Package: L0Learn (via r-universe)

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L0Learn-package

A package for L0-regularized learning

Description

L0Learn fits regularization paths for L0-regularized regression and classification problems. Specifically, it can solve either one of the following problems over a grid of λ and γ values:

$$\min_{\beta_0,\beta} \sum_{i=1}^n \ell(y_i, \beta_0 + \langle x_i, \beta \rangle) + \lambda ||\beta||_0 \qquad (L0)$$

$$\min_{\beta_0,\beta} \sum_{i=1}^n \ell(y_i, \beta_0 + \langle x_i, \beta \rangle) + \lambda ||\beta||_0 + \gamma ||\beta||_1 \quad (L0L1)$$

$$\min_{\beta_0, \beta} \sum_{i=1}^{n} \ell(y_i, \beta_0 + \langle x_i, \beta \rangle) + \lambda ||\beta||_0 + \gamma ||\beta||_2^2 \quad (L0L2)$$

where ℓ is the loss function. We currently support regression using squared error loss and classification using either logistic loss or squared hinge loss. Pathwise optimization can be done using either cyclic coordinate descent (CD) or local combinatorial search. The core of the toolkit is implemented in C++ and employs many computational tricks and heuristics, leading to competitive running times. CD runs very fast and typically leads to relatively good solutions. Local combinatorial search can find higher-quality solutions (at the expense of increased running times). The toolkit has the following six main methods:

- LOLearn.fit: Fits an LO-regularized model.
- LOLearn.cvfit: Performs k-fold cross-validation.
- print: Prints a summary of the path.
- coef: Extracts solutions(s) from the path.
- predict: Predicts response using a solution in the path.
- plot: Plots the regularization path or cross-validation error.

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References

Hazimeh and Mazumder. Fast Best Subset Selection: Coordinate Descent and Local Combinatorial Optimization Algorithms. Operations Research (2020). https://pubsonline.informs.org/doi/10.1287/opre.2019.1919.

coef.L0Learn

Extract Solutions

Description

Extracts a specific solution in the regularization path.

Usage

```
## S3 method for class 'L0Learn'
coef(object, lambda = NULL, gamma = NULL, ...)
## S3 method for class 'L0LearnCV'
coef(object, lambda = NULL, gamma = NULL, ...)
```

Arguments

object The output of L0Learn.fit or L0Learn.cvfit

lambda The value of lambda at which to extract the solution.

The value of gamma at which to extract the solution.

ignore

Value

A sparse Matrix of class dgCMatrix, which contains the model coefficients. If both lambda and gamma are not supplied, then a matrix of coefficients for all the solutions in the regularization path is returned. If lambda is supplied but gamma is not, the smallest value of gamma is used.

```
# Generate synthetic data for this example
data <- GenSynthetic(n=100,p=20,k=10,seed=1)
X = data$X
y = data$y

# Fit an L0L2 Model with 3 values of Gamma ranging from 0.0001 to 10, using coordinate descent
fit <- L0Learn.fit(X, y, penalty="L0L2", nGamma=3, gammaMin=0.0001, gammaMax = 10)
print(fit)
# Extract the coefficients of the solution at lambda = 2.45513e-02 and gamma = 0.0001
coef(fit, lambda=2.45513e-02, gamma=0.0001)
# Extract the coefficients of all the solutions in the path
coef(fit)</pre>
```

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GenSynthetic	Generate Synthetic Data	

Description

Generates a synthetic dataset as follows: 1) Sample every element in data matrix X from N(0,1). 2) Generate a vector B with the first k entries set to 1 and the rest are zeros. 3) Sample every element in the noise vector e from N(0,1). 4) Set y = XB + b0 + e.

