

# Package ‘BiplotML’

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**Title** Biplots Estimation with Algorithms ML

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**Description** Logistic Biplot is a method that allows representing multivariate binary data on a subspace of low dimension, where each individual is represented by a point and each variable as vectors directed through the origin. The orthogonal projection of individuals onto these vectors predicts the expected probability that the characteristic occurs. The package contains new techniques to estimate the model parameters and constructs in each case the 'Logistic-Biplot'. References can be found in the help of each procedure.

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**URL** <https://github.com/jgbabativam/BiplotML>

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bootBLB	<i>Fitting a Binary Logistic Biplot using bootstrap methodology</i>
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## Description

This function estimates the vector  $\mu$ , matrix A and matrix B using the optimization algorithm chosen by the user and applies a bootstrap methodology to determine the confidence ellipses.

## Usage

```
bootBLB(
  x,
  k = 2,
  L = 0,
  method = "CG",
  type = 1,
  plot = TRUE,
  sup = TRUE,
  ellipses = FALSE,
  maxit = NULL,
  resamples = 100,
  conf = 0.9,
  col.ind = NULL
)
```

## Arguments

x	Binary matrix.
k	Dimensions number. By default k = 2.
L	Penalization parameter. By default L = 0.
method	Method to be used to estimate the parameters. By default method="CG"
type	For the conjugate-gradients method. Takes value 1 for the Fletcher–Reeves update, 2 for Polak–Ribiere and 3 for Beale–Sorenson.
plot	Plot the Bootstrap Logistic Biplot.

sup	Boolean, if TRUE, rows that are not selected in each resample are treated as supplementary individuals. See details.
ellipses	Draw confidence ellipses. By default is FALSE.
maxit	The maximum number of iterations. Defaults to 100 for the gradient methods, and 500 without gradient.
resamples	Number of iterations in the bootstrap process. By default 100.
conf	Level confidence in the ellipses. By default conf=0.90
col.ind	Color for the rows.

### Details

Fitting when sup=TRUE ... whereas sup=FALSE ...

### Value

Coordinates of the matrix A and B in resamples and Biplot

### Author(s)

Giovany Babativa <gbativam@gmail.com>

### References

John C. Nash (2011). Unifying Optimization Algorithms to Aid Software System Users:optimx for R. *Journal of Statistical Software*. 43(9). 1–14.

John C. Nash (2014). On Best Practice Optimization Methods in R. *Journal of Statistical Software*. 60(2). 1–14.

Milan, L., & Whittaker, J. (1995). Application of the parametric bootstrap to models that incorporate a singular value decomposition. *Applied Statistics*, 44, 31–49.

Vicente-Villardón, J.L. and Galindo, M. Purificación (2006), *Multiple Correspondence Analysis and related Methods. Chapter: Logistic Biplots*. Chapman-Hall

### See Also

[plotBLB](#), [performanceBLB](#)

### Examples

```
data("Methylation")
set.seed(02052020)
out.sup <- bootBLB(x = Methylation, ellipses = FALSE)
out <- bootBLB(x = Methylation, sup = FALSE, ellipses = TRUE)
```

**Description**

This function run cross-validation for logistic biplot

**Usage**

```
cv_LogBip(  
  data,  
  k = 0:5,  
  K = 7,  
  method = "MM",  
  type = NULL,  
  plot = TRUE,  
  maxit = NULL  
)
```

**Arguments**

data	Binary matrix.
k	Dimensions to analyze. By default k = 1:3.
K	folds. By default K = 7.
method	Method to be used to estimate the parameters. By default method="MM"
type	For the conjugate-gradients method. Takes value 1 for the Fletcher–Reeves update, 2 for Polak–Ribiere and 3 for Beale–Sorenson.
plot	draw the graph. By default plot=TRUE
maxit	The maximum number of iterations. Defaults to 100 for the gradient methods, and 2000 for MM algorithm.

**Value**

Training error and generalization error for a logistic biplot model.

**Author(s)**

Giovany Babativa <gbativam@gmail.com>

**References**

Bro R and Kjeldahl K and Smilde AK. (2008). Cross-validation of component models: a critical look at current methods. *Analytical and bioanalytical chemistry*. 390(5):1241-1251

Wold S. (1978). Cross-validatory estimation of the number of components in factor and principal components models. *Technometrics*. 20(4):397–405.

