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Title The Generalized Semi-Supervised Elastic-Net

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Description Implements the generalized semi-supervised elastic-net. This method extends the supervised elastic-net problem, and thus it is a practical solution to the problem of feature selection in semi-supervised contexts. Its mathematical formulation is presented from a general perspective, covering a wide range of models. We focus on linear and logistic responses, but the implementation could be easily extended to other losses in generalized linear models. We develop a flexible and fast implementation, written in 'C++' using 'RcppArmadillo' and integrated into R via 'Rcpp' modules. See Culp, M. 2013 <doi:10.1080/10618600.2012.657139> for references on the Joint Trained Elastic-Net.

License GPL (>= 2)

Imports Rcpp, methods, MASS

Depends stats

LinkingTo Rcpp, RcppArmadillo

Suggests knitr, rmarkdown, glmnet, Metrics, testthat

VignetteBuilder knitr

URL https://github.com/jlaria/s2net

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NeedsCompilation yes

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`s2net-package` *The Generalized Semi-Supervised Elastic-Net*

Description

Implements the generalized semi-supervised elastic-net. This method extends the supervised elastic-net problem, and thus it is a practical solution to the problem of feature selection in semi-supervised contexts. Its mathematical formulation is presented from a general perspective, covering a wide range of models. We focus on linear and logistic responses, but the implementation could be easily extended to other losses in generalized linear models. We develop a flexible and fast implementation, written in 'C++' using 'RcppArmadillo' and integrated into R via 'Rcpp' modules. See Culp, M. 2013 <doi:10.1080/10618600.2012.657139> for references on the Joint Trained Elastic-Net.

Details

The DESCRIPTION file:

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Version:	1.0.7
Date:	2024-03-04

Authors@R:	c(person("Juan C.", "Laria",, role = c("aut", "cre"), email = "juank.laria@gmail.com", comment = c(ORCI
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License:	GPL (>= 2)
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Author:	Juan C. Laria [aut, cre] (<https://orcid.org/0000-0001-7734-9647>), Line H. Clemmensen [aut]
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Index of help topics:


```
Rcpp_s2net-class        Class 's2net'
auto_mpg                Auto MPG Data Set
predict.s2netR          S3 Methods for 's2netR' objects.
predict_Rcpp_s2net      Predict method for 's2net' C++ class.
print.s2Data            Print methods for S3 objects
s2Data                  Data wrapper for 's2net'.
s2Fista                 Hyper-parameter wrapper for FISTA.
s2Params                Hyper-parameter wrapper for 's2net'
s2net                   The Generalized Semi-Supervised Elastic-Net
s2netR                  Trains a generalized extended linear joint
                        trained model using semi-supervised data.
simulate_extra          Simulate extrapolated data
simulate_groups         Simulate data (two groups design)
```


This package includes a very easy-to-use interface for handling data, with the `s2Data` function. The main function of the package is the `s2netR` function, which is a wrapper for the `Rcpp_s2net` (`s2net`) class.

Author(s)

Juan C. Laria [aut, cre] (<https://orcid.org/0000-0001-7734-9647>), Line H. Clemmensen [aut]

References

Laria, J.C., L. Clemmensen (2019). A generalized elastic-net for semi-supervised learning of sparse features.

Sogaard Larsen, J. et. al. (2019). Semi-supervised covariate shift modelling of spectroscopic data.

Ryan, K. J., & Culp, M. V. (2015). On semi-supervised linear regression in covariate shift problems. *The Journal of Machine Learning Research, 16*(1), 3183-3217.

See Also

s2Data, s2netR, Rcpp_s2net

Examples

```
data("auto_mpg")
train = s2Data(xL = auto_mpg$P1$xL, yL = auto_mpg$P1$yL,  xU = auto_mpg$P1$xU)

model = s2netR(train,
                s2Params(lambda1 = 0.1,
                           lambda2 = 0,
                           gamma1 = 0.1,
                           gamma2 = 100,
                           gamma3 = 0.1))

# here we tell it to transform the valid data as we did with train.
valid = s2Data(auto_mpg$P1$xU, auto_mpg$P1$yU, preprocess = train)
ypred = predict(model, valid$xL)

## Not run:
if(require(ggplot2)){
  ggplot() +
    aes(x = ypred, y = valid$yL) + geom_point() +
    geom_abline(intercept = 0, slope = 1, linetype = 2)
}

## End(Not run)
```

---

auto_mpg *Auto MPG Data Set*

Description

This dataset was taken from the UCI Machine Learning Repository https://archive.ics.uci.edu/ml/datasets/Auto+MPG, and processed for the semi-supervised setting (Ryan and Culp, 2015).

Usage

```
data("auto_mpg")
```

Format

There are two lists that contain partitions from a data frame with 398 observations on the following 9 variables.