Usage

```
GenSynthetic(n, p, k, seed, rho = 0, b0 = 0, snr = 1)
```

Arguments

n	Number of samples
р	Number of features
k	Number of non-zeros in true vector of coefficients
seed	The seed used for randomly generating the data
rho	The threshold for setting values to 0. if $ X(i, j) > \text{rho} => X(i, j) < 0$
b0	intercept value to translate y by.
snr	desired Signal-to-Noise ratio. This sets the magnitude of the error term 'e'. SNR is defined as $SNR = Var(XB)/Var(e)$

Value

A list containing: the data matrix X, the response vector y, the coefficients B, the error vector e, the intercept term b0.

```
data <- GenSynthetic(n=100,p=20,k=10,seed=1) X = data$X  y = data$y
```

GenSyntheticHighCorr Generate Exponential Correlated Synthetic Data

Description

Generates a synthetic dataset as follows: 1) Generate a correlation matrix, SIG, where item $[i, j] = A^{i-j}$. 2) Draw from a Multivariate Normal Distribution using (mu and SIG) to generate X. 3) Generate a vector B with every p/k entry set to 1 and the rest are zeros. 4) Sample every element in the noise vector e from N(0,1). 4) Set y = XB + b0 + e.

Usage

```
GenSyntheticHighCorr(
    n,
    p,
    k,
    seed,
    rho = 0,
    b0 = 0,
    snr = 1,
    mu = 0,
    base_cor = 0.9
)
```

Arguments

n	Number of samples
p	Number of features
k	Number of non-zeros in true vector of coefficients
seed	The seed used for randomly generating the data
rho	The threshold for setting values to 0. if $ X(i, j) > \text{rho} \Rightarrow X(i, j) < 0$
b0	intercept value to scale y by.
snr	desired Signal-to-Noise ratio. This sets the magnitude of the error term 'e'. SNR is defined as SNR = $Var(XB)/Var(e)$
mu	The mean for drawing from the Multivariate Normal Distribution. A scalar of vector of length p.
base_cor	The base correlation, A in $[i, j] = A^i - ji$.

Value

A list containing: the data matrix X, the response vector y, the coefficients B, the error vector e, the intercept term b0.

GenSyntheticLogistic Generate Logistic Synthetic Data

Description

Generates a synthetic dataset as follows: 1) Generate a data matrix, X, drawn from a multivariate Gaussian distribution with mean = 0, sigma = Sigma 2) Generate a vector B with k entries set to 1 and the rest are zeros. 3) Every coordinate yi of the outcome vector y exists in -1, 1^n is sampled independently from a Bernoulli distribution with success probability: P(yi = 1|xi) = 1/(1 + exp(-s < xi, B>)) Source https://arxiv.org/pdf/2001.06471.pdf Section 5.1 Data Generation

Usage

```
GenSyntheticLogistic(
   n,
   p,
   k,
   seed,
   rho = 0,
   s = 1,
   sigma = NULL,
   shuffle_B = FALSE
)
```

Arguments

n	Number of samples
p	Number of features
k	Number of non-zeros in true vector of coefficients
seed	The seed used for randomly generating the data
rho	The threshold for setting values to 0. if $ X(i, j) > \text{rho} \Rightarrow X(i, j) < 0$
S	Signal-to-noise parameter. As s -> $+$ Inf, the data generated becomes linearly separable.
sigma	Correlation matrix, defaults to I.
shuffle_B	A boolean flag for whether or not to randomly shuffle the Beta vector, B. If FALSE, the first k entries in B are set to 1.

Value

A list containing: the data matrix X, the response vector y, the coefficients B.

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L0Learn.cvfit

Cross Validation

Description

Computes a regularization path and performs K-fold cross-validation.

Usage

```
L0Learn.cvfit(
  Х,
  у,
  loss = "SquaredError",
  penalty = "L0",
  algorithm = "CD",
 maxSuppSize = 100,
  nLambda = 100,
  nGamma = 10,
  gammaMax = 10,
  gammaMin = 1e-04,
  partialSort = TRUE,
 maxIters = 200,
  rtol = 1e-06,
  atol = 1e-09,
  activeSet = TRUE,
  activeSetNum = 3,
 maxSwaps = 100,
  scaleDownFactor = 0.8,
  screenSize = 1000,
  autoLambda = NULL,
  lambdaGrid = list(),
  nFolds = 10,
  seed = 1,
  excludeFirstK = 0,
  intercept = TRUE,
  lows = -Inf,
  highs = Inf
)
```

Arguments

loss

x The data matrix.

y The response vector. For classification, we only support binary vectors.