**See Also**

[LogBip](#), [pred\\_LB](#), [fitted\\_LB](#), [simBin](#)

**Examples**

```
set.seed(1234)
x <- simBin(n = 100, p = 50, k = 3, D = 0.5, C = 20)
# cross-validation with coordinate descendent MM algorithm
cv_MM <- cv_LogBip(data = x$X, k=0:5, method = "MM", maxit = 1000)

# cross-validation with CG Fletcher-Reeves algorithm
cv_CG <- cv_LogBip(data = x$X, k=0:5, method = "CG", type = 1)

# cross-validation with projection data and block coordinate descending algorithm
cv_PB <- cv_LogBip(data = x$X, k=0:5, method = "PDLB", maxit = 1000)
```

---

fitted\_LB

*Fitted values using Logistic Biplot*

---

**Description**

Compute the predicted matrix or log-odds for a logistic biplot model

**Usage**

```
fitted_LB(object, type = c("link", "response"))
```

**Arguments**

object	BiplotML object
type	the type of fitting required. type = "link" gives output on the logit scale and type = "response" gives output on the probability scale

**Value**

This function returns the predicted matrix or the log-odds of a binary logistic biplot model.

**Author(s)**

Giovany Babativa <gbativam@gmail.com>

## Examples

```
data("Methylation")
LB <- LogBip(Methylation, plot = FALSE)
Theta <- fitted_LB(LB, type = "link")
Pi <- fitted_LB(LB, type = "response")
```

---

gradientDesc

*Gradient function for Binary Logistic Biplot*

---

## Description

This function computes the parameters of A and B in Binary Logistic Biplot under algorithm of Descendent Gradient.

## Usage

```
gradientDesc(
  x,
  k = 2,
  rate = 0.001,
  converg = 0.001,
  max_iter,
  plot = FALSE,
  ...
)
```

## Arguments

x	Binary matrix.
k	Dimensions number. By default k = 2.
rate	The value of the rate of descent $\alpha$ in the algorithm of descending gradient. By default $\alpha = 0.001$ .
converg	Tolerance limit to achieve convergence. By default converg = 0.001
max_iter	Maximum iterations number.
plot	Plot the Logistic Biplot.
...	other arguments

## Details

We note that the Binary Logistic Biplot is defined as:

$$\text{logit}(\pi_{ij}) = \log\left(\frac{\pi_{ij}}{1 - \pi_{ij}}\right) = \mu_j + \sum_{s=1}^k b_{js} a_{is} = \mu_j + \mathbf{a}_i^T \mathbf{b}_j$$

Also, note that the gradient is:

$$\nabla \ell = \left( \frac{\partial \ell}{\partial \mu}, \frac{\partial \ell}{\partial \mathbf{A}}, \frac{\partial \ell}{\partial \mathbf{B}} \right) == ((\mathbf{\Pi} - \mathbf{X})^T, (\mathbf{\Pi} - \mathbf{X})\mathbf{B}, (\mathbf{\Pi} - \mathbf{X})^T \mathbf{A})$$

### Value

The coefficients of A and B matrix.

### Author(s)

Giovany Babativa <gbativam@gmail.com>

### References

Vicente-Villardón, J.L. and Galindo, M. Purificación (2006), *Multiple Correspondence Analysis and related Methods. Chapter: Logistic Biplots*. Chapman-Hall

### See Also

[plotBLB](#), [performanceBLB](#)

### Examples

```
data('Methylation')
set.seed(02052020)
MatGD <- gradientDesc(x = Methylation, k=2, max_iter=10000)
outGD <- gradientDesc(x = Methylation, k=2, max_iter=10000, plot = TRUE)
```

---

LogBip

*Fitting a Binary Logistic Biplot using optimization methods*

---

### Description

This function estimates the vector  $\mu$ , matrix A and matrix B using the optimization algorithm chosen by the user. The PDLB method allows to enter a binary matrix with missing data

### Usage

```
LogBip(
  x,
  k = 2,
  method = "MM",
  type = NULL,
  plot = TRUE,
  maxit = NULL,
  endsegm = 0.9,
  label.ind = FALSE,
  col.ind = NULL,
```

```

draw = c("biplot", "ind", "var"),
random_start = FALSE,
L = 0,
cv_LogBip = FALSE
)

```

### Arguments

x	Binary matrix.
k	Dimensions number. By default k = 2.
method	Method to be used to estimate the parameters. By default method="CG"
type	For the conjugate-gradients method. Takes value 1 for the Fletcher–Reeves update, 2 for Polak–Ribiere and 3 for Beale–Sorenson.
plot	Plot the Bootstrap Logistic Biplot.
maxit	The maximum number of iterations. Defaults to 100 for the gradient methods, and 500 without gradient.
endsegm	The segment starts at 0.5 and ends at this value. By default endsegm = 0.90.
label.ind	By default the row points are not labelled.
col.ind	Color for the rows marks.
draw	The graph to draw ("ind" for the individuals, "var" for the variables and "biplot" for the row and columns coordinates in the same graph)
random_start	Logical value; whether to randomly initialize the parameters. If FALSE, algorithm will use an SVD as starting value.
L	Penalization parameter. By default L = 0.
cv_LogBip	Indicates if the procedure is being used for cross validation.

