Value

a list with components:

N length of groups
M number of groups

maxLen maximum number of observations in a group

sumLenSq sum of the squares of the number of observations per group

len an integer vector with the number of observations per group

start an integer vector with the starting position for the observations in each group,

beginning from zero

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

Dim.pdMat 77

## See Also

```
Dim, Dim. corSpatial
```

## **Examples**

```
Dim(corAR1(), getGroups(Orthodont))
```

Dim.pdMat

Dimensions of a pdMat Object

# **Description**

This method function returns the dimensions of the matrix represented by object.

# Usage

```
## S3 method for class 'pdMat'
Dim(object, ...)
```

# **Arguments**

object an object inheriting from class "pdMat", representing a positive-definite matrix.

... some methods for this generic require additional arguments. None are used in this method.

# Value

an integer vector with the number of rows and columns of the matrix represented by object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

Dim

```
Dim(pdSymm(diag(3)))
```

78 Earthquake

Earthquake

Earthquake Intensity

## **Description**

The Earthquake data frame has 182 rows and 5 columns.

#### **Format**

This data frame contains the following columns:

**Quake** an ordered factor with levels 20 < 16 < 14 < 10 < 3 < 8 < 23 < 22 < 6 < 13 < 7 < 21 < 18 < 15 < 4 < 12 < 19 < 5 < 9 < 1 < 2 < 17 < 11 indicating the earthquake on which the measurements were made.

**Richter** a numeric vector giving the intensity of the earthquake on the Richter scale.

**distance** the distance from the seismological measuring station to the epicenter of the earthquake (km).

soil a factor with levels 0 and 1 giving the soil condition at the measuring station, either soil or rock.

accel maximum horizontal acceleration observed (g).

# **Details**

Measurements recorded at available seismometer locations for 23 large earthquakes in western North America between 1940 and 1980. They were originally given in Joyner and Boore (1981); are mentioned in Brillinger (1987); and are analyzed in Davidian and Giltinan (1995).

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.8)

Davidian, M. and Giltinan, D. M. (1995), *Nonlinear Models for Repeated Measurement Data*, Chapman and Hall, London.

Joyner and Boore (1981), Peak horizontal acceleration and velocity from strong-motion records including records from the 1979 Imperial Valley, California, earthquake, *Bulletin of the Seismological Society of America*, **71**, 2011-2038.

Brillinger, D. (1987), Comment on a paper by C. R. Rao, Statistical Science, 2, 448-450.

ergoStool 79

ergoStool

Ergometrics experiment with stool types

## Description

The ergoStool data frame has 36 rows and 3 columns.

#### **Format**

This data frame contains the following columns:

effort a numeric vector giving the effort (Borg scale) required to arise from a stool.

Type a factor with levels T1, T2, T3, and T4 giving the stool type.

Subject an ordered factor giving a unique identifier for the subject in the experiment.

### **Details**

Devore (2000) cites data from an article in *Ergometrics* (1993, pp. 519-535) on "The Effects of a Pneumatic Stool and a One-Legged Stool on Lower Limb Joint Load and Muscular Activity."

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.9)

Devore, J. L. (2000), *Probability and Statistics for Engineering and the Sciences (5th ed)*, Duxbury, Boston, MA.

# **Examples**

```
fm1 <-
   lme(effort ~ Type, data = ergoStool, random = ~ 1 | Subject)
anova( fm1 )</pre>
```

Fatigue

Cracks caused by metal fatigue

### **Description**

The Fatigue data frame has 262 rows and 3 columns.

80 fdHess

### **Format**

This data frame contains the following columns:

**Path** an ordered factor with levels 1 < 2 < 3 < 4 < 5 < 6 < 7 < 8 < 9 < 10 < 11 < 12 < 13 < 14 < 15 < 16 < 17 < 18 < 19 < 20 < 21 giving the test path (or test unit) number. The order is in terms of increasing failure time or decreasing terminal crack length.

cycles number of test cycles at which the measurement is made (millions of cycles).

relLength relative crack length (dimensionless).

#### **Details**

These data are given in Lu and Meeker (1993) where they state "We obtained the data in Table 1 visually from figure 4.5.2 on page 242 of Bogdanoff and Kozin (1985)." The data represent the growth of cracks in metal for 21 test units. An initial notch of length 0.90 inches was made on each unit which then was subjected to several thousand test cycles. After every 10,000 test cycles the crack length was measured. Testing was stopped if the crack length exceeded 1.60 inches, defined as a failure, or at 120,000 cycles.

#### **Source**

Lu, C. Joséph, and Meeker, William Q. (1993), Using degradation measures to estimate a time-to-failure distribution, *Technometrics*, **35**, 161-174

fdHess

Finite difference Hessian

### **Description**

Evaluate an approximate Hessian and gradient of a scalar function using finite differences.

### Usage

### **Arguments**

pars	the numeric values of the parameters at which to evaluate the function fun and its derivatives.
fun	a function depending on the parameters pars that returns a numeric scalar.
	Optional additional arguments to fun
.relStep	The relative step size to use in the finite differences. It defaults to the cube root of .Machine $$double.eps$
minAbsPar	The minimum magnitude of a parameter value that is considered non-zero. It defaults to zero meaning that any non-zero value will be considered different from zero.

fitted.glsStruct 81

### **Details**

This function uses a second-order response surface design known as a "Koschal design" to determine the parameter values at which the function is evaluated.

### Value

### A list with components

mean the value of function fun evaluated at the parameter values pars

gradient an approximate gradient (of length length(pars)).

Hessian a matrix whose upper triangle contains an approximate Hessian.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## **Examples**

fitted.glsStruct

Calculate glsStruct Fitted Values

### Description

The fitted values for the linear model represented by object are extracted.

# Usage

```
## S3 method for class 'glsStruct'
fitted(object, glsFit, ...)
```

### Arguments

object	an object inheriting from class "glsStruct", representing a list of linear model components, such as corStruct and "varFunc" objects.
glsFit	an optional list with components logLik (log-likelihood), beta (coefficients), sigma (standard deviation for error term), varBeta (coefficients' covariance matrix), fitted (fitted values), and residuals (residuals). Defaults to attr(object, "glsFit").
	some methods for this generic require additional arguments. None are used in this method.

82 fitted.gnlsStruct

### Value

a vector with the fitted values for the linear model represented by object.

#### Note

This method function is generally only used inside gls and fitted.gls.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
gls, residuals.glsStruct
```

fitted.gnlsStruct

Calculate gnlsStruct Fitted Values

### **Description**

The fitted values for the nonlinear model represented by object are extracted.

## Usage

```
## S3 method for class 'gnlsStruct'
fitted(object, ...)
```

## **Arguments**

object

an object inheriting from class "gnlsStruct", representing a list of model components, such as corStruct and varFunc objects, and attributes specifying the underlying nonlinear model and the response variable.

. . .

some methods for this generic require additional arguments. None are used in this method.

#### Value

a vector with the fitted values for the nonlinear model represented by object.

### Note

This method function is generally only used inside gnls and fitted.gnls.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

fitted.lme 83

### See Also

```
gnls, residuals.gnlsStruct
```

fitted.lme

Extract lme Fitted Values

## **Description**

The fitted values at level i are obtained by adding together the population fitted values (based only on the fixed effects estimates) and the estimated contributions of the random effects to the fitted values at grouping levels less or equal to i. The resulting values estimate the best linear unbiased predictions (BLUPs) at level i.

### Usage

```
## S3 method for class 'lme'
fitted(object, level, asList, ...)
```

## **Arguments**

object	an object inheriting from class " $1me$ ", representing a fitted linear mixed-effects model.
level	an optional integer vector giving the level(s) of grouping to be used in extracting the fitted values from object. Level values increase from outermost to innermost grouping, with level zero corresponding to the population fitted values. Defaults to the highest or innermost level of grouping.
asList	an optional logical value. If TRUE and a single value is given in level, the returned object is a list with the fitted values split by groups; else the returned value is either a vector or a data frame, according to the length of level. Defaults to FALSE.
	some methods for this generic require additional arguments. None are used in this method.

### Value

If a single level of grouping is specified in level, the returned value is either a list with the fitted values split by groups (asList = TRUE) or a vector with the fitted values (asList = FALSE); else, when multiple grouping levels are specified in level, the returned object is a data frame with columns given by the fitted values at different levels and the grouping factors. For a vector or data frame result the napredict method is applied.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

84 fitted.ImeStruct

### References

Bates, D.M. and Pinheiro, J.C. (1998) "Computational methods for multilevel models" available in PostScript or PDF formats at http://nlme.stat.wisc.edu/pub/NLME/

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 235, 397.

#### See Also

```
lme, residuals.lme
```

### **Examples**

```
fm1 <- lme(distance \sim age + Sex, data = Orthodont, random = \sim 1) fitted(fm1, level = 0:1)
```

fitted.lmeStruct

Calculate lmeStruct Fitted Values

## **Description**

The fitted values at level i are obtained by adding together the population fitted values (based only on the fixed effects estimates) and the estimated contributions of the random effects to the fitted values at grouping levels less or equal to i. The resulting values estimate the best linear unbiased predictions (BLUPs) at level i.

### Usage

```
## S3 method for class 'lmeStruct'
fitted(object, level, conLin, lmeFit, ...)
```

### **Arguments**

object	an object inheriting from class "lmeStruct", representing a list of linear mixed-effects model components, such as reStruct, corStruct, and varFunc objects.
level	an optional integer vector giving the level(s) of grouping to be used in extracting the fitted values from object. Level values increase from outermost to innermost grouping, with level zero corresponding to the population fitted values. Defaults to the highest or innermost level of grouping.
conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying lme model. Defaults to attr(object, "conLin").
lmeFit	an optional list with components beta and b containing respectively the fixed effects estimates and the random effects estimates to be used to calculate the fitted values. Defaults to attr(object, "lmeFit").
	some methods for this generic accept other optional arguments.

fitted.lmList 85

## Value

if a single level of grouping is specified in level, the returned value is a vector with the fitted values at the desired level; else, when multiple grouping levels are specified in level, the returned object is a matrix with columns given by the fitted values at different levels.

#### Note

This method function is generally only used inside lme and fitted.lme.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
lme, fitted.lme, residuals.lmeStruct
```

fitted.lmList

Extract lmList Fitted Values

### **Description**

The fitted values are extracted from each 1m component of object and arranged into a list with as many components as object, or combined into a single vector.

## Usage

```
## S3 method for class 'lmList'
fitted(object, subset, asList, ...)
```

## **Arguments**

object	an object inheriting from class "lmList", representing a list of lm objects with a common model.
subset	an optional character or integer vector naming the 1m components of object from which the fitted values are to be extracted. Default is NULL, in which case all components are used.
asList	an optional logical value. If TRUE, the returned object is a list with the fitted values split by groups; else the returned value is a vector. Defaults to FALSE.
• • •	some methods for this generic require additional arguments. None are used in this method.

# Value

a list with components given by the fitted values of each 1m component of object, or a vector with the fitted values for all 1m components of object.

86 fitted.nlmeStruct

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lmList, residuals.lmList
```

### **Examples**

```
fm1 <- lmList(distance \sim age | Subject, Orthodont) fitted(fm1)
```

fitted.nlmeStruct

Calculate nlmeStruct Fitted Values

### **Description**

The fitted values at level i are obtained by adding together the contributions from the estimated fixed effects and the estimated random effects at levels less or equal to i and evaluating the model function at the resulting estimated parameters. The resulting values estimate the predictions at level i.

## Usage

```
## S3 method for class 'nlmeStruct'
fitted(object, level, conLin, ...)
```

# Arguments

object	an object inheriting from class "nlmeStruct", representing a list of mixed- effects model components, such as reStruct, corStruct, and varFunc objects, plus attributes specifying the underlying nonlinear model and the response vari- able.
level	an optional integer vector giving the level(s) of grouping to be used in extracting the fitted values from object. Level values increase from outermost to innermost grouping, with level zero corresponding to the population fitted values. Defaults to the highest or innermost level of grouping.
conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying nlme

additional arguments that could be given to this method. None are used.

model. Defaults to attr(object, "conLin").

### Value

if a single level of grouping is specified in level, the returned value is a vector with the fitted values at the desired level; else, when multiple grouping levels are specified in level, the returned object is a matrix with columns given by the fitted values at different levels.

fixed.effects 87

### Note

This method function is generally only used inside nlme and fitted.nlme.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# References

Bates, D.M. and Pinheiro, J.C. (1998) "Computational methods for multilevel models" available in PostScript or PDF formats at http://nlme.stat.wisc.edu/pub/NLME/

#### See Also

```
nlme, residuals.nlmeStruct
```

fixed.effects

Extract Fixed Effects

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include lmList and lme.

### Usage

```
fixed.effects(object, ...)
fixef(object, ...)
```

# **Arguments**

object any fitted model object from which fixed effects estimates can be extracted.
... some methods for this generic function require additional arguments.

### Value

will depend on the method function used; see the appropriate documentation.

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
fixef.lmList
```

```
## see the method function documentation
```

88 fixef.lmList

fixef.lmList

Extract lmList Fixed Effects

# Description

The average of the coefficients corresponding to the 1m components of object is calculated.

# Usage

```
## S3 method for class 'lmList'
fixef(object, ...)
```

# Arguments

object an object inheriting from class "lmList", representing a list of lm objects with

a common model.

... some methods for this generic require additional arguments. None are used in

this method.

## Value

a vector with the average of the individual 1m coefficients in object.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
lmList, random.effects.lmList
```

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
fixed.effects(fm1)</pre>
```

formula.pdBlocked 89

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Extract pdBlocked Formula

# Description

The formula attributes of the pdMat elements of x are extracted and returned as a list, in case asList=TRUE, or converted to a single one-sided formula when asList=FALSE. If the pdMat elements do not have a formula attribute, a NULL value is returned.

# Usage

```
## S3 method for class 'pdBlocked'
formula(x, asList, ...)
```

# Arguments

х	an object inheriting from class "pdBlocked", representing a positive definite block diagonal matrix.
asList	an optional logical value. If TRUE, a list with the formulas for the individual block diagonal elements of x is returned; else, if FALSE, a one-sided formula combining all individual formulas is returned. Defaults to FALSE.
	some methods for this generic require additional arguments. None are used in this method.

### Value

a list of one-sided formulas, or a single one-sided formula, or NULL.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
pdBlocked, pdMat
```

```
pd1 <- pdBlocked(list(~ age, ~ Sex - 1))
formula(pd1)
formula(pd1, asList = TRUE)</pre>
```

90 formula.pdMat

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Extract pdMat Formula

# Description

This method function extracts the formula associated with a pdMat object, in which the column and row names are specified.

# Usage

```
## S3 method for class 'pdMat'
formula(x, asList, ...)
```

# **Arguments**

X	an object inheriting from class "pdMat", representing a positive definite matrix.
asList	logical. Should the asList argument be applied to each of the components? Never used. $ \\$
• • •	some methods for this generic require additional arguments. None are used in this method.

## Value

if x has a formula attribute, its value is returned, else NULL is returned.

# Note

Because factors may be present in formula(x), the pdMat object needs to have access to a data frame where the variables named in the formula can be evaluated, before it can resolve its row and column names from the formula.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

pdMat

```
pd1 <- pdSymm(~Sex*age)
formula(pd1)</pre>
```

formula.reStruct 91

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Extract reStruct Object Formula

## **Description**

This method function extracts a formula from each of the components of x, returning a list of formulas.

# Usage

```
## S3 method for class 'reStruct'
formula(x, asList, ...)
```

# Arguments

x	an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.
asList	logical. Should the asList argument be applied to each of the components?
	some methods for this generic require additional arguments. None are used in this method.

## Value

a list with the formulas of each component of x.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

formula

```
rs1 <- reStruct(list(A = pdDiag(diag(2), ~age), B = ~1))
formula(rs1)</pre>
```

92 gapply

|--|

# Description

Applies the function to the distinct sets of rows of the data frame defined by groups.

# Usage

```
gapply(object, which, FUN, form, level, groups, ...)
```

# Arguments

object	an object to which the function will be applied - usually a groupedData object or a data.frame. Must inherit from class "data.frame".
which	an optional character or positive integer vector specifying which columns of object should be used with FUN. Defaults to all columns in object.
FUN	function to apply to the distinct sets of rows of the data frame object defined by the values of groups.
form	an optional one-sided formula that defines the groups. When this formula is given the right-hand side is evaluated in object, converted to a factor if necessary, and the unique levels are used to define the groups. Defaults to formula(object).
level	an optional positive integer giving the level of grouping to be used in an object with multiple nested grouping levels. Defaults to the highest or innermost level of grouping.
groups	an optional factor that will be used to split the rows into groups. Defaults to getGroups(object, form, level).
• • •	optional additional arguments to the summary function FUN. Often it is helpful to specify na.rm = TRUE.

## Value

Returns a data frame with as many rows as there are levels in the groups argument.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. sec. 3.4.

# See Also

gsummary

Gasoline 93

### **Examples**

Gasoline

Refinery yield of gasoline

### **Description**

The Gasoline data frame has 32 rows and 6 columns.

#### **Format**

This data frame contains the following columns:

**yield** a numeric vector giving the percentage of crude oil converted to gasoline after distillation and fractionation

**endpoint** a numeric vector giving the temperature (degrees F) at which all the gasoline is vaporized **Sample** an ordered factor giving the inferred crude oil sample number

**API** a numeric vector giving the crude oil gravity (degrees API)

**vapor** a numeric vector giving the vapor pressure of the crude oil (lbf/in<sup>2</sup>)

**ASTM** a numeric vector giving the crude oil 10% point ASTM—the temperature at which 10% of the crude oil has become vapor.

# Details

Prater (1955) provides data on crude oil properties and gasoline yields. Atkinson (1985) uses these data to illustrate the use of diagnostics in multiple regression analysis. Three of the covariates—API, vapor, and ASTM—measure characteristics of the crude oil used to produce the gasoline. The other covariate — endpoint—is a characteristic of the refining process. Daniel and Wood (1980) notice that the covariates characterizing the crude oil occur in only ten distinct groups and conclude that the data represent responses measured on ten different crude oil samples.

### Source

Prater, N. H. (1955), Estimate gasoline yields from crudes, *Petroleum Refiner*, **35** (5).

Atkinson, A. C. (1985), *Plots, Transformations, and Regression*, Oxford Press, New York.

Daniel, C. and Wood, F. S. (1980), Fitting Equations to Data, Wiley, New York

Venables, W. N. and Ripley, B. D. (2002) *Modern Applied Statistics with S (4th ed)*, Springer, New York.

94 getCovariate

getCovariate A	extract Covariate from an Object	bject

## **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include corStruct, corSpatial, data.frame, and varFunc.

## Usage

```
getCovariate(object, form, data)
```

### **Arguments**

object any object with a covariate component

form an optional one-sided formula specifying the covariate(s) to be extracted. De-

faults to formula(object).

data a data frame in which to evaluate the variables defined in form.

### Value

will depend on the method function used; see the appropriate documentation.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. p. 100.

### See Also

 $\tt getCovariate.corStruct, getCovariate.data.frame, getCovariate.varFunc, getCovariateFormula \\$ 

## **Examples**

## see the method function documentation

getCovariate.corStruct 95

```
getCovariate.corStruct
```

Extract corStruct Object Covariate

### **Description**

This method function extracts the covariate(s) associated with object.

## Usage

```
## S3 method for class 'corStruct'
getCovariate(object, form, data)
```

### **Arguments**

object an object inheriting from class corStruct representing a correlation structure.

form this argument is included to make the method function compatible with the

generic. It will be assigned the value of formula(object) and should not be

modified.

data an optional data frame in which to evaluate the variables defined in form, in case

object is not initialized and the covariate needs to be evaluated.

## Value

when the correlation structure does not include a grouping factor, the returned value will be a vector or a matrix with the covariate(s) associated with object. If a grouping factor is present, the returned value will be a list of vectors or matrices with the covariate(s) corresponding to each grouping level. For spatial correlation structures, this extracts the *distances* implied by the covariates, and excludes 1-observation groups.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
getCovariate
```

```
cs1 <- corAR1(form = ~ 1 | Subject)
getCovariate(cs1, data = Orthodont)</pre>
```

```
getCovariate.data.frame
```

Extract Data Frame Covariate

## **Description**

The right hand side of form, stripped of any conditioning expression (i.e. an expression following a | operator), is evaluated in object.

## Usage

```
## S3 method for class 'data.frame'
getCovariate(object, form, data)
```

# Arguments

object an object inheriting from class data.frame.

form an optional formula specifying the covariate to be evaluated in object. Defaults

to formula(object).

data some methods for this generic require a separate data frame. Not used in this

method.

### Value

the value of the right hand side of form, stripped of any conditional expression, evaluated in object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
getCovariateFormula
```

```
getCovariate(Orthodont)
```

getCovariate.varFunc 97

getCovariate.varFunc Extract varFunc Covariate

# Description

This method function extracts the covariate(s) associated with the variance function represented by object, if any is present.

### Usage

```
## S3 method for class 'varFunc'
getCovariate(object, form, data)
```

# Arguments

object an object inheriting from class varFunc, representing a variance function struc-

ture.

form an optional formula specifying the covariate to be evaluated in object. Defaults

to formula(object).

data some methods for this generic require a data object. Not used in this method.

### Value

if object has a covariate attribute, its value is returned; else NULL is returned.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
covariate<-.varFunc
```

```
vf1 <- varPower(1.1, form = ~age)
covariate(vf1) <- Orthodont[["age"]]
getCovariate(vf1)</pre>
```

98 getData

 ${\tt getCovariateFormula}$ 

Extract Covariates Formula

# Description

The right hand side of formula(object), without any conditioning expressions (i.e. any expressions after a | operator) is returned as a one-sided formula.

# Usage

```
getCovariateFormula(object)
```

# **Arguments**

object

any object from which a formula can be extracted.

### Value

a one-sided formula describing the covariates associated with formula(object).

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
getCovariate
```

# **Examples**

```
getCovariateFormula(y ~ x | g)
getCovariateFormula(y ~ x)
```

getData

Extract Data from an Object

## **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include gls, lme, and lmList.

# Usage

```
getData(object)
```

getData.gls 99

# Arguments

object an object from which a data.frame can be extracted, generally a fitted model

object.

### Value

will depend on the method function used; see the appropriate documentation.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
getData.gls, getData.lme, getData.lmList
```

# **Examples**

## see the method function documentation

getData.gls

Extract gls Object Data

## Description

If present in the calling sequence used to produce object, the data frame used to fit the model is obtained.

## Usage

```
## S3 method for class 'gls'
getData(object)
```

### **Arguments**

object

an object inheriting from class gls, representing a generalized least squares fitted linear model.

# Value

if a data argument is present in the calling sequence that produced object, the corresponding data frame (with na.action and subset applied to it, if also present in the call that produced object) is returned; else, NULL is returned.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

100 getData.lme

### See Also

```
gls, getData
```

### **Examples**

getData.lme

Extract lme Object Data

# Description

If present in the calling sequence used to produce object, the data frame used to fit the model is obtained.

### **Usage**

```
## S3 method for class 'lme'
getData(object)
```

### **Arguments**

object

an object inheriting from class 1me, representing a linear mixed-effects fitted model.

#### Value

if a data argument is present in the calling sequence that produced object, the corresponding data frame (with na.action and subset applied to it, if also present in the call that produced object) is returned; else, NULL is returned.

Note that as from version 3.1-102, this only omits rows omitted in the fit if na.action = na.omit, and does not omit at all if na.action = na.exclude. That is generally what is wanted for plotting, the main use of this function.

### Author(s)

José Pinheiro and Douglas Bates <bate="englast: bates@stat.wisc.edu">

#### See Also

```
lme, getData
```

getData.lmList

getData.lmList

Extract lmList Object Data

# Description

If present in the calling sequence used to produce object, the data frame used to fit the model is obtained.

## Usage

```
## S3 method for class 'lmList'
getData(object)
```

## **Arguments**

object

an object inheriting from class lmList, representing a list of lm objects with a common model.

## Value

if a data argument is present in the calling sequence that produced object, the corresponding data frame (with na.action and subset applied to it, if also present in the call that produced object) is returned; else, NULL is returned.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
lmList, getData
```

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
getData(fm1)</pre>
```

102 getGroups

getGroups Extract Grouping Factors from an Object	
---	--

# Description

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include corStruct, data.frame, gls, lme, lmList, and varFunc.

## Usage

```
getGroups(object, form, level, data, sep)
```

## **Arguments**

object	any object
form	an optional formula with a conditioning expression on its right hand side (i.e. an expression involving the   operator). Defaults to formula(object).
level	a positive integer vector with the level(s) of grouping to be used when multiple nested levels of grouping are present. This argument is optional for most methods of this generic function and defaults to all levels of nesting.
data	a data frame in which to interpret the variables named in form. Optional for most methods.
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is '/'.

### Value

will depend on the method function used; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 100, 461.

## See Also

```
getGroupsFormula, getGroups.data.frame, getGroups.gls, getGroups.lmList, getGroups.lme
```

### **Examples**

## see the method function documentation

getGroups.corStruct 103

# Description

This method function extracts the grouping factor associated with object, if any is present.

## Usage

```
## S3 method for class 'corStruct'
getGroups(object, form, level, data, sep)
```

# Arguments

object	an object inheriting from class corStruct representing a correlation structure.
form	this argument is included to make the method function compatible with the generic. It will be assigned the value of formula(object) and should not be modified.
level	this argument is included to make the method function compatible with the generic and is not used.
data	an optional data frame in which to evaluate the variables defined in form, in case object is not initialized and the grouping factor needs to be evaluated.
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is '/'.

### Value

if a grouping factor is present in the correlation structure represented by object, the function returns the corresponding factor vector; else the function returns NULL.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
getGroups
```

```
cs1 <- corAR1(form = ~ 1 | Subject)
getGroups(cs1, data = Orthodont)</pre>
```

104 getGroups.data.frame

## **Description**

Each variable named in the expression after the | operator on the right hand side of form is evaluated in object. If more than one variable is indicated in level they are combined into a data frame; else the selected variable is returned as a vector. When multiple grouping levels are defined in form and level > 1, the levels of the returned factor are obtained by pasting together the levels of the grouping factors of level greater or equal to level, to ensure their uniqueness.

## Usage

```
## S3 method for class 'data.frame'
getGroups(object, form, level, data, sep)
```

# **Arguments**

object	an object inheriting from class data.frame.
form	an optional formula with a conditioning expression on its right hand side (i.e. an expression involving the   operator). Defaults to formula(object).
level	a positive integer vector with the level(s) of grouping to be used when multiple nested levels of grouping are present. Defaults to all levels of nesting.
data	unused
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is '/'.

### Value

either a data frame with columns given by the grouping factors indicated in level, from outer to inner, or, when a single level is requested, a factor representing the selected grouping factor.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 100, 461.

#### See Also

```
getGroupsFormula
```

getGroups.gls 105

# **Examples**

```
getGroups(Pixel)
getGroups(Pixel, level = 2)
```

getGroups.gls

Extract gls Object Groups

# Description

If present, the grouping factor associated to the correlation structure for the linear model represented by object is extracted.

# Usage

```
## S3 method for class 'gls'
getGroups(object, form, level, data, sep)
```

# Arguments

object	an object inheriting from class gls, representing a generalized least squares fitted linear model.
form	an optional formula with a conditioning expression on its right hand side (i.e. an expression involving the   operator). Defaults to formula(object). Not used.
level	a positive integer vector with the level(s) of grouping to be used when multiple nested levels of grouping are present. This argument is optional for most methods of this generic function and defaults to all levels of nesting. Not used.
data	a data frame in which to interpret the variables named in form. Optional for most methods. Not used.
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is '/'. Not used.

# Value

if the linear model represented by object incorporates a correlation structure and the corresponding corStruct object has a grouping factor, a vector with the group values is returned; else, NULL is returned.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
gls, corClasses
```

106 getGroups.lme

### **Examples**

getGroups.lme

Extract lme Object Groups

## **Description**

The grouping factors corresponding to the linear mixed-effects model represented by object are extracted. If more than one level is indicated in level, the corresponding grouping factors are combined into a data frame; else the selected grouping factor is returned as a vector.

# Usage

```
## S3 method for class 'lme'
getGroups(object, form, level, data, sep)
```

### **Arguments**

object	an object inheriting from class $lme$ , representing a fitted linear mixed-effects model.
form	this argument is included to make the method function compatible with the generic and is ignored in this method.
level	an optional integer vector giving the level(s) of grouping to be extracted from object. Defaults to the highest or innermost level of grouping.
data	unused
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is '/'.

### Value

either a data frame with columns given by the grouping factors indicated in level, or, when a single level is requested, a factor representing the selected grouping factor.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

1me

getGroups.lmList 107

# **Examples**

```
fm1 <- lme(pixel ~ day + day^2, Pixel,
  random = list(Dog = ~day, Side = ~1))
getGroups(fm1, level = 1:2)</pre>
```

getGroups.lmList

Extract lmList Object Groups

# Description

The grouping factor determining the partitioning of the observations used to produce the 1m components of object is extracted.

# Usage

```
## S3 method for class 'lmList'
getGroups(object, form, level, data, sep)
```

# **Arguments**

object	an object inheriting from class ${\tt lmList}$ , representing a list of ${\tt lm}$ objects with a common model.
form	an optional formula with a conditioning expression on its right hand side (i.e. an expression involving the   operator). Defaults to formula(object). Not used.
level	a positive integer vector with the level(s) of grouping to be used when multiple nested levels of grouping are present. This argument is optional for most methods of this generic function and defaults to all levels of nesting. Not used.
data	a data frame in which to interpret the variables named in form. Optional for most methods. Not used.
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is '/'. Not used.

# Value

a vector with the grouping factor corresponding to the 1m components of object.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

 ${\tt lmList}$ 

```
fm1 <- lmList(distance \sim age | Subject, Orthodont) getGroups(fm1)
```

108 getGroups.varFunc

# Description

This method function extracts the grouping factor associated with the variance function represented by object, if any is present.

## Usage

```
## S3 method for class 'varFunc'
getGroups(object, form, level, data, sep)
```

# Arguments

object	an object inheriting from class varFunc, representing a variance function structure.
form	an optional formula with a conditioning expression on its right hand side (i.e. an expression involving the   operator). Defaults to formula(object). Not used.
level	a positive integer vector with the level(s) of grouping to be used when multiple nested levels of grouping are present. This argument is optional for most methods of this generic function and defaults to all levels of nesting. Not used.
data	a data frame in which to interpret the variables named in form. Optional for most methods. Not used.
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is '/'. Not used.

### Value

if object has a groups attribute, its value is returned; else NULL is returned.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

```
vf1 <- varPower(form = ~ age | Sex)
vf1 <- Initialize(vf1, Orthodont)
getGroups(vf1)</pre>
```

getGroupsFormula 109

# Description

The conditioning expression associated with formula(object) (i.e. the expression after the | operator) is returned either as a named list of one-sided formulas, or a single one-sided formula, depending on the value of asList. The components of the returned list are ordered from outermost to innermost level and are named after the grouping factor expression.

# Usage

```
getGroupsFormula(object, asList, sep)
```

# Arguments

object	any object from which a formula can be extracted.
asList	an optional logical value. If TRUE the returned value with be a list of formulas; else, if FALSE the returned value will be a one-sided formula. Defaults to FALSE.
sep	character, the separator to use between group levels when multiple levels are collapsed. The default is $'/'$ .

### Value

a one-sided formula, or a list of one-sided formulas, with the grouping structure associated with formula(object). If no conditioning expression is present in formula(object) a NULL value is returned.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

getGroupsFormula. 1mList, getGroupsFormula. 1mList, getGroupsFormula. 1me, getGroupsFormula. reStruct, getGroups

# Examples

```
getGroupsFormula(y \sim x \mid g1/g2)
```

110 getResponseFormula

getResponse

Extract Response Variable from an Object

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include data.frame, gls, lme, and lmList.

# Usage

```
getResponse(object, form)
```

### **Arguments**

object any object

form an optional two-sided formula. Defaults to formula(object).

#### Value

will depend on the method function used; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

getResponseFormula

# **Examples**

getResponse(Orthodont)

getResponseFormula

Extract Formula Specifying Response Variable

# Description

The left hand side of formula{object} is returned as a one-sided formula.

### Usage

```
getResponseFormula(object)
```

# **Arguments**

object

any object from which a formula can be extracted.

getVarCov 111

# Value

a one-sided formula with the response variable associated with formula{object}.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
getResponse
```

### **Examples**

```
getResponseFormula(y \sim x \mid g)
```

getVarCov

Extract variance-covariance matrix

### **Description**

Extract the variance-covariance matrix from a fitted model, such as a mixed-effects model.

# Usage

```
getVarCov(obj, ...)
## S3 method for class 'lme'
getVarCov(obj, individuals,
         type = c("random.effects", "conditional", "marginal"), ...)
## S3 method for class 'gls'
getVarCov(obj, individual = 1, ...)
```

# **Arguments**

obj	A fitted model. Methods are available for models fit by 1me and by g1s
individuals	For models fit by lme a vector of levels of the grouping factor can be specified for the conditional or marginal variance-covariance matrices.
individual	For models fit by gls the only type of variance-covariance matrix provided is the marginal variance-covariance of the responses by group. The optional argument individual specifies the group of responses.
type	For models fit by lme the type argument specifies the type of variance-covariance matrix, either "random.effects" for the random-effects variance-covariance (the default), or "conditional" for the conditional. variance-covariance of the responses or "marginal" for the marginal variance-covariance of the responses.
	Optional arguments for some methods, as described above

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# Value

A variance-covariance matrix or a list of variance-covariance matrices.

### Author(s)

Mary Lindstrom dindstro@biostat.wisc.edu>

### See Also

```
1me, gls
```

# **Examples**

gls

Fit Linear Model Using Generalized Least Squares

# **Description**

This function fits a linear model using generalized least squares. The errors are allowed to be correlated and/or have unequal variances.

### Usage

# Arguments

object	an object inheriting from class "gls", representing a generalized least squares fitted linear model.
model	a two-sided linear formula object describing the model, with the response on the left of a $\sim$ operator and the terms, separated by + operators, on the right.
model.	Changes to the model – see update.formula for details.
data	an optional data frame containing the variables named in model, correlation, weights, and subset. By default the variables are taken from the environment from which gls is called.

gls 113

correlation	an optional corStruct object describing the within-group correlation structure. See the documentation of corClasses for a description of the available corStruct classes. If a grouping variable is to be used, it must be specified in the form argument to the corStruct constructor. Defaults to NULL, corresponding to uncorrelated errors.
weights	an optional varFunc object or one-sided formula describing the within-group heteroscedasticity structure. If given as a formula, it is used as the argument to varFixed, corresponding to fixed variance weights. See the documentation on varClasses for a description of the available varFunc classes. Defaults to NULL, corresponding to homoscedastic errors.
subset	an optional expression indicating which subset of the rows of data should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
method	a character string. If "REML" the model is fit by maximizing the restricted log-likelihood. If "ML" the log-likelihood is maximized. Defaults to "REML".
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes gls to print an error message and terminate if there are any incomplete observations.
control	a list of control values for the estimation algorithm to replace the default values returned by the function glsControl. Defaults to an empty list.
verbose	an optional logical value. If TRUE information on the evolution of the iterative algorithm is printed. Default is FALSE.
• • •	some methods for this generic require additional arguments. None are used in this method.
evaluate	If TRUE evaluate the new call else return the call.

# **Details**

offset terms in model are an error since 3.1-157 (2022-03): previously they were silently ignored.

### Value

an object of class "gls" representing the linear model fit. Generic functions such as print, plot, and summary have methods to show the results of the fit. See glsObject for the components of the fit. The functions resid, coef and fitted, can be used to extract some of its components.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

The different correlation structures available for the correlation argument are described in Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994), Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996), and Venables, W.N. and Ripley, B.D. (2002). The use of variance functions

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for linear and nonlinear models is presented in detail in Carroll, R.J. and Ruppert, D. (1988) and Davidian, M. and Giltinan, D.M. (1995).

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Carroll, R.J. and Ruppert, D. (1988) "Transformation and Weighting in Regression", Chapman and Hall.

Davidian, M. and Giltinan, D.M. (1995) "Nonlinear Mixed Effects Models for Repeated Measurement Data", Chapman and Hall.

Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 100, 461.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

### See Also

```
corClasses, glsControl, glsObject, glsStruct, plot.gls, predict.gls, qqnorm.gls, residuals.gls, summary.gls, varClasses, varFunc
```

### **Examples**

glsControl

Control Values for gls Fit

### Description

The values supplied in the function call replace the defaults and a list with all possible arguments is returned. The returned list is used as the control argument to the gls function.

## Usage

glsControl 115

# Arguments

maxIter	maximum number of iterations for the gls optimization algorithm. Default is 50.
msMaxIter	maximum number of iterations for the optimization step inside the gls optimization. Default is 50.
tolerance	tolerance for the convergence criterion in the gls algorithm. Default is 1e-6.
msTol	tolerance for the convergence criterion of the first outer iteration when optim is used. Default is 1e-7.
msVerbose	a logical value passed as the trace control value to the chosen optimizer (see documentation on that function). Default is FALSE.
singular.ok	a logical value indicating whether non-estimable coefficients (resulting from linear dependencies among the columns of the regression matrix) should be allowed. Default is FALSE.
returnObject	a logical value indicating whether the fitted object should be returned when the maximum number of iterations is reached without convergence of the algorithm. Default is FALSE.
apVar	a logical value indicating whether the approximate covariance matrix of the variance-covariance parameters should be calculated. Default is TRUE.
.relStep	relative step for numerical derivatives calculations. Default is .Machine\$double.eps^(1/3).
opt	the optimizer to be used, either "nlminb" (the current default) or "optim" (the previous default).
optimMethod	character - the optimization method to be used with the optim optimizer. The default is "BFGS". An alternative is "L-BFGS-B".
minAbsParApVar	numeric value - minimum absolute parameter value in the approximate variance calculation. The default is 0.05.
natural	logical. Should the natural parameterization be used for the approximate variance calculations? Default is TRUE.
sigma	optionally a positive number to fix the residual error at. If $NULL$ , as by default, or $\emptyset$ , sigma is estimated.

# Value

a list with components for each of the possible arguments.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>; the sigma option: Siem Heisterkamp and Bert van Willigen.

# See Also

gls

116 glsObject

### **Examples**

# decrease the maximum number of iterations and request tracing
glsControl(msMaxIter = 20, msVerbose = TRUE)

gls0bject

Fitted gls Object

### **Description**

An object returned by the gls function, inheriting from class "gls" and representing a generalized least squares fitted linear model. Objects of this class have methods for the generic functions anova, coef, fitted, formula, getGroups, getResponse, intervals, logLik, plot, predict, print, residuals, summary, and update.

#### Value

The following components must be included in a legitimate "gls" object.

apVar an approximate covariance matrix for the variance-covariance coefficients. If

apVar = FALSE in the list of control values used in the call to gls, this component

is equal to NULL.

call a list containing an image of the gls call that produced the object.

coefficients a vector with the estimated linear model coefficients.

contrasts a list of the contrast matrices used to represent factors in the model formula.

This information is important for making predictions from a new data frame in which not all levels of the original factors are observed. If no factors are used in

the model, this component will be an empty list.

dims a list with basic dimensions used in the model fit, including the components N -

the number of observations in the data and p - the number of coefficients in the

linear model.

fitted a vector with the fitted values.

modelStruct an object inheriting from class glsStruct, representing a list of linear model

components, such as corStruct and varFunc objects.

groups the correlation structure grouping factor, if any is present.

logLik the log-likelihood at convergence.

method the estimation method: either "ML" for maximum likelihood, or "REML" for re-

stricted maximum likelihood.

numIter the number of iterations used in the iterative algorithm.

residuals a vector with the residuals.

sigma the estimated residual standard error.

varBeta an approximate covariance matrix of the coefficients estimates.

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### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
gls, glsStruct
```

glsStruct

Generalized Least Squares Structure

# **Description**

A generalized least squares structure is a list of model components representing different sets of parameters in the linear model. A glsStruct may contain corStruct and varFunc objects. NULL arguments are not included in the glsStruct list.