The loss function. Currently we support the choices "SquaredError" (for regression), "Logistic" (for logistic regression), and "SquaredHinge" (for smooth SVM).

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The type of regularization. This can take either one of the following choices:

penalty

"L0", "L0L2", and "L0L1". algorithm The type of algorithm used to minimize the objective function. Currently "CD" and "CDPSI" are are supported. "CD" is a variant of cyclic coordinate descent and runs very fast. "CDPSI" performs local combinatorial search on top of CD and typically achieves higher quality solutions (at the expense of increased running time). The maximum support size at which to terminate the regularization path. We maxSuppSize recommend setting this to a small fraction of min(n,p) (e.g. 0.05 * min(n,p)) as L0 regularization typically selects a small portion of non-zeros. nLambda The number of Lambda values to select (recall that Lambda is the regularization parameter corresponding to the L0 norm). This value is ignored if 'lambdaGrid' is supplied. The number of Gamma values to select (recall that Gamma is the regularization nGamma parameter corresponding to L1 or L2, depending on the chosen penalty). This value is ignored if 'lambdaGrid' is supplied and will be set to length(lambdaGrid) gammaMax The maximum value of Gamma when using the L0L2 penalty. For the L0L1 penalty this is automatically selected. gammaMin The minimum value of Gamma when using the L0L2 penalty. For the L0L1 penalty, the minimum value of gamma in the grid is set to gammaMin * gammaMax. Note that this should be a strictly positive quantity. partialSort If TRUE partial sorting will be used for sorting the coordinates to do greedy cycling (see our paper for for details). Otherwise, full sorting is used. The maximum number of iterations (full cycles) for CD per grid point. maxIters The relative tolerance which decides when to terminate optimization (based on rtol the relative change in the objective between iterations). atol The absolute tolerance which decides when to terminate optimization (based on the absolute L2 norm of the residuals). activeSet If TRUE, performs active set updates. activeSetNum The number of consecutive times a support should appear before declaring support stabilization. maxSwaps The maximum number of swaps used by CDPSI for each grid point. scaleDownFactor This parameter decides how close the selected Lambda values are. The choice should be strictly between 0 and 1 (i.e., 0 and 1 are not allowed). Larger values lead to closer lambdas and typically to smaller gaps between the support sizes. For details, see our paper - Section 5 on Adaptive Selection of Tuning Parameters). screenSize The number of coordinates to cycle over when performing initial correlation screening. autoLambda Ignored parameter. Kept for backwards compatibility. lambdaGrid A grid of Lambda values to use in computing the regularization path. This is

by default an empty list and is ignored. When specified, LambdaGrid should

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be a list of length 'nGamma', where the ith element (corresponding to the ith gamma) should be a decreasing sequence of lambda values which are used by the algorithm when fitting for the ith value of gamma (see the vignette for details).

nFolds The number of folds for cross-validation.

seed The seed used in randomly shuffling the data for cross-validation.

excludeFirstK This parameter takes non-negative integers. The first excludeFirstK features in

 \boldsymbol{x} will be excluded from variable selection, i.e., the first excludeFirstK variables will not be included in the L0-norm penalty (they will still be included in the L1

or L2 norm penalties.).

intercept If FALSE, no intercept term is included in the model.

lows Lower bounds for coefficients. Either a scalar for all coefficients to have the

same bound or a vector of size p (number of columns of X) where lows[i] is the

lower bound for coefficient i.

highs Upper bounds for coefficients. Either a scalar for all coefficients to have the

same bound or a vector of size p (number of columns of X) where highs[i] is the

upper bound for coefficient i.