`mpg` a numeric vector

`cylinders` an ordered factor with levels $3 < 4 < 5 < 6 < 8$

`displacement` a numeric vector

`horsepower` a numeric vector

`weight` a numeric vector

`acceleration` a numeric vector

`year` a numeric vector

`origin` a factor

Details

This dataset is a slightly modified version of the dataset provided in the StatLib library. In line with the use by Ross Quinlan (1993) in predicting the attribute "mpg", 8 of the original instances were removed because they had unknown values for the "mpg" attribute. "The data concerns city-cycle fuel consumption in miles per gallon, to be predicted in terms of 3 multivalued discrete and 5 continuous attributes." (Quinlan, 1993)

Source

Quinlan,R. (1993). Combining Instance-Based and Model-Based Learning. In Proceedings on the Tenth International Conference of Machine Learning, 236-243, University of Massachusetts, Amherst. Morgan Kaufmann.

Dua, D. and Graff, C. (2019). UCI Machine Learning Repository [http://archive.ics.uci.edu/ml/]. Irvine, CA: University of California, School of Information and Computer Science.

References

Ryan, K. J., & Culp, M. V. (2015). On semi-supervised linear regression in covariate shift problems. *The Journal of Machine Learning Research, 16*(1), 3183-3217.

Examples

```
data(auto_mpg)
head(auto_mpg$P1$xL)
```

---

predict.s2netR *S3 Methods for* s2netR *objects.*

Description

Generic predict method. Wrapper for the C++ class method `s2net$predict`.

Usage

```
## S3 method for class 's2netR'
predict(object, newX, type = "default", ...)
```

Arguments

object	A s2netR object
newX	A matrix with the data to make predictions. It should be in the same scale as the original data. See s2Data to see how to format the data.
type	Type of predictions. One of "default" (figure it out from the train data), "response", "probs", "class".
...	other parameters passed to predict

Value

A column matrix with predictions.

See Also

s2netR, s2net

Examples

```
data("auto_mpg")
train = s2Data(xL = auto_mpg$P1$xL, yL = auto_mpg$P1$yL,  xU = auto_mpg$P1$xU)

model = s2netR(train,
               s2Params(lambda1 = 0.1,
                        lambda2 = 0,
                        gamma1 = 0.1,
                        gamma2 = 100,
                        gamma3 = 0.1),
               loss = "linear",
               frame = "ExtJT",
               proj = "auto",
               fista = s2Fista(5000, 1e-7, 1, 0.8))

valid = s2Data(auto_mpg$P1$xU, auto_mpg$P1$yU, preprocess = train)
ypred = predict(model, valid$xL)
## Not run:
if(require(ggplot2)){
  ggplot() +
    aes(x = ypred, y = valid$yL) + geom_point() +
    geom_abline(intercept = 0, slope = 1, linetype = 2)
}

## End(Not run)
```

predict_Rcpp_s2net *Predict method for* s2net *C++ class.*

Description

This function provides an interface in R for the method predict in C++ class s2net.

Usage

```
predict_Rcpp_s2net(object, newX, type = "default")
```

Arguments

object	An object of class Rcpp_s2net.
newX	Data to make predictions. Could be a s2Data object (field xL is used) or a matrix (in the same space as the original data where the model was fitted).
type	Type of predictions. One of "default": let the method figure it out; "response": the linear predictor; "probs": fitted probabilities; class: fitted class.

Details

This method is included as a high-level wrapper of object$predict().

Value

Returns a column matrix with the same number of rows/observations as newX.

Author(s)

Juan C. Laria

See Also

Rcpp_s2net

print.s2Data *Print methods for S3 objects*

Description

Very simple print methods to show basic information about these simple S3 objects.

Usage

```
## S3 method for class 's2Data'
print(x, ...)
## S3 method for class 's2Fista'
print(x, ...)
```

Arguments

x	S3 object of class s2Data or s2Fista
...	other parameters passed to print

See Also

s2Data

Rcpp_s2net-class *Class* s2net

Description

This is the main class of this library, implemented in C++ and exposed to R using Rcpp modules. It can be used in R directly, although some generic S4 methods have been implemented to make it easier to interact in R.

Methods

predict `signature(object = "Rcpp_s2net")`: See predict_Rcpp_s2net

Fields

`beta`: Object of class `matrix`. The fitted model coefficients.

`intercept`: The model intercept.

Class-Based Methods

`initialize(data, loss)`: `data` `s2Data` object

`loss` Loss function: 0 = linear, 1 = logit

`setupFista(s2Fista)`: Configures the FISTA internal algorithm.

`predict(newX, type)`: `newX` New data `matrix` to make predictions.