# Usage

```
glsStruct(corStruct, varStruct)
```

# Arguments

corStruct an optional corStruct object, representing a correlation structure. Default is

NULL.

varStruct an optional varFunc object, representing a variance function structure. Default

is NULL.

#### Value

a list of model variance-covariance components determining the parameters to be estimated for the associated linear model.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
corClasses, gls, residuals.glsStruct, varFunc
```

# **Examples**

```
gls1 <- glsStruct(corAR1(), varPower())</pre>
```

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Glucose

Glucose levels over time

# **Description**

The Glucose data frame has 378 rows and 4 columns.

#### **Format**

This data frame contains the following columns:

**Subject** an ordered factor with levels 6 < 2 < 3 < 5 < 1 < 4

Time a numeric vector

conc a numeric vector of glucose levels

Meal an ordered factor with levels 2am < 6am < 10am < 2pm < 6pm < 10pm

#### **Source**

Hand, D. and Crowder, M. (1996), *Practical Longitudinal Data Analysis*, Chapman and Hall, London.

Glucose2

Glucose Levels Following Alcohol Ingestion

# Description

The Glucose2 data frame has 196 rows and 4 columns.

### **Format**

This data frame contains the following columns:

Subject a factor with levels 1 to 7 identifying the subject whose glucose level is measured.

Date a factor with levels 1 2 indicating the occasion in which the experiment was conducted.

**Time** a numeric vector giving the time since alcohol ingestion (in min/10).

glucose a numeric vector giving the blood glucose level (in mg/dl).

### **Details**

Hand and Crowder (Table A.14, pp. 180-181, 1996) describe data on the blood glucose levels measured at 14 time points over 5 hours for 7 volunteers who took alcohol at time 0. The same experiment was repeated on a second date with the same subjects but with a dietary additive used for all subjects.

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#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.10)

Hand, D. and Crowder, M. (1996), *Practical Longitudinal Data Analysis*, Chapman and Hall, London.

gnls

Fit Nonlinear Model Using Generalized Least Squares

## **Description**

This function fits a nonlinear model using generalized least squares. The errors are allowed to be correlated and/or have unequal variances.

### Usage

```
gnls(model, data, params, start, correlation, weights, subset,
    na.action, naPattern, control, verbose)
```

#### **Arguments**

model a two-sided formula object describing the model, with the response on the left

of a ~ operator and a nonlinear expression involving parameters and covariates on the right. If data is given, all names used in the formula should be defined

as parameters or variables in the data frame.

data an optional data frame containing the variables named in model, correlation,

weights, subset, and naPattern. By default the variables are taken from the

environment from which gnls is called.

params an optional two-sided linear formula of the form p1+...+pn~x1+...+xm, or list

of two-sided formulas of the form  $p1\sim x1+\ldots+xm$ , with possibly different models for each parameter. The  $p1,\ldots,pn$  represent parameters included on the right hand side of model and  $x1+\ldots+xm$  define a linear model for the parameters (when the left hand side of the formula contains several parameters, they are all assumed to follow the same linear model described by the right hand side expression). A 1 on the right hand side of the formula(s) indicates a single fixed effects for the corresponding parameter(s). By default, the parameters are

obtained from the names of start.

start an optional named list, or numeric vector, with the initial values for the param-

eters in model. It can be omitted when a selfStarting function is used in model, in which case the starting estimates will be obtained from a single call to

the nls function.

correlation an optional corStruct object describing the within-group correlation struc-

ture. See the documentation of corClasses for a description of the available corStruct classes. If a grouping variable is to be used, it must be specified in the form argument to the corStruct constructor. Defaults to NULL, correspond-

ing to uncorrelated errors.

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weights an optional varFunc object or one-sided formula describing the within-group heteroscedasticity structure. If given as a formula, it is used as the argument to varFixed, corresponding to fixed variance weights. See the documentation on varClasses for a description of the available varFunc classes. Defaults to NULL, corresponding to homoscedastic errors. subset an optional expression indicating which subset of the rows of data should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default. na.action a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes gnls to print an error message and terminate if there are any incomplete observations. an expression or formula object, specifying which returned values are to be renaPattern garded as missing. control a list of control values for the estimation algorithm to replace the default values returned by the function gnlsControl. Defaults to an empty list. an optional logical value. If TRUE information on the evolution of the iterative verbose algorithm is printed. Default is FALSE.

#### Value

an object of class gnls, also inheriting from class gls, representing the nonlinear model fit. Generic functions such as print, plot and summary have methods to show the results of the fit. See gnlsObject for the components of the fit. The functions resid, coef, and fitted can be used to extract some of its components.

#### Author(s)

José Pinheiro and Douglas Bates <bate date : du>

## References

The different correlation structures available for the correlation argument are described in Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994), Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996), and Venables, W.N. and Ripley, B.D. (2002). The use of variance functions for linear and nonlinear models is presented in detail in Carrol, R.J. and Rupert, D. (1988) and Davidian, M. and Giltinan, D.M. (1995).

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Carrol, R.J. and Rupert, D. (1988) "Transformation and Weighting in Regression", Chapman and Hall.

Davidian, M. and Giltinan, D.M. (1995) "Nonlinear Mixed Effects Models for Repeated Measurement Data", Chapman and Hall.

Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996) "SAS Systems for Mixed Models", SAS Institute.

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Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

# See Also

corClasses, gnlsControl, gnlsObject, gnlsStruct, predict.gnls, varClasses, varFunc

# Examples

gnlsControl

Control Values for gnls Fit

### **Description**

The values supplied in the function call replace the defaults and a list with all possible arguments is returned. The returned list is used as the control argument to the gnls function.

# Usage

#### **Arguments**

maxIter	maximum number of iterations for the gnls optimization algorithm. Default is 50.
nlsMaxIter	maximum number of iterations for the nls optimization step <i>inside</i> the gnls optimization. Default is 7.
msMaxIter	maximum number of iterations for the optimization step inside the gnls optimization. Default is 50.
minScale	minimum factor by which to shrink the default step size in an attempt to decrease the sum of squares in the nls step. Default 0.001.
tolerance	tolerance for the convergence criterion in the gnls algorithm. Default is 1e-6.
nlsTol	tolerance for the convergence criterion in nls step. Default is 1e-3.
msTol	tolerance for the convergence criterion of the first outer iteration when optim is used. Default is 1e-7.

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a logical value indicating whether the fitted object should be returned with a returnObject warning (instead of an error via stop()) when the maximum number of iterations is reached without convergence of the algorithm. msVerbose a logical value passed as the trace argument to the optimizer chosen by opt; see documentation on that. Default is FALSE. a logical value indicating whether the approximate covariance matrix of the apVar variance-covariance parameters should be calculated. Default is TRUE. .relStep relative step for numerical derivatives calculations. Default is .Machine\$double.eps^(1/3) (about 6e-6). the optimizer to be used, either "nlminb" (the current default) or "optim" (the opt previous default). character - the optimization method to be used with the optim optimizer. The optimMethod default is "BFGS". An alternative is "L-BFGS-B". minAbsParApVar numeric value - minimum absolute parameter value in the approximate variance calculation. The default is 0.05. sigma optionally a positive number to fix the residual error at. If NULL, as by default,

#### Value

a list with components for each of the possible arguments.

or 0, sigma is estimated.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>; the sigma option: Siem Heisterkamp and Bert van Willigen.

### See Also

gnls

#### **Examples**

# decrease the maximum number of iterations and request tracing
gnlsControl(msMaxIter = 20, msVerbose = TRUE)

gnlsObject Fitted gnls Object

### **Description**

An object returned by the gnls function, inheriting from class "gnls" and also from class "gls", and representing a generalized nonlinear least squares fitted model. Objects of this class have methods for the generic functions anova, coef, fitted, formula, getGroups, getResponse, intervals, logLik, plot, predict, print, residuals, summary, and update.

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#### Value

The following components must be included in a legitimate "gnls" object.

apVar an approximate covariance matrix for the variance-covariance coefficients. If

apVar = FALSE in the control values used in the call to gnls, this component is

equal to NULL.

call a list containing an image of the gnls call that produced the object.

coefficients a vector with the estimated nonlinear model coefficients.

contrasts a list of the contrast matrices used to represent factors in the model formula.

This information is important for making predictions from a new data frame in which not all levels of the original factors are observed. If no factors are used in

the model, this component will be an empty list.

dims a list with basic dimensions used in the model fit, including the components N -

the number of observations used in the fit and p - the number of coefficients in

the nonlinear model.

fitted a vector with the fitted values.

modelStruct an object inheriting from class gnlsStruct, representing a list of model com-

ponents, such as corStruct and varFunc objects.

groups a vector with the correlation structure grouping factor, if any is present.

logLik the log-likelihood at convergence.

numIter the number of iterations used in the iterative algorithm.

plist

pmap

residuals a vector with the residuals.

sigma the estimated residual standard error.

varBeta an approximate covariance matrix of the coefficients estimates.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
gnls, gnlsStruct
```

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gnlsStruct (	Generalized Nonlinear Least Squares Structure
--------------	---

# Description

A generalized nonlinear least squares structure is a list of model components representing different sets of parameters in the nonlinear model. A gnlsStruct may contain corStruct and varFunc objects. NULL arguments are not included in the gnlsStruct list.

## Usage

```
gnlsStruct(corStruct, varStruct)
```

# Arguments

corStruct an optional corStruct object, representing a correlation structure. Default is

NULL.

varStruct an optional varFunc object, representing a variance function structure. Default

is NULL.

# Value

a list of model variance-covariance components determining the parameters to be estimated for the associated nonlinear model.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
gnls, corClasses, residuals.gnlsStruct varFunc
```

# **Examples**

```
gnls1 <- gnlsStruct(corAR1(), varPower())</pre>
```

groupedData 125

groupedData

Construct a groupedData Object

# **Description**

An object of the groupedData class is constructed from the formula and data by attaching the formula as an attribute of the data, along with any of outer, inner, labels, and units that are given. If order groups is TRUE the grouping factor is converted to an ordered factor with the ordering determined by FUN. Depending on the number of grouping levels and the type of primary covariate, the returned object will be of one of three classes: nfnGroupedData - numeric covariate, single level of nesting; nffGroupedData - factor covariate, single level of nesting; and nmGroupedData - multiple levels of nesting. Several modeling and plotting functions can use the formula stored with a groupedData object to construct default plots and models.

# Usage

# **Arguments**

object an object inheriting from class groupedData.

formula a formula of the form resp ~ cov | group where resp is the response, cov is

the primary covariate, and group is the grouping factor. The expression 1 can be used for the primary covariate when there is no other suitable candidate. Multiple nested grouping factors can be listed separated by the / symbol as in fact1/fact2. In an expression like this the fact2 factor is nested within the

fact1 factor.

data a data frame in which the expressions in formula can be evaluated. The result-

ing groupedData object will consist of the same data values in the same order

but with additional attributes.

order.groups an optional logical value, or list of logical values, indicating if the grouping

factors should be converted to ordered factors according to the function FUN applied to the response from each group. If multiple levels of grouping are present, this argument can be either a single logical value (which will be repeated for all grouping levels) or a list of logical values. If no names are assigned to the list elements, they are assumed in the same order as the group levels (outermost to innermost grouping). Ordering within a level of grouping is done within the levels of the grouping factors which are outer to it. Changing the grouping factor to an ordered factor does not affect the ordering of the rows in the data frame but it does affect the order of the panels in a trellis display of the data or models

fitted to the data. Defaults to TRUE.

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FUN an

an optional summary function that will be applied to the values of the response for each level of the grouping factor, when order.groups = TRUE, to determine the ordering. Defaults to the max function.

outer

an optional one-sided formula, or list of one-sided formulas, indicating covariates that are outer to the grouping factor(s). If multiple levels of grouping are present, this argument can be either a single one-sided formula, or a list of one-sided formulas. If no names are assigned to the list elements, they are assumed in the same order as the group levels (outermost to innermost grouping). An outer covariate is invariant within the sets of rows defined by the grouping factor. Ordering of the groups is done in such a way as to preserve adjacency of groups with the same value of the outer variables. When plotting a groupedData object, the argument outer = TRUE causes the panels to be determined by the outer formula. The points within the panels are associated by level of the grouping factor. Defaults to NULL, meaning that no outer covariates are present.

inner

an optional one-sided formula, or list of one-sided formulas, indicating covariates that are inner to the grouping factor(s). If multiple levels of grouping are present, this argument can be either a single one-sided formula, or a list of one-sided formulas. If no names are assigned to the list elements, they are assumed in the same order as the group levels (outermost to innermost grouping). An inner covariate can change within the sets of rows defined by the grouping factor. An inner formula can be used to associate points in a plot of a groupedData object. Defaults to NULL, meaning that no inner covariates are present.

labels

an optional list of character strings giving labels for the response and the primary covariate. The label for the primary covariate is named x and that for the response is named y. Either label can be omitted.

units

an optional list of character strings giving the units for the response and the primary covariate. The units string for the primary covariate is named x and that for the response is named y. Either units string can be omitted.

. . .

some methods for this generic require additional arguments. None are used in this method.

### Value

an object of one of the classes nfnGroupedData, nffGroupedData, or nmGroupedData, and also inheriting from classes groupedData and data.frame.

### Author(s)

Douglas Bates and José Pinheiro

#### References

Bates, D.M. and Pinheiro, J.C. (1997), "Software Design for Longitudinal Data Analysis", in "Modelling Longitudinal and Spatially Correlated Data: Methods, Applications and Future Directions", T.G. Gregoire (ed.), Springer-Verlag, New York. doi:10.1007/9781461206996\_4

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

gsummary 127

#### See Also

formula, gapply, gsummary, lme, plot.nffGroupedData, plot.nfnGroupedData, plot.nmGroupedData,
reStruct

### **Examples**

```
Orth.new <- # create a new copy of the groupedData object
 groupedData( distance ~ age | Subject,
              data = as.data.frame( Orthodont ),
             FUN = mean,
              outer = ~ Sex,
              labels = list( x = "Age",
               y = "Distance from pituitary to pterygomaxillary fissure" ),
              units = list(x = "(yr)", y = "(mm)"))
                         # trellis plot by Subject
plot( Orth.new )
formula( Orth.new )
                        # extractor for the formula
gsummary( Orth.new )
                        # apply summary by Subject
fm1 <- lme( Orth.new ) # fixed and groups formulae extracted from object</pre>
Orthodont2 <- update(Orthodont, FUN = mean)
```

gsummary

Summarize by Groups

# Description

Provide a summary of the variables in a data frame by groups of rows. This is most useful with a groupedData object to examine the variables by group.

## Usage

```
gsummary(object, FUN, omitGroupingFactor, form, level,
   groups, invariantsOnly, ...)
```

### Arguments

object FUN an object to be summarized - usually a groupedData object or a data.frame. an optional summary function or a list of summary functions to be applied to each variable in the frame. The function or functions are applied only to variables in object that vary within the groups defined by groups. Invariant variables in object that vary within the groups defined by groups.

ables in object that vary within the groups defined by groups. Invariant variables are always summarized by group using the unique value that they assume within that group. If FUN is a single function it will be applied to each non-invariant variable by group to produce the summary for that variable. If FUN is a list of functions, the names in the list should designate classes of variables in the frame such as ordered, factor, or numeric. The indicated function will be applied to any non-invariant variables of that class. The default functions to be used are mean for numeric factors, and Mode for both factor and ordered. The Mode function, defined internally in gsummary, returns the modal or most popular value of the variable. It is different from the mode function that returns the S-language mode of the variable.

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omitGroupingFactor

an optional logical value. When TRUE the grouping factor itself will be omitted from the group-wise summary but the levels of the grouping factor will continue to be used as the row names for the data frame that is produced by the summary.

Defaults to FALSE.

form an optional one-sided formula that defines the groups. When this formula is

given, the right-hand side is evaluated in object, converted to a factor if neces-

sary, and the unique levels are used to define the groups. Defaults to formula(object).

level an optional positive integer giving the level of grouping to be used in an object

with multiple nested grouping levels. Defaults to the highest or innermost level

of grouping.

groups an optional factor that will be used to split the rows into groups. Defaults to

getGroups(object, form, level).

invariantsOnly an optional logical value. When TRUE only those covariates that are invariant

within each group will be summarized. The summary value for the group is always the unique value taken on by that covariate within the group. The columns in the summary are of the same class as the corresponding columns in object. By definition, the grouping factor itself must be an invariant. When combined with omitGroupingFactor = TRUE, this option can be used to discover is there

are invariant covariates in the data frame. Defaults to FALSE.

.. optional additional arguments to the summary functions that are invoked on the

variables by group. Often it is helpful to specify na.rm = TRUE.

## Value

A data.frame with one row for each level of the grouping factor. The number of columns is at most the number of columns in object.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

summary, groupedData, getGroups

### **Examples**

```
gsummary(Orthodont) # default summary by Subject
## gsummary with invariantsOnly = TRUE and omitGroupingFactor = TRUE
## determines whether there are covariates like Sex that are invariant
## within the repeated observations on the same Subject.
gsummary(Orthodont, invariantsOnly = TRUE, omitGroupingFactor = TRUE)
```

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Gun

Methods for firing naval guns

# **Description**

The Gun data frame has 36 rows and 4 columns.

#### **Format**

This data frame contains the following columns:

rounds a numeric vector

Method a factor with levels M1 M2

**Team** an ordered factor with levels T1S < T3S < T2S < T1A < T2A < T3A < T1H < T3H < T2H

**Physique** an ordered factor with levels Slight < Average < Heavy

#### **Details**

Hicks (p.180, 1993) reports data from an experiment on methods for firing naval guns. Gunners of three different physiques (slight, average, and heavy) tested two firing methods. Both methods were tested twice by each of nine teams of three gunners with identical physique. The response was the number of rounds fired per minute.

### **Source**

Hicks, C. R. (1993), Fundamental Concepts in the Design of Experiments (4th ed), Harcourt Brace, New York.

IGF

Radioimmunoassay of IGF-I Protein

# **Description**

The IGF data frame has 237 rows and 3 columns.

### **Format**

This data frame contains the following columns:

Lot an ordered factor giving the radioactive tracer lot.

age a numeric vector giving the age (in days) of the radioactive tracer.

conc a numeric vector giving the estimated concentration of IGF-I protein (ng/ml)

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### **Details**

Davidian and Giltinan (1995) describe data obtained during quality control radioimmunoassays for ten different lots of radioactive tracer used to calibrate the Insulin-like Growth Factor (IGF-I) protein concentration measurements.

#### Source

Davidian, M. and Giltinan, D. M. (1995), *Nonlinear Models for Repeated Measurement Data*, Chapman and Hall, London.

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.11)

Initialize

Initialize Object

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: corStruct, lmeStruct, reStruct, and varFunc.

# Usage

```
Initialize(object, data, ...)
```

### **Arguments**

object	any object requiring initialization, e.g. "plug-in" structures such as corStruct and varFunc objects.
data	a data frame to be used in the initialization procedure.
	some methods for this generic function require additional arguments.

### Value

an initialized object with the same class as object. Changes introduced by the initialization procedure will depend on the method function used; see the appropriate documentation.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

Initialize.corStruct 131

### See Also

Initialize. corStruct, Initialize. lmeStruct, Initialize. glsStruct, Initialize. varFunc, is Initialized

# **Examples**

## see the method function documentation

# **Description**

This method initializes object by evaluating its associated covariate(s) and grouping factor, if any is present, in data, calculating various dimensions and constants used by optimization algorithms involving corStruct objects (see the appropriate Dim method documentation), and assigning initial values for the coefficients in object, if none were present.

# Usage

```
## S3 method for class 'corStruct'
Initialize(object, data, ...)
```

# Arguments

object	an object inheriting from class "corStruct" representing a correlation structure.
data	a data frame in which to evaluate the variables defined in formula(object).
	this argument is included to make this method compatible with the generic.

### Value

an initialized object with the same class as object representing a correlation structure.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

### See Also

Dim.corStruct

132 Initialize.glsStruct

# **Examples**

```
cs1 <- corAR1(form = ~ 1 | Subject)
cs1 <- Initialize(cs1, data = Orthodont)</pre>
```

# Description

The individual linear model components of the glsStruct list are initialized.

# Usage

```
## S3 method for class 'glsStruct'
Initialize(object, data, control, ...)
```

# Arguments

object	an object inheriting from class "glsStruct", representing a list of linear model components, such as corStruct and varFunc objects.
data	a data frame in which to evaluate the variables defined in formula(object).
control	an optional list with control parameters for the initialization and optimization algorithms used in gls. Defaults to list(singular.ok = FALSE), implying that linear dependencies are not allowed in the model.
	some methods for this generic require additional arguments. None are used in this method.

## Value

a glsStruct object similar to object, but with initialized model components.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
gls, Initialize.corStruct, Initialize.varFunc, Initialize
```

Initialize.lmeStruct 133

# Description

The individual linear mixed-effects model components of the lmeStruct list are initialized.

# Usage

```
## S3 method for class 'lmeStruct'
Initialize(object, data, groups, conLin, control, ...)
```

# **Arguments**

-		
	object	an object inheriting from class "lmeStruct", representing a list of linear mixed-effects model components, such as reStruct, corStruct, and varFunc objects.
	data	a data frame in which to evaluate the variables defined in formula(object).
	groups	a data frame with the grouping factors corresponding to the lme model associated with object as columns, sorted from innermost to outermost grouping level.
	conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying lme model. Defaults to attr(object, "conLin").
	control	an optional list with control parameters for the initialization and optimization algorithms used in lme. Defaults to list(niterEM=20, gradHess=TRUE), implying that 20 EM iterations are to be used in the derivation of initial estimates for the coefficients of the reStruct component of object and, if possible, numerical gradient vectors and Hessian matrices for the log-likelihood function are to be used in the optimization algorithm.
	• • •	some methods for this generic require additional arguments. None are used in this method.

# Value

an 1meStruct object similar to object, but with initialized model components.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

lme, Initialize.reStruct, Initialize.corStruct, Initialize.varFunc, Initialize

134 Initialize.reStruct

# Description

Initial estimates for the parameters in the pdMat objects forming object, which have not yet been initialized, are obtained using the methodology described in Bates and Pinheiro (1998). These estimates may be refined using a series of EM iterations, as described in Bates and Pinheiro (1998). The number of EM iterations to be used is defined in control.

# Usage

```
## S3 method for class 'reStruct'
Initialize(object, data, conLin, control, ...)
```

# Arguments

object	an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.
data	a data frame in which to evaluate the variables defined in formula(object).
conLin	a condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying model.
control	an optional list with a single component niterEM controlling the number of iterations for the EM algorithm used to refine initial parameter estimates. It is given as a list for compatibility with other Initialize methods. Defaults to list(niterEM = 20).
•••	some methods for this generic require additional arguments. None are used in this method.

### Value

an reStruct object similar to object, but with all pdMat components initialized.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
reStruct, pdMat, Initialize
```

Initialize.varFunc 135

Initialize.varFunc Initialize varFunc Object

### **Description**

This method initializes object by evaluating its associated covariate(s) and grouping factor, if any is present, in data; determining if the covariate(s) need to be updated when the values of the coefficients associated with object change; initializing the log-likelihood and the weights associated with object; and assigning initial values for the coefficients in object, if none were present. The covariate(s) will only be initialized if no update is needed when coef(object) changes.

# Usage

```
## S3 method for class 'varFunc'
Initialize(object, data, ...)
```

# **Arguments**

object	an object inheriting from class "varFunc", representing a variance function structure.
data	a data frame in which to evaluate the variables named in formula(object).
	this argument is included to make this method compatible with the generic.

### Value

an initialized object with the same class as object representing a variance function structure.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
Initialize
```

# **Examples**

```
vf1 <- varPower( form = ~ age | Sex )
vf1 <- Initialize( vf1, Orthodont )</pre>
```

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intervals

Confidence Intervals on Coefficients

# **Description**

Confidence intervals on the parameters associated with the model represented by object are obtained. This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: gls, lme, and lmList.

# Usage

```
intervals(object, level, ...)
```

### **Arguments**

object a fitted model object from which parameter estimates can be extracted.

level an optional numeric value for the interval confidence level. Defaults to 0.95.

some methods for the generic may require additional arguments.

#### Value

will depend on the method function used; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bate date : du>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

# See Also

```
intervals.lme, intervals.lmList, intervals.gls
```

# **Examples**

## see the method documentation

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Confidence Intervals on gls Parameters

### **Description**

Approximate confidence intervals for the parameters in the linear model represented by object are obtained, using a normal approximation to the distribution of the (restricted) maximum likelihood estimators (the estimators are assumed to have a normal distribution centered at the true parameter values and with covariance matrix equal to the negative inverse Hessian matrix of the (restricted) log-likelihood evaluated at the estimated parameters). Confidence intervals are obtained in an unconstrained scale first, using the normal approximation, and, if necessary, transformed to the constrained scale.

# Usage

```
## S3 method for class 'gls'
intervals(object, level, which, ...)
```

# **Arguments**

object	an object inheriting from class "gls", representing a generalized least squares fitted linear model.
level	an optional numeric value for the interval confidence level. Defaults to 0.95.
which	an optional character string specifying the subset of parameters for which to construct the confidence intervals. Possible values are "all" for all parameters, "var-cov" for the variance-covariance parameters only, and "coef" for the linear model coefficients only. Defaults to "all".
•••	some methods for this generic require additional arguments. None are used in this method.

### Value

a list with components given by data frames with rows corresponding to parameters and columns lower, est., and upper representing respectively lower confidence limits, the estimated values, and upper confidence limits for the parameters. Possible components are:

coef	linear model coefficients, only present when which is not equal to "var-cov".
corStruct	correlation parameters, only present when which is not equal to "coef" and a correlation structure is used in object.
varFunc	variance function parameters, only present when which is not equal to "coef" and a variance function structure is used in object.
sigma	residual standard error.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

intervals.lme

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
gls, intervals, print.intervals.gls
```

### **Examples**

intervals.lme

Confidence Intervals on lme Parameters

### **Description**

Approximate confidence intervals for the parameters in the linear mixed-effects model represented by object are obtained, using a normal approximation to the distribution of the (restricted) maximum likelihood estimators (the estimators are assumed to have a normal distribution centered at the true parameter values and with covariance matrix equal to the negative inverse Hessian matrix of the (restricted) log-likelihood evaluated at the estimated parameters). Confidence intervals are obtained in an unconstrained scale first, using the normal approximation, and, if necessary, transformed to the constrained scale. The pdNatural parametrization is used for general positive-definite matrices.

# Usage

#### **Arguments**

object	an object inheriting from class "lme", representing a fitted linear mixed-effects model.
level	an optional numeric value with the confidence level for the intervals. Defaults to $0.95$ .
which	an optional character string specifying the subset of parameters for which to construct the confidence intervals. Possible values are "all" for all parameters, "var-cov" for the variance-covariance parameters only, and "fixed" for the fixed effects only. Defaults to "all".
	some methods for this generic require additional arguments. None are used in this method.

intervals.ImList

#### Value

a list with components given by data frames with rows corresponding to parameters and columns lower, est., and upper representing respectively lower confidence limits, the estimated values, and upper confidence limits for the parameters. Possible components are:

fixed fixed effects, only present when which is not equal to "var-cov".

reStruct random effects variance-covariance parameters, only present when which is not

equal to "fixed".

corStruct within-group correlation parameters, only present when which is not equal to

"fixed" and a correlation structure is used in object.

varFunc within-group variance function parameters, only present when which is not

equal to "fixed" and a variance function structure is used in object.

sigma within-group standard deviation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
lme, intervals, print.intervals.lme, pdNatural
```

#### **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)
intervals(fm1)</pre>
```

intervals.lmList

Confidence Intervals on lmList Coefficients

# Description

Confidence intervals on the linear model coefficients are obtained for each 1m component of object and organized into a three dimensional array. The first dimension corresponding to the names of the object components. The second dimension is given by lower, est., and upper corresponding, respectively, to the lower confidence limit, estimated coefficient, and upper confidence limit. The third dimension is given by the coefficients names.

#### Usage

```
## S3 method for class 'lmList'
intervals(object, level = 0.95, pool = attr(object, "pool"), ...)
```

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### **Arguments**

object	an object inheriting from class "lmList", representing a list of lm objects with a common model.
level	an optional numeric value with the confidence level for the intervals. Defaults to 0.95.
pool	an optional logical value indicating whether a pooled estimate of the residual standard error should be used. Default is attr(object, "pool").
	some methods for this generic require additional arguments. None are used in this method.

### Value

a three dimensional array with the confidence intervals and estimates for the coefficients of each 1m component of object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

# See Also

```
{\tt lmList, intervals, plot.intervals.lmList}
```

# **Examples**

```
fm1 <- lmList(distance \sim age | Subject, Orthodont) intervals(fm1)
```

isBalanced

Check a Design for Balance

# **Description**

Check the design of the experiment or study for balance.

# Usage

```
isBalanced(object, countOnly, level)
```

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### **Arguments**

object A groupedData object containing a data frame and a formula that describes the

roles of variables in the data frame. The object will have one or more nested

grouping factors and a primary covariate.

countOnly A logical value indicating if the check for balance should only consider the num-

ber of observations at each level of the grouping factor(s). Defaults to FALSE.

level an optional integer vector specifying the desired prediction levels. Levels in-

crease from outermost to innermost grouping, with level 0 representing the pop-

ulation (fixed effects) predictions. Defaults to the innermost level.

#### **Details**

A design is balanced with respect to the grouping factor(s) if there are the same number of observations at each distinct value of the grouping factor or each combination of distinct levels of the nested grouping factors. If countOnly is FALSE the design is also checked for balance with respect to the primary covariate, which is often the time of the observation. A design is balanced with respect to the grouping factor and the covariate if the number of observations at each distinct level (or combination of levels for nested factors) is constant and the times at which the observations are taken (in general, the values of the primary covariates) also are constant.

#### Value

TRUE or FALSE according to whether the data are balanced or not

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
table, groupedData
```

#### **Examples**

isInitialized

Check if Object is Initialized

### **Description**

Checks if object has been initialized (generally through a call to Initialize), by searching for components and attributes which are modified during initialization.

LDEsysMat

### Usage

```
isInitialized(object)
```

### **Arguments**

object

any object requiring initialization.

# Value

a logical value indicating whether object has been initialized.

#### Author(s)

José Pinheiro and Douglas Bates

### See Also

Initialize

### **Examples**

```
pd1 <- pdDiag(~age)
isInitialized(pd1)</pre>
```

LDEsysMat

Generate system matrix for LDEs

# **Description**

Generate the system matrix for the linear differential equations determined by a compartment model.

# Usage

```
LDEsysMat(pars, incidence)
```

# **Arguments**

pars

a numeric vector of parameter values.

incidence

an integer matrix with columns named From, To, and Par. Values in the Par column must be in the range 1 to length(pars). Values in the From column must be between 1 and the number of compartments. Values in the To column

must be between 0 and the number of compartments.

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#### **Details**

A compartment model describes material transfer between k in a system of k compartments to a linear system of differential equations. Given a description of the system and a vector of parameter values this function returns the system matrix.

This function is intended for use in a general system for solving compartment models, as described in Bates and Watts (1988).

#### Value

A k by k numeric matrix.

#### Author(s)

Douglas Bates <bates@stat.wisc.edu>

#### References

Bates, D. M. and Watts, D. G. (1988), *Nonlinear Regression Analysis and Its Applications*, Wiley, New York.

### **Examples**

```
# incidence matrix for a two compartment open system
incidence <-
   matrix(c(1,1,2,2,2,1,3,2,0), ncol = 3, byrow = TRUE,
   dimnames = list(NULL, c("Par", "From", "To")))
incidence
LDEsysMat(c(1.2, 0.3, 0.4), incidence)</pre>
```

1me

Linear Mixed-Effects Models

### **Description**

This generic function fits a linear mixed-effects model in the formulation described in Laird and Ware (1982) but allowing for nested random effects. The within-group errors are allowed to be correlated and/or have unequal variances.

This page describes the formula method; the methods lme.lmList and lme.groupedData are documented separately.

# Usage

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```
ma.action, control, contrasts = NULL, keep.data = TRUE)
## S3 method for class 'lme'
update(object, fixed., ..., evaluate = TRUE)
```

#### **Arguments**

object an object inheriting from class lme, representing a fitted linear mixed-effects

model.

fixed a two-sided linear formula object describing the fixed-effects part of the model,

with the response on the left of a ~ operator and the terms, separated by + operators, on the right, an "lmList" object, or a "groupedData" object.

There is limited support for formulae such as resp ~ 1 and resp ~ 0, and less

prior to version '3.1-112'.

fixed. Changes to the fixed-effects formula – see update. formula for details.

data an optional data frame containing the variables named in fixed, random, correlation,

weights, and subset. By default the variables are taken from the environment

from which 1me is called.

random optionally, any of the following: (i) a one-sided formula of the form ~ x1 +

... + xn | g1/.../gm, with x1 + ... + xn specifying the model for the random effects and g1/.../gm the grouping structure (m may be equal to 1, in which case no / is required). The random effects formula will be repeated for all levels of grouping, in the case of multiple levels of grouping; (ii) a list of one-sided formulas of the form  $\sim x1 + ... + xn$  | g, with possibly different random effects models for each grouping level. The order of nesting will be assumed the same as the order of the elements in the list; (iii) a one-sided formula of the form  $\sim x1 + ... + xn$ , or a pdMat object with a formula (i.e. a non-NULL value for formula(object)), or a list of such formulas or pdMat objects. In this case, the grouping structure formula will be derived from the data used to fit the linear mixed-effects model, which should inherit from class "groupedData"; (iv) a named list of formulas or pdMat objects as in (iii), with the grouping factors as names. The order of nesting will be assumed the same as the order of the order of the elements in the list; (v) an reStruct object. See the documentation on pdClasses for a description of the available pdMat classes. Defaults to a

formula consisting of the right hand side of fixed.

correlation an optional corStruct object describing the within-group correlation structure. See the documentation of corClasses for a description of the available

corStruct classes. Defaults to NULL, corresponding to no within-group corre-

lations.

weights an optional varFunc object or one-sided formula describing the within-group

heteroscedasticity structure. If given as a formula, it is used as the argument to varFixed, corresponding to fixed variance weights. See the documentation on varClasses for a description of the available varFunc classes. Defaults to

NULL, corresponding to homoscedastic within-group errors.

subset an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which

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	observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
method	a character string. If "REML" the model is fit by maximizing the restricted log-likelihood. If "ML" the log-likelihood is maximized. Defaults to "REML".
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes lme to print an error message and terminate if there are any incomplete observations.
control	a list of control values for the estimation algorithm to replace the default values returned by the function lmeControl. Defaults to an empty list.
contrasts	an optional list. See the contrasts.arg of model.matrix.default.
keep.data	logical: should the data argument (if supplied and a data frame) be saved as part of the model object?
• • •	some methods for this generic require additional arguments. None are used in this method.
evaluate	If TRUE evaluate the new call else return the call.

#### **Details**

offset terms in fixed are an error since 3.1-157 (2022-03): previously they were silently ignored.

## Value

An object of class "lme" representing the linear mixed-effects model fit. Generic functions such as print, plot and summary have methods to show the results of the fit. See lmeObject for the components of the fit. The functions resid, coef, fitted, fixed.effects, and random.effects can be used to extract some of its components.

## Note

The function does not do any scaling internally: the optimization will work best when the response is scaled so its variance is of the order of one.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

The computational methods follow the general framework of Lindstrom and Bates (1988). The model formulation is described in Laird and Ware (1982). The variance-covariance parametrizations are described in Pinheiro and Bates (1996). The different correlation structures available for the correlation argument are described in Box, Jenkins and Reinsel (1994), Littell *et al* (1996), and Venables and Ripley (2002). The use of variance functions for linear and nonlinear mixed effects models is presented in detail in Davidian and Giltinan (1995).

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994). *Time Series Analysis: Forecasting and Control*, 3rd Edition, Holden–Day.

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Davidian, M. and Giltinan, D.M. (1995). *Nonlinear Mixed Effects Models for Repeated Measure-ment Data*, Chapman and Hall. doi:10.1201/9780203745502.

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Lindstrom, M.J. and Bates, D.M. (1988). Newton-Raphson and EM Algorithms for Linear Mixed-Effects Models for Repeated-Measures Data. *Journal of the American Statistical Association* **83**, 1014–1022. doi:10.2307/2290128.

Littell, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996). SAS Systems for Mixed Models, SAS Institute.

Pinheiro, J.C. and Bates., D.M. (1996). Unconstrained Parametrizations for Variance-Covariance Matrices. *Statistics and Computing* **6**, 289–296. doi:10.1007/BF00140873.

Pinheiro, J.C., and Bates, D.M. (2000). *Mixed-Effects Models in S and S-PLUS*, Springer. doi:10.1007/b98882.

Venables, W.N. and Ripley, B.D. (2002). *Modern Applied Statistics with S*, 4th Edition, Springer-Verlag. doi:10.1007/9780387217062.

### See Also

```
corClasses, lme.lmList, lme.groupedData, lmeControl, lmeObject, lmeStruct, lmList, pdClasses, plot.lme, predict.lme, qqnorm.lme, residuals.lme, reStruct, simulate.lme, summary.lme, varClasses, varFunc
```

# **Examples**

```
fm1 <- lme(distance ~ age, data = Orthodont) # random is ~ age
fm2 <- lme(distance ~ age + Sex, data = Orthodont, random = ~ 1)
summary(fm1)
summary(fm2)
```

lme.groupedData

LME fit from groupedData Object

# Description

The response variable and primary covariate in formula(fixed) are used to construct the fixed effects model formula. This formula and the groupedData object are passed as the fixed and data arguments to lme.formula, together with any other additional arguments in the function call. See the documentation on lme.formula for a description of that function.

## Usage