### Details

The methods that can be used to estimate the parameters of a logistic biplot

- For methods based on the conjugate gradient use method = "CG" and

type = 1 for the Fletcher Reeves; type = 2 for Polak Ribiere; type = 3 for Hestenes Stiefel and type = 4 for Dai Yuan.

- To use the iterative coordinate descendent MM algorithm then method = "MM".

- If the binary matrix X has missing data, use method = "PDLB". In case it's required to estimate the row coordinates of other individuals, this method is also the most appropriate. For more details see the paper "Logistic biplot with missing data".

- To use the BFGS formula, method = "BFGS".

### Value

Coordinates of the matrix A and B, threshold for classification rule. Furthermore, for the PDLB method, the imputed matrix is returned.



**Author(s)**

Giovary Babativa <gbabativam@gmail.com>

**References**

- Babativa-Marquez, J. G., & Vicente-Villardón, J. L. (2022). Logistic biplot with missing data. In Process.
- Babativa-Marquez, J. G., & Vicente-Villardón, J. L. (2021). Logistic Biplot by Conjugate Gradient Algorithms and Iterated SVD. *Mathematics*, 9(16).
- John C. Nash (2011). Unifying Optimization Algorithms to Aid Software System Users: `optimx` for R. *Journal of Statistical Software*. 43(9). 1–14.
- John C. Nash (2014). On Best Practice Optimization Methods in R. *Journal of Statistical Software*. 60(2). 1–14.
- Nocedal, J.; Wright, S. (2006). *Numerical optimization*; Springer Science & Business Media.
- Vicente-Villardón, J.L. and Galindo, M. Purificación (2006), *Multiple Correspondence Analysis and related Methods. Chapter: Logistic Biplots*. Chapman-Hall

**See Also**

[plotBLB](#), [pred\\_LB](#), [fitted\\_LB](#)

**Examples**

```
data("Methylation")
# If the binary matrix has no missing data and does not require the projection
# of supplementary individuals, you can use an coordinate descendent MM algorithm
res_MM <- LogBip(x = Methylation, method = "MM", maxit = 1000)
# If the binary matrix has missing data or requires the projection of supplementary
# individuals, use a method based on data projection with a block coordinate descent algorithm
data("Methylation")
set.seed(12345)
n <- nrow(Methylation)
p <- ncol(Methylation)
miss <- matrix(rbinom(n*p, 1, 0.2), n, p) #I simulate some missing data
miss <- ifelse(miss == 1, NA, miss)
x <- Methylation + miss #Matrix containing missing data
out <- LogBip(x, method = "PDLB", maxit = 1000)
```

---

Methylation

*Binary data set of 48 human cell lines.*

---

**Description**

A dataset containing the BRCA (breast invasive carcinoma) for 48 human cell lines, where each variable is a likely cancer driver or suppressor gene. A gene is labeled as '1' when it is classified as mutated in a sample and as '0' when classified as wild type.

**Usage**

Methylation

**Format**

A data frame with 48 rows and 9 variables:

**GSTM1** Glutathione S-Transferase Mu 1, is a Protein Coding gene  
**C1orf70** Chromosome 1 Open Reading Frame 70, Transmembrane Protein  
**DNM3** Dynamin 3, is a Protein Coding gene  
**THY1** Thy-1 Cell Surface Antigen, is a Protein Coding gene  
**ADCY4** Adenylate Cyclase 4, is a Protein Coding gene  
**GSTT1** Glutathione S-Transferase Theta 1, is a Protein Coding gen  
**FILIP1L** Filamin A Interacting Protein 1 Like, is a Protein Coding gene  
**DUSP22** Dual Specificity Phosphatase 22, is a Protein Coding gene  
**NAPRT1** Nicotinic Acid Phosphoribosyltransferase

**Source**

<https://www.cancerrxgene.org>

---

performanceBLB

*Performance comparison of severals estimation algorithms*

---

**Description**

This function computes the estimates of A and B matrix with severals algorithms.