Value

An S3 object of type "L0LearnCV" describing the regularization path. The object has the following members.

cvMeans This is a list, where the ith element is the sequence of cross-validation errors cor-

responding to the ith gamma value, i.e., the sequence cvMeans[[i]] corresponds

to fit\$gamma[i]

cvSDs This a list, where the ith element is a sequence of standard deviations for the

cross-validation errors: cvSDs[[i]] corresponds to cvMeans[[i]].

fit The fitted model with type "L0Learn", i.e., this is the same object returned by

L0Learn.fit.

```
# Generate synthetic data for this example
data <- GenSynthetic(n=100,p=20,k=10,seed=1)
X = data$X
y = data$y
#'
# Perform 3-fold cross-validation on an L0L2 regression model with 3 values of
# Gamma ranging from 0.0001 to 10
fit <- L0Learn.cvfit(X, y, nFolds=3, seed=1, penalty="L0L2", maxSuppSize=20, nGamma=3,
gammaMin=0.0001, gammaMax = 10)
print(fit)
# Plot the graph of cross-validation error versus lambda for gamma = 0.0001
plot(fit, gamma=0.0001)
# Extract the coefficients at lambda = 0.0361829 and gamma = 0.0001
coef(fit, lambda=2.45513e-02, gamma=0.0001)
# Apply the fitted model on X to predict the response
predict(fit, newx = X, lambda=2.45513e-02, gamma=0.0001)</pre>
```

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L0Learn.fit

Fit an L0-regularized model

Description

Computes the regularization path for the specified loss function and penalty function (which can be a combination of the L0, L1, and L2 norms).

Usage

```
L0Learn.fit(
  Х,
  у,
  loss = "SquaredError",
  penalty = "L0",
  algorithm = "CD",
  maxSuppSize = 100,
  nLambda = 100,
  nGamma = 10,
  gammaMax = 10,
  gammaMin = 1e-04,
  partialSort = TRUE,
 maxIters = 200,
  rtol = 1e-06,
  atol = 1e-09,
  activeSet = TRUE,
  activeSetNum = 3,
  maxSwaps = 100,
  scaleDownFactor = 0.8,
  screenSize = 1000,
  autoLambda = NULL,
  lambdaGrid = list(),
  excludeFirstK = 0,
  intercept = TRUE,
  lows = -Inf,
  highs = Inf
)
```

Arguments

x The data matrix.

y The response vector. For classification, we only support binary vectors.

The loss function. Currently we support the choices "SquaredError" (for regression), "Logistic" (for logistic regression), and "SquaredHinge" (for smooth SVM).

L0Learn.fit

The type of regularization. This can take either one of the following choices:

penalty

lambdaGrid

"L0", "L0L2", and "L0L1". algorithm The type of algorithm used to minimize the objective function. Currently "CD" and "CDPSI" are are supported. "CD" is a variant of cyclic coordinate descent and runs very fast. "CDPSI" performs local combinatorial search on top of CD and typically achieves higher quality solutions (at the expense of increased running time). The maximum support size at which to terminate the regularization path. We maxSuppSize recommend setting this to a small fraction of min(n,p) (e.g. 0.05 * min(n,p)) as L0 regularization typically selects a small portion of non-zeros. nLambda The number of Lambda values to select (recall that Lambda is the regularization parameter corresponding to the L0 norm). This value is ignored if 'lambdaGrid' is supplied. The number of Gamma values to select (recall that Gamma is the regularization nGamma parameter corresponding to L1 or L2, depending on the chosen penalty). This value is ignored if 'lambdaGrid' is supplied and will be set to length(lambdaGrid) gammaMax The maximum value of Gamma when using the L0L2 penalty. For the L0L1 penalty this is automatically selected. gammaMin The minimum value of Gamma when using the L0L2 penalty. For the L0L1 penalty, the minimum value of gamma in the grid is set to gammaMin * gammaMax. Note that this should be a strictly positive quantity. partialSort If TRUE partial sorting will be used for sorting the coordinates to do greedy cycling (see our paper for for details). Otherwise, full sorting is used. The maximum number of iterations (full cycles) for CD per grid point. maxIters The relative tolerance which decides when to terminate optimization (based on rtol the relative change in the objective between iterations). The absolute tolerance which decides when to terminate optimization (based on atol the absolute L2 norm of the residuals). activeSet If TRUE, performs active set updates. activeSetNum The number of consecutive times a support should appear before declaring support stabilization. maxSwaps The maximum number of swaps used by CDPSI for each grid point. scaleDownFactor This parameter decides how close the selected Lambda values are. The choice should be strictly between 0 and 1 (i.e., 0 and 1 are not allowed). Larger values lead to closer lambdas and typically to smaller gaps between the support sizes. For details, see our paper - Section 5 on Adaptive Selection of Tuning Parameters). screenSize The number of coordinates to cycle over when performing initial correlation screening. autoLambda Ignored parameter. Kept for backwards compatibility.