```
## S3 method for class 'groupedData'
lme(fixed, data, random, correlation, weights,
    subset, method, na.action, control, contrasts, keep.data = TRUE)
```

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### **Arguments**

fixed a data frame inheriting from class "groupedData".

data this argument is included for consistency with the generic function. It is ignored

in this method function.

random optionally, any of the following: (i) a one-sided formula of the form ~x1+...+xn

| g1/.../gm, with x1+...+xn specifying the model for the random effects and g1/.../gm the grouping structure (m may be equal to 1, in which case no / is required). The random effects formula will be repeated for all levels of grouping, in the case of multiple levels of grouping; (ii) a list of one-sided formulas of the form ~x1+...+xn | g, with possibly different random effects models for each grouping level. The order of nesting will be assumed the same as the order of the elements in the list; (iii) a one-sided formula of the form ~x1+...+xn, or a pdMat object with a formula (i.e. a non-NULL value for formula(object)), or a list of such formulas or pdMat objects. In this case, the grouping structure formula will be derived from the data used to fit the linear mixed-effects model, which should inherit from class groupedData; (iv) a named list of formulas or pdMat objects as in (iii), with the grouping factors as names. The order of nesting will be assumed the same as the order of the order of the elements in the list; (v) an reStruct object. See the documentation on pdClasses for a description of the available pdMat classes. Defaults to a formula consisting of

the right hand side of fixed.

correlation an optional corStruct object describing the within-group correlation struc-

ture. See the documentation of corClasses for a description of the available corStruct classes. Defaults to NULL, corresponding to no within-group corre-

lations.

weights an optional varFunc object or one-sided formula describing the within-group

heteroscedasticity structure. If given as a formula, it is used as the argument to varFixed, corresponding to fixed variance weights. See the documentation on varClasses for a description of the available varFunc classes. Defaults to

NULL, corresponding to homoscedastic within-group errors.

subset an optional expression indicating the subset of the rows of data that should be

used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names

to be included. All observations are included by default.

method a character string. If "REML" the model is fit by maximizing the restricted log-

likelihood. If "ML" the log-likelihood is maximized. Defaults to "REML".

na.action a function that indicates what should happen when the data contain NAs. The

default action (na.fail) causes 1me to print an error message and terminate if

there are any incomplete observations.

control a list of control values for the estimation algorithm to replace the default values

returned by the function lmeControl. Defaults to an empty list.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

keep.data logical: should the data argument (if supplied and a data frame) be saved as

part of the model object?

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### Value

an object of class 1me representing the linear mixed-effects model fit. Generic functions such as print, plot and summary have methods to show the results of the fit. See 1meObject for the components of the fit. The functions resid, coef, fitted, fixed.effects, and random.effects can be used to extract some of its components.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

The computational methods follow on the general framework of Lindstrom, M.J. and Bates, D.M. (1988). The model formulation is described in Laird, N.M. and Ware, J.H. (1982). The variance-covariance parametrizations are described in Pinheiro, J.C. and Bates., D.M. (1996). The different correlation structures available for the correlation argument are described in Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994), Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996), and Venables, W.N. and Ripley, B.D. (2002). The use of variance functions for linear and nonlinear mixed effects models is presented in detail in Davidian, M. and Giltinan, D.M. (1995).

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

Davidian, M. and Giltinan, D.M. (1995) "Nonlinear Mixed Effects Models for Repeated Measurement Data", Chapman and Hall.

Laird, N.M. and Ware, J.H. (1982) "Random-Effects Models for Longitudinal Data", Biometrics, 38, 963-974.

Lindstrom, M.J. and Bates, D.M. (1988) "Newton-Raphson and EM Algorithms for Linear Mixed-Effects Models for Repeated-Measures Data", Journal of the American Statistical Association, 83, 1014-1022.

Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C. and Bates., D.M. (1996) "Unconstrained Parametrizations for Variance-Covariance Matrices", Statistics and Computing, 6, 289-296.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

### See Also

lme, groupedData, lmeObject

```
fm1 <- lme(Orthodont)
summary(fm1)</pre>
```

Ime.ImList

lme.lmList

LME fit from lmList Object

## **Description**

If the random effects names defined in random are a subset of the lmList object coefficient names, initial estimates for the covariance matrix of the random effects are obtained (overwriting any values given in random). formula(fixed) and the data argument in the calling sequence used to obtain fixed are passed as the fixed and data arguments to lme.formula, together with any other additional arguments in the function call. See the documentation on lme.formula for a description of that function.

# Usage

### **Arguments**

fixed	an object inheriting from class "lmList.", representing a list of lm fits with a common model.
data	this argument is included for consistency with the generic function. It is ignored in this method function.
random	an optional one-sided linear formula with no conditioning expression, or a pdMat object with a formula attribute. Multiple levels of grouping are not allowed with this method function. Defaults to a formula consisting of the right hand side of formula(fixed).
correlation	an optional corStruct object describing the within-group correlation structure. See the documentation of corClasses for a description of the available corStruct classes. Defaults to NULL, corresponding to no within-group correlations.
weights	an optional varFunc object or one-sided formula describing the within-group heteroscedasticity structure. If given as a formula, it is used as the argument to varFixed, corresponding to fixed variance weights. See the documentation on varClasses for a description of the available varFunc classes. Defaults to NULL, corresponding to homoscedastic within-group errors.
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subset an optional expression indicating the subset of the rows of data that should be

used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names

to be included. All observations are included by default.

method a character string. If "REML" the model is fit by maximizing the restricted log-

likelihood. If "ML" the log-likelihood is maximized. Defaults to "REML".

na.action a function that indicates what should happen when the data contain NAs. The

default action (na.fail) causes lme to print an error message and terminate if

there are any incomplete observations.

lme.lmList

control a list of control values for the estimation algorithm to replace the default values

returned by the function lmeControl. Defaults to an empty list.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

keep.data logical: should the data argument (if supplied and a data frame) be saved as

part of the model object?

### Value

an object of class 1me representing the linear mixed-effects model fit. Generic functions such as print, plot and summary have methods to show the results of the fit. See 1meObject for the components of the fit. The functions resid, coef, fitted, fixed.effects, and random.effects can be used to extract some of its components.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

The computational methods follow the general framework of Lindstrom and Bates (1988). The model formulation is described in Laird and Ware (1982). The variance-covariance parametrizations are described in Pinheiro and Bates (1996). The different correlation structures available for the correlation argument are described in Box, Jenkins and Reinse (1994), Littel *et al* (1996), and Venables and Ripley, (2002). The use of variance functions for linear and nonlinear mixed effects models is presented in detail in Davidian and Giltinan (1995).

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden–Day.

Davidian, M. and Giltinan, D.M. (1995) "Nonlinear Mixed Effects Models for Repeated Measurement Data", Chapman and Hall.

Laird, N.M. and Ware, J.H. (1982) "Random-Effects Models for Longitudinal Data", Biometrics, 38, 963–974.

Lindstrom, M.J. and Bates, D.M. (1988) "Newton-Raphson and EM Algorithms for Linear Mixed-Effects Models for Repeated-Measures Data", Journal of the American Statistical Association, 83, 1014–1022.

Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C. and Bates., D.M. (1996) "Unconstrained Parametrizations for Variance-Covariance Matrices", Statistics and Computing, 6, 289–296.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

#### See Also

lme, lmList, lmeObject

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# **Examples**

```
fm1 <- lmList(Orthodont)
fm2 <- lme(fm1)
summary(fm1)
summary(fm2)</pre>
```

lmeControl

Specifying Control Values for lme Fit

# Description

The values supplied in the lmeControl() call replace the defaults, and a list with all settings (i.e., values for all possible arguments) is returned. The returned list is used as the control argument to the lme function.

# Usage

# **Arguments**

maxIter	maximum number of iterations for the $1me$ optimization algorithm. Default is $50$ .
msMaxIter	maximum number of iterations for the optimization step inside the lme optimization. Default is $50$ .
tolerance	tolerance for the convergence criterion in the 1me algorithm. Default is 1e-6.
niterEM	number of iterations for the EM algorithm used to refine the initial estimates of the random effects variance-covariance coefficients. Default is 25.
msMaxEval	maximum number of evaluations of the objective function permitted for nlminb. Default is 200.
msTol	tolerance for the convergence criterion on the first iteration when optim is used. Default is 1e-7.
msVerbose	a logical value passed as the trace argument to ${\tt nlminb}$ or ${\tt optim}$ . Default is FALSE.
returnObject	a logical value indicating whether the fitted object should be returned with a warning (instead of an error via stop()) when the maximum number of iterations is reached without convergence of the algorithm. Default is FALSE.

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gradHess	a logical value indicating whether numerical gradient vectors and Hessian matrices of the log-likelihood function should be used in the internal optimization. This option is only available when the correlation structure (corStruct) and the variance function structure (varFunc) have no "varying" parameters and the pdMat classes used in the random effects structure are pdSymm (general positive-definite), pdDiag (diagonal), pdIdent (multiple of the identity), or pdCompSymm (compound symmetry). Default is TRUE.
apVar	a logical value indicating whether the approximate covariance matrix of the variance-covariance parameters should be calculated. Default is TRUE.
.relStep	$relative \ step \ for \ numerical \ derivatives \ calculations. \ Default \ is \ . Machine \$ double . eps \^(1/3).$
opt	the optimizer to be used, either "nlminb" (the default) or "optim".
optimMethod	character - the optimization method to be used with the optim optimizer. The default is "BFGS". An alternative is "L-BFGS-B".
minAbsParApVar	numeric value - minimum absolute parameter value in the approximate variance calculation. The default is 0.05.
natural	a logical value indicating whether the pdNatural parametrization should be used for general positive-definite matrices (pdSymm) in reStruct, when the approximate covariance matrix of the estimators is calculated. Default is TRUE.
sigma	optionally a positive number to fix the residual error at. If NULL, as by default, or 0, sigma is estimated.
allow.n.lt.q	logical indicating if it is ok to have less observations than random effects for each group. The default, FALSE signals an error; if NA, such a situation only gives a warning, as in <b>nlme</b> versions prior to 2019; if true, no message is given at all.
•••	further named control arguments to be passed, depending on opt, to nlminb (those from abs.tol down) or optim (those except trace and maxit; reltol is used only from the second iteration).

# Value

a list with components for each of the possible arguments.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>; the sigma option: Siem Heisterkamp and Bert van Willigen.

## See Also

lme, nlminb, optim

```
# decrease the maximum number iterations in the ms call and
# request that information on the evolution of the ms iterations be printed
str(lCtr <- lmeControl(msMaxIter = 20, msVerbose = TRUE))
## This should always work:
do.call(lmeControl, lCtr)</pre>
```

ImeObject 153

|--|

# **Description**

An object returned by the lme function, inheriting from class "lme" and representing a fitted linear mixed-effects model. Objects of this class have methods for the generic functions anova, coef, fitted, fixed.effects, formula, getGroups, getResponse, intervals, logLik, pairs, plot, predict, print, random.effects, residuals, sigma, summary, update, and vcov.

#### Value

The following components must be included in a legitimate "lme" object.

apVar	an approximate				

apVar = FALSE in the control values used in the call to 1me, this component is

NULL.

call a list containing an image of the lme call that produced the object.

coefficients a list with two components, fixed and random, where the first is a vector con-

taining the estimated fixed effects and the second is a list of matrices with the estimated random effects for each level of grouping. For each matrix in the random list, the columns refer to the random effects and the rows to the groups.

contrasts a list of the contrast matrices used to represent factors in the fixed effects for-

mula and/or random effects formula. This information is important for making predictions from a new data frame in which not all levels of the original factors are observed. If no factors are used in the lme model, this component will be an

empty list.

dims a list with basic dimensions used in the lme fit, including the components N - the

number of observations in the data, Q - the number of grouping levels, qvec - the number of random effects at each level from innermost to outermost (last two values are equal to zero and correspond to the fixed effects and the response), ngrps - the number of groups at each level from innermost to outermost (last two values are one and correspond to the fixed effects and the response), and ncol - the number of columns in the model matrix for each level of grouping from innermost to outermost (last two values are equal to the number of fixed

effects and one).

fitted a data frame with the fitted values as columns. The leftmost column corresponds

to the population fixed effects (corresponding to the fixed effects only) and successive columns from left to right correspond to increasing levels of grouping.

fixDF a list with components X and terms specifying the denominator degrees of free-

dom for, respectively, t-tests for the individual fixed effects and F-tests for the

fixed-effects terms in the models.

groups a data frame with the grouping factors as columns. The grouping level increases

from left to right.

logLik the (restricted) log-likelihood at convergence.

154 ImeStruct

method the estimation method: either "ML" for maximum likelihood, or "REML" for re-

stricted maximum likelihood.

modelStruct an object inheriting from class lmeStruct, representing a list of mixed-effects

model components, such as reStruct, corStruct, and varFunc objects.

numIter the number of iterations used in the iterative algorithm.

residuals a data frame with the residuals as columns. The leftmost column corresponds to

the population residuals and successive columns from left to right correspond to

increasing levels of grouping.

terms the terms, including formula, see also terms.object. sigma the estimated within-group error standard deviation.

varFix an approximate covariance matrix of the fixed effects estimates.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

lme, lmeStruct

lmeStruct	Linear Mixed-Effects Structure
-----------	--------------------------------

## **Description**

A linear mixed-effects structure is a list of model components representing different sets of parameters in the linear mixed-effects model. An lmeStruct list must contain at least a reStruct object, but may also contain corStruct and varFunc objects. NULL arguments are not included in the lmeStruct list.

### **Usage**

```
lmeStruct(reStruct, corStruct, varStruct)
```

## **Arguments**

reStruct a reStruct representing a random effects structure.

construct an optional construct object, representing a correlation structure. Default is

NULL.

varStruct an optional varFunc object, representing a variance function structure. Default

is NULL.

## Value

a list of model components determining the parameters to be estimated for the associated linear mixed-effects model.

**lmList** 155

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
corClasses, lme, residuals.lmeStruct, reStruct, varFunc
```

# **Examples**

```
lms1 <- lmeStruct(reStruct(~age), corAR1(), varPower())</pre>
```

**lmList** 

List of lm Objects with a Common Model

## **Description**

Data is partitioned according to the levels of the grouping factor g and individual 1m fits are obtained for each data partition, using the model defined in object.

# Usage

```
lmList(object, data, level, subset, na.action = na.fail,
       pool = TRUE, warn.lm = TRUE)
## S3 method for class 'formula'
lmList(object, data, level, subset, na.action = na.fail,
       pool = TRUE, warn.lm = TRUE)
## S3 method for class 'lmList'
update(object, formula., ..., evaluate = TRUE)
## S3 method for class 'lmList'
print(x, pool, ...)
```

## **Arguments**

object

For lmList, either a linear formula object of the form  $y \sim x1+...+xn \mid g$  or a groupedData object. In the formula object, y represents the response, x1, ..., xn the covariates, and g the grouping factor specifying the partitioning of the data according to which different 1m fits should be performed. The grouping factor g may be omitted from the formula, in which case the grouping structure will be obtained from data, which must inherit from class groupedData. The method function lmList.groupedData is documented separately. For the method update.lmList, object is an object inheriting from class lmList.

formula

(used in update.lmList only) a two-sided linear formula with the common model for the individuals 1m fits.

formula.

Changes to the formula – see update. formula for details.

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data	a data frame in which to interpret the variables named in object.
level	an optional integer specifying the level of grouping to be used when multiple nested levels of grouping are present.
subset	an optional expression indicating which subset of the rows of data should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes lmList to print an error message and terminate if there are any incomplete observations.
pool	an optional logical value indicating whether a pooled estimate of the residual standard error should be used in calculations of standard deviations or standard errors for summaries.
warn.lm	logical indicating if $lm()$ errors (all of which are caught by tryCatch) should be signalled as a "summarizing" warning.
x	an object inheriting from class 1mList to be printed.
• • •	some methods for this generic require additional arguments. None are used in this method.
evaluate	If TRUE evaluate the new call else return the call.

# Value

a list of lm objects with as many components as the number of groups defined by the grouping factor. Generic functions such as coef, fixed.effects, lme, pairs, plot, predict, random.effects, summary, and update have methods that can be applied to an lmList object.

# References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

```
lm, lme.lmList, plot.lmList, pooledSD, predict.lmList, residuals.lmList, summary.lmList
```

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
summary(fm1)</pre>
```

lmList.groupedData 157

lmList.groupedData

lmList Fit from a groupedData Object

## **Description**

The response variable and primary covariate in formula(object) are used to construct the linear model formula. This formula and the groupedData object are passed as the object and data arguments to lmList.formula, together with any other additional arguments in the function call. See the documentation on lmList.formula for a description of that function.

## Usage

# **Arguments**

object	a data frame inheriting from class "groupedData".
data	this argument is included for consistency with the generic function. It is ignored in this method function.
level	an optional integer specifying the level of grouping to be used when multiple nested levels of grouping are present.
subset	an optional expression indicating which subset of the rows of data should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes lmList to print an error message and terminate if there are any incomplete observations.
pool,warn.lm	optional logicals, see lmList.

## Value

a list of lm objects with as many components as the number of groups defined by the grouping factor. Generic functions such as coef, fixed.effects, lme, pairs, plot, predict, random.effects, summary, and update have methods that can be applied to an lmList object.

# See Also

```
groupedData, lm, lme.lmList, lmList, lmList.formula
```

```
fm1 <- lmList(Orthodont)
summary(fm1)</pre>
```

logDet.corStruct

logDet

Extract the Logarithm of the Determinant

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: corStruct, several pdMat classes, and reStruct.

# Usage

```
logDet(object, ...)
```

# **Arguments**

object any object from which a matrix, or list of matrices, can be extracted some methods for this generic function require additional arguments.

### Value

will depend on the method function used; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
logLik, logDet.corStruct, logDet.pdMat, logDet.reStruct
```

## **Examples**

## see the method function documentation

logDet.corStruct

Extract corStruct Log-Determinant

# **Description**

This method function extracts the logarithm of the determinant of a square-root factor of the correlation matrix associated with object, or the sum of the log-determinants of square-root factors of the list of correlation matrices associated with object.

#### Usage

```
## S3 method for class 'corStruct'
logDet(object, covariate, ...)
```

logDet.pdMat 159

# **Arguments**

object an object inheriting from class	s "corStruct", representing a correlation struc-
--	--

ture.

covariate an optional covariate vector (matrix), or list of covariate vectors (matrices), at

which values the correlation matrix, or list of correlation matrices, are to be

evaluated. Defaults to getCovariate(object).

... some methods for this generic require additional arguments. None are used in

this method.

## Value

the log-determinant of a square-root factor of the correlation matrix associated with object, or the sum of the log-determinants of square-root factors of the list of correlation matrices associated with object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
logLik.corStruct, corMatrix.corStruct, logDet
```

## **Examples**

```
cs1 <- corAR1(0.3)
logDet(cs1, covariate = 1:4)</pre>
```

logDet.pdMat

Extract Log-Determinant from a pdMat Object

# Description

This method function extracts the logarithm of the determinant of a square-root factor of the positive-definite matrix represented by object.

## Usage

```
## S3 method for class 'pdMat'
logDet(object, ...)
```

## Arguments

object an object inheriting from class "pdMat", representing a positive definite matrix.

... some methods for this generic require additional arguments. None are used in

this method.

logDet.reStruct

## Value

the log-determinant of a square-root factor of the positive-definite matrix represented by object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
pdMat, logDet
```

## **Examples**

```
pd1 <- pdSymm(diag(1:3))
logDet(pd1)</pre>
```

logDet.reStruct

Extract reStruct Log-Determinants

## Description

Calculates, for each of the pdMat components of object, the logarithm of the determinant of a square-root factor.

# Usage

```
## S3 method for class 'reStruct'
logDet(object, ...)
```

### **Arguments**

object an object inheriting from class "reStruct", representing a random effects struc-

ture and consisting of a list of pdMat objects.

... some methods for this generic require additional arguments. None are used in

this method.

## Value

a vector with the log-determinants of square-root factors of the pdMat components of object.

## Author(s)

José Pinheiro

## See Also

```
reStruct, pdMat, logDet
```

logLik.corStruct 161

## **Examples**

```
rs1 <- reStruct(list(A = pdSymm(diag(1:3), form = ~Score),
   B = pdDiag(2 * diag(4), form = ~Educ)))
logDet(rs1)</pre>
```

logLik.corStruct

Extract corStruct Log-Likelihood

## **Description**

This method function extracts the component of a Gaussian log-likelihood associated with the correlation structure, which is equal to the negative of the logarithm of the determinant (or sum of the logarithms of the determinants) of the matrix (or matrices) represented by object.

## Usage

```
## S3 method for class 'corStruct'
logLik(object, data, ...)
```

# Arguments

object	an object inheriting from class "corStruct", representing a correlation structure.
data	this argument is included to make this method function compatible with other logLik methods and will be ignored.
	some methods for this generic require additional arguments. None are used in this method.

# Value

the negative of the logarithm of the determinant (or sum of the logarithms of the determinants) of the correlation matrix (or matrices) represented by object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
logDet.corStruct, logLik.lme,
```

```
cs1 <- corAR1(0.2)
cs1 <- Initialize(cs1, data = Orthodont)
logLik(cs1)</pre>
```

logLik.glsStruct

	logLik.glsStruct	Log-Likelihood of a glsStruct Object
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# **Description**

Pars is used to update the coefficients of the model components of object and the individual (restricted) log-likelihood contributions of each component are added together. The type of log-likelihood (restricted or not) is determined by the settings attribute of object.

# Usage

```
## S3 method for class 'glsStruct'
logLik(object, Pars, conLin, ...)
```

# Arguments

object	an object inheriting from class "glsStruct", representing a list of linear model components, such as corStruct and "varFunc" objects.
Pars	the parameter values at which the (restricted) log-likelihood is to be evaluated.
conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying linear model. Defaults to attr(object, "conLin").
	some methods for this generic require additional arguments. None are used in this method.

# Value

the (restricted) log-likelihood for the linear model described by object, evaluated at Pars.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
{\tt gls, glsStruct, logLik.lme}
```

logLik.gnls 163

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Log-Likelihood of a gnls Object

# **Description**

Returns the log-likelihood value of the nonlinear model represented by object evaluated at the estimated coefficients.

# Usage

```
## S3 method for class 'gnls'
logLik(object, REML, ...)
```

# Arguments

object	an object inheriting from class "gnls", representing a generalized nonlinear least squares fitted model.
REML	an logical value for consistency with logLik, gls, but only FALSE is accepted
•••	some methods for this generic require additional arguments. None are used in this method.

## Value

the log-likelihood of the linear model represented by object evaluated at the estimated coefficients.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
gnls, logLik.lme
```

logLik.gnlsStruct

logLik.gnlsStruct	Log-Likelihood of a gnlsStruct Object

# **Description**

Pars is used to update the coefficients of the model components of object and the individual log-likelihood contributions of each component are added together.

# Usage

```
## S3 method for class 'gnlsStruct'
logLik(object, Pars, conLin, ...)
```

## **Arguments**

object	an object inheriting from class gnlsStruct, representing a list of model com-

ponents, such as corStruct and varFunc objects, and attributes specifying the

underlying nonlinear model and the response variable.

Pars the parameter values at which the log-likelihood is to be evaluated.

conLin an optional condensed linear model object, consisting of a list with components

"Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying

nonlinear model. Defaults to attr(object, "conLin").

... some methods for this generic require additional arguments. None are used in

this method.

### Value

the log-likelihood for the linear model described by object, evaluated at Pars.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
gnls, gnlsStruct, logLik.gnls
```

logLik.lme 165

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Log-Likelihood of an lme Object

# **Description**

If REML=FALSE, returns the log-likelihood value of the linear mixed-effects model represented by object evaluated at the estimated coefficients; else, the restricted log-likelihood evaluated at the estimated coefficients is returned.

## Usage

```
## S3 method for class 'lme'
logLik(object, REML, ...)
```

# Arguments

object an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

REML an optional logical value. If TRUE the restricted log-likelihood is returned, else, if

FALSE, the log-likelihood is returned. Defaults to the method of estimation used, that is TRUE if and only object was fitted with method = "REML" (the default for

these fitting functions).

... some methods for this generic require additional arguments. None are used in

this method.

### Value

the (restricted) log-likelihood of the model represented by object evaluated at the estimated coefficients.

## Author(s)

José Pinheiro and Douglas Bates

## References

Harville, D.A. (1974) "Bayesian Inference for Variance Components Using Only Error Contrasts", *Biometrika*, **61**, 383–385.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

lme,gls, logLik.corStruct, logLik.glsStruct, logLik.lmeStruct, logLik.lmList, logLik.reStruct,
logLik.varFunc,

logLik.lmeStruct

## **Examples**

```
fm1 <- lme(distance \sim Sex * age, Orthodont, random = \sim age, method = "ML") logLik(fm1) logLik(fm1, REML = TRUE)
```

logLik.lmeStruct

Log-Likelihood of an lmeStruct Object

# Description

Pars is used to update the coefficients of the model components of object and the individual (restricted) log-likelihood contributions of each component are added together. The type of log-likelihood (restricted or not) is determined by the settings attribute of object.

# Usage

```
## S3 method for class 'lmeStruct'
logLik(object, Pars, conLin, ...)
```

# **Arguments**

object	an object inheriting from class "lmeStruct", representing a list of linear mixed-effects model components, such as reStruct, corStruct, and varFunc objects.
Pars	the parameter values at which the (restricted) log-likelihood is to be evaluated.
conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying lme model. Defaults to attr(object, "conLin").
	some methods for this generic require additional arguments. None are used in this method.

### Value

the (restricted) log-likelihood for the linear mixed-effects model described by object, evaluated at Pars.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
lme, lmeStruct, logLik.lme
```

logLik.lmList

logLik.lmList	Log-Likelihood of an lmList Object	
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# **Description**

If pool=FALSE, the (restricted) log-likelihoods of the lm components of object are summed together. Else, the (restricted) log-likelihood of the lm fit with different coefficients for each level of the grouping factor associated with the partitioning of the object components is obtained.

# Usage

```
## S3 method for class 'lmList'
logLik(object, REML, pool, ...)
```

# **Arguments**

object	an object inheriting from class " $lmList$ ", representing a list of $lm$ objects with a common model.
REML	an optional logical value. If TRUE the restricted log-likelihood is returned, else, if FALSE, the log-likelihood is returned. Defaults to FALSE.
pool	an optional logical value indicating whether all 1m components of object may be assumed to have the same error variance. Default is attr(object, "pool").
	some methods for this generic require additional arguments. None are used in this method.

## Value

either the sum of the (restricted) log-likelihoods of each 1m component in object, or the (restricted) log-likelihood for the 1m fit with separate coefficients for each component of object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
lmList, logLik.lme,
```

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
logLik(fm1)  # returns NA when it should not</pre>
```

logLik.reStruct

|--|

# Description

Calculates the log-likelihood, or restricted log-likelihood, of the Gaussian linear mixed-effects model represented by object and conLin (assuming spherical within-group covariance structure), evaluated at coef(object). The settings attribute of object determines whether the log-likelihood, or the restricted log-likelihood, is to be calculated. The computational methods are described in Bates and Pinheiro (1998).

# Usage

```
## S3 method for class 'reStruct'
logLik(object, conLin, ...)
```

## **Arguments**

object	an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.
conLin	a condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying model.
	some methods for this generic require additional arguments. None are used in this method.

#### Value

the log-likelihood, or restricted log-likelihood, of linear mixed-effects model represented by object and conLin, evaluated at coef{object}.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
reStruct, pdMat, logLik.lme
```

logLik.varFunc 169

# Description

This method function extracts the component of a Gaussian log-likelihood associated with the variance function structure represented by object, which is equal to the sum of the logarithms of the corresponding weights.

# Usage

```
## S3 method for class 'varFunc'
logLik(object, data, ...)
```

# Arguments

object	an object inheriting from class "varFunc", representing a variance function structure.
data	this argument is included to make this method function compatible with other logLik methods and will be ignored.
	some methods for this generic require additional arguments. None are used in this method.

## Value

the sum of the logarithms of the weights corresponding to the variance function structure represented by object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
logLik.lme
```

```
vf1 <- varPower(form = ~age)
vf1 <- Initialize(vf1, Orthodont)
coef(vf1) <- 0.1
logLik(vf1)</pre>
```

170 MathAchieve

Machines

Productivity Scores for Machines and Workers

## **Description**

The Machines data frame has 54 rows and 3 columns.

#### **Format**

This data frame contains the following columns:

Worker an ordered factor giving the unique identifier for the worker.

Machine a factor with levels A, B, and C identifying the machine brand.

**score** a productivity score.

#### **Details**

Data on an experiment to compare three brands of machines used in an industrial process are presented in Milliken and Johnson (p. 285, 1992). Six workers were chosen randomly among the employees of a factory to operate each machine three times. The response is an overall productivity score taking into account the number and quality of components produced.

### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.14)

Milliken, G. A. and Johnson, D. E. (1992), *Analysis of Messy Data, Volume I: Designed Experiments*, Chapman and Hall, London.

MathAchieve

Mathematics achievement scores

## Description

The MathAchieve data frame has 7185 rows and 6 columns.

# Format

This data frame contains the following columns:

School an ordered factor identifying the school that the student attends

**Minority** a factor with levels No Yes indicating if the student is a member of a minority racial group.

Sex a factor with levels Male Female

SES a numeric vector of socio-economic status.

**MathAch** a numeric vector of mathematics achievement scores.

MEANSES a numeric vector of the mean SES for the school.

MathAchSchool 171

### **Details**

Each row in this data frame contains the data for one student.

## **Examples**

summary(MathAchieve)

MathAchSchool

School demographic data for MathAchieve

## **Description**

The MathAchSchool data frame has 160 rows and 7 columns.

### **Format**

This data frame contains the following columns:

**School** a factor giving the school on which the measurement is made.

Size a numeric vector giving the number of students in the school

**Sector** a factor with levels Public Catholic

**PRACAD** a numeric vector giving the percentage of students on the academic track

**DISCLIM** a numeric vector measuring the discrimination climate

**HIMINTY** a factor with levels 0 1

**MEANSES** a numeric vector giving the mean SES score.

### **Details**

These variables give the school-level demographic data to accompany the MathAchieve data.

Matrix

Assign Matrix Values

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include pdMat, pdBlocked, and reStruct.

# Usage

```
matrix(object) <- value</pre>
```

172 Matrix.pdMat

### **Arguments**

object any object to which as.matrix can be applied.

value a matrix, or list of matrices, with the same dimensions as as.matrix(object)

with the new values to be assigned to the matrix associated with object.

### Value

will depend on the method function; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
as.matrix, also for examples, matrix<-.pdMat, matrix<-.reStruct.
```

Matrix.pdMat

Assign Matrix to a pdMat or pdBlocked Object

## **Description**

The positive-definite matrix represented by object is replaced by value. If the original matrix had row and/or column names, the corresponding names for value can either be NULL, or a permutation of the original names.

## Usage

```
## S3 replacement method for class 'pdMat'
matrix(object) <- value
## S3 replacement method for class 'pdBlocked'
matrix(object) <- value</pre>
```

# **Arguments**

object an object inheriting from class "pdMat", representing a positive definite matrix.

value a matrix with the new values to be assigned to the positive-definite matrix represented by object. Must have the same dimensions as as.matrix(object).

## Value

a pdMat or pdBlocked object similar to object, but with its coefficients modified to produce the matrix in value.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

Matrix.reStruct 173

## See Also

```
pdMat, "matrix<-"
```

## **Examples**

```
class(pd1 <- pdSymm(diag(3))) # "pdSymm" "pdMat"
matrix(pd1) <- diag(1:3)
pd1</pre>
```

Matrix.reStruct

Assign reStruct Matrices

# **Description**

The individual matrices in value are assigned to each pdMat component of object, in the order they are listed. The new matrices must have the same dimensions as the matrices they are meant to replace.

## Usage

```
## S3 replacement method for class 'reStruct'
matrix(object) <- value</pre>
```

## **Arguments**

object an object inheriting from class "reStruct", representing a random effects struc-

ture and consisting of a list of pdMat objects.

value a matrix, or list of matrices, with the new values to be assigned to the matrices

associated with the pdMat components of object.

### Value

an reStruct object similar to object, but with the coefficients of the individual pdMat components modified to produce the matrices listed in value.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
reStruct, pdMat, "matrix<-"
```

```
rs1 <- reStruct(list(Dog = ~day, Side = ~1), data = Pixel)
matrix(rs1) <- list(diag(2), 3)</pre>
```

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Meat

Tenderness of meat

# Description

The Meat data frame has 30 rows and 4 columns.

### **Format**

This data frame contains the following columns:

**Storage** an ordered factor specifying the storage treatment - 1 (0 days), 2 (1 day), 3 (2 days), 4 (4 days), 5 (9 days), and 6 (18 days)

score a numeric vector giving the tenderness score of beef roast.

**Block** an ordered factor identifying the muscle from which the roast was extracted with levels II < V < I < III < IV

Pair an ordered factor giving the unique identifier for each pair of beef roasts with levels II-1 < ... < IV-1

#### **Details**

Cochran and Cox (section 11.51, 1957) describe data from an experiment conducted at Iowa State College (Paul, 1943) to compare the effects of length of cold storage on the tenderness of beef roasts. Six storage periods ranging from 0 to 18 days were used. Thirty roasts were scored by four judges on a scale from 0 to 10, with the score increasing with tenderness. The response was the sum of all four scores. Left and right roasts from the same animal were grouped into pairs, which were further grouped into five blocks, according to the muscle from which they were extracted. Different storage periods were applied to each roast within a pair according to a balanced incomplete block design.

# Source

Cochran, W. G. and Cox, G. M. (1957), Experimental Designs, Wiley, New York.

Milk

Protein content of cows' milk

### **Description**

The Milk data frame has 1337 rows and 4 columns.

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### **Format**

This data frame contains the following columns:

protein a numeric vector giving the protein content of the milk.

**Time** a numeric vector giving the time since calving (weeks).

Cow an ordered factor giving a unique identifier for each cow.

Diet a factor with levels barley, barley+lupins, and lupins identifying the diet for each cow.

### **Details**

Diggle, Liang, and Zeger (1994) describe data on the protein content of cows' milk in the weeks following calving. The cattle are grouped according to whether they are fed a diet with barley alone, with barley and lupins, or with lupins alone.

## Source

Diggle, Peter J., Liang, Kung-Yee and Zeger, Scott L. (1994), Analysis of longitudinal data, Oxford University Press, Oxford.

```
model.matrix.reStruct reStruct Model Matrix
```

# **Description**

The model matrices for each element of formula(object), calculated using data, are bound together column-wise. When multiple grouping levels are present (i.e. when length(object) > 1), the individual model matrices are combined from innermost (at the leftmost position) to outermost (at the rightmost position).

## Usage

```
## S3 method for class 'reStruct'
model.matrix(object, data, contrast, ...)
```

# Arguments

object	an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.	
data	a data frame in which to evaluate the variables defined in formula(object).	
contrast	an optional named list specifying the contrasts to be used for representing the factor variables in data. The components names should match the names of the variables in data for which the contrasts are to be specified. The components	

of this list will be used as the contrasts attribute of the corresponding factor.

If missing, the default contrast specification is used.

some methods for this generic require additional arguments. None are used in

this method.

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## Value

a matrix obtained by binding together, column-wise, the model matrices for each element of formula(object).

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
model.matrix, contrasts, reStruct, formula.reStruct
```

# **Examples**

```
rs1 <- reStruct(list(Dog = ~day, Side = ~1), data = Pixel)
model.matrix(rs1, Pixel)</pre>
```

Muscle

Contraction of heart muscle sections

# **Description**

The Muscle data frame has 60 rows and 3 columns.

### **Format**

This data frame contains the following columns:

**Strip** an ordered factor indicating the strip of muscle being measured.

conc a numeric vector giving the concentration of CaCl2

**length** a numeric vector giving the shortening of the heart muscle strip.

## **Details**

Baumann and Waldvogel (1963) describe data on the shortening of heart muscle strips dipped in a CaCl<sub>2</sub> solution. The muscle strips are taken from the left auricle of a rat's heart.

## **Source**

Baumann, F. and Waldvogel, F. (1963), La restitution pastsystolique de la contraction de l'oreillette gauche du rat. Effets de divers ions et de l'acetylcholine, *Helvetica Physiologica Acta*, **21**.

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Names

Names Associated with an Object

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: formula, modelStruct, pdBlocked, pdMat, and reStruct.

# Usage

```
Names(object, ...)
Names(object, ...) <- value
```

# **Arguments**

object any object for which names can be extracted and/or assigned.
... some methods for this generic function require additional arguments.
value names to be assigned to object.

### Value

will depend on the method function used; see the appropriate documentation.

## SIDE EFFECTS

On the left side of an assignment, sets the names associated with object to value, which must have an appropriate length.

## Note

If names were generic, there would be no need for this generic function.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
Names.formula, Names.pdMat
```

```
## see the method function documentation
```

Names.formula

Names.f	ormula
---------	--------

Extract Names from a formula

# Description

This method function returns the names of the terms corresponding to the right hand side of object (treated as a linear formula), obtained as the column names of the corresponding model.matrix.

# Usage

```
## S3 method for class 'formula'
Names(object, data, exclude, ...)
```

# Arguments

object	an object inheriting from class "formula".
data	an optional data frame containing the variables specified in object. By default the variables are taken from the environment from which Names.formula is called.
exclude	an optional character vector with names to be excluded from the returned value. Default is $c("pi", ".")$ .
	some methods for this generic require additional arguments. None are used in this method.

## Value

a character vector with the column names of the model.matrix corresponding to the right hand side of object which are not listed in excluded.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
model.matrix, terms, Names
```

```
Names(distance ~ Sex * age, data = Orthodont)
```

Names.pdBlocked 179

Names.pdBlocked	Names of a pdBlocked Object

# Description

This method function extracts the first element of the Dimnames attribute, which contains the column names, for each block diagonal element in the matrix represented by object.

# Usage

```
## S3 method for class 'pdBlocked'
Names(object, asList, ...)
```

# **Arguments**

object	an object inheriting from class "pdBlocked" representing a positive-definite matrix with block diagonal structure
asList	a logical value. If TRUE a list with the names for each block diagonal element is returned. If FALSE a character vector with all column names is returned. Defaults to FALSE.
	some methods for this generic require additional arguments. None are used in this method.

## Value

if asList is FALSE, a character vector with column names of the matrix represented by object; otherwise, if asList is TRUE, a list with components given by the column names of the individual block diagonal elements in the matrix represented by object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
Names, Names.pdMat
```

```
pd1 <- pdBlocked(list(\simSex - 1, \simage - 1), data = Orthodont)
Names(pd1)
```

Names.pdMat

Names.pdMat

Names of a pdMat Object

## **Description**

This method function returns the fist element of the Dimnames attribute of object, which contains the column names of the matrix represented by object.

# Usage

```
## $3 method for class 'pdMat'
Names(object, ...)
## $3 replacement method for class 'pdMat'
Names(object, ...) <- value</pre>
```

## Arguments

object an object inheriting from class "pdMat", representing a positive-definite matrix.

value a character vector with the replacement values for the column and row names of the matrix represented by object. It must have length equal to the dimension of the matrix represented by object and, if names have been previously assigned to object, it must correspond to a permutation of the original names.

some methods for this generic require additional arguments. None are used in this method.

### Value

if object has a Dimnames attribute then the first element of this attribute is returned; otherwise NULL.

## SIDE EFFECTS

On the left side of an assignment, sets the Dimnames attribute of object to list(value, value).

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
Names, Names.pdBlocked
```

```
pd1 <- pdSymm(~age, data = Orthodont)
Names(pd1)</pre>
```

Names.reStruct 181

Names.reStruct	Names of an reStruct Object	

# Description

This method function extracts the column names of each of the positive-definite matrices represented the pdMat elements of object.

