

# Package ‘gomp’

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**Description** The gamma-Orthogonal Matching Pursuit (gamma-OMP) is a recently suggested modification of the OMP feature selection algorithm for a wide range of response variables. The package offers many alternative regression models, such linear, robust, survival, multivariate etc., including k-fold cross-validation. References: Tsagris M., Papadovasilakis Z., Lakiotaki K. and Tsamardinos I. (2018). ``Efficient feature selection on gene expression data: Which algorithm to use?" BioRxiv. <[doi:10.1101/431734](https://doi.org/10.1101/431734)>. Tsagris M., Papadovasilakis Z., Lakiotaki K. and Tsamardinos I. (2022). ``The gamma-OMP algorithm for feature selection with application to gene expression data". IEEE/ACM Transactions on Computational Biology and Bioinformatics 19(2): 1214--1224. <[doi:10.1109/TCBB.2020.3029952](https://doi.org/10.1109/TCBB.2020.3029952)>.

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gomp-package

*The gamma-OMP Feature Selection Algorithm*

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## Description

The gamma-Orthogonal Matching Pursuit (gamma-OMP) is a recently suggested modification of the OMP feature selection algorithm for a wide range of response variables. The package offers many alternative regression models, such linear, robust, survival, multivariate etc., including k-fold cross-validation. References: Tsagris M., Papadovasilakis Z., Lakiotaki K. and Tsamardinos I. (2018). "Efficient feature selection on gene expression data: Which algorithm to use?" *BioRxiv*. <doi:10.1101/431734>. Tsagris M., Papadovasilakis Z., Lakiotaki K. and Tsamardinos I. (2022). "The gamma-OMP algorithm for feature selection with application to gene expression data". *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 19(2): 1214–1224.

## Details

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## Maintainers

Michail Tsagris <mtsagris@uoc.gr>.

## Author(s)

Michail Tsagris <mtsagris@uoc.gr>.

## References

Tsagris M., Papadovasilakis Z., Lakiotaki K. and Tsamardinos I. (2018). Efficient feature selection on gene expression data: Which algorithm to use? *BioRxiv*.

Tsagris M., Papadovasilakis Z., Lakiotaki K. and Tsamardinos I. (2022). The  $\gamma$ -OMP algorithm for feature selection with application to gene expression data". *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 19(2): 1214–1224.

Alharbi N. (2024). Variable selection with time-to-event data: Cox or Weibull regression? *Communications in Statistics: Case Studies, Data Analysis and Applications* (accepted for publication).

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Bootstrap bias correction for the performance of the cross-validation procedure

*Bootstrap bias correction for the performance of the cross-validation procedure*

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## Description

Bootstrap bias correction for the performance of the cross-validation procedure.

## Usage

```
bbc(predictions, y, metric = "auc.gomp", conf = 0.95, B = 1000)
```

## Arguments

predictions	A matrix with the predicted values.
y	A vector with the response variable, survival object, factor (ordered or unordered) or a numerical vector.
metric	<p>The possible values are:</p> <p>a) Binary response: "auc.gomp" (area under the curve), "fscore.gomp" (F-score), "prec.gomp" (precision), "euclid_sens.spec.gomp" (Euclidean distance of sensitivity and specificity), "spec.gomp" (specificity), "sens.gomp" (sensitivity), "acc.gomp" (accuracy, proportion of correct classification).</p> <p>b) Multinomial response: "acc_multinom.gomp" (accuracy, proportion of correct classification).</p> <p>c) Ordinal response: "ord_mae.gomp" (mean absolute error).</p> <p>d) Continuous response: "mae.gomp" (MAE with continuous response), "mse.gomp" (mean squared error), "pve.gomp" (percentage of variance explained).</p> <p>e) Survival response "ci.gomp" (concordance index for Cox regression), "ciwr.gomp" (concordance index for Weibull regression).</p> <p>g) Count response "poisdev.gomp".</p> <p>h) Binomial response "binomdev.gomp" (deviance of binomial regression).</p> <p>The "nbdev.gomp" (negative binomial deviance) is missing. For more information on these see <a href="#">cv.gomp</a>. <b>Note</b> that they come with "".</p>
conf	A number between 0 and 1, the confidence level.
B	The number of bootstrap replicates. The default number is 1000.