`type` 0 = default, 1 = response, 2 = probs, 3 = class

`fit(params, frame, proj)`: `params` `s2Params` object

`frame` 0 = "JT", 1 = "ExtJT"

`proj` 0 = no, 1 = yes, 2 = auto

Author(s)

Juan C. Laria

Examples

```
data("auto_mpg")
train = s2Data(xL = auto_mpg$P1$xL, yL = auto_mpg$P1$yL,  xU = auto_mpg$P1$xU)

# We create the C++ object calling the new method (constructor)
obj = new(s2net, train, 0) # 0 = regression
obj

# We call directly the $fit method of obj,
obj$fit(s2Params(lambda1 = 0.01,
                 lambda2 = 0.01,
                 gamma1 = 0.05,
                 gamma2 = 100,
                 gamma3 = 0.05), 1, 2)
# fitted model
obj$beta

# We can test the results using the unlabeled data
test = s2Data(xL = auto_mpg$P1$xU, yL = auto_mpg$P1$yU,  preprocess = train)
ypred = obj$predict(test$xL, 0)

## Not run:
if(require(ggplot2)){
  ggplot() +
    aes(x = ypred, y = test$yL) + geom_point() +
    geom_abline(intercept = 0, slope = 1, linetype = 2)
}

## End(Not run)
```

s2Data *Data wrapper for* s2net.

Description

This function preprocess the data to fit a semi-supervised linear joint trained model.

Usage

```
s2Data(xL, yL, xU = NULL, preprocess = T)
```

Arguments

xL	The labeled data. Could be a matrix or data.frame.
yL	The labels associated with xL. Could be a vector, matrix or data.frame, of factor or numeric types.
xU	The unlabeled data (optional). Could be a matrix or data.frame.
preprocess	Should the input data be pre-processed? Possible values are: TRUE (default) The data is converted to a matrix. Factor variables are automatically coded using model.matrix. The data is scaled, and constant columns are removed. FALSE Do nothing. Keep in mind that the theoretical framework assumes that xL is centered. Unless you are absolutely sure, avoid this. Another object of class s2Data that was obtained from similar data (same original variables). This is useful when using train/validation sets, to apply the validation data the same transformation as train data.

Value

Returns an object of S3 class s2Data with fields

xL	Transformed labeled data
yL	Transformed labels. If yL was a factor, it is converted to numeric, and the base category is kept in base
xU	Tranformed unlabeled data
type	Type of task. This one is inferred from the response labels.
base	Base category for classification 0 = base

In addition the following attributes are stored.

pr:rm_cols	logical vector of removed columns
pr:center	column center
pr:scale	column scale
pr:ycenter	yL center. Regression
pr:yscale	yL scale. Regression

Author(s)

Juan C. Laria

See Also

s2Fista

Examples

```
data("auto_mpg")

train = s2Data( xL = auto_mpg$P1$xL,
                  yL = auto_mpg$P1$yL,
                  xU = auto_mpg$P1$xU,
                  preprocess = TRUE )
show(train)

# Notice how ordered factor variable $cylinders is handled
# .L (linear) .Q (quadratic) .C (cubic) and .^4
head(train$xL)


#if you want to do validation with the unlabeled data
idx = sample(length(auto_mpg$P1$yU), 200)

train = s2Data(xL = auto_mpg$P1$xL, yL = auto_mpg$P1$yL, xU = auto_mpg$P1$xU[idx, ])

valid = s2Data(xL = auto_mpg$P1$xU[-idx, ], yL = auto_mpg$P1$yU[-idx], preprocess = train)

test = s2Data(xL = auto_mpg$P1$xU[idx, ], yL = auto_mpg$P1$yU[idx], preprocess = train)

train
valid
test
```

---

s2Fista *Hyper-parameter wrapper for FISTA.*

Description

This is a very simple function that supplies the hyper-parameters for the Fast Iterative Soft-Threshold Algorithm (FISTA) that solves the s2net minimization problem.

Usage

```
s2Fista(MAX_ITER_INNER = 5000, TOL = 1e-07, t0 = 2, step = 0.1, use_warmstart = FALSE)
```

Arguments

MAX_ITER_INNER	Number of iterations of FISTA
TOL	The relative tolerance. The algorith stops when the objective does not improve more than TOL*the null model's objective function evaluation, after two successive iterations.
t0	The initial stepsize for backtracking.
step	The scale factor in the stepsize to backtrack until a valid step is found.
use_warmstart	Should we use a warm beta to fit the model? This is useful to speed-up hyper-parameter searching methods.

Value

Returns an object of S3 class s2Fista with the input arguments as fields.

References

Beck, A., & Teboulle, M. (2009). A fast iterative shrinkage-thresholding algorithm for linear inverse problems. *SIAM journal on imaging sciences*, 2(1), 183-202. doi:10.1137/080716542

See Also

s2Params, s2Data

---

s2netR *Trains a generalized extended linear joint trained model using semi-supervised data.*

Description

This function is a wrapper for the class s2net. It creates the C++ object and fits the model using input data.