## Usage

```
## S3 method for class 'reStruct'
Names(object, ...)
## S3 replacement method for class 'reStruct'
Names(object, ...) <- value</pre>
```

### **Arguments**

object	an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.
value	a list of character vectors with the replacement values for the names of the individual pdMat objects that form object. It must have the same length as object.
	some methods for this generic require additional arguments. None are used in this method.

#### Value

a list containing the column names of each of the positive-definite matrices represented by the pdMat elements of object.

### SIDE EFFECTS

On the left side of an assignment, sets the Names of the pdMat elements of object to the corresponding element of value.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
reStruct, pdMat, Names.pdMat
```

```
rs1 <- reStruct(list(Dog = ~day, Side = ~1), data = Pixel)
Names(rs1)</pre>
```

needUpdate

Check if Update is Needed

### **Description**

This function is generic; method functions can be written to handle specific classes of objects. By default, it tries to extract a needUpdate attribute of object. If this is NULL or FALSE it returns FALSE; else it returns TRUE. Updating of objects usually takes place in iterative algorithms in which auxiliary quantities associated with the object, and not being optimized over, may change.

## Usage

```
needUpdate(object)
```

# **Arguments**

object

any object

#### Value

a logical value indicating whether object needs to be updated.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
needUpdate.modelStruct
```

## **Examples**

```
vf1 <- varExp()
vf1 <- Initialize(vf1, data = Orthodont)
needUpdate(vf1)</pre>
```

needUpdate.modelStruct

Check if a modelStruct Object Needs Updating

## **Description**

This method function checks if any of the elements of object needs to be updated. Updating of objects usually takes place in iterative algorithms in which auxiliary quantities associated with the object, and not being optimized over, may change.

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### Usage

```
## S3 method for class 'modelStruct'
needUpdate(object)
```

## Arguments

object

an object inheriting from class "modelStruct", representing a list of model components, such as corStruct and varFunc objects.

## Value

a logical value indicating whether any element of object needs to be updated.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

needUpdate

## **Examples**

```
lms1 <- lmeStruct(reStruct = reStruct(pdDiag(diag(2), ~age)),
    varStruct = varPower(form = ~age))
needUpdate(lms1)</pre>
```

Nitrendipene

Assay of nitrendipene

### **Description**

The Nitrendipene data frame has 89 rows and 4 columns.

## Format

This data frame contains the following columns:

```
activity a numeric vector
NIF a numeric vector
Tissue an ordered factor with levels 2 < 1 < 3 < 4</li>
log.NIF a numeric vector
```

## **Source**

Bates, D. M. and Watts, D. G. (1988), *Nonlinear Regression Analysis and Its Applications*, Wiley, New York.

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nlme

Nonlinear Mixed-Effects Models

## Description

This generic function fits a nonlinear mixed-effects model in the formulation described in Lindstrom and Bates (1990) but allowing for nested random effects. The within-group errors are allowed to be correlated and/or have unequal variances.

### Usage

```
nlme(model, data, fixed, random, groups, start, correlation, weights,
     subset, method, na.action, naPattern, control, verbose)
## S3 method for class 'formula'
nlme(model, data, fixed, random, groups, start, correlation, weights,
    subset, method, na.action, naPattern, control, verbose)
```

## **Arguments**

model

a nonlinear model formula, with the response on the left of a ~ operator and an expression involving parameters and covariates on the right, or an nlsList object. If data is given, all names used in the formula should be defined as parameters or variables in the data frame. The method function nlme.nlsList is documented separately.

data

an optional data frame containing the variables named in model, fixed, random, correlation, weights, subset, and naPattern. By default the variables are taken from the environment from which nlme is called.

fixed

a two-sided linear formula of the form f1+...+fn~x1+...+xm, or a list of twosided formulas of the form f1~x1+...+xm, with possibly different models for different parameters. The f1, ..., fn are the names of parameters included on the right hand side of model and the x1+...+xm expressions define linear models for these parameters (when the left hand side of the formula contains several parameters, they all are assumed to follow the same linear model, described by the right hand side expression). A 1 on the right hand side of the formula(s) indicates a single fixed effects for the corresponding parameter(s).

optionally, any of the following: (i) a two-sided formula of the form r1+...+rn~x1+...+xm | g1/.../gQ, with r1,...,rn naming parameters included on the right hand side of model, x1+...+xm specifying the random-effects model for these parameters and g1/.../g0 the grouping structure (0 may be equal to 1, in which case no / is required). The random effects formula will be repeated for all levels of grouping, in the case of multiple levels of grouping; (ii) a two-sided formula of the form r1+...+rn~x1+..+xm, a list of two-sided formulas of the form r1~x1+...+xm, with possibly different random-effects models for different parameters, a pdMat object with a two-sided formula, or list of two-sided

random

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> formulas (i.e. a non-NULL value for formula (random)), or a list of pdMat objects with two-sided formulas, or lists of two-sided formulas. In this case, the grouping structure formula will be given in groups, or derived from the data used to fit the nonlinear mixed-effects model, which should inherit from class groupedData; (iii) a named list of formulas, lists of formulas, or pdMat objects as in (ii), with the grouping factors as names. The order of nesting will be assumed the same as the order of the order of the elements in the list; (iv) an reStruct object. See the documentation on pdClasses for a description of the available pdMat classes. Defaults to fixed, resulting in all fixed effects having also random effects.

groups

an optional one-sided formula of the form ~g1 (single level of nesting) or ~g1/.../gQ (multiple levels of nesting), specifying the partitions of the data over which the random effects vary. g1, ..., gQ must evaluate to factors in data. The order of nesting, when multiple levels are present, is taken from left to right (i.e. g1 is the first level, g2 the second, etc.).

start

an optional numeric vector, or list of initial estimates for the fixed effects and random effects. If declared as a numeric vector, it is converted internally to a list with a single component fixed, given by the vector. The fixed component is required, unless the model function inherits from class selfStart, in which case initial values will be derived from a call to nlsList. An optional random component is used to specify initial values for the random effects and should consist of a matrix, or a list of matrices with length equal to the number of grouping levels. Each matrix should have as many rows as the number of groups at the corresponding level and as many columns as the number of random effects in that level.

correlation

an optional corStruct object describing the within-group correlation structure. See the documentation of corClasses for a description of the available corStruct classes. Defaults to NULL, corresponding to no within-group correlations.

weights

an optional varFunc object or one-sided formula describing the within-group heteroscedasticity structure. If given as a formula, it is used as the argument to varFixed, corresponding to fixed variance weights. See the documentation on varClasses for a description of the available varFunc classes. Defaults to NULL, corresponding to homoscedastic within-group errors.

subset

an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.

method

a character string. If "REML" the model is fit by maximizing the restricted loglikelihood. If "ML" the log-likelihood is maximized. Defaults to "ML".

na.action

a function that indicates what should happen when the data contain NAs. The default action (na. fail) causes nlme to print an error message and terminate if there are any incomplete observations.

naPattern

an expression or formula object, specifying which returned values are to be regarded as missing.

control

a list of control values for the estimation algorithm to replace the default values returned by the function nlmeControl. Defaults to an empty list.

nlme

verbose

an optional logical value. If TRUE information on the evolution of the iterative algorithm is printed. Default is FALSE.

#### Value

an object of class nlme representing the nonlinear mixed-effects model fit. Generic functions such as print, plot and summary have methods to show the results of the fit. See nlmeObject for the components of the fit. The functions resid, coef, fitted, fixed.effects, and random.effects can be used to extract some of its components.

#### Note

The function does not do any scaling internally: the optimization will work best when the response is scaled so its variance is of the order of one.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

The model formulation and computational methods are described in Lindstrom, M.J. and Bates, D.M. (1990). The variance-covariance parametrizations are described in Pinheiro and Bates (1996).

Lindstrom, M.J. and Bates, D.M. (1990) "Nonlinear Mixed Effects Models for Repeated Measures Data", Biometrics, 46, 673-687.

Pinheiro, J.C. and Bates., D.M. (1996) "Unconstrained Parametrizations for Variance-Covariance Matrices", Statistics and Computing, 6, 289-296.

For the different correlation structures, variance functions and links, see 'References' in 1me.

### See Also

 $\verb|nlmeControl|, \verb|nlme.nlsList|, \verb|nlmeObject|, \verb|nlsList|, \verb|nlmeStruct|, \verb|pdClasses|, \verb|reStruct|, \verb|varFunc|, \verb|corClasses|, \verb|varClasses|, \|varClasses|, \|varClass$ 

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nlme.nlsList

NLME fit from nlsList Object

### **Description**

If the random effects names defined in random are a subset of the lmList object coefficient names, initial estimates for the covariance matrix of the random effects are obtained (overwriting any values given in random). formula(fixed) and the data argument in the calling sequence used to obtain fixed are passed as the fixed and data arguments to nlme.formula, together with any other additional arguments in the function call. See the documentation on nlme.formula for a description of that function.

# Usage

### **Arguments**

٤	suments	
	model	an object inheriting from class "nlsList", representing a list of nls fits with a common model.
	data	this argument is included for consistency with the generic function. It is ignored in this method function.
	fixed	this argument is included for consistency with the generic function. It is ignored in this method function.
	random	an optional one-sided linear formula with no conditioning expression, or a pdMat object with a formula attribute. Multiple levels of grouping are not allowed with this method function. Defaults to a formula consisting of the right hand side of formula(fixed).
	groups	an optional one-sided formula of the form $^g1$ (single level of nesting) or $^g1/\dots/gQ$ (multiple levels of nesting), specifying the partitions of the data over which the random effects vary. $g1,\dots,gQ$ must evaluate to factors in data. The order of nesting, when multiple levels are present, is taken from left to right (i.e. $g1$ is the first level, $g2$ the second, etc.).
	start	an optional numeric vector, or list of initial estimates for the fixed effects and random effects. If declared as a numeric vector, it is converted internally to a list with a single component fixed, given by the vector. The fixed component is required, unless the model function inherits from class selfStart, in which case initial values will be derived from a call to nlsList. An optional random

in that level.

component is used to specify initial values for the random effects and should consist of a matrix, or a list of matrices with length equal to the number of grouping levels. Each matrix should have as many rows as the number of groups at the corresponding level and as many columns as the number of random effects

nlme.nlsList

correlation an optional corStruct object describing the within-group correlation structure. See the documentation of corClasses for a description of the available corStruct classes. Defaults to NULL, corresponding to no within-group correlations. weights an optional varFunc object or one-sided formula describing the within-group heteroscedasticity structure. If given as a formula, it is used as the argument to varFixed, corresponding to fixed variance weights. See the documentation on varClasses for a description of the available varFunc classes. Defaults to NULL, corresponding to homoscedastic within-group errors. subset an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default. method a character string. If "REML" the model is fit by maximizing the restricted loglikelihood. If "ML" the log-likelihood is maximized. Defaults to "ML". a function that indicates what should happen when the data contain NAs. The na.action default action (na.fail) causes nlme to print an error message and terminate if there are any incomplete observations. naPattern an expression or formula object, specifying which returned values are to be regarded as missing. control a list of control values for the estimation algorithm to replace the default values returned by the function nlmeControl. Defaults to an empty list. an optional logical value. If TRUE information on the evolution of the iterative verbose algorithm is printed. Default is FALSE.

# Value

an object of class nlme representing the linear mixed-effects model fit. Generic functions such as print, plot and summary have methods to show the results of the fit. See nlmeObject for the components of the fit. The functions resid, coef, fitted, fixed.effects, and random.effects can be used to extract some of its components.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

The computational methods follow on the general framework of Lindstrom, M.J. and Bates, D.M. (1988). The model formulation is described in Laird, N.M. and Ware, J.H. (1982). The variance-covariance parametrizations are described in <Pinheiro, J.C. and Bates., D.M. (1996). The different correlation structures available for the correlation argument are described in Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994), Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996), and Venables, W.N. and Ripley, B.D. (2002). The use of variance functions for linear and nonlinear mixed effects models is presented in detail in Davidian, M. and Giltinan, D.M. (1995).

Box, G.E.P., Jenkins, G.M., and Reinsel G.C. (1994) "Time Series Analysis: Forecasting and Control", 3rd Edition, Holden-Day.

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Davidian, M. and Giltinan, D.M. (1995) "Nonlinear Mixed Effects Models for Repeated Measurement Data", Chapman and Hall.

Laird, N.M. and Ware, J.H. (1982) "Random-Effects Models for Longitudinal Data", Biometrics, 38, 963-974.

Lindstrom, M.J. and Bates, D.M. (1988) "Newton-Raphson and EM Algorithms for Linear Mixed-Effects Models for Repeated-Measures Data", Journal of the American Statistical Association, 83, 1014-1022.

Littel, R.C., Milliken, G.A., Stroup, W.W., and Wolfinger, R.D. (1996) "SAS Systems for Mixed Models", SAS Institute.

Pinheiro, J.C. and Bates., D.M. (1996) "Unconstrained Parametrizations for Variance-Covariance Matrices", Statistics and Computing, 6, 289-296.

Venables, W.N. and Ripley, B.D. (2002) "Modern Applied Statistics with S", 4th Edition, Springer-Verlag.

#### See Also

```
nlme, lmList, nlmeObject
```

### **Examples**

```
fm1 <- nlsList(SSasymp, data = Loblolly)
fm2 <- nlme(fm1, random = Asym ~ 1)
summary(fm1)
summary(fm2)</pre>
```

nlmeControl

Control Values for nlme Fit

### **Description**

The values supplied in the function call replace the defaults and a list with all possible arguments is returned. The returned list is used as the control argument to the nlme function.

### Usage

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### **Arguments**

maxIter maximum number of iterations for the nlme optimization algorithm. Default is pnlsMaxIter maximum number of iterations for the PNLS optimization step inside the nlme optimization. Default is 7. msMaxIter maximum number of iterations for nlminb (iter.max) or the nlm (iterlim, from the 10-th step) optimization step inside the nlme optimization. Default is 50 (which may be too small for e.g. for overparametrized cases). minScale minimum factor by which to shrink the default step size in an attempt to decrease the sum of squares in the PNLS step. Default 0.001. tolerance tolerance for the convergence criterion in the nlme algorithm. Default is 1e-6. number of iterations for the EM algorithm used to refine the initial estimates of niterEM the random effects variance-covariance coefficients. Default is 25. pnlsTol tolerance for the convergence criterion in PNLS step. Default is 1e-3. msTol tolerance for the convergence criterion in nlm, passed as the gradtol argument to the function (see documentation on nlm). Default is 1e-7. returnObject a logical value indicating whether the fitted object should be returned when the maximum number of iterations is reached without convergence of the algorithm. Default is FALSE. msVerbose a logical value passed as the trace to nlminb(.., control=list(trace = \*, ..)) or as argument print.level to nlm(). Default is FALSE. msWarnNoConv logical indicating if a warning should be signalled whenever the minimization (by opt) in the LME step does not converge; defaults to TRUE. gradHess a logical value indicating whether numerical gradient vectors and Hessian matrices of the log-likelihood function should be used in the nlm optimization. This option is only available when the correlation structure (corStruct) and the variance function structure (varFunc) have no "varying" parameters and the pdMat classes used in the random effects structure are pdSymm (general positivedefinite), pdDiag (diagonal), pdIdent (multiple of the identity), or pdCompSymm (compound symmetry). Default is TRUE. apVar a logical value indicating whether the approximate covariance matrix of the variance-covariance parameters should be calculated. Default is TRUE. .relStep relative step for numerical derivatives calculations. Default is .Machine\$double.eps^(1/3). minAbsParApVar numeric value - minimum absolute parameter value in the approximate variance calculation. The default is 0.05. opt the optimizer to be used, either "nlminb" (the default) or "nlm". natural a logical value indicating whether the pdNatural parametrization should be used for general positive-definite matrices (pdSymm) in reStruct, when the approximate covariance matrix of the estimators is calculated. Default is TRUE. optionally a positive number to fix the residual error at. If NULL, as by default, sigma or 0, sigma is estimated. Further, named control arguments to be passed to nlminb (apart from trace and iter.max mentioned above), where used (eval.max and those from abs.tol

down).

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#### Value

a list with components for each of the possible arguments.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>; the sigma option: Siem Heisterkamp and Bert van Willigen.

#### See Also

```
nlme, nlm, optim, nlmeStruct
```

## **Examples**

```
# decrease the maximum number of iterations and request tracing
nlmeControl(msMaxIter = 20, msVerbose = TRUE)
```

nlmeObject

Fitted nlme Object

## Description

An object returned by the nlme function, inheriting from class "nlme", also inheriting from class "lme", and representing a fitted nonlinear mixed-effects model. Objects of this class have methods for the generic functions anova, coef, fitted, fixed.effects, formula, getGroups, getResponse, intervals, logLik, pairs, plot, predict, print, random.effects, residuals, summary, and update.

#### Value

The following components must be included in a legitimate "nlme" object.

apVar an approximate covariance matrix for the variance-covariance coefficients. If

apVar = FALSE in the control values used in the call to nlme, this component is

NULL.

call a list containing an image of the nlme call that produced the object.

coefficients a list with two components, fixed and random, where the first is a vector con-

taining the estimated fixed effects and the second is a list of matrices with the estimated random effects for each level of grouping. For each matrix in the random list, the columns refer to the random effects and the rows to the groups.

contrasts a list of the contrast matrices used to represent factors in the fixed effects for-

mula and/or random effects formula. This information is important for making predictions from a new data frame in which not all levels of the original factors are observed. If no factors are used in the nlme model, this component will be

an empty list.

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dims	a list with basic dimensions used in the nlme fit, including the components N - the number of observations in the data, Q - the number of grouping levels, qvec - the number of random effects at each level from innermost to outermost (last two values are equal to zero and correspond to the fixed effects and the response), ngrps - the number of groups at each level from innermost to outermost (last two values are one and correspond to the fixed effects and the response), and ncol - the number of columns in the model matrix for each level of grouping from innermost to outermost (last two values are equal to the number of fixed effects and one).
fitted	a data frame with the fitted values as columns. The leftmost column corresponds to the population fixed effects (corresponding to the fixed effects only) and successive columns from left to right correspond to increasing levels of grouping.
fixDF	a list with components X and terms specifying the denominator degrees of freedom for, respectively, t-tests for the individual fixed effects and F-tests for the fixed-effects terms in the models.
groups	a data frame with the grouping factors as columns. The grouping level increases from left to right.
logLik	the (restricted) log-likelihood at convergence.
map	a list with components fmap, rmap, rmapRel, and bmap, specifying various mappings for the fixed and random effects, used to generate predictions from the fitted object.
method	the estimation method: either "ML" for maximum likelihood, or "REML" for restricted maximum likelihood.
modelStruct	an object inheriting from class nlmeStruct, representing a list of mixed-effects model components, such as reStruct, corStruct, and varFunc objects.
numIter	the number of iterations used in the iterative algorithm.
residuals	a data frame with the residuals as columns. The leftmost column corresponds to

increasing levels of grouping.

sigma the estimated within-group error standard deviation.

varFix an approximate covariance matrix of the fixed effects estimates.

the population residuals and successive columns from left to right correspond to

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

nlme, nlmeStruct

nlmeStruct 193

nlmeStruct	ruct Nonlinear Mixed-Effects Structure

# Description

A nonlinear mixed-effects structure is a list of model components representing different sets of parameters in the nonlinear mixed-effects model. An nlmeStruct list must contain at least a reStruct object, but may also contain corStruct and varFunc objects. NULL arguments are not included in the nlmeStruct list.

### Usage

```
nlmeStruct(reStruct, corStruct, varStruct)
```

## **Arguments**

reStruct a reStruct representing a random effects structure.

corStruct an optional corStruct object, representing a correlation structure. Default is

NULL.

varStruct an optional varFunc object, representing a variance function structure. Default

is NULL.

## Value

a list of model components determining the parameters to be estimated for the associated nonlinear mixed-effects model.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
corClasses, nlme, residuals.nlmeStruct, reStruct, varFunc
```

```
nlms1 <- nlmeStruct(reStruct(~age), corAR1(), varPower())</pre>
```

194 nlsList

nlsList

List of nls Objects with a Common Model

# Description

Data is partitioned according to the levels of the grouping factor defined in model and individual nls fits are obtained for each data partition, using the model defined in model.

## Usage

# **Arguments**

object	an object inheriting from class nlsList, representing a list of fitted nls objects.
model	either a nonlinear model formula, with the response on the left of a ~ operator and an expression involving parameters, covariates, and a grouping factor separated by the   operator on the right, or a selfStart function. The method function nlsList.selfStart is documented separately.
model.	changes to the model – see update.formula for details.
data	a data frame in which to interpret the variables named in model.
start	an optional named list with initial values for the parameters to be estimated in model. It is passed as the start argument to each nls call and is required when the nonlinear function in model does not inherit from class selfStart.
control	a list of control values passed as the control argument to nls. Defaults to an empty list.
level	an optional integer specifying the level of grouping to be used when multiple nested levels of grouping are present.
subset	an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes nlsList to print an error message and terminate if there are any incomplete observations.

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pool	an optional logical value that is preserved as an attribute of the returned value. This will be used as the default for pool in calculations of standard deviations or standard errors for summaries.
warn.nls	logical indicating if nls() errors (all of which are caught by tryCatch) should be signalled as a "summarizing" warning.
• • •	some methods for this generic require additional arguments. None are used in this method.
evaluate	If TRUE evaluate the new call else return the call.

#### **Details**

As nls(.) is called on each sub group, and convergence of these may be problematic, these calls happen with error catching.

Since **nlme** version 3.1–127 (2016-04), all the errors are caught (via tryCatch) and if present, a "summarizing" warning is stored as attribute of the resulting "nlsList" object and signalled unless suppressed by warn.nls = FALSE or currently also when warn.nls = NA (default) and getOption("show.error.messages" is false.

nlsList() originally had used try(\*) (with its default silent=FALSE) and hence all errors were printed to the console *unless* the global option show.error.messages was set to true. This still works, but has been *deprecated*.

### Value

a list of nls objects with as many components as the number of groups defined by the grouping factor. Generic functions such as coef, fixed.effects, lme, pairs, plot, predict, random.effects, summary, and update have methods that can be applied to an nlsList object.

#### References

Pinheiro, J.C., and Bates, D.M. (2000), Mixed-Effects Models in S and S-PLUS, Springer.

#### See Also

```
nls, nlme.nlsList, nlsList.selfStart, summary.nlsList
```

nlsList.selfStart

## **Description**

The response variable and primary covariate in formula(data) are used together with model to construct the nonlinear model formula. This is used in the nls calls and, because a self-starting model function can calculate initial estimates for its parameters from the data, no starting estimates need to be provided.

# Usage

### **Arguments**

model	a "selfStart" model function, which calculates initial estimates for the model parameters from data.
data	a data frame in which to interpret the variables in model. Because no grouping factor can be specified in model, data must inherit from class "groupedData".
start	an optional named list with initial values for the parameters to be estimated in model. It is passed as the start argument to each nls call and is required when the nonlinear function in model does not inherit from class selfStart.
control	a list of control values passed as the control argument to nls. Defaults to an empty list.
level	an optional integer specifying the level of grouping to be used when multiple nested levels of grouping are present.
subset	an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes nlsList to print an error message and terminate if there are any incomplete observations.
pool,warn.nls	optional logicals, see nlsList.

### Value

a list of nls objects with as many components as the number of groups defined by the grouping factor. A NULL value is assigned to the components corresponding to clusters for which the nls algorithm failed to converge. Generic functions such as coef, fixed.effects, lme, pairs, plot, predict, random.effects, summary, and update have methods that can be applied to an nlsList object.

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### See Also

```
selfStart, groupedData, nls, nlsList, nlme.nlsList, nlsList.formula
```

## **Examples**

```
fm1 <- nlsList(SSasympOff, CO2)
summary(fm1)</pre>
```

0ats

Split-plot Experiment on Varieties of Oats

## **Description**

The Oats data frame has 72 rows and 4 columns.

#### **Format**

This data frame contains the following columns:

```
Block an ordered factor with levels VI < V < III < IV < II < I

Variety a factor with levels Golden Rain Marvellous Victory

nitro a numeric vector

yield a numeric vector
```

#### **Details**

These data have been introduced by Yates (1935) as an example of a split-plot design. The treatment structure used in the experiment was a  $3 \times 4$  full factorial, with three varieties of oats and four concentrations of nitrogen. The experimental units were arranged into six blocks, each with three whole-plots subdivided into four subplots. The varieties of oats were assigned randomly to the whole-plots and the concentrations of nitrogen to the subplots. All four concentrations of nitrogen were used on each whole-plot.

### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.15)

Venables, W. N. and Ripley, B. D. (2002) *Modern Applied Statistics with S. (4th ed)*, Springer, New York.

198 Orthodont

Orthodont

Growth curve data on an orthdontic measurement

### **Description**

The Orthodont data frame has 108 rows and 4 columns of the change in an orthdontic measurement over time for several young subjects.

#### **Format**

This data frame contains the following columns:

**distance** a numeric vector of distances from the pituitary to the pterygomaxillary fissure (mm). These distances are measured on x-ray images of the skull.

age a numeric vector of ages of the subject (yr).

**Subject** an ordered factor indicating the subject on which the measurement was made. The levels are labelled M01 to M16 for the males and F01 to F13 for the females. The ordering is by increasing average distance within sex.

Sex a factor with levels Male and Female

### **Details**

Investigators at the University of North Carolina Dental School followed the growth of 27 children (16 males, 11 females) from age 8 until age 14. Every two years they measured the distance between the pituitary and the pterygomaxillary fissure, two points that are easily identified on x-ray exposures of the side of the head.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.17)

Potthoff, R. F. and Roy, S. N. (1964), "A generalized multivariate analysis of variance model useful especially for growth curve problems", *Biometrika*, **51**, 313–326.

#### **Examples**

formula(Orthodont)
plot(Orthodont)

Ovary 199

Counts of Ovarian Follicles 0vary

## **Description**

The Ovary data frame has 308 rows and 3 columns.

#### **Format**

This data frame contains the following columns:

**Mare** an ordered factor indicating the mare on which the measurement is made.

Time time in the estrus cycle. The data were recorded daily from 3 days before ovulation until 3 days after the next ovulation. The measurement times for each mare are scaled so that the ovulations for each mare occur at times 0 and 1.

**follicles** the number of ovarian follicles greater than 10 mm in diameter.

#### **Details**

Pierson and Ginther (1987) report on a study of the number of large ovarian follicles detected in different mares at several times in their estrus cycles.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), Mixed-Effects Models in S and S-PLUS, Springer, New York. (Appendix A.18)

Pierson, R. A. and Ginther, O. J. (1987), Follicular population dynamics during the estrus cycle of the mare, Animal Reproduction Science, 14, 219-231.

0xboys Heights of Boys in Oxford

### **Description**

The Oxboys data frame has 234 rows and 4 columns.

### **Format**

This data frame contains the following columns:

**Subject** an ordered factor giving a unique identifier for each boy in the experiment

age a numeric vector giving the standardized age (dimensionless)

**height** a numeric vector giving the height of the boy (cm)

Occasion an ordered factor - the result of converting age from a continuous variable to a count so these slightly unbalanced data can be analyzed as balanced.

200 Oxide

#### **Details**

These data are described in Goldstein (1987) as data on the height of a selection of boys from Oxford, England versus a standardized age.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.19)

0xide

Variability in Semiconductor Manufacturing

## **Description**

The Oxide data frame has 72 rows and 5 columns.

#### **Format**

This data frame contains the following columns:

**Source** a factor with levels 1 and 2

Lot a factor giving a unique identifier for each lot.

**Wafer** a factor giving a unique identifier for each wafer within a lot.

Site a factor with levels 1, 2, and 3

**Thickness** a numeric vector giving the thickness of the oxide layer.

### **Details**

These data are described in Littell et al. (1996, p. 155) as coming "from a passive data collection study in the semiconductor industry where the objective is to estimate the variance components to determine the assignable causes of the observed variability." The observed response is the thickness of the oxide layer on silicon wafers, measured at three different sites of each of three wafers selected from each of eight lots sampled from the population of lots.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.20)

Littell, R. C., Milliken, G. A., Stroup, W. W. and Wolfinger, R. D. (1996), SAS System for Mixed Models, SAS Institute, Cary, NC.

pairs.compareFits 201

pairs.compareFits

Pairs Plot of compareFits Object

## Description

Scatter plots of the values being compared are generated for each pair of coefficients in x. Different symbols (colors) are used for each object being compared and values corresponding to the same group are joined by a line, to facilitate comparison of fits. If only two coefficients are present, the trellis function xyplot is used; otherwise the trellis function splom is used.

## Usage

```
## S3 method for class 'compareFits'
pairs(x, subset, key, ...)
```

## **Arguments**

x an object of class compareFits.

subset an optional logical or integer vector specifying which rows of x should be used

in the plots. If missing, all rows are used.

key an optional logical value, or list. If TRUE, a legend is included at the top of

the plot indicating which symbols (colors) correspond to which objects being compared. If FALSE, no legend is included. If given as a list, key is passed down as an argument to the trellis function generating the plots (splom or xyplot).

Defaults to TRUE.

... optional arguments passed down to the trellis function generating the plots.

## Value

Pairwise scatter plots of the values being compared, with different symbols (colors) used for each object under comparison.

### Author(s)

José Pinheiro and Douglas Bates

### See Also

```
compareFits, plot.compareFits, pairs.lme, pairs.lmList, xyplot, splom
```

```
example(compareFits) # cF12 <- compareFits(coef(lmList(Orthodont)), .. lme(*))
pairs(cF12)</pre>
```

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pairs.lme

Pairs Plot of an lme Object

#### **Description**

Diagnostic plots for the linear mixed-effects fit are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a Trellis display. The expression on the right hand side of the formula, before a operator, must evaluate to a data frame with at least two columns. If the data frame has two columns, a scatter plot of the two variables is displayed (the Trellis function xyplot is used). Otherwise, if more than two columns are present, a scatter plot matrix with pairwise scatter plots of the columns in the data frame is displayed (the Trellis function splom is used).

### Usage

```
## S3 method for class 'lme'
pairs(x, form, label, id, idLabels, grid, ...)
```

### **Arguments**

form

an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

an optional one-sided formula specifying the desired type of plot. Any variable present in the original data frame used to obtain x can be referenced. In addition, x itself can be referenced in the formula using the symbol ".". Conditional expressions on the right of a | operator can be used to define separate panels in a Trellis display. The expression on the right hand side of form, and to the left of the | operator, must evaluate to a data frame with at least two columns. Default is ~ coef(.), corresponding to a pairs plot of the coefficients evaluated at the

innermost level of nesting.

label an optional character vector of labels for the variables in the pairs plot.

> an optional numeric value, or one-sided formula. If given as a value, it is used as a significance level for an outlier test based on the Mahalanobis distances of the estimated random effects. Groups with random effects distances greater than the 1-value percentile of the appropriate chi-square distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify

points in the plot. If missing, no points are identified.

idLabels an optional vector, or one-sided formula. If given as a vector, it is converted

> to character and used to label the points identified according to id. If given as a one-sided formula, its right hand side must evaluate to a vector which is converted to character and used to label the identified points. Default is the

innermost grouping factor.

grid an optional logical value indicating whether a grid should be added to plot. De-

fault is FALSE.

optional arguments passed to the Trellis plot function.

id

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#### Value

a diagnostic Trellis plot.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lme, pairs.compareFits, pairs.lmList, xyplot, splom
```

## **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)
# scatter plot of coefficients by gender, identifying unusual subjects
pairs(fm1, ~coef(., augFrame = TRUE) | Sex, id = 0.1, adj = -0.5)
# scatter plot of estimated random effects :
pairs(fm1, ~ranef(.))</pre>
```

pairs.lmList

Pairs Plot of an lmList Object

### **Description**

Diagnostic plots for the linear model fits corresponding to the x components are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a Trellis display. The expression on the right hand side of the formula, before a | operator, must evaluate to a data frame with at least two columns. If the data frame has two columns, a scatter plot of the two variables is displayed (the Trellis function xyplot is used). Otherwise, if more than two columns are present, a scatter plot matrix with pairwise scatter plots of the columns in the data frame is displayed (the Trellis function splom is used).

#### Usage

```
## S3 method for class 'lmList'
pairs(x, form, label, id, idLabels, grid, ...)
```

## Arguments

x an object inheriting from class "lmList", representing a list of lm objects with a common model.

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form an optional one-sided formula specifying the desired type of plot. Any variable

present in the original data frame used to obtain x can be referenced. In addition, x itself can be referenced in the formula using the symbol ".". Conditional expressions on the right of a | operator can be used to define separate panels in a Trellis display. The expression on the right hand side of form, and to the left of the | operator, must evaluate to a data frame with at least two columns. Default

is ~ coef(.), corresponding to a pairs plot of the coefficients of x.

label an optional character vector of labels for the variables in the pairs plot.

id an optional numeric value, or one-sided formula. If given as a value, it is used

as a significance level for an outlier test based on the Mahalanobis distances of the estimated random effects. Groups with random effects distances greater than the 1-value percentile of the appropriate chi-square distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify

points in the plot. If missing, no points are identified.

idLabels an optional vector, or one-sided formula. If given as a vector, it is converted

to character and used to label the points identified according to id. If given as a one-sided formula, its right hand side must evaluate to a vector which is converted to character and used to label the identified points. Default is the

innermost grouping factor.

grid an optional logical value indicating whether a grid should be added to plot. De-

fault is FALSE.

... optional arguments passed to the Trellis plot function.

#### Value

a diagnostic Trellis plot.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lmList, pairs.lme, pairs.compareFits, xyplot, splom
```

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
# scatter plot of coefficients by gender, identifying unusual subjects
pairs(fm1, ~coef(.) | Sex, id = 0.1, adj = -0.5)
# scatter plot of estimated random effects -- "bivariate Gaussian (?)"
pairs(fm1, ~ranef(.))</pre>
```

PBG 205

PBG

Effect of Phenylbiguanide on Blood Pressure

## **Description**

The PBG data frame has 60 rows and 5 columns.

#### **Format**

This data frame contains the following columns:

deltaBP a numeric vector

dose a numeric vector

**Run** an ordered factor with levels T5 < T4 < T3 < T2 < T1 < P5 < P3 < P2 < P4 < P1

Treatment a factor with levels MDL 72222 Placebo

**Rabbit** an ordered factor with levels 5 < 3 < 2 < 4 < 1

### **Details**

Data on an experiment to examine the effect of a antagonist MDL 72222 on the change in blood pressure experienced with increasing dosage of phenylbiguanide are described in Ludbrook (1994) and analyzed in Venables and Ripley (2002, section 10.3). Each of five rabbits was exposed to increasing doses of phenylbiguanide after having either a placebo or the HD5-antagonist MDL 72222 administered.

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.21)

Venables, W. N. and Ripley, B. D. (2002) *Modern Applied Statistics with S (4th ed)*, Springer, New York.

Ludbrook, J. (1994), Repeated measurements and multiple comparisons in cardiovascular research, *Cardiovascular Research*, **28**, 303-311.

pdBlocked

Positive-Definite Block Diagonal Matrix

206 pdBlocked

## **Description**

This function is a constructor for the pdBlocked class, representing a positive-definite block-diagonal matrix. Each block-diagonal element of the underlying matrix is itself a positive-definite matrix and is represented internally as an individual pdMat object. When value is numeric(0), a list of uninitialized pdMat objects, a list of one-sided formulas, or a list of vectors of character strings, object is returned as an uninitialized pdBlocked object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions. If value is a list of initialized pdMat objects, object will be constructed from the list obtained by applying as.matrix to each of the pdMat elements of value. Finally, if value is a list of numeric vectors, they are assumed to represent the unrestricted coefficients of the block-diagonal elements of the underlying positive-definite matrix.

## Usage

pdBlocked(value, form, nam, data, pdClass)

#### **Arguments**

value an optional list with elements to be used as the value argument to other pdMat

constructors. These include: pdMat objects, positive-definite matrices, one-sided linear formulas, vectors of character strings, or numeric vectors. All elements in the list must be similar (e.g. all one-sided formulas, or all numeric vectors). Defaults to numeric(0), corresponding to an uninitialized object.

form an optional list of one-sided linear formulas specifying the row/column name

an optional list of one-sided linear formulas specifying the row/column names for the block-diagonal elements of the matrix represented by object. Because factors may be present in form, the formulas needs to be evaluated on a data.frame to resolve the names they define. This argument is ignored when value is a list

of one-sided formulas. Defaults to NULL.

nam an optional list of vector of character strings specifying the row/column names

for the block-diagonal elements of the matrix represented by object. Each of its components must have length equal to the dimension of the corresponding block-diagonal element and unreplicated elements. This argument is ignored

when value is a list of vector of character strings. Defaults to NULL.

data an optional data frame in which to evaluate the variables named in value and

form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on any factors appearing in the formulas. Defaults to the

parent frame from which the function was called.

pdClass an optional vector of character strings naming the pdMat classes to be assigned

to the individual blocks in the underlying matrix. If a single class is specified, it is used for all block-diagonal elements. This argument will only be used when value is missing, or its elements are not pdMat objects. Defaults to "pdSymm".

## Value

a pdBlocked object representing a positive-definite block-diagonal matrix, also inheriting from class pdMat.

pdClasses 207

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. p. 162.

#### See Also

```
as.matrix.pdMat, coef.pdMat, pdClasses, matrix<-.pdMat
```

### **Examples**

pdClasses

Positive-Definite Matrix Classes

## Description

Standard classes of positive-definite matrices (pdMat) structures available in the nlme package.

#### Value

Available standard classes:

pdSymm general positive-definite matrix, with no additional structure

pdLogChol general positive-definite matrix, with no additional structure, using a log-Cholesky

parameterization

pdDiag diagonal

pdIdent multiple of an identity

pdCompSymm compound symmetry structure (constant diagonal and constant off-diagonal el-

ements)

pdBlocked block-diagonal matrix, with diagonal blocks of any "atomic" pdMat class

pdNatural general positive-definite matrix in natural parametrization (i.e. parametrized in

terms of standard deviations and correlations). The underlying coefficients are

not unrestricted, so this class should NOT be used for optimization.

#### Note

Users may define their own pdMat classes by specifying a constructor function and, at a minimum, methods for the functions pdConstruct, pdMatrix and coef. For examples of these functions, see the methods for classes pdSymm and pdDiag.

208 pdCompSymm

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

pdBlocked, pdCompSymm, pdDiag, pdFactor, pdIdent, pdMatrix, pdNatural, pdSymm, pdLogChol

pdCompSymm

Positive-Definite Matrix with Compound Symmetry Structure

# **Description**

This function is a constructor for the pdCompSymm class, representing a positive-definite matrix with compound symmetry structure (constant diagonal and constant off-diagonal elements). The underlying matrix is represented by 2 unrestricted parameters. When value is numeric(0), an uninitialized pdMat object, a one-sided formula, or a vector of character strings, object is returned as an uninitialized pdCompSymm object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions. If value is an initialized pdMat object, object will be constructed from as.matrix(value). Finally, if value is a numeric vector of length 2, it is assumed to represent the unrestricted coefficients of the underlying positive-definite matrix.

#### Usage

pdCompSymm(value, form, nam, data)

#### **Arguments**

value an optional initialization value, which can be any of the following: a pdMat ob-

ject, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric vector of length 2. De-

faults to numeric(0), corresponding to an uninitialized object.

form an optional one-sided linear formula specifying the row/column names for the

matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL.

nam an optional vector of character strings specifying the row/column names for the

matrix represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is

ignored when value is a vector of character strings. Defaults to NULL.

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data

an optional data frame in which to evaluate the variables named in value and form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to the parent frame from which the function was called.

#### Value

a pdCompSymm object representing a positive-definite matrix with compound symmetry structure, also inheriting from class pdMat.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. p. 161.

#### See Also

```
as.matrix.pdMat, coef.pdMat, matrix<-.pdMat, pdClasses
```

### **Examples**

```
pd1 <- pdCompSymm(diag(3) + 1, nam = c("A","B","C"))
pd1</pre>
```

pdConstruct

Construct pdMat Objects

## **Description**

This function is an alternative constructor for the pdMat class associated with object and is mostly used internally in other functions. See the documentation on the principal constructor function, generally with the same name as the pdMat class of object.

### Usage

```
pdConstruct(object, value, form, nam, data, ...)
```

#### **Arguments**

object an object inheriting from class pdMat, representing a positive definite matrix. value an optional initialization value, which can be any of the following: a pdMat object, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric vector. Defaults to numeric(0), corresponding to an uninitialized object. form an optional one-sided linear formula specifying the row/column names for the matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL. nam an optional vector of character strings specifying the row/column names for the matrix represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is ignored when value is a vector of character strings. Defaults to NULL. an optional data frame in which to evaluate the variables named in value and data

form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to the parent frame from which the function was called.

optional arguments for some methods.

### Value

a pdMat object representing a positive-definite matrix, inheriting from the same classes as object.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
pdCompSymm, pdDiag, pdIdent, pdNatural, pdSymm
```

### **Examples**

```
pd1 <- pdSymm()
pdConstruct(pd1, diag(1:4))
```

pdConstruct.pdBlocked Construct pdBlocked Objects

## **Description**

This function give an alternative constructor for the pdBlocked class, representing a positive-definite block-diagonal matrix. Each block-diagonal element of the underlying matrix is itself a positive-definite matrix and is represented internally as an individual pdMat object. When value is numeric(0), a list of uninitialized pdMat objects, a list of one-sided formulas, or a list of vectors of character strings, object is returned as an uninitialized pdBlocked object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions. If value is a list of initialized pdMat objects, object will be constructed from the list obtained by applying as .matrix to each of the pdMat elements of value. Finally, if value is a list of numeric vectors, they are assumed to represent the unrestricted coefficients of the block-diagonal elements of the underlying positive-definite matrix.