## Details

Upon completion of the cross-validation, the predicted values produced by all predictive models across all folds is collected in a matrix  $P$  of dimensions  $n \times M$ , where  $n$  is the number of samples and  $M$  the number of trained models or configurations. Sampled with replacement a fraction of rows (predictions) from  $P$  are denoted as the in-sample values. On average, the newly created set

will be comprised by 63.2% of the original individuals (The probability of sampling, with replacement, a sample of  $n$  numbers from a set of  $n$  numbers is  $1 - (1 - \frac{1}{n})^n \simeq 1 - \frac{1}{e} = 0.632$ ), whereas the rest 36.8% will be random copies of them. The non re-sampled rows are denoted as out-of-sample values. The performance of each model in the in-sample rows is calculated and the model (or configuration) with the optimal performance is selected, followed by the calculation of performance in the out-of-sample values. This process is repeated  $B$  times and the average performance is returned.

Note, that the only computational overhead is with the repetitive re-sampling and calculation of the predictive performance, i.e. no model is fitted nor trained. The final estimated performance usually underestimates the true performance, but this negative bias is smaller than the optimistic uncorrected performance.

Note, that all metrics are for maximization. For this reason "mse.gomp", "mae.gomp", "ord\_mae.gomp", "poisdev.gomp", "binomdev.gomp" are multiplied by -1.

### Value

A list including:

out.perf	The $B$ out sampled performances. Their mean is the "bbc.perf" given above.
bbc.perf	The bootstrap bias corrected performance of the chosen algorithm, model or configuration.
ci	The (1- conf)% confidence interval of the BBC performance. It is based on the empirical or percentile method for bootstrap samples. The lower and upper 2.5% of the "out.perf".

### Author(s)

Michail Tsagris

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Ioannis Tsamardinos, Elissavet Greasidou and Giorgos Borboudakis (2018). Bootstrapping the out-of-sample predictions for efficient and accurate cross-validation. *Machine Learning*, 107: 1895–1922.

### See Also

[cv.gomp](#), [gomp](#)

### Examples

```
predictions <- matrix( rbinom(200 * 50, 1, 0.7), ncol = 50)
y <- rbinom(200, 1, 0.5)
gomp::bbc(predictions, y, metric = "auc.gomp")
```

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Cross-validation for gamma-Orthogonal Matching Pursuit (gamma-OMP) algorithm

*Cross-validation for the gamma-Orthogonal Matching Pursuit (gamma-OMP) algorithm*

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## Description

The function performs a k-fold cross-validation for identifying the best tolerance values for the  $\gamma$ -Orthogonal Matching Pursuit ( $\gamma$ -OMP) algorithm.

## Usage

```
cv.gomp(y, x, kfolds = 10, folds = NULL, tol = seq(4, 9, by = 1),
task = "C", metric = NULL, metricbbc = NULL, modeler = NULL, test = NULL,
method = "ar2", B = 1)
```