**Usage**

```
performanceBLB(xi, k = 2, L = 0, method = NULL, maxit = NULL)
```

**Arguments**

<code>xi</code>	Binary matrix.
<code>k</code>	Dimensions number. By default $k = 2$ .
<code>L</code>	Penalization parameter. By default $L = 0$ .
<code>method</code>	use value 1 for algorithms without gradient, 2 with gradient, 3 quasi-newton methods or 4 for all methods. By default <code>method = 2</code> .
<code>maxit</code>	The maximum number of iterations. Defaults to 100 for the gradient methods, and 500 without gradient.

**Details**

This function compare the process time and convergence of different algorithms without gradient, with gradient or quasi-newton method for estimating the parameters in a Binary Logistic Biplot

**Value**

data frame with method, time of process, convergence and number of evaluations

**Author(s)**

Giovany Babativa <gbabativam@gmail.com>

**References**

John C. Nash (2011). Unifying Optimization Algorithms to Aid Software System Users:optimx for R. *Journal of Statistical Software*. 43(9). 1–14.

John C. Nash (2014). On Best Practice Optimization Methods in R. *Journal of Statistical Software*. 60(2). 1–14.

Vicente-Villardón, J.L. and Galindo, M. Purificación (2006), *Multiple Correspondence Analysis and related Methods. Chapter: Logistic Biplots*. Chapman-Hall

**See Also**

[gradientDesc](#)

**Examples**

```
data('Methylation')
set.seed(123456)
##### Gradient Methods
performanceBLB(xi = Methylation)
performanceBLB(xi = Methylation, maxit = 150)

##### Without Gradient Methods
performanceBLB(xi = Methylation, method = 1)
performanceBLB(xi = Methylation, method = 1, maxit = 100)

##### Quasi-Newton Methods
performanceBLB(xi = Methylation, method = 3)
performanceBLB(xi = Methylation, method = 3, maxit = 100)

##### All methods
performanceBLB(x = Methylation, method = 4)
```

plotBLB

*Plot a Binary Logistic Biplot using a BiplotML object***Description**

Plot the bootstrap binary logistic biplot and draw confidence ellipses on the individuals of an object BiplotML.

**Usage**

```
plotBLB(
  x,
  dim = c(1, 2),
  col.ind = NULL,
  col.var = "#0E185F",
  label.ind = FALSE,
  draw = c("biplot", "ind", "var"),
  titles = NULL,
  ellipses = FALSE,
  endsegm = 0.75,
  repel = FALSE,
  xlim = NULL
)
```

**Arguments**

x	Object class BiplotML.
dim	Dimensions plot. By default Dim1 and Dim2.
col.ind	Color for the individuals.
col.var	Color for the variables.
label.ind	By default the row points are not labelled.
draw	The graph to draw ("ind" for the individuals, "var" for the variables and "biplot" for the row and columns coordinates in the same graph)
titles	Title for the Biplot
ellipses	If ellipses=TRUE, draw confidence ellipses around the rows.
endsegm	Represents where the segment of a variable ends on the logit probability scale. By default endsegm=0.75
repel	Repel overlapping text labels.
xylim	vector specifying the minimum and maximum of the x-axis and y-axis. For example, you can use xlim=c(-10, 10).

**Details**

If draw = "ind", then the biplot is plotted only for individuals and if draw = "var" then is plotted only for the variables.

**Value**

Returns the Biplot of the individuals and variables.

**Author(s)**

Giovany Babativa <gbabativam@gmail.com>

**References**

Meulman, J. J., & Heiser, W. J. (1983). The display of bootstrap solutions in multidimensional scaling. Murray Hill, NJ: Bell Laboratories. (Technical memorandum)

Vicente-Villardón, J.L. and Galindo, M. Purificación (2006), *Multiple Correspondence Analysis and related Methods. Chapter: Logistic Biplots*. Chapman-Hall

**See Also**

[bootBLB](#)

**Examples**

```
data("Methylation")
set.seed(123456)
outBLB <- bootBLB(x = Methylation, sup = TRUE, plot=FALSE)
plotBLB(x = outBLB, titles = "Methylation Logistic Biplot", ellipses = FALSE)
plotBLB(x = outBLB, titles = "Methylation LogBiplot", endsegm = 0.95)
plotBLB(x = outBLB, label.ind = TRUE, titles = "Methylation LogBiplot")
```

---

pred\_LB

*Predict logistic biplot and thresholds by variable*

---

**Description**

Predicts the binary matrix and calculates the optimal thresholds per variable that minimize the Balanced Accuracy (BACC)

**Usage**

```
pred_LB(object, x, ncuts = 100)
```

**Arguments**

object	BiplotML object
x	Binary matrix.
ncuts	Number of equidistant cuts between 0 and 1 that will be evaluated. By default ncuts = 100

**Details**

The threshold for each variable is lowered to minimize the Balanced Accuracy (BACC).

$$BACC = \frac{1}{2} \left( \frac{TP}{TP + FN} + \frac{TN}{TN + FP} \right),$$

where TP is the number of true positives, TN is the number of true negatives, FP is the number of false positives and FN is the number of false negatives

**Value**

This function returns the thresholds per variable, the predicted matrix, the confusion matrix and the BACC.