#### Usage

```
## S3 method for class 'pdBlocked'
pdConstruct(object, value, form, nam, data, pdClass,
...)
```

#### **Arguments**

object an object inheriting from class "pdBlocked", representing a positive definite

block-diagonal matrix.

value an optional list with elements to be used as the value argument to other pdMat

constructors. These include: pdMat objects, positive-definite matrices, one-sided linear formulas, vectors of character strings, or numeric vectors. All elements in the list must be similar (e.g. all one-sided formulas, or all numeric

vectors). Defaults to numeric(0), corresponding to an uninitialized object.

form an optional list of one-sided linear formula specifying the row/column names for the block-diagonal elements of the matrix represented by object. Because fac-

tors may be present in form, the formulas needs to be evaluated on a data.frame to resolve the names they defines. This argument is ignored when value is a list

of one-sided formulas. Defaults to NULL.

nam an optional list of vector of character strings specifying the row/column names

for the block-diagonal elements of the matrix represented by object. Each of its components must have length equal to the dimension of the corresponding block-diagonal element and unreplicated elements. This argument is ignored

when value is a list of vector of character strings. Defaults to NULL.

data an optional data frame in which to evaluate the variables named in value and

form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to

the parent frame from which the function was called.

pdClass an optional vector of character strings naming the pdMat classes to be assigned

to the individual blocks in the underlying matrix. If a single class is specified, it is used for all block-diagonal elements. This argument will only be used when value is missing, or its elements are not pdMat objects. Defaults to "pdSymm".

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... some methods for this generic require additional arguments. None are used in this method.

### Value

a pdBlocked object representing a positive-definite block-diagonal matrix, also inheriting from class pdMat.

#### Author(s)

José Pinheiro and Douglas Bates <bate="englast: bates@stat.wisc.edu">

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
as.matrix.pdMat, coef.pdMat, pdBlocked, pdClasses, pdConstruct, matrix<-.pdMat
```

# **Examples**

```
pd1 <- pdBlocked(list(c("A","B"), c("a1", "a2", "a3")))
pdConstruct(pd1, list(diag(1:2), diag(c(0.1, 0.2, 0.3))))</pre>
```

pdDiag

Diagonal Positive-Definite Matrix

# **Description**

This function is a constructor for the pdDiag class, representing a diagonal positive-definite matrix. If the matrix associated with object is of dimension n, it is represented by n unrestricted parameters, given by the logarithm of the square-root of the diagonal values. When value is numeric(0), an uninitialized pdMat object, a one-sided formula, or a vector of character strings, object is returned as an uninitialized pdDiag object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions. If value is an initialized pdMat object, object will be constructed from as .matrix(value). Finally, if value is a numeric vector, it is assumed to represent the unrestricted coefficients of the underlying positive-definite matrix.

#### Usage

```
pdDiag(value, form, nam, data)
```

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### Arguments

value an optional initialization value, which can be any of the following: a pdMat

object, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric vector of length equal to the dimension of the underlying positive-definite matrix. Defaults to

numeric(0), corresponding to an uninitialized object.

form an optional one-sided linear formula specifying the row/column names for the

matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL.

nam an optional vector of character strings specifying the row/column names for the

matrix represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is

ignored when value is a vector of character strings. Defaults to NULL.

data an optional data frame in which to evaluate the variables named in value and

form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to

the parent frame from which the function was called.

#### Value

a pdDiag object representing a diagonal positive-definite matrix, also inheriting from class pdMat.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
as.matrix.pdMat, coef.pdMat, pdClasses, matrix<-.pdMat
```

```
pd1 <- pdDiag(diag(1:3), nam = c("A","B","C"))
pd1
```

214 pdFactor

pdFactor

Square-Root Factor of a Positive-Definite Matrix

### **Description**

A square-root factor of the positive-definite matrix represented by object is obtained. Letting  $\Sigma$  denote a positive-definite matrix, a square-root factor of  $\Sigma$  is any square matrix L such that  $\Sigma = L'L$ . This function extracts L.

### Usage

```
pdFactor(object)
```

### **Arguments**

object

an object inheriting from class pdMat, representing a positive definite matrix, which must have been initialized (i.e. length(coef(object)) > 0).

#### Value

a vector with a square-root factor of the positive-definite matrix associated with object stacked column-wise.

### Note

This function is used intensively in optimization algorithms and its value is returned as a vector for efficiency reasons. The pdMatrix function can be used to obtain square-root factors in matrix form.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

```
pdMatrix
```

```
pd1 <- pdCompSymm(4 * diag(3) + 1)
pdFactor(pd1)</pre>
```

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pdFactor.reStruct

Extract Square-Root Factor from Components of an reStruct Object

### Description

This method function extracts square-root factors of the positive-definite matrices corresponding to the pdMat elements of object.

## Usage

```
## S3 method for class 'reStruct'
pdFactor(object)
```

### **Arguments**

object

an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.

#### Value

a vector with square-root factors of the positive-definite matrices corresponding to the elements of object stacked column-wise.

### Note

This function is used intensively in optimization algorithms and its value is returned as a vector for efficiency reasons. The pdMatrix function can be used to obtain square-root factors in matrix form.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

```
pdFactor, pdMatrix.reStruct, pdFactor.pdMat
```

```
rs1 <- reStruct(pdSymm(diag(3), ~age+Sex, data = Orthodont))
pdFactor(rs1)</pre>
```

216 pdIdent

pdIdent

Multiple of the Identity Positive-Definite Matrix

## **Description**

This function is a constructor for the pdIdent class, representing a multiple of the identity positive-definite matrix. The matrix associated with object is represented by 1 unrestricted parameter, given by the logarithm of the square-root of the diagonal value. When value is numeric(0), an uninitialized pdMat object, a one-sided formula, or a vector of character strings, object is returned as an uninitialized pdIdent object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions. If value is an initialized pdMat object, object will be constructed from as.matrix(value). Finally, if value is a numeric value, it is assumed to represent the unrestricted coefficient of the underlying positive-definite matrix.

### Usage

```
pdIdent(value, form, nam, data)
```

## **Arguments**

value	an optional initialization value, which can be any of the following: a pdMat object, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric value. Defaults to numeric(0), corresponding to an uninitialized object.
form	an optional one-sided linear formula specifying the row/column names for the matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data.frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL.
nam	an optional vector of character strings specifying the row/column names for the matrix represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is ignored when value is a vector of character strings. Defaults to NULL.
data	an optional data frame in which to evaluate the variables named in value and form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to the parent frame from which the function was called.

#### Value

a pdIdent object representing a multiple of the identity positive-definite matrix, also inheriting from class pdMat.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

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#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
as.matrix.pdMat, coef.pdMat, pdClasses, matrix<-.pdMat
```

### **Examples**

```
pd1 <- pdIdent(4 * diag(3), nam = c("A","B","C"))
pd1</pre>
```

pdLogChol

General Positive-Definite Matrix

### **Description**

This function is a constructor for the pdLogChol class, representing a general positive-definite matrix. If the matrix associated with object is of dimension n, it is represented by n(n+1)/2 unrestricted parameters, using the log-Cholesky parametrization described in Pinheiro and Bates (1996).

- When value is numeric(0), an uninitialized pdMat object, a one-sided formula, or a character vector, object is returned as an *uninitialized* pdLogChol object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions.
- If value is an initialized pdMat object, object will be constructed from as.matrix(value).
- Finally, if value is a numeric vector, it is assumed to represent the unrestricted coefficients of the matrix-logarithm parametrization of the underlying positive-definite matrix.

#### Usage

```
pdLogChol(value, form, nam, data)
```

#### **Arguments**

value

an optional initialization value, which can be any of the following: a pdMat object, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric vector. Defaults to numeric(0), corresponding to an uninitialized object.

form

an optional one-sided linear formula specifying the row/column names for the matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL.

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nam an optional character vector specifying the row/column names for the matrix

represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is

ignored when value is a character vector. Defaults to NULL.

data an optional data frame in which to evaluate the variables named in value and

form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to

the parent frame from which the function was called.

#### **Details**

Internally, the pdLogChol representation of a symmetric positive definite matrix is a vector starting with the logarithms of the diagonal of the Choleski factorization of that matrix followed by its upper triangular portion.

#### Value

a pdLogChol object representing a general positive-definite matrix, also inheriting from class pdMat.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C. and Bates., D.M. (1996) Unconstrained Parametrizations for Variance-Covariance Matrices, *Statistics and Computing* **6**, 289–296.

Pinheiro, J.C., and Bates, D.M. (2000) Mixed-Effects Models in S and S-PLUS, Springer.

#### See Also

```
as.matrix.pdMat, coef.pdMat, pdClasses, matrix<-.pdMat
```

#### **Examples**

```
(pd1 <- pdLogChol(diag(1:3), nam = c("A","B","C")))
(pd4 <- pdLogChol(1:6))
(pd4c <- chol(pd4)) # -> upper-tri matrix with off-diagonals  4 5 6
pd4c[upper.tri(pd4c)]
log(diag(pd4c)) # 1 2 3
```

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pdMat	Positive-Definite Matrix	

# Description

This function gives an alternative way of constructing an object inheriting from the pdMat class named in pdClass, or from data.class(object) if object inherits from pdMat, and is mostly used internally in other functions. See the documentation on the principal constructor function, generally with the same name as the pdMat class of object.

# Usage

```
pdMat(value, form, nam, data, pdClass)
```

### **Arguments**

value	an optional initialization value, which can be any of the following: a pdMat object, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric vector. Defaults to numeric(0), corresponding to an uninitialized object.
form	an optional one-sided linear formula specifying the row/column names for the matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data.frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL.
nam	an optional vector of character strings specifying the row/column names for the matrix represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is ignored when value is a vector of character strings. Defaults to NULL.
data	an optional data frame in which to evaluate the variables named in value and form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to the parent frame from which the function was called.
pdClass	an optional character string naming the pdMat class to be assigned to the returned object. This argument will only be used when value is not a pdMat object. Defaults to "pdSymm".

### Value

a pdMat object representing a positive-definite matrix, inheriting from the class named in pdClass, or from class(object), if object inherits from pdMat.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

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#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

pdClasses, pdCompSymm, pdDiag, pdIdent, pdNatural, pdSymm, reStruct, solve.pdMat, summary.pdMat

# Examples

```
pd1 <- pdMat(diag(1:4), pdClass = "pdDiag")
pd1
str(pd1)</pre>
```

pdMatrix

Extract Matrix or Square-Root Factor from a pdMat Object

# **Description**

The positive-definite matrix represented by object, or a square-root factor of it is obtained. Letting  $\Sigma$  denote a positive-definite matrix, a square-root factor of  $\Sigma$  is any square matrix L such that  $\Sigma = L'L$ . This function extracts  $\Sigma$  or L.

#### Usage

```
pdMatrix(object, factor)
```

#### **Arguments**

object an object inheriting from class pdMat, representing a positive definite matrix.

factor an optional logical value. If TRUE, a square-root factor of the positive-definite

matrix represented by object is returned; else, if FALSE, the positive-definite

matrix is returned. Defaults to FALSE.

#### Value

if factor is FALSE the positive-definite matrix represented by object is returned; else a square-root of the positive-definite matrix is returned.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. p. 162.

pdMatrix.reStruct 221

### See Also

```
as.matrix.pdMat,pdClasses,pdFactor,pdMat,pdMatrix.reStruct,corMatrix
```

### **Examples**

```
pd1 <- pdSymm(diag(1:4))
pdMatrix(pd1)</pre>
```

pdMatrix.reStruct

Extract Matrix or Square-Root Factor from Components of an reStruct Object

### **Description**

This method function extracts the positive-definite matrices corresponding to the pdMat elements of object, or square-root factors of the positive-definite matrices.

### Usage

```
## S3 method for class 'reStruct'
pdMatrix(object, factor)
```

#### **Arguments**

object an object inheriting from class "reStruct", representing a random effects struc-

ture and consisting of a list of pdMat objects.

factor an optional logical value. If TRUE, square-root factors of the positive-definite

matrices represented by the elements of object are returned; else, if FALSE, the

positive-definite matrices are returned. Defaults to FALSE.

#### Value

a list with components given by the positive-definite matrices corresponding to the elements of object, or square-root factors of the positive-definite matrices.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. p. 162.

### See Also

```
as.matrix.reStruct, reStruct, pdMat, pdMatrix, pdMatrix.pdMat
```

222 pdNatural

### **Examples**

```
rs1 <- reStruct(pdSymm(diag(3), ~age+Sex, data = Orthodont))
pdMatrix(rs1)</pre>
```

pdNatural

General Positive-Definite Matrix in Natural Parametrization

# Description

This function is a constructor for the pdNatural class, representing a general positive-definite matrix, using a natural parametrization . If the matrix associated with object is of dimension n, it is represented by n(n+1)/2 parameters. Letting  $\sigma_{ij}$  denote the ij-th element of the underlying positive definite matrix and  $\rho_{ij} = \sigma_i/\sqrt{\sigma_{ii}\sigma_{jj}}, \ i \neq j$  denote the associated "correlations", the "natural" parameters are given by  $\sqrt{\sigma_{ii}}, \ i = 1, \ldots, n$  and  $\log((1+\rho_{ij})/(1-\rho_{ij})), \ i \neq j$ . Note that all natural parameters are individually unrestricted, but not jointly unrestricted (meaning that not all unrestricted vectors would give positive-definite matrices). Therefore, this parametrization should NOT be used for optimization. It is mostly used for deriving approximate confidence intervals on parameters following the optimization of an objective function. When value is numeric(0), an uninitialized pdMat object, a one-sided formula, or a vector of character strings, object is returned as an uninitialized pdSymm object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions. If value is an initialized pdMat object, object will be constructed from as .matrix(value). Finally, if value is a numeric vector, it is assumed to represent the natural parameters of the underlying positive-definite matrix.

### Usage

```
pdNatural(value, form, nam, data)
```

#### **Arguments**

value	an optional initialization value, which can be any of the following: a pdMat object, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric vector. Defaults to numeric(0), corresponding to an uninitialized object.
form	an optional one-sided linear formula specifying the row/column names for the matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL.
nam	an optional vector of character strings specifying the row/column names for the matrix represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is ignored when value is a vector of character strings. Defaults to NULL.
data	an optional data frame in which to evaluate the variables named in value and form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to the parent frame from which the function was called.

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#### Value

a pdNatural object representing a general positive-definite matrix in natural parametrization, also inheriting from class pdMat.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. p. 162.

#### See Also

```
as.matrix.pdMat, coef.pdMat, pdClasses, matrix<-.pdMat
```

### **Examples**

```
pdNatural(diag(1:3))
```

pdSymm

General Positive-Definite Matrix

# Description

This function is a constructor for the pdSymm class, representing a general positive-definite matrix. If the matrix associated with object is of dimension n, it is represented by n(n+1)/2 unrestricted parameters, using the matrix-logarithm parametrization described in Pinheiro and Bates (1996). When value is numeric(0), an uninitialized pdMat object, a one-sided formula, or a vector of character strings, object is returned as an uninitialized pdSymm object (with just some of its attributes and its class defined) and needs to have its coefficients assigned later, generally using the coef or matrix replacement functions. If value is an initialized pdMat object, object will be constructed from as .matrix(value). Finally, if value is a numeric vector, it is assumed to represent the unrestricted coefficients of the matrix-logarithm parametrization of the underlying positive-definite matrix.

```
pdSymm(value, form, nam, data)
```

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#### **Arguments**

value an optional initialization value, which can be any of the following: a pdMat object, a positive-definite matrix, a one-sided linear formula (with variables separated by +), a vector of character strings, or a numeric vector. Defaults to

numeric(0), corresponding to an uninitialized object.

form an optional one-sided linear formula specifying the row/column names for the

matrix represented by object. Because factors may be present in form, the formula needs to be evaluated on a data frame to resolve the names it defines. This argument is ignored when value is a one-sided formula. Defaults to NULL.

nam an optional vector of character strings specifying the row/column names for the

matrix represented by object. It must have length equal to the dimension of the underlying positive-definite matrix and unreplicated elements. This argument is

ignored when value is a vector of character strings. Defaults to NULL.

data an optional data frame in which to evaluate the variables named in value and

form. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying matrix. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to

the parent frame from which the function was called.

#### Value

a pdSymm object representing a general positive-definite matrix, also inheriting from class pdMat.

### Author(s)

José Pinheiro and Douglas Bates <bate dates@stat.wisc.edu>

#### References

Pinheiro, J.C. and Bates., D.M. (1996) "Unconstrained Parametrizations for Variance-Covariance Matrices", Statistics and Computing, 6, 289-296.

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

### See Also

```
as.matrix.pdMat, coef.pdMat, pdClasses, matrix<-.pdMat
```

### **Examples**

```
pd1 <- pdSymm(diag(1:3), nam = c("A","B","C"))
pd1</pre>
```

Phenobarb 225

Phenobarb

Phenobarbitol Kinetics

### **Description**

The Phenobarb data frame has 744 rows and 7 columns.

#### **Format**

This data frame contains the following columns:

**Subject** an ordered factor identifying the infant.

Wt a numeric vector giving the birth weight of the infant (kg).

**Apgar** an ordered factor giving the 5-minute Apgar score for the infant. This is an indication of health of the newborn infant.

**ApgarInd** a factor indicating whether the 5-minute Apgar score is < 5 or >= 5.

time a numeric vector giving the time when the sample is drawn or drug administered (hr).

dose a numeric vector giving the dose of drug administered (ug/kg).

**conc** a numeric vector giving the phenobarbital concentration in the serum (ug/L).

#### **Details**

Data from a pharmacokinetics study of phenobarbital in neonatal infants. During the first few days of life the infants receive multiple doses of phenobarbital for prevention of seizures. At irregular intervals blood samples are drawn and serum phenobarbital concentrations are determined. The data were originally given in Grasela and Donn(1985) and are analyzed in Boeckmann, Sheiner and Beal (1994), in Davidian and Giltinan (1995), and in Littell et al. (1996).

### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.23)

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phenoModel phenoModel

phenoModel Model function for the Phenobarb data
--

# Description

A model function for a model used with the Phenobarb data. This function uses compiled C code to improve execution speed.

# Usage

```
phenoModel(Subject, time, dose, 1Cl, 1V)
```

# Arguments

Subject	an integer vector of subject identifiers. These should be sorted in increasing order.
time	numeric. A vector of the times at which the sample was drawn or the drug administered (hr).
dose	numeric. A vector of doses of drug administered (ug/kg).
1C1	numeric. A vector of values of the natural log of the clearance parameter according to Subject and time.
1V	numeric. A vector of values of the natural log of the effective volume of distribution according to Subject and time.

### **Details**

See the details section of Phenobarb for a description of the model function that phenoModel evaluates.

#### Value

a numeric vector of predicted phenobarbital concentrations.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J. C. and Bates, D. M. (2000) *Mixed-effects Models in S and S-PLUS*, Springer. (section 6.4)

Pixel 227

Pixel

*X-ray pixel intensities over time* 

### **Description**

The Pixel data frame has 102 rows and 4 columns of data on the pixel intensities of CT scans of dogs over time

#### **Format**

This data frame contains the following columns:

Dog a factor with levels 1 to 10 designating the dog on which the scan was made

Side a factor with levels L and R designating the side of the dog being scanned

day a numeric vector giving the day post injection of the contrast on which the scan was made

pixel a numeric vector of pixel intensities

#### Source

Pinheiro, J. C. and Bates, D. M. (2000) Mixed-effects Models in S and S-PLUS, Springer.

#### **Examples**

plot.ACF

Plot an ACF Object

# Description

an xyplot of the autocorrelations versus the lags, with type = "h", is produced. If alpha > 0, curves representing the critical limits for a two-sided test of level alpha for the autocorrelations are added to the plot.

```
## S3 method for class 'ACF'
plot(x, alpha, xlab, ylab, grid, ...)
```

228 plot.augPred

#### **Arguments**

an optional numeric value with the significance level for testing if the autocorrelations are zero. Lines corresponding to the lower and upper critical values for a test of level alpha are added to the plot. Default is 0, in which case no lines are plotted.  xlab, ylab optional character strings with the x- and y-axis labels. Default respectively to "Lag" and "Autocorrelation".  grid an optional logical value indicating whether a grid should be added to plot. Default is FALSE.	lations are zero. Lines corresponding to the lower and upper critical values for a test of level alpha are added to the plot. Default is 0, in which case no lines are plotted.  xlab, ylab optional character strings with the x- and y-axis labels. Default respectively to "Lag" and "Autocorrelation".  grid an optional logical value indicating whether a grid should be added to plot. De-	X	an object inheriting from class ACF, consisting of a data frame with two columns named lag and ACF, representing the autocorrelation values and the corresponding lags.
"Lag" and "Autocorrelation".  grid an optional logical value indicating whether a grid should be added to plot. Default is FALSE.	"Lag" and "Autocorrelation".  grid an optional logical value indicating whether a grid should be added to plot. Default is FALSE.	alpha	lations are zero. Lines corresponding to the lower and upper critical values for a test of level alpha are added to the plot. Default is $\theta$ , in which case no lines are
fault is FALSE.	fault is FALSE.	xlab, ylab	
	optional arguments passed to the xyplot function.	grid	
optional arguments passed to the xyplot function.			optional arguments passed to the xyplot function.

### Value

an xyplot Trellis plot.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
ACF, xyplot
```

### **Examples**

```
fm1 <- lme(follicles ~ sin(2*pi*Time) + cos(2*pi*Time), Ovary) plot(ACF(fm1, maxLag = 10), alpha = 0.01)
```

plot.augPred

Plot an augPred Object

# Description

A Trellis xyplot of predictions versus the primary covariate is generated, with a different panel for each value of the grouping factor. Predicted values are joined by lines, with different line types (colors) being used for each level of grouping. Original observations are represented by circles.

```
## S3 method for class 'augPred'
plot(x, key, grid, ...)
```

plot.compareFits 229

### **Arguments**

X	an object of class "augPred".
key	an optional logical value, or list. If TRUE, a legend is included at the top of the plot indicating which symbols (colors) correspond to which prediction levels. If FALSE, no legend is included. If given as a list, key is passed down as an argument to the trellis function generating the plots (xyplot). Defaults to TRUE.
grid	an optional logical value indicating whether a grid should be added to plot. Default is FALSE.
	optional arguments passed down to the trellis function generating the plots.

### Value

A Trellis plot of predictions versus the primary covariate, with panels determined by the grouping factor.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
augPred, xyplot
```

# **Examples**

```
fm1 <- lme(Orthodont)
plot(augPred(fm1, level = 0:1, length.out = 2))</pre>
```

plot.compareFits

Plot a compareFits Object

# Description

A Trellis dotplot of the values being compared, with different rows per group, is generated, with a different panel for each coefficient. Different symbols (colors) are used for each object being compared.

```
## S3 method for class 'compareFits'
plot(x, subset, key, mark, ...)
```

plot.gls

#### **Arguments**

x	an object of class "compareFits".
subset	an optional logical or integer vector specifying which rows of $\boldsymbol{x}$ should be used in the plots. If missing, all rows are used.
key	an optional logical value, or list. If TRUE, a legend is included at the top of the plot indicating which symbols (colors) correspond to which objects being compared. If FALSE, no legend is included. If given as a list, key is passed down as an argument to the trellis function generating the plots (dotplot). Defaults to TRUE.
mark	an optional numeric vector, of length equal to the number of coefficients being compared, indicating where vertical lines should be drawn in the plots. If missing, no lines are drawn.
	optional arguments passed down to the trellis function generating the plots.

#### Value

A Trellis dotplot of the values being compared, with rows determined by the groups and panels by the coefficients.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
compareFits, pairs.compareFits, dotplot
```

#### **Examples**

```
example(compareFits) # cF12 <- compareFits(coef(lmList(Orthodont)), .. lme(*))
plot(cF12)</pre>
```

plot.gls

Plot a gls Object

### **Description**

Diagnostic plots for the linear model fit are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a Trellis display. If form is a one-sided formula, histograms of the variable on the right hand side of the formula, before a | operator, are displayed (the Trellis function histogram is used). If form is two-sided and both its left and right hand side variables are numeric, scatter plots are displayed (the Trellis function xyplot is used). Finally, if form is two-sided and its left had side variable is a factor, box-plots of the right hand side variable by the levels of the left hand side variable are displayed (the Trellis function bwplot is used).

plot.gls 231

#### Usage

```
## S3 method for class 'gls'
plot(x, form, abline, id, idLabels, idResType, grid, ...)
```

#### **Arguments**

form

abline

id

idLabels

idResType

x an object inheriting from class "gls", representing a generalized least squares fitted linear model.

an optional formula specifying the desired type of plot. Any variable present in the original data frame used to obtain x can be referenced. In addition, x itself can be referenced in the formula using the symbol ".". Conditional expressions on the right of a | operator can be used to define separate panels in a Trellis display. Default is resid(., type = "p") ~ fitted(.), corresponding to a plot of the standardized residuals versus fitted values, both evaluated at the innermost

level of nesting.

an optional numeric value, or numeric vector of length two. If given as a single value, a horizontal line will be added to the plot at that coordinate; else, if given as a vector, its values are used as the intercept and slope for a line added to the

plot. If missing, no lines are added to the plot.

an optional numeric value, or one-sided formula. If given as a value, it is used as a significance level for a two-sided outlier test for the standardized residuals. Observations with absolute standardized residuals greater than the 1-value/2 quantile of the standard normal distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify observations.

vations in the plot. If missing, no observations are identified.

an optional vector, or one-sided formula. If given as a vector, it is converted to character mode and used to label the observations identified according to id. If given as a one-sided formula, its right hand side must evaluate to a vector which is converted to character mode and used to label the identified observations.

Default is the innermost grouping factor.

an optional character string specifying the type of residuals to be used in identifying outliers, when id is a numeric value. If "pearson", the standardized residuals (row residuals divided by the corresponding standard errors) are used:

residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals premultiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the first charac-

ter needs to be provided. Defaults to "pearson".

grid an optional logical value indicating whether a grid should be added to plot. De-

fault depends on the type of Trellis plot used: if xyplot defaults to TRUE, else

defaults to FALSE.

... optional arguments passed to the Trellis plot function.

### Value

a diagnostic Trellis plot.

232 plot.intervals.lmList

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
gls, xyplot, bwplot, histogram
```

### **Examples**

plot.intervals.lmList Plot lmList Confidence Intervals

# Description

A Trellis dot-plot of the confidence intervals on the linear model coefficients is generated, with a different panel for each coefficient. Rows in the dot-plot correspond to the names of the 1m components of the 1mList object used to produce x. The lower and upper confidence limits are connected by a line segment and the estimated coefficients are marked with a "+".

This is based on function dotplot() from package lattice.

#### Usage

## **Arguments**

```
an object inheriting from class "intervals.lmList", representing confidence intervals and estimates for the coefficients in the lm components of the lmList object used to produce x.

xlab, ylab axis labels, each with a sensible default.

strip a function or FALSE, see dotplot() from package lattice.

optional arguments passed to the dotplot function (see above).
```

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#### Value

a Trellis plot with the confidence intervals on the coefficients of the individual 1m components of the 1mList that generated x.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
intervals.lmList, lmList, dotplot
```

### **Examples**

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
plot(intervals(fm1))</pre>
```

plot.lme

Plot an lme or nls object

### **Description**

Diagnostic plots for the linear mixed-effects fit are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a Trellis display. If form is a one-sided formula, histograms of the variable on the right hand side of the formula, before a | operator, are displayed (the Trellis function histogram is used). If form is two-sided and both its left and right hand side variables are numeric, scatter plots are displayed (the Trellis function xyplot is used). Finally, if form is two-sided and its left had side variable is a factor, box-plots of the right hand side variable by the levels of the left hand side variable are displayed (the Trellis function bwplot is used).

#### Usage

```
## S3 method for class 'lme'
plot(x, form, abline, id, idLabels, idResType, grid, ...)
## S3 method for class 'nls'
plot(x, form, abline, id, idLabels, idResType, grid, ...)
```

### **Arguments**

v

an object inheriting from class "lme", representing a fitted linear mixed-effects model, or from nls, representing an fitted nonlinear least squares model.

form

an optional formula specifying the desired type of plot. Any variable present in the original data frame used to obtain x can be referenced. In addition, x itself can be referenced in the formula using the symbol ".". Conditional expressions

plot.lme

on the right of a | operator can be used to define separate panels in a Trellis display. Default is resid(., type = "p") ~ fitted(.), corresponding to a plot of the standardized residuals versus fitted values, both evaluated at the innermost level of nesting.

abline

an optional numeric value, or numeric vector of length two. If given as a single value, a horizontal line will be added to the plot at that coordinate; else, if given as a vector, its values are used as the intercept and slope for a line added to the plot. If missing, no lines are added to the plot.

id

an optional numeric value, or one-sided formula. If given as a value, it is used as a significance level for a two-sided outlier test for the standardized, or normalized residuals. Observations with absolute standardized (normalized) residuals greater than the 1-value/2 quantile of the standard normal distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify observations in the plot. If missing, no observations are identified.

idLabels

an optional vector, or one-sided formula. If given as a vector, it is converted to character and used to label the observations identified according to id. If given as a one-sided formula, its right hand side must evaluate to a vector which is converted to character and used to label the identified observations. Default is the innermost grouping factor.

idResType

an optional character string specifying the type of residuals to be used in identifying outliers, when id is a numeric value. If "pearson", the standardized residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals premultiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the first character needs to be provided. Defaults to "pearson".

grid

an optional logical value indicating whether a grid should be added to plot. Default depends on the type of Trellis plot used: if xyplot defaults to TRUE, else defaults to FALSE.

. .

optional arguments passed to the Trellis plot function.

### Value

a diagnostic Trellis plot.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lme, xyplot, bwplot, histogram
```

### **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)
# standardized residuals versus fitted values by gender</pre>
```

plot.lmList 235

```
plot(fm1, resid(., type = "p") ~ fitted(.) | Sex, abline = 0)
# box-plots of residuals by Subject
plot(fm1, Subject ~ resid(.))
# observed versus fitted values by Subject
plot(fm1, distance ~ fitted(.) | Subject, abline = c(0,1))
```

plot.lmList

Plot an lmList Object

#### **Description**

Diagnostic plots for the linear model fits corresponding to the x components are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a Trellis display. If form is a one-sided formula, histograms of the variable on the right hand side of the formula, before a | operator, are displayed (the Trellis function histogram is used). If form is two-sided and both its left and right hand side variables are numeric, scatter plots are displayed (the Trellis function xyplot is used). Finally, if form is two-sided and its left had side variable is a factor, box-plots of the right hand side variable by the levels of the left hand side variable are displayed (the Trellis function bwplot is used).

### Usage

```
## S3 method for class 'lmList'
plot(x, form, abline, id, idLabels, grid, ...)
```

## **Arguments**

Х

an object inheriting from class "lmList", representing a list of lm objects with a common model.

form

an optional formula specifying the desired type of plot. Any variable present in the original data frame used to obtain x can be referenced. In addition, x itself can be referenced in the formula using the symbol ".". Conditional expressions on the right of a | operator can be used to define separate panels in a Trellis display. Default is  $resid(., type = "pool") \sim fitted(.)$ , corresponding to a plot of the standardized residuals (using a pooled estimate for the residual standard error) versus fitted values.

abline

an optional numeric value, or numeric vector of length two. If given as a single value, a horizontal line will be added to the plot at that coordinate; else, if given as a vector, its values are used as the intercept and slope for a line added to the plot. If missing, no lines are added to the plot.

id

an optional numeric value, or one-sided formula. If given as a value, it is used as a significance level for a two-sided outlier test for the standardized residuals. Observations with absolute standardized residuals greater than the 1-value/2 quantile of the standard normal distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify observations in the plot. If missing, no observations are identified.

236 plot.nffGroupedData

idLabels	an optional vector, or one-sided formula. If given as a vector, it is converted to
	character and used to label the observations identified according to id. If given

as a one-sided formula, its right hand side must evaluate to a vector which is converted to character and used to label the identified observations. Default is

getGroups(x).

grid an optional logical value indicating whether a grid should be added to plot. De-

fault depends on the type of Trellis plot used: if xyplot defaults to TRUE, else

defaults to FALSE.

... optional arguments passed to the Trellis plot function.

#### Value

a diagnostic Trellis plot.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lmList,predict.lm, xyplot, bwplot, histogram
```

#### **Examples**

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
# standardized residuals versus fitted values by gender
plot(fm1, resid(., type = "pool") ~ fitted(.) | Sex, abline = 0, id = 0.05)
# box-plots of residuals by Subject
plot(fm1, Subject ~ resid(.))
# observed versus fitted values by Subject
plot(fm1, distance ~ fitted(.) | Subject, abline = c(0,1))</pre>
```

plot.nffGroupedData

Plot an nffGroupedData Object

### **Description**

A Trellis dot-plot of the response by group is generated. If outer variables are specified, the combination of their levels are used to determine the panels of the Trellis display. The Trellis function dotplot is used.

plot.nffGroupedData 237

# Arguments

X	an object inheriting from class nffGroupedData, representing a groupedData object with a factor primary covariate and a single grouping level.
outer	an optional logical value or one-sided formula, indicating covariates that are outer to the grouping factor, which are used to determine the panels of the Trellis plot. If equal to TRUE, attr(object, "outer") is used to indicate the outer covariates. An outer covariate is invariant within the sets of rows defined by the grouping factor. Ordering of the groups is done in such a way as to preserve adjacency of groups with the same value of the outer variables. Defaults to NULL, meaning that no outer covariates are to be used.
inner	an optional logical value or one-sided formula, indicating a covariate that is inner to the grouping factor, which is used to associate points within each panel of the Trellis plot. If equal to TRUE, attr(object, "inner") is used to indicate the inner covariate. An inner covariate can change within the sets of rows defined by the grouping factor. Defaults to NULL, meaning that no inner covariate is present.
innerGroups	an optional one-sided formula specifying a factor to be used for grouping the levels of the inner covariate. Different colors, or symbols, are used for each level of the innerGroups factor. Default is NULL, meaning that no innerGroups covariate is present.
xlab	an optional character string with the label for the horizontal axis. Default is the y elements of attr(object, "labels") and attr(object, "units") pasted together.
ylab	an optional character string with the label for the vertical axis. Default is the grouping factor name.
strip	an optional function passed as the strip argument to the dotplot function. Default is strip.default(, style = 1) (see trellis.args).
panel	an optional function used to generate the individual panels in the Trellis display, passed as the panel argument to the dotplot function.
key	an optional logical function or function. If TRUE and either inner or innerGroups are non-NULL, a legend for the different inner (innerGroups) levels is included at the top of the plot. If given as a function, it is passed as the key argument to the dotplot function. Default is TRUE is either inner or innerGroups are non-NULL and FALSE otherwise.
grid	this argument is included for consistency with the plot.nfnGroupedData method calling sequence. It is ignored in this method function.
	optional arguments passed to the dotplot function.

# Value

a Trellis dot-plot of the response by group.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

238 plot.nfnGroupedData

#### References

Bates, D.M. and Pinheiro, J.C. (1997), "Software Design for Longitudinal Data", in "Modelling Longitudinal and Spatially Correlated Data: Methods, Applications and Future Directions", T.G. Gregoire (ed.), Springer-Verlag, New York.

#### See Also

```
groupedData, dotplot
```

### **Examples**

```
plot(Machines)
plot(Machines, inner = TRUE)
```

plot.nfnGroupedData

Plot an nfnGroupedData Object

### **Description**

A Trellis plot of the response versus the primary covariate is generated. If outer variables are specified, the combination of their levels are used to determine the panels of the Trellis display. Otherwise, the levels of the grouping variable determine the panels. A scatter plot of the response versus the primary covariate is displayed in each panel, with observations corresponding to same inner group joined by line segments. The Trellis function xyplot is used.

### Usage