## Arguments

y	The response variable.
x	A matrix with the predictor variables.
kfolds	The number of the folds in the k-fold Cross Validation (integer).
folds	The folds of the data to use. If NULL the folds are created internally with the same function.
tol	A vector of tolerance values.
task	A character ("C", "R" or "S"). It can be "C" for classification (logistic, multinomial or ordinal regression), "R" for regression (robust and non robust linear regression, median regression, (zero inflated) poisson and negative binomial regression, beta regression), "S" for survival regression (Cox, Weibull or exponential regression).
metric	A metric function provided by the user. If NULL the following functions will be used: auc.gomp, mse.gomp, ci.gomp for classification, regression and survival analysis tasks, respectively. See details for more. If you know what you have put it here to avoid the function choosing something else. <b>Note</b> that you put these words as they are, without "".
metricbbc	This is the same argument as "metric" with the difference that " " must be placed. If for example, metric = auc.mxm, here metricbbc = "auc.mxm". The same value must be given here. This argument is to be used with the function <code>bbc</code> which does bootstrap bias correction of the estimated performance (Tsamardinos, Greasidou and Borboudakis, 2018). This argument is valid if the last argument (B) is more than 1.
modeler	A modeling function provided by the user. If NULL the following functions will be used: glm.gomp, lm.gomp, coxph.gomp for classification, regression and survival analysis tasks, respectively. See details for more. If you know what you have put it here to avoid the function choosing something else. <b>Note</b> that you put these words as they are, without "".

test	A function object that defines the conditional independence test used in the SES function (see also SES help page). If NULL, "cor", "logistic" and "cox" are used for classification, regression and survival analysis tasks, respectively. If you know what you have put it here to avoid the function choosing something else. Not all tests can be included here. "mv", "gamma", and "tobit" are not available.
method	This is only for the "cor". You can either specify, "ar2" for the adjusted R-square or "sse" for the sum of squares of errors. The tolerance value in both cases must be a number between 0 and 1. That will denote a percentage. If the percentage increase or decrease is less than the number the algorithm stops. An alternative is "BIC" for BIC and the tolerance values are like in all other regression models.
B	How many bootstrap re-samples to draw. This argument is to be used with the function <code>bbc</code> which does bootstrap bias correction of the estimated performance (Tsamardinos, Greasidou and Borboudakis, 2018). If you have thousands of observations then this might not be necessary, as there is no optimistic bias to be corrected. What is the lower limit cannot be told beforehand however. SES and MMPC however were designed for the low sample cases, hence, bootstrap bias correction is perhaps a must thing to do.

### Details

For more details see also [gomp](#).

### Value

A list including:

cv_results_all	A list with predictions, performances and selected variables for each fold and each tolerance value. The elements are called "preds", "performances" and "selectedVars".
best_performance	A numeric value that represents the best average performance.
best_configuration	A numeric value that represents the best tolerance value.
bbc_best_performance	The bootstrap bias corrected best performance if B was more than 1, otherwise this is NULL.
runtime	The runtime of the cross-validation procedure.

Bear in mind that the values can be extracted with the \$ symbol, i.e. this is an S3 class output.

### Author(s)

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

## References

Tsamardinos I., Greasidou E. and Borboudakis G. (2018). Bootstrapping the out-of-sample predictions for efficient and accurate cross-validation. *Machine Learning*, 107: 1895–1922. <https://link.springer.com/article/10.1007/s10994-018-5714-4>

Tsagris M., Papadovasilakis Z., Lakiotaki K. and Tsamardinos, I. (2022). The  $\gamma$ -OMP algorithm for feature selection with application to gene expression data. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 19(2): 1214–1224.

## See Also

[gomp](#), [gomp.path](#), [bbc](#)

## Examples

```
# simulate a dataset with continuous data
x <- matrix( rnorm(200 * 50), ncol = 50 )
# the target feature is the last column of the dataset as a vector
y <- x[, 50]
x <- x[, -50]
# run a 10 fold CV for the regression task
best_model <- cv.gomp(y, x, kfolds = 5, task = "R",
  tol = seq(0.001, 0.01, by = 0.001), method = "ar2" )
```

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Generate random folds for cross-validation

*Generate random folds for cross-validation*

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## Description

Random folds for use in a cross validation are generated. There is the option for stratified splitting as well.