Usage

```
s2netR(data, params, loss = "default", frame = "ExtJT", proj = "auto",
        fista = NULL, S3 = TRUE)
```

Arguments

data	A s2Data object with the (training) data.
params	A s2Params object with the model hyper-parameters.
loss	Loss function. One of "default" (figure it out from the data), "linear" or "logit".
frame	The semi-supervised frame: "ExtJT" (the extended linear joint trained model), "JT" (the linear joint trained model from Ryan and Culp. 2015)

proj	Should the unlabeled data be shifted to remove the model's effect? One of "no", "yes", "auto" (option auto shifts the unlabeled data if the angle betwen beta and the center of the data is important)
fista	Fista setup parameters. An object of class s2Fista.
S3	Boolean: should the method return an S3 object (default) or a C++ object?

Value

Returns an object of S3 class s2netR or a C++ object of class s2net

Author(s)

Juan C. Laria

References

Ryan, K. J., & Culp, M. V. (2015). On semi-supervised linear regression in covariate shift problems. *The Journal of Machine Learning Research, 16*(1), 3183-3217.

See Also

s2net

Examples

```
data("auto_mpg")
train = s2Data(xL = auto_mpg$P1$xL, yL = auto_mpg$P1$yL,  xU = auto_mpg$P1$xU)

model = s2netR(train,
               s2Params(lambda1 = 0.1,
                        lambda2 = 0,
                        gamma1 = 0.1,
                        gamma2 = 100,
                        gamma3 = 0.1),
               loss = "linear",
               frame = "ExtJT",
               proj = "auto",
               fista = s2Fista(5000, 1e-7, 1, 0.8))

valid = s2Data(auto_mpg$P1$xU, auto_mpg$P1$yU, preprocess = train)
ypred = predict(model, valid$xL)

## Not run:
if(require(ggplot2)){
  ggplot() +
    aes(x = ypred, y = valid$yL) + geom_point() +
    geom_abline(intercept = 0, slope = 1, linetype = 2)
}

## End(Not run)
```

s2Params *Hyper-parameter wrapper for* s2net

Description

This is a very simple function that collapses the input parameters into a named vector to supply to C++ methods.

Usage

```
s2Params(lambda1, lambda2 = 0, gamma1 = 0, gamma2 = 0, gamma3 = 0)
```

Arguments

lambda1	elastic-net regularization parameter - l_1 norm.
lambda2	elastic-net regularization parameter - l_2 norm.
gamma1	s2net weight hyper-parameter.
gamma2	s2net covariance hyper-parameter (between 1 and Inf).
gamma3	s2net shift hyper-parameter (between 0 and 1).

Value

Returns a named vector of S3 class s2Params.

See Also

s2Data, s2Fista

simulate_extra *Simulate extrapolated data*

Description

Simulated data scenarios described in the paper from Ryan and Culp (2015).

Usage

```
simulate_extra(n_source = 100, n_target = 100, p = 1000, shift = 10,
               scenario = "same", response = "linear", sigma2 = 2.5)
```

Arguments

n_source	Number of source samples (labeled)
n_target	Number of target samples (unlabeled)
p	Number of variables (p > 10)
shift	The shift applied to the first 10 columns of xU.
scenario	Simulation scenario. One of "same" (same distribution), "lucky" (extrapolation with lucky β), "unlucky" (extrapolation with unlucky β)
response	Type of response: "linear" or "logit"
sigma2	The variance of the error term, linear response case.

Value

A list, with

xL data frame with the labeled (source) data

yL labels associated with xL

xU data frame with the unlabeled (target) data

yU labels associated with xU (for validation/testing)

References

Ryan, K. J., & Culp, M. V. (2015). On semi-supervised linear regression in covariate shift problems. *The Journal of Machine Learning Research, 16*(1), 3183-3217.

See Also

simulate_groups

Examples

```
set.seed(0)
data = simulate_extra()

train = s2Data(data$xL, data$yL, data$xU)
valid = s2Data(data$xU, data$yU, preprocess = train)

model = s2netR(train, s2Params(0.1))
ypred = predict(model, valid$xL)
plot(ypred, valid$yL)
```

`simulate_groups` *Simulate data (two groups design)*

Description

Simulated data scenario described in paper [citation here].

Usage

```
simulate_groups(n_source = 100, n_target = 100, p = 200, response = "linear")
```

Arguments

`n_source`	Number of labeled observations
`n_target`	Number of unlabeled (target) observations
`p`	Number of variables
`response`	Type of response: `"linear"` or `"logit"`

Value

A list, with

xL data frame with the labeled (source) data

yL labels associated with `xL`

xU data frame with the unlabeled (target) data

yU labels associated with `xU` (for validation/testing)

Author(s)

Juan C. Laria

See Also

`simulate_extra`

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