```
## S3 method for class 'nfnGroupedData'
plot(x, outer, inner, innerGroups, xlab, ylab, strip, aspect, panel,
    key, grid, ...)
```

#### **Arguments**

Χ

an object inheriting from class nfnGroupedData, representing a groupedData object with a numeric primary covariate and a single grouping level.

outer

an optional logical value or one-sided formula, indicating covariates that are outer to the grouping factor, which are used to determine the panels of the Trellis plot. If equal to TRUE, attr(object, "outer") is used to indicate the outer covariates. An outer covariate is invariant within the sets of rows defined by the grouping factor. Ordering of the groups is done in such a way as to preserve adjacency of groups with the same value of the outer variables. Defaults to NULL, meaning that no outer covariates are to be used.

inner

an optional logical value or one-sided formula, indicating a covariate that is inner to the grouping factor, which is used to associate points within each panel of the Trellis plot. If equal to TRUE, attr(object, "inner") is used to indicate the inner covariate. An inner covariate can change within the sets of rows defined by the grouping factor. Defaults to NULL, meaning that no inner covariate is present.

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innerGroups	an optional one-sided formula specifying a factor to be used for grouping the levels of the inner covariate. Different colors, or line types, are used for each level of the innerGroups factor. Default is NULL, meaning that no innerGroups covariate is present.
xlab, ylab	optional character strings with the labels for the plot. Default is the corresponding elements of attr(object, "labels") and attr(object, "units") pasted together.
strip	an optional function passed as the strip argument to the xyplot function. Default is strip.default(, style = 1) (see trellis.args).
aspect	an optional character string indicating the aspect ratio for the plot passed as the aspect argument to the xyplot function. Default is "xy" (see trellis.args).
panel	an optional function used to generate the individual panels in the Trellis display, passed as the panel argument to the xyplot function.
key	an optional logical function or function. If TRUE and innerGroups is non-NULL, a legend for the different innerGroups levels is included at the top of the plot. If given as a function, it is passed as the key argument to the xyplot function. Default is TRUE if innerGroups is non-NULL and FALSE otherwise.
grid	an optional logical value indicating whether a grid should be added to plot. Default is TRUE.
	optional arguments passed to the xyplot function.

#### Value

a Trellis plot of the response versus the primary covariate.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Bates, D.M. and Pinheiro, J.C. (1997), "Software Design for Longitudinal Data", in "Modelling Longitudinal and Spatially Correlated Data: Methods, Applications and Future Directions", T.G. Gregoire (ed.), Springer-Verlag, New York.

## See Also

```
groupedData, xyplot
```

## **Examples**

```
# different panels per Subject
plot(Orthodont)
# different panels per gender
plot(Orthodont, outer = TRUE)
```

240 plot.nmGroupedData

plot.nmGroupedData

Plot an nmGroupedData Object

#### **Description**

The groupedData object is summarized by the values of the displayLevel grouping factor (or the combination of its values and the values of the covariate indicated in preserve, if any is present). The collapsed data is used to produce a new groupedData object, with grouping factor given by the displayLevel factor, which is plotted using the appropriate plot method for groupedData objects with single level of grouping.

#### Usage

```
## S3 method for class 'nmGroupedData'
plot(x, collapseLevel, displayLevel, outer, inner,
    preserve, FUN, subset, key, grid, ...)
```

#### **Arguments**

x an object inheriting from class nmGroupedData, representing a groupedData

object with multiple grouping factors.

collapseLevel an optional positive integer or character string indicating the grouping level to

use when collapsing the data. Level values increase from outermost to innermost  $\,$ 

grouping. Default is the highest or innermost level of grouping.

displayLevel an optional positive integer or character string indicating the grouping level to

use for determining the panels in the Trellis display, when outer is missing.

Default is collapseLevel.

outer an optional logical value or one-sided formula, indicating covariates that are

outer to the displayLevel grouping factor, which are used to determine the panels of the Trellis plot. If equal to TRUE, the displayLevel element attr(object, "outer") is used to indicate the outer covariates. An outer covariate is invariant within the sets of rows defined by the grouping factor. Ordering of the groups is done in such a way as to preserve adjacency of groups with the same value of the outer variables. Defaults to NULL, meaning that no outer covariates are to be

used.

inner an optional logical value or one-sided formula, indicating a covariate that is

inner to the displayLevel grouping factor, which is used to associate points within each panel of the Trellis plot. If equal to TRUE, attr(object, "outer") is used to indicate the inner covariate. An inner covariate can change within the sets of rows defined by the grouping factor. Defaults to NULL, meaning that no

inner covariate is present.

preserve an optional one-sided formula indicating a covariate whose levels should be

preserved when collapsing the data according to the collapseLevel grouping factor. The collapsing factor is obtained by pasting together the levels of the collapseLevel grouping factor and the values of the covariate to be preserved.

Default is NULL, meaning that no covariates need to be preserved.

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**FUN** 

an optional summary function or a list of summary functions to be used for collapsing the data. The function or functions are applied only to variables in object that vary within the groups defined by collapseLevel. Invariant variables are always summarized by group using the unique value that they assume within that group. If FUN is a single function it will be applied to each non-invariant variable by group to produce the summary for that variable. If FUN is a list of functions, the names in the list should designate classes of variables in the data such as ordered, factor, or numeric. The indicated function will be applied to any non-invariant variables of that class. The default functions to be used are mean for numeric factors, and Mode for both factor and ordered. The Mode function, defined internally in gsummary, returns the modal or most popular value of the variable. It is different from the mode function that returns the S-language mode of the variable.

subset

an optional named list. Names can be either positive integers representing grouping levels, or names of grouping factors. Each element in the list is a vector indicating the levels of the corresponding grouping factor to be used for plotting the data. Default is NULL, meaning that all levels are used.

key

an optional logical value, or list. If TRUE, a legend is included at the top of the plot indicating which symbols (colors) correspond to which prediction levels. If FALSE, no legend is included. If given as a list, key is passed down as an argument to the trellis function generating the plots (xyplot). Defaults to

grid

an optional logical value indicating whether a grid should be added to plot. De-

fault is TRUE.

... optional arguments passed to the Trellis plot function.

#### Value

a Trellis display of the data collapsed over the values of the collapseLevel grouping factor and grouped according to the displayLevel grouping factor.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Bates, D.M. and Pinheiro, J.C. (1997), "Software Design for Longitudinal Data", in "Modelling Longitudinal and Spatially Correlated Data: Methods, Applications and Future Directions", T.G. Gregoire (ed.), Springer-Verlag, New York.

### See Also

groupedData, collapse.groupedData, plot.nfnGroupedData, plot.nffGroupedData

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#### **Examples**

```
# no collapsing, panels by Dog
plot(Pixel, displayLevel = "Dog", inner = ~Side)
# collapsing by Dog, preserving day
plot(Pixel, collapseLevel = "Dog", preserve = ~day)
```

plot.ranef.lme

Plot a ranef.lme Object

### **Description**

Plots (class "Trellis" from package lattice) of the random effects from linear mixed effects model, i.e., the result of ranef(lme(\*)) (of class "ranef.lme").

# Usage

```
## S3 method for class 'ranef.lme'
plot(x, form = NULL, omitFixed = TRUE, level = Q,
     grid = TRUE, control, xlab, ylab, strip,
     ...)
```

#### **Arguments**

Х

an object inheriting from class "ranef.lme", representing the estimated coefficients or estimated random effects for the 1me object from which it was produced.

form

an optional formula specifying the desired type of plot.

- If given as a one-sided formula, a dotplot() of the estimated random effects (coefficients) grouped according to all combinations of the levels of the factors named in form is returned.
- If given as a two-sided formula (or by default, NULL), an xyplot() Trellis display of the random effect (coefficient) versus the named covariates is returned. In NULL case the row names of the random effects (coefficients) are used (as covariates).

See also 'Details:'.

omitFixed

an optional logical value indicating whether columns with values that are constant across groups should be omitted. Default is TRUE.

level

an optional integer value giving the level of grouping to be used for x. Only used when x is a list with different components for each grouping level. Defaults to the highest or innermost level of grouping.

grid

an optional logical value indicating whether a grid should be added to plot. Only applies to plots associated with two-sided formulas in form. Default is TRUE.

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control

an optional list with control values for the plot, when form is given as a two-sided formula. The control values are referenced by name in the control list and only the ones to be modified from the default need to be specified. Available values include: drawLine, a logical value indicating whether a loess smoother should be added to the scatter plots and a line connecting the medians should be added to the boxplots (default is TRUE); span.loess, used as the span argument in the call to panel.loess (default is 2/3); degree.loess, used as the degree argument in the call to panel.loess (default is 1); cex.axis, the character expansion factor for the x-axis (default is 0.8); srt.axis, the rotation factor for the x-axis (default is 0); and mgp.axis, the margin parameters for the x-axis (default is c(2, 0.5, 0)).

xlab, ylab axis labels, each with a sensible default.
strip a function or FALSE, see dotplot() from package lattice.
... optional arguments passed to the Trellis dotplot function.

#### **Details**

If form is missing, or is given as a one-sided formula, a Trellis dot-plot (via dotplot() from pkg lattice) of the random effects is generated, with a different panel for each random effect (coefficient). Rows in the dot-plot are determined by the form argument (if not missing) or by the row names of the random effects (coefficients). Single factors (~g) or crossed factors (~g1\*g2) are allowed. For a single factor, its levels determine the dot-plot rows (with possibly multiple dots per row); otherwise, if form specifies a crossing of factors, the dot-plot rows are determined by all combinations of the levels of the individual factors in the formula.

If form is a two-sided formula, the left hand side must be a single random effect (coefficient) and the right hand side is formed by covariates in x separated by +. An xyplot() Trellis display is generated, with a different panel for each variable listed in the right hand side of form. Scatter plots are generated for numeric variables and boxplots are generated for categorical (factor or ordered) variables.

#### Value

a Trellis plot of the estimated random-effects (coefficients) versus covariates, or groups.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
ranef.lme, lme, dotplot.
```

## **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)
plot(ranef(fm1))
fm1RE <- ranef(fm1, augFrame = TRUE)
plot(fm1RE, form = ~ Sex)
plot(fm1RE, form = age ~ Sex) # "connected" boxplots</pre>
```

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plot.ranef.lmList

Plot a ranef.lmList Object

### **Description**

If form is missing, or is given as a one-sided formula, a Trellis dot-plot of the random effects is generated, with a different panel for each random effect (coefficient). Rows in the dot-plot are determined by the form argument (if not missing) or by the row names of the random effects (coefficients). If a single factor is specified in form, its levels determine the dot-plot rows (with possibly multiple dots per row); otherwise, if form specifies a crossing of factors, the dot-plot rows are determined by all combinations of the levels of the individual factors in the formula. The Trellis function dotplot is used in this method function.

If form is a two-sided formula, a Trellis display is generated, with a different panel for each variable listed in the right hand side of form. Scatter plots are generated for numeric variables and boxplots are generated for categorical (factor or ordered) variables.

#### Usage

```
## S3 method for class 'ranef.lmList'
plot(x, form, grid, control, ...)
```

#### **Arguments**

Х

an object inheriting from class "ranef.lmList", representing the estimated coefficients or estimated random effects for the lmList object from which it was produced.

form

an optional formula specifying the desired type of plot. If given as a one-sided formula, a dotplot of the estimated random effects (coefficients) grouped according to all combinations of the levels of the factors named in form is returned. Single factors (~g) or crossed factors (~g1\*g2) are allowed. If given as a two-sided formula, the left hand side must be a single random effects (coefficient) and the right hand side is formed by covariates in x separated by +. A Trellis display of the random effect (coefficient) versus the named covariates is returned in this case. Default is NULL, in which case the row names of the random effects (coefficients) are used.

grid

an optional logical value indicating whether a grid should be added to plot. Only applies to plots associated with two-sided formulas in form. Default is FALSE.

control

an optional list with control values for the plot, when form is given as a two-sided formula. The control values are referenced by name in the control list and only the ones to be modified from the default need to be specified. Available values include: drawLine, a logical value indicating whether a loess smoother should be added to the scatter plots and a line connecting the medians should be added to the boxplots (default is TRUE); span.loess, used as the span argument in the call to panel.loess (default is 2/3); degree.loess, used as the degree argument in the call to panel.loess (default is 1); cex.axis, the character expansion factor for the x-axis (default is 0.8); srt.axis, the rotation factor

.

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for the x-axis (default is 0); and mgp.axis, the margin parameters for the x-axis (default is c(2, 0.5, 0)).

... optional arguments passed to the Trellis dotplot function.

#### Value

a Trellis plot of the estimated random-effects (coefficients) versus covariates, or groups.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lmList, dotplot
```

### **Examples**

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
plot(ranef(fm1))
fm1RE <- ranef(fm1, augFrame = TRUE)
plot(fm1RE, form = ~ Sex)
plot(fm1RE, form = age ~ Sex)</pre>
```

plot.Variogram

Plot a Variogram Object

## **Description**

an xyplot of the semi-variogram versus the distances is produced. If smooth = TRUE, a loess smoother is added to the plot. If showModel = TRUE and x includes an "modelVariog" attribute, the corresponding semi-variogram is added to the plot.

## Usage

```
## S3 method for class 'Variogram'
plot(x, smooth, showModel, sigma, span, xlab,
    ylab, type, ylim, grid, ...)
```

# **Arguments**

Х

an object inheriting from class "Variogram", consisting of a data frame with two columns named variog and dist, representing the semi-variogram values and the corresponding distances.

smooth

an optional logical value controlling whether a loess smoother should be added to the plot. Defaults to TRUE, when showModel is FALSE.

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showModel	an optional logical value controlling whether the semi-variogram corresponding to an "modelVariog" attribute of $x$ , if any is present, should be added to the plot. Defaults to TRUE, when the "modelVariog" attribute is present.
sigma	an optional numeric value used as the height of a horizontal line displayed in the plot. Can be used to represent the process standard deviation. Default is NULL, implying that no horizontal line is drawn.
span	an optional numeric value with the smoothing parameter for the loess fit. Default is $0.6$ .
xlab, ylab	optional character strings with the x- and y-axis labels. Default respectively to "Distance" and "SemiVariogram".
type	an optional character indicating the type of plot. Defaults to "p".
ylim	an optional numeric vector with the limits for the y-axis. Defaults to $c(0, max(x\$variog))$ .
grid	an optional logical value indicating whether a grid should be added to plot. Default is FALSE.
	optional arguments passed to the Trellis xyplot function.

#### Value

an xyplot Trellis plot.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
Variogram, xyplot, loess
```

# **Examples**

```
fm1 <- lme(follicles ~ sin(2*pi*Time) + cos(2*pi*Time), Ovary) plot(Variogram(fm1, form = ~ Time | Mare, maxDist = 0.7))
```

pooledSD

Extract Pooled Standard Deviation

# Description

The pooled estimated standard deviation is obtained by adding together the residual sum of squares for each non-null element of object, dividing by the sum of the corresponding residual degrees-of-freedom, and taking the square-root.

```
pooledSD(object)
```

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### **Arguments**

object an object inheriting from class lmList.

#### Value

the pooled standard deviation for the non-null elements of object, with an attribute df with the number of degrees-of-freedom used in the estimation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
1mList, 1m
```

### **Examples**

```
fm1 <- lmList(Orthodont)
pooledSD(fm1)</pre>
```

predict.gls

Predictions from a gls Object

# Description

The predictions for the linear model represented by object are obtained at the covariate values defined in newdata.

### Usage

```
## S3 method for class 'gls'
predict(object, newdata, na.action, ...)
```

### **Arguments**

object	an object inheriting from class "gls", representing a generalized least squares fitted linear model.
newdata	an optional data frame to be used for obtaining the predictions. All variables used in the linear model must be present in the data frame. If missing, the fitted values are returned.
na.action	a function that indicates what should happen when newdata contains NAs. The default action (na.fail) causes the function to print an error message and terminate if there are any incomplete observations.
	some methods for this generic require additional arguments. None are used in this method.

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### Value

a vector with the predicted values.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

gls

#### **Examples**

```
fm1 <- gls(follicles \sim sin(2*pi*Time) + cos(2*pi*Time), Ovary, correlation = corAR1(form = \sim 1 | Mare)) newOvary <- data.frame(Time = c(-0.75, -0.5, 0, 0.5, 0.75)) predict(fm1, newOvary)
```

predict.gnls

Predictions from a gnls Object

# Description

The predictions for the nonlinear model represented by object are obtained at the covariate values defined in newdata.

# Usage

```
## S3 method for class 'gnls'
predict(object, newdata, na.action, naPattern, ...)
```

# **Arguments**

object	an object inheriting from class "gnls", representing a generalized nonlinear least squares fitted model.
newdata	an optional data frame to be used for obtaining the predictions. All variables used in the nonlinear model must be present in the data frame. If missing, the fitted values are returned.
na.action	a function that indicates what should happen when newdata contains NAs. The default action (na.fail) causes the function to print an error message and terminate if there are any incomplete observations.
naPattern	an expression or formula object, specifying which returned values are to be regarded as missing.
	some methods for this generic require additional arguments. None are used in this method

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#### Value

a vector with the predicted values.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

gnls

### **Examples**

predict.lme

Predictions from an Ime Object

## **Description**

The predictions at level i are obtained by adding together the population predictions (based only on the fixed effects estimates) and the estimated contributions of the random effects to the predictions at grouping levels less or equal to i. The resulting values estimate the best linear unbiased predictions (BLUPs) at level i. If group values not included in the original grouping factors are present in newdata, the corresponding predictions will be set to NA for levels greater or equal to the level at which the unknown groups occur.

#### Usage

### **Arguments**

object an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

newdata an optional data frame to be used for obtaining the predictions. All variables

used in the fixed and random effects models, as well as the grouping factors,

must be present in the data frame. If missing, the fitted values are returned.

level an optional integer vector giving the level(s) of grouping to be used in obtaining

the predictions. Level values increase from outermost to innermost grouping, with level zero corresponding to the population predictions. Defaults to the

highest or innermost level of grouping.

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asList	an optional logical value. If TRUE and a single value is given in level, the returned object is a list with the predictions split by groups; else the returned value is either a vector or a data frame, according to the length of level.
na.action	a function that indicates what should happen when newdata contains NAs. The default action (na.fail) causes the function to print an error message and terminate if there are any incomplete observations.
•••	some methods for this generic require additional arguments. None are used in this method.

#### Value

if a single level of grouping is specified in level, the returned value is either a list with the predictions split by groups (asList = TRUE) or a vector with the predictions (asList = FALSE); else, when multiple grouping levels are specified in level, the returned object is a data frame with columns given by the predictions at different levels and the grouping factors.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lme, fitted.lme
```

#### **Examples**

predict.lmList

Predictions from an lmList Object

### **Description**

If the grouping factor corresponding to object is included in newdata, the data frame is partitioned according to the grouping factor levels; else, newdata is repeated for all 1m components. The predictions and, optionally, the standard errors for the predictions, are obtained for each 1m component of object, using the corresponding element of the partitioned newdata, and arranged into a list with as many components as object, or combined into a single vector or data frame (if se.fit=TRUE).

```
## S3 method for class 'lmList'
predict(object, newdata, subset, pool, asList, se.fit, ...)
```

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#### **Arguments**

object	an object inheriting from class "lmList", representing a list of lm objects with a common model.
newdata	an optional data frame to be used for obtaining the predictions. All variables used in the object model formula must be present in the data frame. If missing, the same data frame used to produce object is used.
subset	an optional character or integer vector naming the ${\tt lm}$ components of object from which the predictions are to be extracted. Default is NULL, in which case all components are used.
asList	an optional logical value. If TRUE, the returned object is a list with the predictions split by groups; else the returned value is a vector. Defaults to FALSE.
pool	an optional logical value indicating whether a pooled estimate of the residual standard error should be used. Default is attr(object, "pool").
se.fit	an optional logical value indicating whether pointwise standard errors should be computed along with the predictions. Default is FALSE.
	some methods for this generic require additional arguments. None are used in this method.

### Value

a list with components given by the predictions (and, optionally, the standard errors for the predictions) from each 1m component of object, a vector with the predictions from all 1m components of object, or a data frame with columns given by the predictions and their corresponding standard errors.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
lmList, predict.lm
```

# **Examples**

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
predict(fm1, se.fit = TRUE)</pre>
```

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predict.nlme	Predictions from an nlme Object	

### Description

The predictions at level i are obtained by adding together the contributions from the estimated fixed effects and the estimated random effects at levels less or equal to i and evaluating the model function at the resulting estimated parameters. If group values not included in the original grouping factors are present in newdata, the corresponding predictions will be set to NA for levels greater or equal to the level at which the unknown groups occur.

# Usage

# Arguments

object	an object inheriting from class "nlme", representing a fitted nonlinear mixed-effects model.
newdata	an optional data frame to be used for obtaining the predictions. All variables used in the nonlinear model, the fixed and the random effects models, as well as the grouping factors, must be present in the data frame. If missing, the fitted values are returned.
level	an optional integer vector giving the level(s) of grouping to be used in obtaining the predictions. Level values increase from outermost to innermost grouping, with level zero corresponding to the population predictions. Defaults to the highest or innermost level of grouping (and is object\$dims\$Q).
asList	an optional logical value. If TRUE and a single value is given in level, the returned object is a list with the predictions split by groups; else the returned value is either a vector or a data frame, according to the length of level.
na.action	a function that indicates what should happen when newdata contains NAs. The default action (na.fail) causes the function to print an error message and terminate if there are any incomplete observations.
naPattern	an expression or formula object, specifying which returned values are to be regarded as missing.
	some methods for this generic require additional arguments. None are used in this method.

#### Value

if a single level of grouping is specified in level, the returned value is either a list with the predictions split by groups (asList = TRUE) or a vector with the predictions (asList = FALSE); else, when multiple grouping levels are specified in level, the returned object is a data frame with columns given by the predictions at different levels and the grouping factors.

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### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
nlme, fitted.lme
```

### **Examples**

```
head(Loblolly) # groupedData w/ 'Seed' is grouping variable :
## Grouped Data: height ~ age | Seed
## height age Seed
## 1
       4.51 3 301
## 15 10.89 5 301
## .. ..... . ...
fm1 <- nlme(height ~ SSasymp(age, Asym, R0, lrc), data = Loblolly,</pre>
            fixed = Asym + R0 + lrc \sim 1,
            random = Asym ~ 1, ## <---grouping---> Asym ~ 1 | Seed
            start = c(Asym = 103, R0 = -8.5, 1rc = -3.3))
fm1
age. <- seq(from = 2, to = 30, by = 2)
newLL.301 <- data.frame(age = age., Seed = 301)</pre>
newLL.329 <- data.frame(age = age., Seed = 329)</pre>
(p301 <- predict(fm1, newLL.301, level = 0:1))
(p329 <- predict(fm1, newLL.329, level = 0:1))</pre>
## Prediction are the same at level 0 :
all.equal(p301[,"predict.fixed"],
          p329[, "predict.fixed"])
## and differ by the 'Seed' effect at level 1 :
p301[,"predict.Seed"] -
p329[,"predict.Seed"]
```

### **Description**

The standard deviations and correlations associated with the positive-definite matrix represented by object (considered as a variance-covariance matrix) are printed, together with the formula and the grouping level associated object, if any are present.

## Usage

```
## S3 method for class 'summary.pdMat'
print(x, sigma, rdig, Level, resid, ...)
```

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# **Arguments**

X	an object inheriting from class "summary.pdMat", generally resulting from applying summary to an object inheriting from class "pdMat".
sigma	an optional numeric value used as a multiplier for the square-root factor of the positive-definite matrix represented by object (usually the estimated withingroup standard deviation from a mixed-effects model). Defaults to 1.
rdig	an optional integer value with the number of significant digits to be used in printing correlations. Defaults to 3.
Level	an optional character string with a description of the grouping level associated with object (generally corresponding to levels of grouping in a mixed-effects model). Defaults to NULL.
resid	an optional logical value. If TRUE an extra row with the "residual" standard deviation given in sigma will be included in the output. Defaults to FALSE.
•••	optional arguments passed to print.default; see the documentation on that method function.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
summary.pdMat,pdMat
```

# **Examples**

print.varFunc

Print a varFunc Object

# **Description**

The class and the coefficients associated with x are printed.

# Usage

```
## S3 method for class 'varFunc'
print(x, ...)
```

# Arguments

X	an object inheriting from class "varFunc", representing a variance function
	structure.
	optional arguments passed to print.default; see the documentation on that

method function.

255 qqnorm.gls

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
summary.varFunc
```

#### **Examples**

```
vf1 <- varPower(0.3, form = ~age)
vf1 <- Initialize(vf1, Orthodont)</pre>
print(vf1)
```

qqnorm.gls

Normal Plot of Residuals from a gls Object

### **Description**

Diagnostic plots for assessing the normality of residuals the generalized least squares fit are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a Trellis display.

### Usage

```
## S3 method for class 'gls'
qqnorm(y, form, abline, id, idLabels, grid, ...)
```

### **Arguments**

an object inheriting from class "gls", representing a generalized least squares У fitted model.

an optional one-sided formula specifying the desired type of plot. Any variable present in the original data frame used to obtain y can be referenced. In addition, y itself can be referenced in the formula using the symbol ".". Conditional expressions on the right of a | operator can be used to define separate panels in a Trellis display. The expression on the right hand side of form and to the left of a | operator must evaluate to a residuals vector. Default is ~ resid(., type = "p"), corresponding to a normal plot of the standardized residuals.

an optional numeric value, or numeric vector of length two. If given as a single value, a horizontal line will be added to the plot at that coordinate; else, if given as a vector, its values are used as the intercept and slope for a line added to the

plot. If missing, no lines are added to the plot.

abline

form

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id an optional numeric value, or one-sided formula. If given as a value, it is used

as a significance level for a two-sided outlier test for the standardized residuals (random effects). Observations with absolute standardized residuals (random effects) greater than the 1-value/2 quantile of the standard normal distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify observations in the plot. If missing, no observations are iden-

tified.

idLabels an optional vector, or one-sided formula. If given as a vector, it is converted to

character and used to label the observations identified according to id. If given as a one-sided formula, its right hand side must evaluate to a vector which is converted to character and used to label the identified observations. Default is

the innermost grouping factor.

grid an optional logical value indicating whether a grid should be added to plot. De-

fault depends on the type of Trellis plot used: if xyplot defaults to TRUE, else

defaults to FALSE.

... optional arguments passed to the Trellis plot function.

#### Value

a diagnostic Trellis plot for assessing normality of residuals.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
gls, plot.gls
```

### **Examples**

qqnorm.lme

Normal Plot of Residuals or Random Effects from an lme Object

# **Description**

Diagnostic plots for assessing the normality of residuals and random effects in the linear mixed-effects fit are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a Trellis display.

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#### Usage

```
## S3 method for class 'lme'
qqnorm(y, form, abline, id, idLabels, grid, ...)
```

### **Arguments**

У

an object inheriting from class "lme", representing a fitted linear mixed-effects model or from class "lmList", representing a list of lm objects, or from class "lm", representing a fitted linear model, or from class "nls", representing a nonlinear least squares fitted model.

form

an optional one-sided formula specifying the desired type of plot. Any variable present in the original data frame used to obtain y can be referenced. In addition, y itself can be referenced in the formula using the symbol ".". Conditional expressions on the right of a | operator can be used to define separate panels in a Trellis display. The expression on the right hand side of form and to the left of a | operator must evaluate to a residuals vector, or a random effects matrix. Default is ~ resid(., type = "p"), corresponding to a normal plot of the standardized residuals evaluated at the innermost level of nesting.

abline

an optional numeric value, or numeric vector of length two. If given as a single value, a horizontal line will be added to the plot at that coordinate; else, if given as a vector, its values are used as the intercept and slope for a line added to the plot. If missing, no lines are added to the plot.

id

an optional numeric value, or one-sided formula. If given as a value, it is used as a significance level for a two-sided outlier test for the standardized residuals (random effects). Observations with absolute standardized residuals (random effects) greater than the 1-value/2 quantile of the standard normal distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify observations in the plot. If missing, no observations are identified.

idLabels

an optional vector, or one-sided formula. If given as a vector, it is converted to character and used to label the observations identified according to id. If given as a one-sided formula, its right hand side must evaluate to a vector which is converted to character and used to label the identified observations. Default is the innermost grouping factor.

grid

an optional logical value indicating whether a grid should be added to plot. Default is FALSE.

. . .

optional arguments passed to the Trellis plot function.

#### Value

a diagnostic Trellis plot for assessing normality of residuals or random effects.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

258 Quinidine

#### See Also

```
lme, plot.lme
```

#### **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)
## normal plot of standardized residuals by gender
qqnorm(fm1, ~ resid(., type = "p") | Sex, abline = c(0, 1))
## normal plots of random effects
qqnorm(fm1, ~ranef(.))</pre>
```

Quinidine

Quinidine Kinetics

### **Description**

The Quinidine data frame has 1471 rows and 14 columns.

#### **Format**

This data frame contains the following columns:

**Subject** a factor identifying the patient on whom the data were collected.

**time** a numeric vector giving the time (hr) at which the drug was administered or the blood sample drawn. This is measured from the time the patient entered the study.

**conc** a numeric vector giving the serum quinidine concentration (mg/L).

**dose** a numeric vector giving the dose of drug administered (mg). Although there were two different forms of quinidine administered, the doses were adjusted for differences in salt content by conversion to milligrams of quinidine base.

**interval** a numeric vector giving the when the drug has been given at regular intervals for a sufficiently long period of time to assume steady state behavior, the interval is recorded.

**Age** a numeric vector giving the age of the subject on entry to the study (yr).

**Height** a numeric vector giving the height of the subject on entry to the study (in.).

Weight a numeric vector giving the body weight of the subject (kg).

Race a factor with levels Caucasian, Latin, and Black identifying the race of the subject.

**Smoke** a factor with levels no and yes giving smoking status at the time of the measurement.

**Ethanol** a factor with levels none, current, former giving ethanol (alcohol) abuse status at the time of the measurement.

**Heart** a factor with levels No/Mild, Moderate, and Severe indicating congestive heart failure for the subject.

**Creatinine** an ordered factor with levels < 50 < >= 50 indicating the creatinine clearance (mg/min).

**glyco** a numeric vector giving the alpha-1 acid glycoprotein concentration (mg/dL). Often measured at the same time as the quinidine concentration.

quinModel 259

### **Details**

Verme et al. (1992) analyze routine clinical data on patients receiving the drug quinidine as a treatment for cardiac arrhythmia (atrial fibrillation or ventricular arrhythmias). All patients were receiving oral quinidine doses. At irregular intervals blood samples were drawn and serum concentrations of quinidine were determined. These data are analyzed in several publications, including Davidian and Giltinan (1995, section 9.3).

### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.25)

Davidian, M. and Giltinan, D. M. (1995), *Nonlinear Models for Repeated Measurement Data*, Chapman and Hall, London.

Verme, C. N., Ludden, T. M., Clementi, W. A. and Harris, S. C. (1992), Pharmacokinetics of quinidine in male patients: A population analysis, *Clinical Pharmacokinetics*, **22**, 468-480.

quinModel

Model function for the Quinidine data

### **Description**

A model function for a model used with the Quinidine data. This function calls compiled C code.

# Usage

```
quinModel(Subject, time, conc, dose, interval, 1V, 1Ka, 1Cl)
```

Subject	a factor identifying the patient on whom the data were collected.
time	a numeric vector giving the time (hr) at which the drug was administered or the blood sample drawn. This is measured from the time the patient entered the study.
conc	a numeric vector giving the serum quinidine concentration (mg/L).
dose	a numeric vector giving the dose of drug administered (mg). Although there were two different forms of quinidine administered, the doses were adjusted for differences in salt content by conversion to milligrams of quinidine base.
interval	a numeric vector giving the when the drug has been given at regular intervals for a sufficiently long period of time to assume steady state behavior, the interval is recorded.
1V	numeric. A vector of values of the natural $\log$ of the effective volume of distribution according to Subject and time.
lKa	numeric. A vector of values of the natural $\log$ of the absorption rate constant according to Subject and time.
1C1	numeric. A vector of values of the natural $\log$ of the clearance parameter according to Subject and time.

260 Rail

#### **Details**

See the details section of Quinidine for a description of the model function that quinModel evaluates.

#### Value

a numeric vector of predicted quinidine concentrations.

### Author(s)

### References

Pinheiro, J. C. and Bates, D. M. (2000) *Mixed-effects Models in S and S-PLUS*, Springer. (section 8.2)

Rail

Evaluation of Stress in Railway Rails

# **Description**

The Rail data frame has 18 rows and 2 columns.

#### **Format**

This data frame contains the following columns:

Rail an ordered factor identifying the rail on which the measurement was made.

**travel** a numeric vector giving the travel time for ultrasonic head-waves in the rail (nanoseconds). The value given is the original travel time minus 36,100 nanoseconds.

### **Details**

Devore (2000, Example 10.10, p. 427) cites data from an article in *Materials Evaluation* on "a study of travel time for a certain type of wave that results from longitudinal stress of rails used for railroad track."

#### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.26)

Devore, J. L. (2000), *Probability and Statistics for Engineering and the Sciences (5th ed)*, Duxbury, Boston, MA.

random.effects 261

random.effects

Extract Random Effects

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include lmList and lme.

### Usage

```
random.effects(object, ...)
ranef(object, ...)
```

# Arguments

object any fitted model object from which random effects estimates can be extracted.
... some methods for this generic function require additional arguments.

#### Value

will depend on the method function used; see the appropriate documentation.

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 100, 461.

#### See Also

```
ranef.lmList.ranef.lme
```

# **Examples**

## see the method function documentation

ranef.lme

Extract lme Random Effects

### **Description**

The estimated random effects at level i are represented as a data frame with rows given by the different groups at that level and columns given by the random effects. If a single level of grouping is specified, the returned object is a data frame; else, the returned object is a list of such data frames. Optionally, the returned data frame(s) may be augmented with covariates summarized over groups.

262 ranef.lme

### Usage

#### **Arguments**

object an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

augFrame an optional logical value. If TRUE, the returned data frame is augmented with

variables defined in data; else, if FALSE, only the coefficients are returned. De-

faults to FALSE.

level an optional vector of positive integers giving the levels of grouping to be used

in extracting the random effects from an object with multiple nested grouping

levels. Defaults to all levels of grouping.

data an optional data frame with the variables to be used for augmenting the returned

data frame when augFrame = TRUE. Defaults to the data frame used to fit object.

which an optional positive integer vector specifying which columns of data should be

used in the augmentation of the returned data frame. Defaults to all columns in

data.

FUN an optional summary function or a list of summary functions to be applied to

group-varying variables, when collapsing data by groups. Group-invariant variables are always summarized by the unique value that they assume within that group. If FUN is a single function it will be applied to each non-invariant variable by group to produce the summary for that variable. If FUN is a list of functions, the names in the list should designate classes of variables in the frame such as ordered, factor, or numeric. The indicated function will be applied to any group-varying variables of that class. The default functions to be used are mean for numeric factors, and Mode for both factor and ordered. The Mode function, defined internally in gsummary, returns the modal or most popular value of the variable. It is different from the mode function that returns the S-language mode

of the variable.

standard an optional logical value indicating whether the estimated random effects should

be "standardized" (i.e. divided by the estimate of the standard deviation of that

group of random effects). Defaults to FALSE.

omitGroupingFactor

an optional logical value. When TRUE the grouping factor itself will be omitted from the group-wise summary of data but the levels of the grouping factor will continue to be used as the row names for the returned data frame. Defaults to

FALSE.

subset an optional expression indicating for which rows the random effects should be

extracted

some methods for this generic require additional arguments. None are used in

this method.

ranef.lmList 263

# Value

a data frame, or list of data frames, with the estimated random effects at the grouping level(s) specified in level and, optionally, other covariates summarized over groups. The returned object inherits from classes random.effects.lme and data.frame.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 100, 461.

#### See Also

```
coef.lme, gsummary, lme, plot.ranef.lme, random.effects
```

### **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject)
ranef(fm1)
random.effects(fm1)  # same as above
random.effects(fm1, augFrame = TRUE)</pre>
```

ranef.lmList

Extract lmList Random Effects

### **Description**

The difference between the individual 1m components coefficients and their average is calculated.

# Usage

object	an object inheriting from class "lmList", representing a list of lm objects with a common model.
augFrame	an optional logical value. If TRUE, the returned data frame is augmented with variables defined in data; else, if FALSE, only the coefficients are returned. Defaults to FALSE.
data	an optional data frame with the variables to be used for augmenting the returned data frame when augFrame = TRUE. Defaults to the data frame used to fit object.

264 ranef.lmList

which

an optional positive integer vector specifying which columns of data should be used in the augmentation of the returned data frame. Defaults to all columns in data.

FUN

an optional summary function or a list of summary functions to be applied to group-varying variables, when collapsing data by groups. Group-invariant variables are always summarized by the unique value that they assume within that group. If FUN is a single function it will be applied to each non-invariant variable by group to produce the summary for that variable. If FUN is a list of functions, the names in the list should designate classes of variables in the frame such as ordered, factor, or numeric. The indicated function will be applied to any group-varying variables of that class. The default functions to be used are mean for numeric factors, and Mode for both factor and ordered. The Mode function, defined internally in gsummary, returns the modal or most popular value of the variable. It is different from the mode function that returns the S-language mode of the variable.

standard

an optional logical value indicating whether the estimated random effects should be "standardized" (i.e. divided by the corresponding estimated standard error). Defaults to FALSE.

omitGroupingFactor

an optional logical value. When TRUE the grouping factor itself will be omitted from the group-wise summary of data but the levels of the grouping factor will continue to be used as the row names for the returned data frame. Defaults to FALSE.

. . .

some methods for this generic require additional arguments. None are used in this method.

### Value

a vector with the differences between the individual 1m coefficients in object and their average.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer, esp. pp. 100, 461.

#### See Also

```
fixed.effects.lmList, lmList, random.effects
```

### **Examples**

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
ranef(fm1)
random.effects(fm1)  # same as above</pre>
```

RatPupWeight 265

RatPupWeight	The weight of rat pups	
--------------	------------------------	--

# **Description**

The RatPupWeight data frame has 322 rows and 5 columns.

#### **Format**

This data frame contains the following columns:

weight a numeric vector

sex a factor with levels Male Female

**Litter** an ordered factor with levels 9 < 8 < 7 < 4 < 2 < 10 < 1 < 3 < 5 < 6 < 21 < 22 < 24 < 27 < 26 < 25 < 23 < 17 < 11 < 14 < 13 < 15 < 16 < 20 < 19 < 18 < 12

Lsize a numeric vector

**Treatment** an ordered factor with levels Control < Low < High

### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York

recalc

Recalculate Condensed Linear Model Object

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include: corStruct, modelStruct, reStruct, and varFunc.

#### Usage

```
recalc(object, conLin, ...)
```

object	any object which induces a recalculation of the condensed linear model object conLin.
conLin	a condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying model.
	some methods for this generic can take additional arguments.

266 recalc.corStruct

### Value

the recalculated condensed linear model object.

#### Note

This function is only used inside model fitting functions, such as lme and gls, that require recalculation of a condensed linear model object.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
recalc.corStruct, recalc.modelStruct, recalc.reStruct, recalc.varFunc
```

# **Examples**

## see the method function documentation

recalc.corStruct

Recalculate for corStruct Object

# **Description**

This method function pre-multiples the "Xy" component of conLin by the transpose square-root factor(s) of the correlation matrix (matrices) associated with object and adds the log-likelihood contribution of object, given by logLik(object), to the "logLik" component of conLin.