> A grid of Lambda values to use in computing the regularization path. This is by default an empty list and is ignored. When specified, LambdaGrid should

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be a list of length 'nGamma', where the ith element (corresponding to the ith gamma) should be a decreasing sequence of lambda values which are used by the algorithm when fitting for the ith value of gamma (see the vignette for details).

excludeFirstK This parameter takes non-negative integers. The first excludeFirstK features in

 \boldsymbol{x} will be excluded from variable selection, i.e., the first excludeFirstK variables will not be included in the L0-norm penalty (they will still be included in the L1

or L2 norm penalties.).

intercept If FALSE, no intercept term is included in the model.

lows Lower bounds for coefficients. Either a scalar for all coefficients to have the

same bound or a vector of size p (number of columns of X) where lows[i] is the

lower bound for coefficient i.

highs Upper bounds for coefficients. Either a scalar for all coefficients to have the

same bound or a vector of size p (number of columns of X) where highs[i] is the

upper bound for coefficient i.

Value

An S3 object of type "L0Learn" describing the regularization path. The object has the following members.

a0 is a list of intercept sequences. The ith element of the list (i.e., a0[[i]]) is the

sequence of intercepts corresponding to the ith gamma value (i.e., gamma[i]).

beta This is a list of coefficient matrices. The ith element of the list is a p x length(lambda)

matrix which corresponds to the ith gamma value. The jth column in each coef-

ficient matrix is the vector of coefficients for the jth lambda value.

lambda This is the list of lambda sequences used in fitting the model. The ith element

of lambda (i.e., lambda[[i]]) is the sequence of Lambda values corresponding to

the ith gamma value.

gamma This is the sequence of gamma values used in fitting the model.

suppSize This is a list of support size sequences. The ith element of the list is a sequence

of support sizes (i.e., number of non-zero coefficients) corresponding to the ith

gamma value.

converged This is a list of sequences for checking whether the algorithm has converged at

every grid point. The ith element of the list is a sequence corresponding to the ith value of gamma, where the jth element in each sequence indicates whether

the algorithm has converged at the jth value of lambda.

```
# Generate synthetic data for this example
data <- GenSynthetic(n=100,p=20,k=10,seed=1)
X = data$X
y = data$y

# Fit an L0 regression model with a maximum of 20 non-zeros using coordinate descent (CD)
fit1 <- L0Learn.fit(X, y, penalty="L0", maxSuppSize=20)
print(fit1)</pre>
```

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```
# Extract the coefficients at lambda = 2.28552e-02
coef(fit1, lambda=2.28552e-02)
# Apply the fitted model on X to predict the response
predict(fit1, newx = X, lambda=2.28552e-02)
# Fit an L0 regression model with a maximum of 20 non-zeros using CD and local search
fit2 <- L0Learn.fit(X, y, penalty="L0", algorithm="CDPSI", maxSuppSize=20)</pre>
print(fit2)
# Fit an L0L2 regression model with 3 values of Gamma ranging from 0.0001 to 10, using CD
fit3 <- L0Learn.fit(X, y, penalty="L0L2", maxSuppSize=20, nGamma=3, gammaMin=0.0001, gammaMax = 10)
# Extract the coefficients at lambda = 2.45513e-02 and gamma = 0.0001
coef(fit3, lambda=2.45513e-02, gamma=0.0001)
# Apply the fitted model on X to predict the response
predict(fit3, newx = X, lambda=2.45513e-02, gamma=0.0001)
# Fit an L0 logistic regression model
# First, convert the response to binary
fit4 <- L0Learn.fit(X, y, loss="Logistic", maxSuppSize=10)</pre>
print(fit4)
```

plot.L0Learn

Plot Regularization Path

Description

Plots the regularization path for a given gamma.

Usage