## Usage

```
makefolds(ina, nfolds = 10, stratified = TRUE, seed = NULL)
```

## Arguments

<code>ina</code>	A variable indicating the groupings.
<code>nfolds</code>	The number of folds to produce.
<code>stratified</code>	A boolean variable specifying whether stratified random (TRUE) or simple random (FALSE) sampling is to be used when producing the folds.
<code>seed</code>	You can specify your own seed number here or leave it NULL.

## Details

I was inspired by the command in the package **TunePareto** in order to do the stratified version.

**Value**

A list with `nfolds` elements where each element is a fold containing the indices of the data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**See Also**

[cv.gomp](#)

**Examples**

```
a <- gomp::makefolds(iris[, 5], nfolds = 5, stratified = TRUE)
table(iris[a[[1]], 5]) ## 10 values from each group
```

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The gamma-Orthogonal Matching Pursuit (gamma-OMP) algorithm

*The gamma-Orthogonal Matching Pursuit (gamma-OMP) algorithm*

---

**Description**

The  $\gamma$ -Orthogonal Matching Pursuit ( $\gamma$ -OMP) algorithm.

**Usage**

```
gomp(y, x, xstand = TRUE, tol = qchisq(0.95, 1), test = "logistic", method = "ar2" )
```

```
gomp.path(y, x, xstand = TRUE, tol = c(4, 5, 6), test = "logistic", method = "ar2" )
```

```
boot.gomp(y, x, tol = qchisq(0.95, 1), test = "logistic", method = "ar2",
B = 500, ncores = 1)
```

**Arguments**

<code>y</code>	The response variable, a numeric vector, a matrix or a Surv object.
<code>x</code>	A matrix with continuous data, where the rows denote the observations and the columns are the variables.
<code>xstand</code>	If this is TRUE the independent variables are standardised.
<code>tol</code>	The tolerance value to terminate the algorithm. This is the change in the criterion value between two successive steps. The default value is the 95% quantile of the $\chi^2$ distribution with 1 degree of freedom. For <code>test = "normal"</code> the BIC is already calculated.  In the case of "gomp.path" this is a vector of values. For each tolerance value the result of the gOMP is returned. It returns the whole path of solutions.

test	This denotes the parametric model to be used each time. It depends upon the nature of the target variable. The possible values are "normal" (or "cor" for the same purpose), "logistic", "poisson", "qpoisson", "qlogistic", "normlog", "mvreg", "negbin", "beta", "gamma", "mm", "quantreg", "ordinal", "tobit", "cox", "weibull", "log-logistic" and "multinom".
method	This is only for the "testIndFisher". You can either specify, "ar2" for the adjusted R-square or "sse" for the sum of squares of errors. The tolerance value in both cases must a number between 0 and 1. That will denote a percentage. If the percentage increase or decrease is less than the nubmer the algorithm stops. An alternative is "BIC" for BIC and the tolerance values are like in all other regression models.
B	How many bootstrap samples to generate. The gOMP will be performed for each of these samples.
ncores	How many cores to use. This argument is valid only if you have a multi-threaded machine.

### Value

A list including:

runtime	The runtime of the algorithm
phi	The <i>phi</i> coefficient, returned in the quasi binomial (qlogistic), quasi Poisson (qpoisson), Gamma (gamma) and Gaussian with log link (normlog). In all other cases this is NULL.
res	For the case of "gomp" a matrix with two columns. The selected variable(s) and the criterion value at every step. For the case of "gomp.path" a matrix with many columns. Every column contains the selected variables for each tolerance caue, starting from the smallest value (which selected most variables). The final column is the deviance of the model at each step. For the "boot.gomp" this is a matrix with two columns. The first one is the selected variables and the second column is their proportion of selection.

### Author(s)

Michail Tsagris

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

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### See Also

[cv.gomp](#)

### Examples

```
x <- matrix( rnorm(500 * 50), ncol = 50)
y <- rnorm(500)
b <- gomp::gomp(y, x, test = "cor")
```

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