**Examples**

```
data("Methylation")
LB <- LogBip(Methylation, plot = FALSE)
out <- pred_LB(LB, Methylation)
```

---

proj\_LogBip

*Fitting a Binary Logistic Biplot with Missing Data Using Data Projection and a Block Coordinate Descending Algorithm*

---

**Description**

This function impute the missing values of a binary dataset  $X$ , and estimates the vector  $\mu$ , matrix A and matrix B using data projection model with a block coordinate descending algorithm.

**Usage**

```
proj_LogBip(x, k = 2, max_iters = 1000, random_start = FALSE, epsilon = 1e-05)
```

**Arguments**

x	binary matrix.
k	dimensions number. By default k = 2.
max_iters	maximum iterations.
random_start	random initialization
epsilon	convergence criteria

**Value**

Imputed  $X$  matrix and coordinates of the matrix A and B, and  $\mu$

**Author(s)**

Giovany Babativa <gbabativam@gmail.com>

**References**

Babativa-Marquez, J. G., & Vicente-Villardón, J. L. (2022). Logistic biplot with missing data.  
Babativa-Marquez, J. G., & Vicente-Villardón, J. L. (2021). Logistic Biplot by Conjugate Gradient Algorithms and Iterated SVD. *Mathematics*, 9(16).  
Vicente-Villardón, J.L. and Galindo, M. Purificación (2006), *Multiple Correspondence Analysis and related Methods. Chapter: Logistic Biplots*. Chapman-Hall

**See Also**

[cv\\_LogBip](#)

**Examples**

```
data("Methylation")
set.seed(12345)
n <- nrow(Methylation)
p <- ncol(Methylation)
miss <- matrix(rbinom(n*p, 1, 0.2), n, p) #I simulate some missing data
miss <- ifelse(miss == 1, NA, miss)
x <- Methylation + miss #Matrix containing missing data
out <- LogBip(x, method = "PDLB", maxit = 1000)
```

---

sdv\_MM

*Fitting a Binary Logistic Biplot using coordinate descendent MM algorithm*

---

**Description**

This function estimates the vector  $\mu$ , matrix A and matrix B using coordinate descendent MM algorithm.

**Usage**

```
sdv_MM(  
  x,  
  k = 2,  
  iterations = 1000,  
  truncated = TRUE,  
  random = FALSE,  
  epsilon = 1e-04  
)
```

**Arguments**

x	binary matrix.
k	dimensions number. By default k = 2.
iterations	maximum iterations.
truncated	if TRUE, find the k largest singular values and vectors of a matrix.
random	random initialization
epsilon	convergence criteria

**Value**

Coordinates of the matrix A and B, and  $\mu$

**Author(s)**

Giovany Babativa <gbabativam@gmail.com>

**References**

Babativa-Marquez, J. G., & Vicente-Villardón, J. L. (2021). Logistic Biplot by Conjugate Gradient Algorithms and Iterated SVD. *Mathematics*, 9(16).

Vicente-Villardón, J.L. and Galindo, M. Purificación (2006), *Multiple Correspondence Analysis and related Methods. Chapter: Logistic Biplots*. Chapman-Hall

**See Also**

[cv\\_LogBip](#)

**Examples**

```
data("Methylation")
out <- sdv_MM(x = Methylation)
```

---

simBin

*Multivariate binary data*

---

**Description**

Simulate a binary data matrix based on a latent variables model

**Usage**

```
simBin(n, p, k, D, C = 1)
```



**Arguments**

n	number of rows
p	number of columns
k	number of underlying dimensions in the model
D	sparsity control
C	variance control

**Value**

X: binary matrix, P: predicted matrix, Theta: matrix of natural parameters, A: row markers, B: column markers, mu: offset term, D: sparsity level, n: number of rows, p: number of columns

**Author(s)**

Giovany Babativa <gbabativam@gmail.com>

**See Also**

[cv\\_LogBip](#)

**Examples**

```
x <- simBin(n = 100, p = 50, k = 3, D = 0.5)
```

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