# Usage

```
## S3 method for class 'corStruct'
recalc(object, conLin, ...)
```

# Arguments

object	an object inheriting from class "corStruct", representing a correlation structure.
conLin	a condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying model.
	some methods for this generic require additional arguments. None are used in this method.

# Value

the recalculated condensed linear model object.

recalc.modelStruct 267

# Note

This method function is only used inside model fitting functions, such as lme and gls, that allow correlated error terms.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
{\tt corFactor}, {\tt logLik.corStruct}
```

recalc.modelStruct

Recalculate for a modelStruct Object

# Description

This method function recalculates the condensed linear model object using each element of object sequentially from last to first.

# Usage

```
## S3 method for class 'modelStruct'
recalc(object, conLin, ...)
```

### Arguments

object	an object inheriting from class "modelStruct", representing a list of model components, such as corStruct and varFunc objects.
conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying model. Defaults to attr(object, "conLin").
• • •	some methods for this generic require additional arguments. None are used in this method.

# Value

the recalculated condensed linear model object.

#### Note

This method function is generally only used inside model fitting functions, such as 1me and g1s, that allow model components, such as correlated error terms and variance functions.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

268 recalc.reStruct

### See Also

```
recalc.corStruct, recalc.reStruct, recalc.varFunc
```

recalc.reStruct

Recalculate for an reStruct Object

# **Description**

The log-likelihood, or restricted log-likelihood, of the Gaussian linear mixed-effects model represented by object and conLin (assuming spherical within-group covariance structure), evaluated at coef(object) is calculated and added to the logLik component of conLin. The settings attribute of object determines whether the log-likelihood, or the restricted log-likelihood, is to be calculated. The computational methods for the (restricted) log-likelihood calculations are described in Bates and Pinheiro (1998).

# Usage

```
## S3 method for class 'reStruct'
recalc(object, conLin, ...)
```

# Arguments

object	an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.
conLin	a condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying model.
	some methods for this generic require additional arguments. None are used in this method.

### Value

the condensed linear model with its logLik component updated.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
logLik, lme, recalc, reStruct
```

recalc.varFunc 269

recalc.varFunc Recalcu	late for varFunc Object
------------------------	-------------------------

# Description

This method function pre-multiples the "Xy" component of conLin by a diagonal matrix with diagonal elements given by the weights corresponding to the variance structure represented by objecte and adds the log-likelihood contribution of object, given by logLik(object), to the "logLik" component of conLin.

# Usage

```
## S3 method for class 'varFunc'
recalc(object, conLin, ...)
```

# **Arguments**

object	an object inheriting from class "varFunc", representing a variance function structure.
conLin	a condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying model.
	some methods for this generic require additional arguments. None are used in this method.

#### Value

the recalculated condensed linear model object.

# Note

This method function is only used inside model fitting functions, such as lme and gls, that allow heteroscedastic error terms.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
recalc, varWeights, logLik.varFunc
```

270 Remifentanil

Relaxin

Assay for Relaxin

# **Description**

The Relaxin data frame has 198 rows and 3 columns.

#### **Format**

This data frame contains the following columns:

```
Run an ordered factor with levels 5 < 8 < 9 < 3 < 4 < 2 < 7 < 1 < 6
```

**conc** a numeric vector **cAMP** a numeric vector

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

Remifentanil

Pharmacokinetics of Remifentanil

### **Description**

Intravenous infusion of remifentanil (a strong analgesic) in different rates over varying time periods was applied to a total of 65 patients. Concentration measurements of remifentanil were taken along with several covariates resulting in the Remifentanil data frame with 2107 rows and 12 columns.

### Usage

```
data("Remifentanil", package = "nlme")
```

# **Format**

This data frame (of class "groupedData", specifically "nfnGroupedData") contains the following columns:

```
ID: numerical (patient) IDs.
```

```
Subject: an ordered factor with 65 levels (of the IDs): 30 < 21 < 25 < 23 < 29 < \dots < 36 < 6 < 5 < 10 < 9.
```

```
Time: time from beginning of infusion in minutes (numeric).
```

conc: remifentanil concentration in [ng / ml] (numeric).

Rate: infusion rate in [µg / min].

Remifentanil 271

```
Amt: amount of remifentanil given in the current time interval in [µg].  
Age: age of the patient in years.  
Sex: gender of the patient, a factor with levels Female and Male.  
Ht: height of the patient in cm.  
Wt: weight of the patient in kg.  
BSA: body surface area (DuBois and DuBois 1916): BSA := Wt^{0.425} \cdot Ht^{0.725} \cdot 0.007184.  
LBM: lean body mass (James 1976), with slightly different formula for men LBM_m := 1.1Wt - 128(Wt/Ht)^2, and women LBM_f := 1.07Wt - 148(Wt/Ht)^2.
```

#### Author(s)

of this help page: Niels Hagenbuch and Martin Maechler, SfS ETH Zurich.

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000). *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

#### References

Minto CF, Schnider TW, Egan TD, Youngs E, Lemmens HJM, Gambus PL, Billard V, Hoke JF, Moore KHP, Hermann DJ, Muir KT, Mandema JW, Shafer SL (1997). Influence of age and gender on the pharmacokinetics and pharmacodynamics of remifentanil: I. Model development. *Anesthesiology* **86** 1, 10–23. doi:10.1097/0000054219970100000004

Charles F. Minto, Thomas W. Schnider and Steven L. Shafer (1997). Pharmacokinetics and Pharmacodynamics of Remifentanil: II. Model Application. *Anesthesiology* **86** 1, 24–33. doi:10.1097/0000054219970100000005

### **Examples**

272 residuals.gls

residuals.gls

Extract gls Residuals

# Description

The residuals for the linear model represented by object are extracted.

# Usage

```
## S3 method for class 'gls'
residuals(object, type, ...)
```

### **Arguments**

object

an object inheriting from class "gls", representing a generalized least squares fitted linear model, or from class gnls, representing a generalized nonlinear least squares fitted linear model.

type

an optional character string specifying the type of residuals to be used. If "response", the "raw" residuals (observed - fitted) are used; else, if "pearson", the standardized residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals pre-multiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the first character needs to be provided. Defaults to "response".

. . .

some methods for this generic function require additional arguments. None are used in this method.

#### Value

a vector with the residuals for the linear model represented by object.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

gls

residuals.glsStruct 273

### **Examples**

residuals.glsStruct

Calculate glsStruct Residuals

# Description

The residuals for the linear model represented by object are extracted.

# Usage

```
## S3 method for class 'glsStruct'
residuals(object, glsFit, ...)
```

# Arguments

object	an object inheriting from class "glsStruct", representing a list of linear model components, such as corStruct and "varFunc" objects.
glsFit	an optional list with components logLik (log-likelihood), beta (coefficients), sigma (standard deviation for error term), varBeta (coefficients' covariance matrix), fitted (fitted values), and residuals (residuals). Defaults to attr(object, "glsFit").
• • •	some methods for this generic require additional arguments. None are used in this method.

### Value

a vector with the residuals for the linear model represented by object.

### Note

This method function is primarily used inside gls and residuals.gls.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
gls, glsStruct, residuals.gls, fitted.glsStruct
```

274 residuals.gnlsStruct

```
residuals.gnlsStruct Calculate gnlsStruct Residuals
```

# Description

The residuals for the nonlinear model represented by object are extracted.

# Usage

```
## S3 method for class 'gnlsStruct'
residuals(object, ...)
```

# Arguments

object an object inheriting from class "gnlsStruct", representing a list of model com-

ponents, such as corStruct and varFunc objects, and attributes specifying the

underlying nonlinear model and the response variable.

... some methods for this generic require additional arguments. None are used in

this method.

### Value

a vector with the residuals for the nonlinear model represented by object.

#### Note

This method function is primarily used inside gnls and residuals.gnls.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
gnls, residuals.gnls, fitted.gnlsStruct
```

residuals.lme 275

residuals.lme

Extract lme Residuals

### **Description**

The residuals at level i are obtained by subtracting the fitted levels at that level from the response vector (and dividing by the estimated within-group standard error, if type="pearson"). The fitted values at level i are obtained by adding together the population fitted values (based only on the fixed effects estimates) and the estimated contributions of the random effects to the fitted values at grouping levels less or equal to i.

# Usage

```
## S3 method for class 'lme'
residuals(object, level = Q,
          type = c("response", "pearson", "normalized"), asList = FALSE, ...)
```

#### Arg

rguments	
object	an object inheriting from class "lme", representing a fitted linear mixed-effects model.
level	an optional integer vector giving the level(s) of grouping to be used in extracting the residuals from object. Level values increase from outermost to innermost grouping, with level zero corresponding to the population residuals. Defaults to the highest or innermost level of grouping.
type	an optional character string specifying the type of residuals to be used. If "response", as by default, the "raw" residuals (observed - fitted) are used; else, if "pearson", the standardized residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals pre-multiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the first character needs to be provided.
asList	an optional logical value. If TRUE and a single value is given in level, the returned object is a list with the residuals split by groups; else the returned value is either a vector or a data frame, according to the length of level. Defaults to FALSE.

### Value

if a single level of grouping is specified in level, the returned value is either a list with the residuals split by groups (asList = TRUE) or a vector with the residuals (asList = FALSE); else, when multiple grouping levels are specified in level, the returned object is a data frame with columns given by the residuals at different levels and the grouping factors. For a vector or data frame result the naresid method is applied.

this method.

some methods for this generic require additional arguments. None are used in

276 residuals.ImeStruct

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
lme, fitted.lme
```

# **Examples**

residuals.lmeStruct

Calculate lmeStruct Residuals

# **Description**

The residuals at level i are obtained by subtracting the fitted values at that level from the response vector. The fitted values at level i are obtained by adding together the population fitted values (based only on the fixed effects estimates) and the estimated contributions of the random effects to the fitted values at grouping levels less or equal to i.

# Usage

```
## S3 method for class 'lmeStruct'
residuals(object, level, conLin, lmeFit, ...)
```

object	an object inheriting from class "lmeStruct", representing a list of linear mixed-effects model components, such as reStruct, corStruct, and varFunc objects.
level	an optional integer vector giving the level(s) of grouping to be used in extracting the residuals from object. Level values increase from outermost to innermost grouping, with level zero corresponding to the population fitted values. Defaults to the highest or innermost level of grouping.
conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying lme model. Defaults to attr(object, "conLin").
lmeFit	an optional list with components beta and b containing respectively the fixed effects estimates and the random effects estimates to be used to calculate the residuals. Defaults to attr(object, "lmeFit").
	some methods for this generic accept optional arguments.

residuals.lmList 277

# Value

if a single level of grouping is specified in level, the returned value is a vector with the residuals at the desired level; else, when multiple grouping levels are specified in level, the returned object is a matrix with columns given by the residuals at different levels.

#### Note

This method function is primarily used within the 1me function.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

```
lme, residuals.lme, fitted.lmeStruct
```

residuals.lmList

Extract lmList Residuals

# **Description**

The residuals are extracted from each 1m component of object and arranged into a list with as many components as object, or combined into a single vector.

# Usage

```
## S3 method for class 'lmList'
residuals(object, type, subset, asList, ...)
```

object	an object inheriting from class "lmList", representing a list of lm objects with a common model.
subset	an optional character or integer vector naming the 1m components of object from which the residuals are to be extracted. Default is NULL, in which case all components are used.
type	an optional character string specifying the type of residuals to be extracted. Options include "response" for the "raw" residuals (observed - fitted), "pearson" for the standardized residuals (raw residuals divided by the estimated residual standard error) using different standard errors for each lm fit, and "pooled.pearson" for the standardized residuals using a pooled estimate of the residual standard error. Partial matching of arguments is used, so only the first character needs to be provided. Defaults to "response".
asList	an optional logical value. If TRUE, the returned object is a list with the residuals split by groups; else the returned value is a vector. Defaults to FALSE.
	some methods for this generic require additional arguments. None are used in this method.

278 residuals.nlmeStruct

# Value

a list with components given by the residuals of each 1m component of object, or a vector with the residuals for all 1m components of object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
lmList, fitted.lmList
```

# **Examples**

```
fm1 <- lmList(distance \sim age | Subject, Orthodont) residuals(fm1)
```

residuals.nlmeStruct Calculate nlmeStruct Residuals

### **Description**

The residuals at level i are obtained by subtracting the fitted values at that level from the response vector. The fitted values at level i are obtained by adding together the contributions from the estimated fixed effects and the estimated random effects at levels less or equal to i and evaluating the model function at the resulting estimated parameters.

# Usage

```
## S3 method for class 'nlmeStruct'
residuals(object, level, conLin, ...)
```

object	an object inheriting from class "nlmeStruct", representing a list of mixed-effects model components, such as reStruct, corStruct, and varFunc objects.
level	an optional integer vector giving the level(s) of grouping to be used in extracting the residuals from object. Level values increase from outermost to innermost grouping, with level zero corresponding to the population fitted values. Defaults to the highest or innermost level of grouping.
conLin	an optional condensed linear model object, consisting of a list with components "Xy", corresponding to a regression matrix (X) combined with a response vector (y), and "logLik", corresponding to the log-likelihood of the underlying nlme model. Defaults to attr(object, "conLin").
	optional arguments to the residuals generic. Not used.

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#### Value

if a single level of grouping is specified in level, the returned value is a vector with the residuals at the desired level; else, when multiple grouping levels are specified in level, the returned object is a matrix with columns given by the residuals at different levels.

#### Note

This method function is primarily used within the nlme function.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Bates, D.M. and Pinheiro, J.C. (1998) "Computational methods for multilevel models" available in PostScript or PDF formats at http://nlme.stat.wisc.edu

#### See Also

```
nlme, fitted.nlmeStruct
```

reStruct

Random Effects Structure

# Description

This function is a constructor for the reStruct class, representing a random effects structure and consisting of a list of pdMat objects, plus a settings attribute containing information for the optimization algorithm used to fit the associated mixed-effects model.

### Usage

```
reStruct(object, pdClass, REML, data)
## S3 method for class 'reStruct'
print(x, sigma, reEstimates, verbose, ...)
```

### **Arguments**

object

any of the following: (i) a one-sided formula of the form  $\sim x1+\ldots+xn \mid g1/\ldots/gm$ , with  $x1+\ldots+xn$  specifying the model for the random effects and  $g1/\ldots/gm$  the grouping structure (m may be equal to 1, in which case no / is required). The random effects formula will be repeated for all levels of grouping, in the case of multiple levels of grouping; (ii) a list of one-sided formulas of the form  $\sim x1+\ldots+xn \mid g$ , with possibly different random effects models for each grouping level. The order of nesting will be assumed the same as the order of the elements in the list; (iii) a one-sided formula of the form  $\sim x1+\ldots+xn$ , or a

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pdMat object with a formula (i.e. a non-NULL value for formula(object)), or a list of such formulas or pdMat objects. In this case, the grouping structure formula will be derived from the data used to to fit the mixed-effects model, which should inherit from class groupedData; (iv) a named list of formulas or pdMat objects as in (iii), with the grouping factors as names. The order of nesting will be assumed the same as the order of the order of the elements in the list; (v) an reStruct object.

pdClass an optional character string with the name of the pdMat class to be used for the

formulas in object. Defaults to "pdLogCho1" which corresponds to a general

positive-definite matrix (Log-Cholesky parametrization).

REML an optional logical value. If TRUE, the associated mixed-effects model will be

fitted using restricted maximum likelihood; else, if FALSE, maximum likelihood

will be used. Defaults to FALSE.

data an optional data frame in which to evaluate the variables used in the random

effects formulas in object. It is used to obtain the levels for factors, which affect the dimensions and the row/column names of the underlying pdMat objects. If NULL, no attempt is made to obtain information on factors appearing in the formulas. Defaults to the parent frame from which the function was called.

x an object inheriting from class reStruct to be printed.

sigma an optional numeric value used as a multiplier for the square-root factors of the

pdMat components (usually the estimated within-group standard deviation from

a mixed-effects model). Defaults to 1.

reEstimates an optional list with the random effects estimates for each level of grouping.

Only used when verbose = TRUE.

verbose an optional logical value determining if the random effects estimates should be

printed. Defaults to FALSE.

... Optional arguments can be given to other methods for this generic. None are

used in this method.

#### Value

an object inheriting from class reStruct, representing a random effects structure.

### Author(s)

José Pinheiro and Douglas Bates <bate="englast: bates@stat.wisc.edu">

#### See Also

```
groupedData, lme, pdMat, solve.reStruct, summary.reStruct, update.reStruct
```

# **Examples**

```
rs1 <- reStruct(list(Dog = ~day, Side = ~1), data = Pixel)
rs1 # 2 entries "Uninitialized"
str(rs1) # a bit more</pre>
```

simulate.lme 281

simulate.lme	Simulate Results from 1me Models
--------------	----------------------------------

### **Description**

The model object is fit to the data. Using the fitted values of the parameters, nsim new data vectors from this model are simulated. Both object and m2 are fit by maximum likelihood (ML) and/or by restricted maximum likelihood (REML) to each of the simulated data vectors.

# Usage

### **Arguments**

object	an object inheriting from class "lme", representing a fitted linear mixed-effects model, or a list containing an lme model specification. If given as a list, it should contain components fixed, data, and random with values suitable for a call to lme. This argument defines the null model.
m2	an "lme" object or a list, like object containing a second lme model specification. This argument defines the alternative model. If given as a list, only those parts of the specification that change between model object and m2 need to be specified.
seed	an optional integer that is passed to set.seed. Defaults to a random integer.
method	an optional character array. If it includes "REML" the models are fit by maximizing the restricted log-likelihood. If it includes "ML" the log-likelihood is maximized. Defaults to c("REML", "ML"), in which case both methods are used.
nsim	an optional positive integer specifying the number of simulations to perform. Defaults to 1. <b>This has changed. Previously the default was 1000.</b>
niterEM	an optional integer vector of length 2 giving the number of iterations of the EM algorithm to apply when fitting the object and m2 to each simulated set of data. Defaults to $c(40,200)$ .
useGen	an optional logical value. If TRUE, the nlminb optimizer is used with numerical derivatives of the log-likelihood. If FALSE, the nlm algorithm is used with an analytic gradient. The default depends on the "pdMat" classes used in object and m2: if both are standard classes (see pdClasses) then defaults to FALSE, otherwise defaults to TRUE.
	optional additional arguments. None are used.

### Value

an object of class simulate. Ime with components null and alt. Each of these has components ML and/or REML which are matrices. An attribute called seed contains the seed that was used for the random number generator.

282 solve.pdMat

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) Mixed-Effects Models in S and S-PLUS, Springer.

#### See Also

```
lme, set.seed
```

# **Examples**

solve.pdMat

Calculate Inverse of a Positive-Definite Matrix

# **Description**

The positive-definite matrix represented by a is inverted and assigned to a.

### Usage

```
## S3 method for class 'pdMat'
solve(a, b, ...)
```

#### **Arguments**

a an object inheriting from class "pdMat", representing a positive definite matrix.
b this argument is only included for consistency with the generic function and is not used in this method function.

some methods for this generic require additional arguments. None are used in

... some methods for this generic require additional arguments. None are used in this method.

# Value

a pdMat object similar to a, but with coefficients corresponding to the inverse of the positive-definite matrix represented by a.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

solve.reStruct 283

### See Also

```
pdMat
```

### **Examples**

```
pd1 <- pdCompSymm(3 * diag(3) + 1)
solve(pd1)</pre>
```

solve.reStruct

Apply Solve to an reStruct Object

# **Description**

Solve is applied to each pdMat component of a, which results in inverting the positive-definite matrices they represent.

### Usage

```
## S3 method for class 'reStruct'
solve(a, b, ...)
```

### **Arguments**

a an object inheriting from class "reStruct", representing a random effects structure and consisting of a list of pdMat objects.

b this argument is only included for consistency with the generic function and is not used in this method function.

some methods for this generic require additional arguments. None are used in this method.

# Value

an reStruct object similar to a, but with the pdMat components representing the inverses of the matrices represented by the components of a.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
solve.pdMat, reStruct
```

#### **Examples**

```
rs1 <- reStruct(list(A = pdSymm(diag(1:3), form = ~Score),
   B = pdDiag(2 * diag(4), form = ~Educ)))
solve(rs1)</pre>
```

284 splitFormula

Soybean

Growth of soybean plants

# Description

The Soybean data frame has 412 rows and 5 columns.

#### **Format**

This data frame contains the following columns:

Plot a factor giving a unique identifier for each plot.

Variety a factor indicating the variety; Forrest (F) or Plant Introduction #416937 (P).

Year a factor indicating the year the plot was planted.

**Time** a numeric vector giving the time the sample was taken (days after planting).

weight a numeric vector giving the average leaf weight per plant (g).

### **Details**

These data are described in Davidian and Giltinan (1995, 1.1.3, p.7) as "Data from an experiment to compare growth patterns of two genotypes of soybeans: Plant Introduction #416937 (P), an experimental strain, and Forrest (F), a commercial variety."

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.27)

Davidian, M. and Giltinan, D. M. (1995), *Nonlinear Models for Repeated Measurement Data*, Chapman and Hall, London.

## **Examples**

```
summary(fm1 <- nlsList(SSlogis, data = Soybean))</pre>
```

splitFormula

Split a Formula

### **Description**

Splits the right hand side of form into a list of subformulas according to the presence of sep. The left hand side of form, if present, will be ignored. The length of the returned list will be equal to the number of occurrences of sep in form plus one.

Spruce 285

### Usage

```
splitFormula(form, sep)
```

### **Arguments**

form a formula object.

sep an optional character string specifying the separator to be used for splitting the

formula. Defaults to "/".

#### Value

a list of formulas, corresponding to the split of form according to sep.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### See Also

formula

# **Examples**

```
splitFormula(~ g1/g2/g3)
```

Spruce

Growth of Spruce Trees

# **Description**

The Spruce data frame has 1027 rows and 4 columns.

# **Format**

This data frame contains the following columns:

Tree a factor giving a unique identifier for each tree.

days a numeric vector giving the number of days since the beginning of the experiment.

logSize a numeric vector giving the logarithm of an estimate of the volume of the tree trunk.

**plot** a factor identifying the plot in which the tree was grown.

### **Details**

Diggle, Liang, and Zeger (1994, Example 1.3, page 5) describe data on the growth of spruce trees that have been exposed to an ozone-rich atmosphere or to a normal atmosphere.

286 summary.corStruct

### Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York. (Appendix A.28)

Diggle, Peter J., Liang, Kung-Yee and Zeger, Scott L. (1994), *Analysis of longitudinal data*, Oxford University Press, Oxford.

summary.corStruct

Summarize a corStruct Object

### **Description**

This method function prepares object to be printed using the print. summary method, by changing its class and adding a structName attribute to it.

## Usage

```
## S3 method for class 'corStruct'
summary(object, structName, ...)
```

# **Arguments**

object an object inheriting from class "corStruct", representing a correlation struc-

ture.

structName an optional character string defining the type of correlation structure associated

with object, to be used in the print.summary method. Defaults to class(object)[1].

... some methods for this generic require additional arguments. None are used in

this method.

#### Value

an object identical to object, but with its class changed to summary.corStruct and an additional attribute structName. The returned value inherits from the same classes as object.

### Author(s)

José Pinheiro and Douglas Bates

#### See Also

```
corClasses, corNatural, Initialize.corStruct, summary
```

# **Examples**

```
cs1 <- corAR1(0.2)
summary(cs1)</pre>
```

summary.gls 287

summary.gls Summarize a Generalized Least Squares gls Object	summary.gls	Summarize a Generalized Least Squares gls Object
--	-------------	--

### **Description**

Additional information about the linear model fit represented by object is extracted and included as components of object.

# Usage

```
## S3 method for class 'gls'
summary(object, verbose, ...)
```

# Arguments

object an object inheriting from class "gls", representing a generalized least squares

fitted linear model.

verbose an optional logical value used to control the amount of output when the object

is printed. Defaults to FALSE.

... some methods for this generic require additional arguments. None are used in

this method.

#### Value

an object inheriting from class summary.gls with all components included in object (see glsObject for a full description of the components) plus the following components:

corBeta approximate correlation matrix for the coefficients estimates

tTable a matrix with columns Value, Std. Error, t-value, and p-value representing

respectively the coefficients estimates, their approximate standard errors, the ratios between the estimates and their standard errors, and the associated p-value

under a t approximation. Rows correspond to the different coefficients.

residuals if more than five observations are used in the gls fit, a vector with the minimum,

first quartile, median, third quartile, and maximum of the residuals distribution;

else the residuals.

AIC the Akaike Information Criterion corresponding to object.

BIC the Bayesian Information Criterion corresponding to object.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
AIC, BIC, gls, summary
```

288 summary.lme

#### **Examples**

summary.1me

Summarize an lme Object

### **Description**

Additional information about the linear mixed-effects fit represented by object is extracted and included as components of object. The returned object has a print and a coef method, the latter returning the coefficient's tTtable.

### Usage

```
## S3 method for class 'lme'
summary(object, adjustSigma, verbose, ...)
## S3 method for class 'summary.lme'
print(x, verbose = FALSE, ...)
```

#### **Arguments**

.

x

#### Value

an object inheriting from class summary. 1me with all components included in object (see 1meObject for a full description of the components) plus the following components:

corFixed approximate correlation matrix for the fixed effects estimates.

a "summary.lme" object.

tTable a matrix with

a matrix with columns named Value, Std. Error, DF, t-value, and p-value representing respectively the fixed effects estimates, their approximate standard errors, the denominator degrees of freedom, the ratios between the estimates and their standard errors, and the associated p-value from a t distribution. Rows correspond to the different fixed effects.

summary.lmList 289

residuals	if more than five observations are used in the 1me fit, a vector with the minimum, first quartile, median, third quartile, and maximum of the innermost grouping level residuals distribution; else the innermost grouping level residuals.
AIC	the Akaike Information Criterion corresponding to object.
BIC	the Bayesian Information Criterion corresponding to object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
AIC, BIC, 1me.
```

# **Examples**

```
fm1 <- lme(distance ~ age, Orthodont, random = ~ age | Subject) (s1 <- summary(fm1)) coef(s1) # the (coef | Std.E | t | P-v ) matrix
```

summary.lmList

Summarize an lmList Object

# Description

The summary.lm method is applied to each lm component of object to produce summary information on the individual fits, which is organized into a list of summary statistics. The returned object is suitable for printing with the print.summary.lmList method.

# Usage

```
## S3 method for class 'lmList'
summary(object, pool, ...)
```

object	an object inheriting from class "lmList", representing a list of lm fitted objects.
pool	an optional logical value indicating whether a pooled estimate of the residual standard error should be used. Default is attr(object, "pool").
	some methods for this generic require additional arguments. None are used in this method.

290 summary.lmList

#### Value

a list with summary statistics obtained by applying summary. Im to the elements of object, inheriting from class summary. ImList. The components of value are:

call a list containing an image of the lmList call that produced object.

coefficients a three dimensional array with summary information on the lm coefficients. The

first dimension corresponds to the names of the object components, the second dimension is given by "Value", "Std. Error", "t value", and "Pr(>|t|)", corresponding, respectively, to the coefficient estimates and their associated standard errors, t-values, and p-values. The third dimension is given by the

coefficients names.

correlation a three dimensional array with the correlations between the individual 1m coef-

ficient estimates. The first dimension corresponds to the names of the object components. The third dimension is given by the coefficients names. For each coefficient, the rows of the associated array give the correlations between that

coefficient and the remaining coefficients, by 1m component.

cov.unscaled a three dimensional array with the unscaled variances/covariances for the in-

dividual 1m coefficient estimates (giving the estimated variance/covariance for the coefficients, when multiplied by the estimated residual errors). The first dimension corresponds to the names of the object components. The third dimension is given by the coefficients names. For each coefficient, the rows of the associated array give the unscaled covariances between that coefficient and the

remaining coefficients, by 1m component.

df an array with the number of degrees of freedom for the model and for residuals,

for each 1m component.

df.residual the total number of degrees of freedom for residuals, corresponding to the sum

of residuals df of all 1m components.

fstatistics an array with the F test statistics and corresponding degrees of freedom, for each

1m component.

pool the value of the pool argument to the function.

r.squared a vector with the multiple R-squared statistics for each 1m component.
residuals a list with components given by the residuals from individual 1m fits.

RSE the pooled estimate of the residual standard error.

sigma a vector with the residual standard error estimates for the individual 1m fits.

terms the terms object used in fitting the individual 1m components.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

lmList, summary

summary.modelStruct 291

## **Examples**

```
fm1 <- lmList(distance ~ age | Subject, Orthodont)
summary(fm1)</pre>
```

summary.modelStruct

Summarize a modelStruct Object

# Description

This method function applies summary to each element of object.

# Usage

```
## S3 method for class 'modelStruct'
summary(object, ...)
```

# **Arguments**

object

an object inheriting from class "modelStruct", representing a list of model

components, such as reStruct, corStruct and varFunc objects.

. . .

some methods for this generic require additional arguments. None are used in

this method.

## Value

a list with elements given by the summarized components of object. The returned value is of class summary.modelStruct, also inheriting from the same classes as object.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# See Also

```
reStruct, summary
```

# **Examples**

```
lms1 <- lmeStruct(reStruct = reStruct(pdDiag(diag(2), ~age)),
    corStruct = corAR1(0.3))
summary(lms1)</pre>
```

292 summary.nlsList

summary.nlsList

Summarize an nlsList Object

### **Description**

The summary function is applied to each nls component of object to produce summary information on the individual fits, which is organized into a list of summary statistics. The returned object is suitable for printing with the print.summary.nlsList method.

## Usage

```
## S3 method for class 'nlsList'
summary(object, ...)
```

### **Arguments**

object an object inheriting from class "nlsList", representing a list of nls fitted ob-

jects.

optional arguments to the summary.lmList method. One such optional argu-

ment is pool, a logical value indicating whether a pooled estimate of the residual

standard error should be used. Default is attr(object, "pool").

### Value

a list with summary statistics obtained by applying summary to the elements of object, inheriting from class summary.nlsList. The components of value are:

call a list containing an image of the nlsList call that produced object.

parameters a three dimensional array with summary information on the nls coefficients.

The first dimension corresponds to the names of the object components, the second dimension is given by "Value", "Std. Error", "t value", and "Pr(>|t|)", corresponding, respectively, to the coefficient estimates and their associated standard errors, t-values, and p-values. The third dimension is given by the

coefficients names.

correlation a three dimensional array with the correlations between the individual nls co-

efficient estimates. The first dimension corresponds to the names of the object components. The third dimension is given by the coefficients names. For each coefficient, the rows of the associated array give the correlations between that

coefficient and the remaining coefficients, by nls component.

cov.unscaled a three dimensional array with the unscaled variances/covariances for the in-

dividual 1m coefficient estimates (giving the estimated variance/covariance for the coefficients, when multiplied by the estimated residual errors). The first dimension corresponds to the names of the object components. The third dimension is given by the coefficients names. For each coefficient, the rows of the associated array give the unscaled covariances between that coefficient and the

remaining coefficients, by nls component.

summary.pdMat 293

df an array with the number of degrees of freedom for the model and for residuals,

for each nls component.

df.residual the total number of degrees of freedom for residuals, corresponding to the sum

of residuals df of all nls components.

pool the value of the pool argument to the function.

RSE the pooled estimate of the residual standard error.

sigma a vector with the residual standard error estimates for the individual 1m fits.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
nlsList, summary
```

## **Examples**

```
fm1 <- nlsList(SSasymp, Loblolly)
summary(fm1)</pre>
```

summary.pdMat

Summarize a pdMat Object

## **Description**

Attributes structName and noCorrelation, with the values of the corresponding arguments to the method function, are appended to object and its class is changed to summary.pdMat.

## Usage

```
## S3 method for class 'pdMat'
summary(object, structName, noCorrelation, ...)
```

## **Arguments**

an object inheriting from class "pdMat", representing a positive definite matrix.

structName an optional character string with a description of the pdMat class. Default depends on the method function: "Blocked" for pdBlocked, "Compound Symmetry" for pdCompSymm, "Diagonal" for pdDiag, "Multiple of an Identity" for pdIdent, "General Positive-Definite, Natural Parametrization" for pdNatural, "General Positive-Definite" for pdSymm, and data.class(object) for pdMat.

noCorrelation an optional logical value indicating whether correlations are to be printed in print.summary.pdMat. Default depends on the method function: FALSE for pdDiag and pdIdent, and TRUE for all other classes.

some methods for this generic require additional arguments. None are used in

this method.

294 summary.varFunc

#### Value

an object similar to object, with additional attributes structName and noCorrelation, inheriting from class summary.pdMat.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

```
print.summary.pdMat, pdMat
```

# **Examples**

```
summary(pdSymm(diag(4)))
```

summary.varFunc

Summarize "varFunc" Object

## **Description**

A structName attribute, with the value of corresponding argument, is appended to object and its class is changed to summary.varFunc.

# Usage

```
## S3 method for class 'varFunc'
summary(object, structName, ...)
```

## **Arguments**

object an object inheriting from class "varFunc", representing a variance function

structure.

structName an optional character string with a description of the varFunc class. Default

depends on the method function:

for varComb: "Combination of variance functions",

for varConstPower: "Constant plus power of variance covariate",

for varConstProp: "Constant plus proportion of variance covariate",

for varExp: "Exponential of variance covariate",

for varIdent: "Different standard deviations per stratum",

for varPower: "Power of variance covariate",

for varFunc: data.class(object).

... some methods for this generic require additional arguments. None are used in

this method.

Tetracycline1 295

# Value

an object similar to object, with an additional attribute structName, inheriting from class summary.varFunc.

# Author(s)

José Pinheiro and Douglas Bates <bate=0.000 | José Pinheiro and Douglas Bates | State | José Pinheiro and Douglas Bates | José Pinheiro and Pinheiro a

#### See Also

```
varClasses, varFunc
```

# **Examples**

```
vf1 <- varPower(0.3, form = ~age)
vf1 <- Initialize(vf1, Orthodont)
summary(vf1)</pre>
```

Tetracycline1

Pharmacokinetics of tetracycline

# **Description**

The Tetracycline1 data frame has 40 rows and 4 columns.

### **Format**

This data frame contains the following columns:

conc a numeric vector

Time a numeric vector

**Subject** an ordered factor with levels 5 < 3 < 2 < 4 < 1

Formulation a factor with levels tetrachel tetracyn

# Source

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

296 update.modelStruct

# **Description**

The Tetracycline2 data frame has 40 rows and 4 columns.

## **Format**

This data frame contains the following columns:

```
conc a numeric vector
Time a numeric vector
Subject an ordered factor with levels 4 < 5 < 2 < 1 < 3</li>
Formulation a factor with levels Berkmycin tetramycin
```

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

```
update.modelStruct Update a modelStruct Object
```

# Description

This method function updates each element of object, allowing the access to data.

# Usage

```
## S3 method for class 'modelStruct'
update(object, data, ...)
```

## **Arguments**

object	an object inheriting from class "modelStruct", representing a list of model components, such as corStruct and varFunc objects.
data	a data frame in which to evaluate the variables needed for updating the elements of object.
	some methods for this generic require additional arguments. None are used in this method.

## Value

an object similar to object (same class, length, and names), but with updated elements.

update.varFunc 297

# Note

This method function is primarily used within model fitting functions, such as lme and gls, that allow model components such as variance functions.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### See Also

reStruct

update.varFunc

Update varFunc Object

## **Description**

If the formula(object) includes a "." term, representing a fitted object, the variance covariate needs to be updated upon completion of an optimization cycle (in which the variance function weights are kept fixed). This method function allows a reevaluation of the variance covariate using the current fitted object and, optionally, other variables in the original data.

# Usage

```
## S3 method for class 'varFunc'
update(object, data, ...)
```

## **Arguments**

object	an object inheriting from class "varFunc", representing a variance function structure.
data	a list with a component named "." with the current version of the fitted object (from which fitted values, coefficients, and residuals can be extracted) and, if necessary, other variables used to evaluate the variance covariate(s).
	some methods for this generic require additional arguments. None are used in this method.

### Value

if formula(object) includes a "." term, an varFunc object similar to object, but with the variance covariate reevaluated at the current fitted object value; else object is returned unchanged.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

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## See Also

needUpdate, covariate<-.varFunc</pre>

varClasses Variance Function Classes

# Description

Standard classes of variance function structures (varFunc) available in the nlme package. Covariates included in the variance function, denoted by variance covariates, may involve functions of the fitted model object, such as the fitted values and the residuals. Different coefficients may be assigned to the levels of a classification factor.

#### Value

Available standard classes:

varExp exponential of a variance covariate.

varPower power of a variance covariate.

varConstPower constant plus power of a variance covariate.

varConstProp constant plus proportion of a variance covariate.

varIdent constant variance(s), generally used to allow different variances according to the

levels of a classification factor.

varFixed fixed weights, determined by a variance covariate.

varComb combination of variance functions.

### Note

Users may define their own varFunc classes by specifying a constructor function and, at a minimum, methods for the functions coef, coef<-, and initialize. For examples of these functions, see the methods for class varPower.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

varComb, varConstPower, varConstProp, varExp, varFixed, varIdent, varPower, summary.varFunc

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varComb

Combination of Variance Functions

# **Description**

This function is a constructor for the varComb class, representing a combination of variance functions. The corresponding variance function is equal to the product of the variance functions of the varFunc objects listed in . . . .

# Usage

```
varComb(...)
```

# **Arguments**

... objects inheriting from class varFunc representing variance function structures.

#### Value

a varComb object representing a combination of variance functions, also inheriting from class varFunc.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

# See Also

```
varClasses, varWeights.varComb, coef.varComb
```

# **Examples**

```
vf1 <- varComb(varIdent(form = ~1|Sex), varPower())</pre>
```

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varConstPower

Constant Plus Power Variance Function

### Description

This function is a constructor for the varConstPower class, representing a constant plus power variance function structure. Letting v denote the variance covariate and  $\sigma^2(v)$  denote the variance function evaluated at v, the constant plus power variance function is defined as  $\sigma^2(v) = (\theta_1 + |v|_2^\theta)^2$ , where  $\theta_1, \theta_2$  are the variance function coefficients. When a grouping factor is present, different  $\theta_1, \theta_2$  are used for each factor level.

# Usage

varConstPower(const, power, form, fixed)

## Arguments

const, power

optional numeric vectors, or lists of numeric values, with, respectively, the coefficients for the constant and the power terms. Both arguments must have length one, unless a grouping factor is specified in form. If either argument has length greater than one, it must have names which identify its elements to the levels of the grouping factor defined in form. If a grouping factor is present in form and the argument has length one, its value will be assigned to all grouping levels. Only positive values are allowed for const. Default is numeric(0), which results in a vector of zeros of appropriate length being assigned to the coefficients when object is initialized (corresponding to constant variance equal to one).

form

an optional one-sided formula of the form  $\sim v$ , or  $\sim v \mid g$ , specifying a variance covariate v and, optionally, a grouping factor g for the coefficients. The variance covariate must evaluate to a numeric vector and may involve expressions using ".", representing a fitted model object from which fitted values (fitted(.)) and residuals (resid(.)) can be extracted (this allows the variance covariate to be updated during the optimization of an object function). When a grouping factor is present in form, a different coefficient value is used for each of its levels. Several grouping variables may be simultaneously specified, separated by the \* operator, as in  $\sim v \mid g1 * g2 * g3$ . In this case, the levels of each grouping variable are pasted together and the resulting factor is used to group the observations. Defaults to  $\sim$  fitted(.) representing a variance covariate given by the fitted values of a fitted model object and no grouping factor.

fixed

an optional list with components const and/or power, consisting of numeric vectors, or lists of numeric values, specifying the values at which some or all of the coefficients in the variance function should be fixed. If a grouping factor is specified in form, the components of fixed must have names identifying which coefficients are to be fixed. Coefficients included in fixed are not allowed to vary during the optimization of an objective function. Defaults to NULL, corresponding to no fixed coefficients.

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## Value

a varConstPower object representing a constant plus power variance function structure, also inheriting from class varFunc.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

### See Also