```
## S3 method for class 'L0Learn'
plot(x, gamma = 0, showLines = FALSE, ...)
```

Arguments

x The output of L0Learn.fit
 gamma The value of gamma at which to plot.
 showLines If TRUE, the lines connecting the points in the plot are shown.
 ignore

Value

A ggplot object.

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Examples

```
# Generate synthetic data for this example
data <- GenSynthetic(n=100,p=20,k=10,seed=1)
X = data$X
y = data$y
# Fit an L0 Model
fit <- L0Learn.fit(X, y, penalty="L0")
plot(fit, gamma=0)</pre>
```

plot.L0LearnCV

Plot Cross-validation Errors

Description

Plots cross-validation errors for a given gamma.

Usage

```
## S3 method for class 'L0LearnCV'
plot(x, gamma = 0, ...)
```

Arguments

x The output of L0Learn.cvfit
gamma The value of gamma at which to plot.
... ignore

Value

A ggplot object.

```
# Generate synthetic data for this example
data <- GenSynthetic(n=100,p=20,k=10,seed=1)
X = data$X
y = data$y

# Perform 3-fold cross-validation on an L0L2 Model with 3 values of
# Gamma ranging from 0.0001 to 10
fit <- L0Learn.cvfit(X, y, nFolds=3, seed=1, penalty="L0L2",
maxSuppSize=20, nGamma=3, gammaMin=0.0001, gammaMax = 10)
# Plot the graph of cross-validation error versus lambda for gamma = 0.0001
plot(fit, gamma=0.0001)</pre>
```

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Description

Predicts the response for a given sample.

Usage

```
## S3 method for class 'L0Learn'
predict(object, newx, lambda = NULL, gamma = NULL, ...)
## S3 method for class 'L0LearnCV'
predict(object, newx, lambda = NULL, gamma = NULL, ...)
```

Arguments

object	The output of L0Learn.fit or L0Learn.cvfit
newx	A matrix on which predictions are made. The matrix should have p columns.
lambda	The value of lambda to use for prediction. A summary of the lambdas in the regularization path can be obtained using print(fit).
gamma	The value of gamma to use for prediction. A summary of the gammas in the regularization path can be obtained using print(fit).
• • •	ignore

Value

A Matrix of class dgeMatrix, which contains the model predictions. If both lambda and gamma are not supplied, then a matrix of predictions for all the solutions in the regularization path is returned. If lambda is supplied but gamma is not, the smallest value of gamma is used. In case of logistic regression, probability values are returned.

```
# Generate synthetic data for this example
data <- GenSynthetic(n=100,p=20,k=10,seed=1)
X = data$X
y = data$y

# Fit an L0L2 Model with 3 values of Gamma ranging from 0.0001 to 10, using coordinate descent
fit <- L0Learn.fit(X,y, penalty="L0L2", nGamma=3, gammaMin=0.0001, gammaMax = 10)
print(fit)
# Apply the fitted model with lambda=2.45513e-02 and gamma=0.0001 on X to predict the response
predict(fit, newx = X, lambda=2.45513e-02, gamma=0.0001)
# Apply the fitted model on X to predict the response for all the solutions in the path
predict(fit, newx = X)</pre>
```

print.L0Learn

print.L0Learn

Print L0Learn.fit object

Description

Prints a summary of L0Learn.fit

Usage

```
## S3 method for class 'L0Learn'
print(x, ...)
## S3 method for class 'L0LearnCV'
print(x, ...)
```

Arguments

```
x The output of L0Learn.fit or L0Learn.cvfit
... ignore
```

Value

Prints a summary of the models to the console.

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