```
varClasses, varWeights.varFunc, coef.varConstPower
```

## **Examples**

```
vf1 <- varConstPower(1.2, 0.2, form = ~age|Sex)
```

varConstProp

Constant Plus Proportion Variance Function

# **Description**

This function is a constructor for the varConstProp class, representing a variance function structure corresponding to a two-component error model (additive and proportional error). Letting v denote the variance covariate and  $\sigma^2(v)$  denote the variance function evaluated at v, the two-component variance function is defined as  $\sigma^2(v) = a^2 + b^2 * v^2$ , where a is the additive component and b is the relative error component. In order to avoid overparameterisation of the model, it is recommended to use the possibility to fix sigma, preferably to a value of 1 (see examples).

## Usage

```
varConstProp(const, prop, form, fixed)
```

## Arguments

const, prop

optional numeric vectors, or lists of numeric values, with, respectively, the coefficients for the constant and the proportional error terms. Both arguments must have length one, unless a grouping factor is specified in form. If either argument has length greater than one, it must have names which identify its elements to the levels of the grouping factor defined in form. If a grouping factor is present in form and the argument has length one, its value will be assigned to all grouping levels. Only positive values are allowed for const. Default is 0.1 for both const and prop.

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form

an optional one-sided formula of the form  $\sim v$ , or  $\sim v \mid g$ , specifying a variance covariate v and, optionally, a grouping factor g for the coefficients. The variance covariate must evaluate to a numeric vector and may involve expressions using ".", representing a fitted model object from which fitted values (fitted(.)) and residuals (resid(.)) can be extracted (this allows the variance covariate to be updated during the optimization of an object function). When a grouping factor is present in form, a different coefficient value is used for each of its levels. Several grouping variables may be simultaneously specified, separated by the  $\star$  operator, as in  $\sim v \mid g1 \star g2 \star g3$ . In this case, the levels of each grouping variable are pasted together and the resulting factor is used to group the observations. Defaults to  $\sim$  fitted(.) representing a variance covariate given by the fitted values of a fitted model object and no grouping factor.

fixed

an optional list with components const and/or power, consisting of numeric vectors, or lists of numeric values, specifying the values at which some or all of the coefficients in the variance function should be fixed. If a grouping factor is specified in form, the components of fixed must have names identifying which coefficients are to be fixed. Coefficients included in fixed are not allowed to vary during the optimization of an objective function. Defaults to NULL, corresponding to no fixed coefficients.

#### Value

a varConstProp object representing a constant plus proportion variance function structure, also inheriting from class varFunc.

#### Note

The error model underlying this variance function structure can be understood to result from two uncorrelated sequences of standardized random variables (Lavielle(2015), p. 55) and has been proposed for use in analytical chemistry (Werner et al. (1978), Wilson et al. (2004)) and chemical degradation kinetics (Ranke and Meinecke (2019)). Note that the two-component error model proposed by Rocke and Lorenzato (1995) assumed a log-normal distribution of residuals at high absolute values, which is not compatible with the varFunc structures in package **nlme**.

## Author(s)

José Pinheiro and Douglas Bates (for varConstPower) and Johannes Ranke (adaptation to varConstProp()).

## References

Lavielle, M. (2015) *Mixed Effects Models for the Population Approach: Models, Tasks, Methods and Tools*, Chapman and Hall/CRC. doi:10.1201/b17203

Pinheiro, J.C., and Bates, D.M. (2000) *Mixed-Effects Models in S and S-PLUS*, Springer. doi:10.1007/b98882

Ranke, J., and Meinecke, S. (2019) Error Models for the Kinetic Evaluation of Chemical Degradation Data. *Environments* **6**(12), 124 doi:10.3390/environments6120124

Rocke, David M. and Lorenzato, Stefan (1995) A Two-Component Model for Measurement Error in Analytical Chemistry. *Technometrics* **37**(2), 176–184. doi:10.1080/00401706.1995.10484302

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Werner, Mario, Brooks, Samuel H., and Knott, Lancaster B. (1978) Additive, Multiplicative, and Mixed Analytical Errors. *Clinical Chemistry* **24**(11), 1895–1898. doi:10.1093/clinchem/24.11.1895

Wilson, M.D., Rocke, D.M., Durbin, B. and Kahn, H.D (2004) Detection Limits and Goodness-of-Fit Measures for the Two-Component Model of Chemical Analytical Error. *Analytica Chimica Acta* 2004, 509, 197–208 doi:10.1016/j.aca.2003.12.047

#### See Also

varClasses, varWeights.varFunc, coef.varFunc

## **Examples**

```
# Generate some synthetic data using the two-component error model and use
# different variance functions, also with fixed sigma in order to avoid
# overparameterisation in the case of a constant term in the variance function
times < c(0, 1, 3, 7, 14, 28, 56, 120)
pred <- 100 * exp(- 0.03 * times)
sd_pred <- sqrt(3^2 + 0.07^2 * pred^2)
n_replicates <- 2
set.seed(123456)
syn_data <- data.frame(</pre>
 time = rep(times, each = n_replicates),
 value = rnorm(length(times) * n_replicates,
    rep(pred, each = n_replicates),
    rep(sd_pred, each = n_replicates)))
syn_data$value <- ifelse(syn_data$value < 0, NA, syn_data$value)</pre>
f_const <- gnls(value ~ SSasymp(time, 0, parent_0, lrc),</pre>
 data = syn_data, na.action = na.omit,
 start = list(parent_0 = 100, lrc = -3))
f_varPower <- gnls(value ~ SSasymp(time, 0, parent_0, lrc),</pre>
 data = syn_data, na.action = na.omit,
 start = list(parent_0 = 100, lrc = -3),
 weights = varPower())
f_varConstPower <- gnls(value ~ SSasymp(time, 0, parent_0, lrc),</pre>
 data = syn_data, na.action = na.omit,
 start = list(parent_0 = 100, lrc = -3),
 weights = varConstPower())
f_varConstPower_sf <- gnls(value ~ SSasymp(time, 0, parent_0, lrc),</pre>
 data = syn_data, na.action = na.omit,
 control = list(sigma = 1),
 start = list(parent_0 = 100, lrc = -3),
 weights = varConstPower())
f_varConstProp <- gnls(value ~ SSasymp(time, 0, parent_0, lrc),</pre>
 data = syn_data, na.action = na.omit,
 start = list(parent_0 = 100, lrc = -3),
 weights = varConstProp())
f_varConstProp_sf <- gnls(value ~ SSasymp(time, 0, parent_0, lrc),</pre>
 data = syn_data, na.action = na.omit,
 start = list(parent_0 = 100, lrc = -3),
 control = list(sigma = 1),
```

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```
weights = varConstProp())

AIC(f_const, f_varPower, f_varConstPower, f_varConstPower_sf,
    f_varConstProp, f_varConstProp_sf)

# The error model parameters 3 and 0.07 are approximately recovered intervals(f_varConstProp_sf)
```

VarCorr

Extract variance and correlation components

# **Description**

This function calculates the estimated variances, standard deviations, and correlations between the random-effects terms in a linear mixed-effects model, of class "lme", or a nonlinear mixed-effects model, of class "nlme". The within-group error variance and standard deviation are also calculated.

# Usage

```
VarCorr(x, sigma = 1, ...)
## S3 method for class 'lme'
VarCorr(x, sigma = x$sigma, rdig = 3, ...)
## S3 method for class 'pdMat'
VarCorr(x, sigma = 1, rdig = 3, ...)
## S3 method for class 'pdBlocked'
VarCorr(x, sigma = 1, rdig = 3, ...)
```

## **Arguments**

X	a fitted model object, usually an object inheriting from class "lme".
sigma	an optional numeric value used as a multiplier for the standard deviations. The default is x\$sigma or 1 depending on class(x).
rdig	an optional integer value specifying the number of digits used to represent correlation estimates. Default is 3.
	further optional arguments passed to other methods (none for the methods documented here).

## Value

a matrix with the estimated variances, standard deviations, and correlations for the random effects. The first two columns, named Variance and StdDev, give, respectively, the variance and the standard deviations. If there are correlation components in the random effects model, the third column, named Corr, and the remaining unnamed columns give the estimated correlations among random effects within the same level of grouping. The within-group error variance and standard deviation are included as the last row in the matrix.

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### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) *Mixed-Effects Models in S and S-PLUS*, Springer, esp. pp. 100, 461.

### See Also

lme, nlme

## **Examples**

```
fm1 <- lme(distance ~ age, data = Orthodont, random = ~age)
VarCorr(fm1)</pre>
```

varExp

Exponential Variance Function

## Description

This function is a constructor for the varExp class, representing an exponential variance function structure. Letting v denote the variance covariate and  $\sigma^2(v)$  denote the variance function evaluated at v, the exponential variance function is defined as  $\sigma^2(v) = \exp(2\theta v)$ , where  $\theta$  is the variance function coefficient. When a grouping factor is present, a different  $\theta$  is used for each factor level.

## Usage

```
varExp(value, form, fixed)
```

### **Arguments**

value

an optional numeric vector, or list of numeric values, with the variance function coefficients. Value must have length one, unless a grouping factor is specified in form. If value has length greater than one, it must have names which identify its elements to the levels of the grouping factor defined in form. If a grouping factor is present in form and value has length one, its value will be assigned to all grouping levels. Default is numeric(0), which results in a vector of zeros of appropriate length being assigned to the coefficients when object is initialized (corresponding to constant variance equal to one).

form

an optional one-sided formula of the form  $\sim v$ , or  $\sim v \mid g$ , specifying a variance covariate v and, optionally, a grouping factor g for the coefficients. The variance covariate must evaluate to a numeric vector and may involve expressions using ".", representing a fitted model object from which fitted values (fitted(.)) and residuals (resid(.)) can be extracted (this allows the variance covariate to be updated during the optimization of an object function). When a grouping

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factor is present in form, a different coefficient value is used for each of its levels. Several grouping variables may be simultaneously specified, separated by the  $\star$  operator, like in  $\sim v \mid g1 \star g2 \star g3$ . In this case, the levels of each grouping variable are pasted together and the resulting factor is used to group the observations. Defaults to  $\sim$  fitted(.) representing a variance covariate given by the fitted values of a fitted model object and no grouping factor.

fixed

an optional numeric vector, or list of numeric values, specifying the values at which some or all of the coefficients in the variance function should be fixed. If a grouping factor is specified in form, fixed must have names identifying which coefficients are to be fixed. Coefficients included in fixed are not allowed to vary during the optimization of an objective function. Defaults to NULL, corresponding to no fixed coefficients.

#### Value

a varExp object representing an exponential variance function structure, also inheriting from class varFunc.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

### See Also

```
varClasses, varWeights.varFunc, coef.varExp
```

## **Examples**

```
vf1 <- varExp(0.2, form = ~age|Sex)
```

varFixed

Fixed Variance Function

#### **Description**

This function is a constructor for the varFixed class, representing a variance function with fixed variances. Letting v denote the variance covariate defined in value, the variance function  $\sigma^2(v)$  for this class is  $\sigma^2(v) = |v|$ . The variance covariate v is evaluated once at initialization and remains fixed thereafter. No coefficients are required to represent this variance function.

## Usage

varFixed(value)

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## **Arguments**

value

a one-sided formula of the form ~ v specifying a variance covariate v. Grouping factors are ignored.

### Value

a varFixed object representing a fixed variance function structure, also inheriting from class varFunc.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
varClasses, varWeights.varFunc, varFunc
```

# **Examples**

```
vf1 <- varFixed(~age)
```

varFunc

Variance Function Structure

## **Description**

If object is a one-sided formula, it is used as the argument to varFixed and the resulting object is returned. Else, if object inherits from class varFunc, it is returned unchanged.

# Usage

```
varFunc(object)
```

# Arguments

object

either an one-sided formula specifying a variance covariate, or an object inheriting from class varFunc, representing a variance function structure.

### Value

an object from class varFunc, representing a variance function structure.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

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### See Also

summary.varFunc, varFixed, varWeights.varFunc, coef.varFunc

## **Examples**

vf1 <- varFunc(~age)

varIdent

Constant Variance Function

## **Description**

This function is a constructor for the varIdent class, representing a constant variance function structure. If no grouping factor is present in form, the variance function is constant and equal to one, and no coefficients required to represent it. When form includes a grouping factor with M>1 levels, the variance function allows M different variances, one for each level of the factor. For identifiability reasons, the coefficients of the variance function represent the ratios between the variances and a reference variance (corresponding to a reference group level). Therefore, only M-1 coefficients are needed to represent the variance function. By default, if the elements in value are unnamed, the first group level is taken as the reference level.

# Usage

```
varIdent(value, form, fixed)
```

### **Arguments**

value

an optional numeric vector, or list of numeric values, with the variance function coefficients. If no grouping factor is present in form, this argument is ignored, as the resulting variance function contains no coefficients. If value has length one, its value is repeated for all coefficients in the variance function. If value has length greater than one, it must have length equal to the number of grouping levels minus one and names which identify its elements to the levels of the grouping factor. Only positive values are allowed for this argument. Default is numeric(0), which results in a vector of zeros of appropriate length being assigned to the coefficients when object is initialized (corresponding to constant variance equal to one).

form

an optional one-sided formula of the form  $\sim v$ , or  $\sim v \mid g$ , specifying a variance covariate v and, optionally, a grouping factor g for the coefficients. The variance covariate is ignored in this variance function. When a grouping factor is present in form, a different coefficient value is used for each of its levels less one reference level. Several grouping variables may be simultaneously specified, separated by the \* operator, like in  $\sim v \mid g1 * g2 * g3$ . In this case, the levels of each grouping variable are pasted together and the resulting factor is used to group the observations. Defaults to  $\sim 1$ .

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fixed

an optional numeric vector, or list of numeric values, specifying the values at which some or all of the coefficients in the variance function should be fixed. It must have names identifying which coefficients are to be fixed. Coefficients included in fixed are not allowed to vary during the optimization of an objective function. Defaults to NULL, corresponding to no fixed coefficients.

#### Value

a varIdent object representing a constant variance function structure, also inheriting from class varFunc.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

```
varClasses, varWeights.varFunc, coef.varIdent
```

## **Examples**

```
vf1 <- varIdent(c(Female = 0.5), form = ~ 1 | Sex)</pre>
```

Variogram

Calculate Semi-variogram

# **Description**

This function is generic; method functions can be written to handle specific classes of objects. Classes which already have methods for this function include default, gls and lme. See the appropriate method documentation for a description of the arguments.

#### Usage

```
Variogram(object, distance, ...)
```

## Arguments

object	a numeric vector with the values to be used for calculating the semi-variogram, usually a residual vector from a fitted model.
distance	a numeric vector with the pairwise distances corresponding to the elements of object. The order of the elements in distance must correspond to the pairs $(1,2), (1,3), \ldots, (n-1,n)$ , with n representing the length of object, and must have length $n(n-1)/2$ .

... some methods for this generic function require additional arguments.

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## Value

will depend on the method function used; see the appropriate documentation.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

```
Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons. Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.
```

#### See Also

```
Variogram.corExp, Variogram.corGaus, Variogram.corLin, Variogram.corRatio, Variogram.corSpatial, Variogram.corSpher, Variogram.default, Variogram.gls, Variogram.lme, plot.Variogram
```

# **Examples**

## see the method function documentation

Variogram.corExp

Calculate Semi-variogram for a corExp Object

# **Description**

This method function calculates the semi-variogram values corresponding to the Exponential correlation model, using the estimated coefficients corresponding to object, at the distances defined by distance.

# Usage

```
## S3 method for class 'corExp'
Variogram(object, distance, sig2, length.out, ...)
```

object	an object inheriting from class "corExp", representing an exponential spatial correlation structure.
distance	an optional numeric vector with the distances at which the semi-variogram is to be calculated. Defaults to NULL, in which case a sequence of length length.out between the minimum and maximum values of getCovariate(object) is used.
sig2	an optional numeric value representing the process variance. Defaults to 1.
length.out	an optional integer specifying the length of the sequence of distances to be used for calculating the semi-variogram, when distance = NULL. Defaults to 50.
• • •	some methods for this generic require additional arguments. None are used in this method.

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## Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. The returned value inherits from class Variogram.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

```
Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.
```

#### See Also

```
corExp, plot. Variogram, Variogram
```

## **Examples**

```
stopifnot(require("stats", quietly = TRUE))
cs1 <- corExp(3, form = ~ Time | Rat)
cs1 <- Initialize(cs1, BodyWeight)
Variogram(cs1)[1:10,]</pre>
```

Variogram.corGaus

Calculate Semi-variogram for a corGaus Object

# **Description**

This method function calculates the semi-variogram values corresponding to the Gaussian correlation model, using the estimated coefficients corresponding to object, at the distances defined by distance.

## Usage

```
## S3 method for class 'corGaus'
Variogram(object, distance, sig2, length.out, ...)
```

object	an object inheriting from class "corGaus", representing an Gaussian spatial correlation structure.
distance	an optional numeric vector with the distances at which the semi-variogram is to be calculated. Defaults to NULL, in which case a sequence of length length.out between the minimum and maximum values of getCovariate(object) is used.
sig2	an optional numeric value representing the process variance. Defaults to 1.
length.out	an optional integer specifying the length of the sequence of distances to be used for calculating the semi-variogram, when distance = NULL. Defaults to 50.
•••	some methods for this generic require additional arguments. None are used in this method.

312 Variogram.corLin

## Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. The returned value inherits from class Variogram.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

```
Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.
```

#### See Also

```
corGaus, plot. Variogram, Variogram
```

# **Examples**

```
cs1 <- corGaus(3, form = ~ Time | Rat)
cs1 <- Initialize(cs1, BodyWeight)
Variogram(cs1)[1:10,]</pre>
```

Variogram.corLin

Calculate Semi-variogram for a corLin Object

## **Description**

This method function calculates the semi-variogram values corresponding to the Linear correlation model, using the estimated coefficients corresponding to object, at the distances defined by distance.

## Usage

```
## S3 method for class 'corLin'
Variogram(object, distance, sig2, length.out, ...)
```

object	an object inheriting from class "corLin", representing an Linear spatial correlation structure.
distance	an optional numeric vector with the distances at which the semi-variogram is to be calculated. Defaults to NULL, in which case a sequence of length length out between the minimum and maximum values of getCovariate(object) is used.
sig2	an optional numeric value representing the process variance. Defaults to 1.
length.out	an optional integer specifying the length of the sequence of distances to be used for calculating the semi-variogram, when distance = NULL. Defaults to 50.
	some methods for this generic require additional arguments. None are used in this method.

Variogram.corRatio 313

# Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. The returned value inherits from class Variogram.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

```
Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.
```

#### See Also

```
corLin, plot. Variogram, Variogram
```

# **Examples**

```
cs1 <- corLin(15, form = ~ Time | Rat)
cs1 <- Initialize(cs1, BodyWeight)
Variogram(cs1)[1:10,]</pre>
```

Variogram.corRatio

Calculate Semi-variogram for a corRatio Object

## **Description**

This method function calculates the semi-variogram values corresponding to the Rational Quadratic correlation model, using the estimated coefficients corresponding to object, at the distances defined by distance.

## Usage

```
## S3 method for class 'corRatio'
Variogram(object, distance, sig2, length.out, ...)
```

object	an object inheriting from class "corRatio", representing an Rational Quadratic spatial correlation structure.
distance	an optional numeric vector with the distances at which the semi-variogram is to be calculated. Defaults to NULL, in which case a sequence of length length out between the minimum and maximum values of getCovariate(object) is used.
sig2	an optional numeric value representing the process variance. Defaults to 1.
length.out	an optional integer specifying the length of the sequence of distances to be used for calculating the semi-variogram, when distance = NULL. Defaults to 50.
	some methods for this generic require additional arguments. None are used in this method.

314 Variogram.corSpatial

## Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. The returned value inherits from class Variogram.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

```
Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.
```

## See Also

```
corRatio, plot. Variogram Variogram
```

# **Examples**

```
cs1 <- corRatio(7, form = ~ Time | Rat)
cs1 <- Initialize(cs1, BodyWeight)
Variogram(cs1)[1:10,]</pre>
```

 ${\tt Variogram.corSpatial} \quad \textit{Calculate Semi-variogram for a corSpatial Object}$ 

# **Description**

This method function calculates the semi-variogram values corresponding to the model defined in FUN, using the estimated coefficients corresponding to object, at the distances defined by distance.

# Usage

```
## S3 method for class 'corSpatial'
Variogram(object, distance, sig2, length.out, FUN, ...)
```

object	an object inheriting from class "corSpatial", representing spatial correlation structure.
distance	an optional numeric vector with the distances at which the semi-variogram is to be calculated. Defaults to NULL, in which case a sequence of length length.out between the minimum and maximum values of getCovariate(object) is used.
sig2	an optional numeric value representing the process variance. Defaults to 1.
length.out	an optional integer specifying the length of the sequence of distances to be used for calculating the semi-variogram, when distance = NULL. Defaults to 50.
FUN	a function of two arguments, the distance and the range corresponding to object, specifying the semi-variogram model.
• • •	some methods for this generic require additional arguments. None are used in this method.

Variogram.corSpher 315

## Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. The returned value inherits from class Variogram.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

#### See Also

corSpatial, Variogram, Variogram.default, Variogram.corExp, Variogram.corGaus, Variogram.corLin, Variogram.corRatio, Variogram.corSpher, plot.Variogram

## **Examples**

```
cs1 <- corExp(3, form = ~ Time | Rat)
cs1 <- Initialize(cs1, BodyWeight)
Variogram(cs1, FUN = function(x, y) (1 - exp(-x/y)))[1:10,]</pre>
```

Variogram.corSpher

Calculate Semi-variogram for a corSpher Object

# Description

This method function calculates the semi-variogram values corresponding to the Spherical correlation model, using the estimated coefficients corresponding to object, at the distances defined by distance.

## Usage

```
## S3 method for class 'corSpher'
Variogram(object, distance, sig2, length.out, ...)
```

object	an object inheriting from class "corSpher", representing an Spherical spatial correlation structure.
distance	an optional numeric vector with the distances at which the semi-variogram is to be calculated. Defaults to NULL, in which case a sequence of length length.out between the minimum and maximum values of getCovariate(object) is used.
sig2	an optional numeric value representing the process variance. Defaults to 1.
length.out	an optional integer specifying the length of the sequence of distances to be used for calculating the semi-variogram, when distance = NULL. Defaults to 50.
•••	some methods for this generic require additional arguments. None are used in this method.

316 Variogram.default

#### Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. The returned value inherits from class Variogram.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

```
Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.
```

#### See Also

```
corSpher, plot. Variogram, Variogram
```

## **Examples**

```
cs1 <- corSpher(15, form = ~ Time | Rat)
cs1 <- Initialize(cs1, BodyWeight)
Variogram(cs1)[1:10,]</pre>
```

Variogram.default

Calculate Semi-variogram

# **Description**

This method function calculates the semi-variogram for an arbitrary vector object, according to the distances in distance. For each pair of elements x, y in object, the corresponding semi-variogram is  $(x-y)^2/2$ . The semi-variogram is useful for identifying and modeling spatial correlation structures in observations with constant expectation and constant variance.

## Usage

```
## Default S3 method:
Variogram(object, distance, ...)
```

## **Arguments**

object	a numeric vector with the values to be used for calculating the semi-variogram,
-	

usually a residual vector from a fitted model.

distance a numeric vector with the pairwise distances corresponding to the elements of

object. The order of the elements in distance must correspond to the pairs (1,2), (1,3), ..., (n-1,n), with n representing the length of object, and

must have length n(n-1)/2.

... some methods for this generic require additional arguments. None are used in

this method.

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#### Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. The returned value inherits from class Variogram.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

## See Also

```
Variogram, Variogram.gls, Variogram.lme, plot.Variogram
```

### **Examples**

Variogram.gls

Calculate Semi-variogram for Residuals from a gls Object

## **Description**

This method function calculates the semi-variogram for the residuals from a gls fit. The semi-variogram values are calculated for pairs of residuals within the same group level, if a grouping factor is present. If collapse is different from "none", the individual semi-variogram values are collapsed using either a robust estimator (robust = TRUE) defined in Cressie (1993), or the average of the values within the same distance interval. The semi-variogram is useful for modeling the error term correlation structure.

# Usage

## **Arguments**

object

an object inheriting from class "gls", representing a generalized least squares fitted model.

318 Variogram.gls

distance an optional numeric vector with the distances between residual pairs. If a group-

ing variable is present, only the distances between residual pairs within the same group should be given. If missing, the distances are calculated based on the values of the arguments form, data, and metric, unless object includes a corSpatial element, in which case the associated covariate (obtained with the

getCovariate method) is used.

form an optional one-sided formula specifying the covariate(s) to be used for calcu-

lating the distances between residual pairs and, optionally, a grouping factor for partitioning the residuals (which must appear to the right of a | operator in form). Default is ~1, implying that the observation order within the groups is

used to obtain the distances.

resType an optional character string specifying the type of residuals to be used. If

"response", the "raw" residuals (observed - fitted) are used; else, if "pearson", the standardized residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals pre-multiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the

first character needs to be provided. Defaults to "pearson".

data an optional data frame in which to interpret the variables in form. By default,

the same data used to fit object is used.

na.action a function that indicates what should happen when the data contain NAs. The

default action (na.fail) causes an error message to be printed and the function

to terminate, if there are any incomplete observations.

maxDist an optional numeric value for the maximum distance used for calculating the

semi-variogram between two residuals. By default all residual pairs are in-

cluded.

length.out an optional integer value. When object includes a corSpatial element, its

semi-variogram values are calculated and this argument is used as the length.out

argument to the corresponding Variogram method. Defaults to 50.

collapse an optional character string specifying the type of collapsing to be applied to the

individual semi-variogram values. If equal to "quantiles", the semi-variogram values are split according to quantiles of the distance distribution, with equal number of observations per group, with possibly varying distance interval lengths. Else, if "fixed", the semi-variogram values are divided according to distance intervals of equal lengths, with possibly different number of observations per interval. Else, if "none", no collapsing is used and the individual semi-variogram

values are returned. Defaults to "quantiles".

nint an optional integer with the number of intervals to be used when collapsing the

semi-variogram values. Defaults to 20.

robust an optional logical value specifying if a robust semi-variogram estimator should

be used when collapsing the individual values. If TRUE the robust estimator is

used. Defaults to FALSE.

breaks an optional numeric vector with the breakpoints for the distance intervals to

be used in collapsing the semi-variogram values. If not missing, the option

specified in collapse is ignored.

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metric an optional character string specifying the distance metric to be used. The cur-

rently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the

first three characters need to be provided. Defaults to "euclidean".

.. some methods for this generic require additional arguments. None are used in

this method.

#### Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. If the semi-variogram values are collapsed, an extra column, n.pairs, with the number of residual pairs used in each semi-variogram calculation, is included in the returned data frame. If object includes a corSpatial element, a data frame with its corresponding semi-variogram is included in the returned value, as an attribute "modelVariog". The returned value inherits from class Variogram.

### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

### See Also

```
gls, Variogram, Variogram.default, Variogram.lme, plot.Variogram
```

## **Examples**

```
fm1 <- gls(weight ~ Time * Diet, BodyWeight)
Vm1 <- Variogram(fm1, form = ~ Time | Rat)
print(head(Vm1), digits = 3)</pre>
```

Variogram.lme

Calculate Semi-variogram for Residuals from an Ime Object

## **Description**

This method function calculates the semi-variogram for the within-group residuals from an lme fit. The semi-variogram values are calculated for pairs of residuals within the same group. If collapse is different from "none", the individual semi-variogram values are collapsed using either a robust estimator (robust = TRUE) defined in Cressie (1993), or the average of the values within the same distance interval. The semi-variogram is useful for modeling the error term correlation structure.

320 Variogram.lme

## Usage

# **Arguments**

object an object inheriting from class "lme", representing a fitted linear mixed-effects

model.

distance an optional numeric vector with the distances between residual pairs. If a group-

ing variable is present, only the distances between residual pairs within the same group should be given. If missing, the distances are calculated based on the values of the arguments form, data, and metric, unless object includes a corSpatial element, in which case the associated covariate (obtained with the

getCovariate method) is used.

form an optional one-sided formula specifying the covariate(s) to be used for calcu-

lating the distances between residual pairs and, optionally, a grouping factor for partitioning the residuals (which must appear to the right of a | operator in form). Default is ~1, implying that the observation order within the groups is

used to obtain the distances.

resType an optional character string specifying the type of residuals to be used. If

"response", the "raw" residuals (observed - fitted) are used; else, if "pearson", the standardized residuals (raw residuals divided by the corresponding standard errors) are used; else, if "normalized", the normalized residuals (standardized residuals pre-multiplied by the inverse square-root factor of the estimated error correlation matrix) are used. Partial matching of arguments is used, so only the

first character needs to be provided. Defaults to "pearson".

data an optional data frame in which to interpret the variables in form. By default,

the same data used to fit object is used.

na.action a function that indicates what should happen when the data contain NAs. The

default action (na.fail) causes an error message to be printed and the function

to terminate, if there are any incomplete observations.

maxDist an optional numeric value for the maximum distance used for calculating the

semi-variogram between two residuals. By default all residual pairs are in-

luded.

length.out an optional integer value. When object includes a corSpatial element, its

semi-variogram values are calculated and this argument is used as the length out

argument to the corresponding Variogram method. Defaults to 50.

collapse an optional character string specifying the type of collapsing to be applied to the

individual semi-variogram values. If equal to "quantiles", the semi-variogram values are split according to quantiles of the distance distribution, with equal number of observations per group, with possibly varying distance interval lengths. Else, if "fixed", the semi-variogram values are divided according to distance intervals of equal lengths, with possibly different number of observations per interval. Else, if "none", no collapsing is used and the individual semi-variogram

values are returned. Defaults to "quantiles".

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nint	an optional integer with the number of intervals to be used when collapsing the semi-variogram values. Defaults to 20.
robust	an optional logical value specifying if a robust semi-variogram estimator should be used when collapsing the individual values. If TRUE the robust estimator is used. Defaults to FALSE.
breaks	an optional numeric vector with the breakpoints for the distance intervals to be used in collapsing the semi-variogram values. If not missing, the option specified in collapse is ignored.
metric	an optional character string specifying the distance metric to be used. The currently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the first three characters need to be provided. Defaults to "euclidean".
	some methods for this generic require additional arguments. None are used in this method.

#### Value

a data frame with columns variog and dist representing, respectively, the semi-variogram values and the corresponding distances. If the semi-variogram values are collapsed, an extra column, n.pairs, with the number of residual pairs used in each semi-variogram calculation, is included in the returned data frame. If object includes a corSpatial element, a data frame with its corresponding semi-variogram is included in the returned value, as an attribute "modelVariog". The returned value inherits from class Variogram.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

### References

Cressie, N.A.C. (1993), "Statistics for Spatial Data", J. Wiley & Sons.

#### See Also

lme, Variogram, Variogram.default, Variogram.gls, plot.Variogram

## **Examples**

322 varPower

varPower

Power Variance Function

## **Description**

This function is a constructor for the varPower class, representing a power variance function structure. Letting v denote the variance covariate and  $\sigma^2(v)$  denote the variance function evaluated at v, the power variance function is defined as  $\sigma^2(v) = |v|^{2\theta}$ , where  $\theta$  is the variance function coefficient. When a grouping factor is present, a different  $\theta$  is used for each factor level.

## Usage

varPower(value, form, fixed)

## **Arguments**

value

an optional numeric vector, or list of numeric values, with the variance function coefficients. Value must have length one, unless a grouping factor is specified in form. If value has length greater than one, it must have names which identify its elements to the levels of the grouping factor defined in form. If a grouping factor is present in form and value has length one, its value will be assigned to all grouping levels. Default is numeric(0), which results in a vector of zeros of appropriate length being assigned to the coefficients when object is initialized (corresponding to constant variance equal to one).

form

an optional one-sided formula of the form ~ v, or ~ v | g, specifying a variance covariate v and, optionally, a grouping factor g for the coefficients. The variance covariate must evaluate to a numeric vector and may involve expressions using ".", representing a fitted model object from which fitted values (fitted(.)) and residuals (resid(.)) can be extracted (this allows the variance covariate to be updated during the optimization of an object function). When a grouping factor is present in form, a different coefficient value is used for each of its levels. Several grouping variables may be simultaneously specified, separated by the  $\star$  operator, like in  $\sim v \mid g1 \star g2 \star g3$ . In this case, the levels of each grouping variable are pasted together and the resulting factor is used to group the observations. Defaults to ~fitted(.) representing a variance covariate given by the fitted values of a fitted model object and no grouping factor.

fixed

an optional numeric vector, or list of numeric values, specifying the values at which some or all of the coefficients in the variance function should be fixed. If a grouping factor is specified in form, fixed must have names identifying which coefficients are to be fixed. Coefficients included in fixed are not allowed to vary during the optimization of an objective function. Defaults to NULL, corresponding to no fixed coefficients.

## Value

a varPower object representing a power variance function structure, also inheriting from class varFunc.

varWeights 323

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

```
varWeights.varFunc, coef.varPower
```

# **Examples**

```
vf1 <- varPower(0.2, form = ~age|Sex)</pre>
```

varWeights

Extract Variance Function Weights

# **Description**

The inverse of the standard deviations corresponding to the variance function structure represented by object are returned.

# Usage

```
varWeights(object)
```

## **Arguments**

object

an object inheriting from class varFunc, representing a variance function structure.

# Value

if object has a weights attribute, its value is returned; else NULL is returned.

## Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

# References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

```
logLik.varFunc, varWeights
```

324 varWeights.glsStruct

## **Examples**

```
vf1 <- varPower(form=~age)
vf1 <- Initialize(vf1, Orthodont)
coef(vf1) <- 0.3
varWeights(vf1)[1:10]</pre>
```

varWeights.glsStruct Variance Weights for glsStruct Object

# **Description**

If object includes a varStruct component, the inverse of the standard deviations of the variance function structure represented by the corresponding varFunc object are returned; else, a vector of ones of length equal to the number of observations in the data frame used to fit the associated linear model is returned.

# Usage

```
## S3 method for class 'glsStruct'
varWeights(object)
```

## **Arguments**

object

an object inheriting from class "glsStruct", representing a list of linear model components, such as corStruct and "varFunc" objects.

## Value

if object includes a varStruct component, a vector with the corresponding variance weights; else, or a vector of ones.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

## See Also

varWeights

varWeights.lmeStruct 325

varWeights.lmeStruct Variance Weights for lmeStruct Object

# Description

If object includes a varStruct component, the inverse of the standard deviations of the variance function structure represented by the corresponding varFunc object are returned; else, a vector of ones of length equal to the number of observations in the data frame used to fit the associated linear mixed-effects model is returned.

#### Usage

```
## S3 method for class 'lmeStruct'
varWeights(object)
```

## **Arguments**

object

an object inheriting from class "lmeStruct", representing a list of linear mixed-effects model components, such as reStruct, corStruct, and varFunc objects.

#### Value

if object includes a varStruct component, a vector with the corresponding variance weights; else, or a vector of ones.

#### Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

#### References

Pinheiro, J.C., and Bates, D.M. (2000) "Mixed-Effects Models in S and S-PLUS", Springer.

#### See Also

varWeights

326 Wheat

Wafer

Modeling of Analog MOS Circuits

## **Description**

The Wafer data frame has 400 rows and 4 columns.

#### **Format**

This data frame contains the following columns:

Wafer a factor with levels 1 2 3 4 5 6 7 8 9 10

Site a factor with levels 1 2 3 4 5 6 7 8

voltage a numeric vector
current a numeric vector

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

Wheat

Yields by growing conditions

## **Description**

The Wheat data frame has 48 rows and 4 columns.

## **Format**

This data frame contains the following columns:

**Tray** an ordered factor with levels 3 < 1 < 2 < 4 < 5 < 6 < 8 < 9 < 7 < 12 < 11 < 10

Moisture a numeric vector fertilizer a numeric vector DryMatter a numeric vector

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

Wheat2 327

Wheat2

Wheat Yield Trials

## Description

The Wheat2 data frame has 224 rows and 5 columns.

#### **Format**

This data frame contains the following columns:

**Block** an ordered factor with levels 4 < 2 < 3 < 1

variety a factor with levels ARAPAHOE BRULE BUCKSKIN CENTURA CENTURK78 CHEYENNE CODY COLT GAGE HOMESTEAD KS831374 LANCER LANCOTA NE83404 NE83406 NE83407 NE83432 NE83498 NE83T12 NE84557 NE85556 NE85623 NE86482 NE86501 NE86503 NE86507 NE86509 NE86527 NE86582 NE86606 NE86607 NE86T666 NE87403 NE87408 NE87409 NE87446 NE87451 NE87457 NE87463 NE87499 NE87512 NE87513 NE87522 NE87612 NE87613 NE87615 NE87619 NE87627 NORKAN REDLAND ROUGHRIDER SCOUT66 SIOUXLAND TAM107 TAM200 VONA

yield a numeric vector

latitude a numeric vector longitude a numeric vector

#### **Source**

Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, Springer, New York.

[.pdMat

Subscript a pdMat Object

# Description

This method function extracts sub-matrices from the positive-definite matrix represented by x.

# Usage

```
## S3 method for class 'pdMat'
x[i, j, drop = TRUE]
## S3 replacement method for class 'pdMat'
x[i, j] <- value</pre>
```

328 [.pdMat

# Arguments

x	an object inheriting from class "pdMat" representing a positive-definite matrix.
i, j	optional subscripts applying respectively to the rows and columns of the positive-definite matrix represented by object. When i (j) is omitted, all rows (columns) are extracted.
drop	a logical value. If TRUE, single rows or columns are converted to vectors. If FALSE the returned value retains its matrix representation.
value	a vector, or matrix, with the replacement values for the relevant piece of the matrix represented by x.

#### Value

if i and j are identical, the returned value will be pdMat object with the same class as x. Otherwise, the returned value will be a matrix. In the case a single row (or column) is selected, the returned value may be converted to a vector, according to the rules above.

# Author(s)

José Pinheiro and Douglas Bates <bates@stat.wisc.edu>

## See Also

```
[, pdMat
```

# **Examples**

```
pd1 <- pdSymm(diag(3))
pd1[1, , drop = FALSE]
pd1[1:2, 1:2] <- 3 * diag(2)</pre>
```

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