

# Package ‘o2plsda’

July 22, 2025

**Type** Package

**Title** Multiomics Data Integration

**Version** 0.0.25

**Description** Provides functions to do 'O2PLS-DA' analysis for multiple omics data integration. The algorithm came from ``O2-PLS, a two-block ( $X \pm Y$ ) latent variable regression (LVR) method with an integral OSC filter" which published by Johan Trygg and Svante Wold at 2003 <[doi:10.1002/cem.775](https://doi.org/10.1002/cem.775)>. 'O2PLS' is a bidirectional multivariate regression method that aims to separate the covariance between two data sets (it was recently extended to multiple data sets) (Löfstedt and Trygg, 2011 <[doi:10.1002/cem.1388](https://doi.org/10.1002/cem.1388)>; Löfstedt et al., 2012 <[doi:10.1016/j.aca.2013.06.026](https://doi.org/10.1016/j.aca.2013.06.026)>) from the systematic sources of variance being specific for each data set separately.

**License** GPL-3

**Imports** Rcpp (>= 1.0.7), dplyr, magrittr, parallel, ggplot2, ggrepel, methods, stats

**Encoding** UTF-8

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**VignetteBuilder** knitr

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**NeedsCompilation** yes

**Repository** CRAN

**Author** Kai Guo [aut, cre],  
Jungk Hur [aut],  
Eva Feldman [aut]

**Maintainer** Kai Guo <[guokai8@gmail.com](mailto:guokai8@gmail.com)>

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---

|          |                                               |
|----------|-----------------------------------------------|
| loadings | <i>Extract the loadings from an O2PLS fit</i> |
|----------|-----------------------------------------------|

---

Description

This function extracts loading parameters from an O2PLS fit  
This function extracts loading parameters from an O2PLS fit

Usage

```
loadings(x, ...)

## S3 method for class 'O2pls'
loadings(x, loading = c("Xjoint", "Yjoint", "Xorth", "Yorth"), ...)
```

Arguments

|         |                                                              |
|---------|--------------------------------------------------------------|
| x       | Object of class O2pls                                        |
| ...     | For consistency                                              |
| loading | the loadings for one of "Xjoint", "Yjoint", "Xorth", "Yorth" |

**Value**

Loading matrix

Loading matrix

---

|                  |                                                            |
|------------------|------------------------------------------------------------|
| loadings.o2plsda | <i>extract the loading value from the O2PLSDA analysis</i> |
|------------------|------------------------------------------------------------|

---

**Description**

extract the loading value from the O2PLSDA analysis

**Usage**

```
## S3 method for class 'o2plsda'  
loadings(x, loading = "Xloading", ...)
```

**Arguments**

|         |                                                              |
|---------|--------------------------------------------------------------|
| x       | Object of class o2plsda                                      |
| loading | the loadings for one of "Xjoint", "Yjoint", "Xorth", "Yorth" |
| ...     | For consistency                                              |

---

|                |                                                          |
|----------------|----------------------------------------------------------|
| loadings.plsda | <i>extract the loading value from the PLSDA analysis</i> |
|----------------|----------------------------------------------------------|

---

**Description**

extract the loading value from the PLSDA analysis

**Usage**

```
## S3 method for class 'plsda'  
loadings(x, ...)
```

**Arguments**

|     |                       |
|-----|-----------------------|
| x   | Object of class plsda |
| ... | For consistency       |

---

`o2cv`*Cross validation for O2PLS*

---

**Description**

Cross validation for O2PLS

**Usage**

```
o2cv(  
  X,  
  Y,  
  nc,  
  nx,  
  ny,  
  group = NULL,  
  nr_folds = 5,  
  ncores = 1,  
  scale = FALSE,  
  center = FALSE  
)
```

**Arguments**

|                       |                                                              |
|-----------------------|--------------------------------------------------------------|
| <code>X</code>        | a Numeric matrix (input)                                     |
| <code>Y</code>        | a Numeric matrix (input)                                     |
| <code>nc</code>       | Integer. Number of joint PLS components.                     |
| <code>nx</code>       | Integer. Number of orthogonal components in X                |
| <code>ny</code>       | Integer. Number of orthogonal components in Y                |
| <code>group</code>    | a vector to indicate the group for Y                         |
| <code>nr_folds</code> | Integer to indicate the folds for cross validation           |
| <code>ncores</code>   | Integer. Number of CPUs to use for cross validation          |
| <code>scale</code>    | boolean values determining if data should be scaled or not   |
| <code>center</code>   | boolean values determining if data should be centered or not |

**Value**

a data frame with the Q and RMSE values

**Author(s)**

Kai Guo

**Examples**

```

set.seed(123)
X = matrix(rnorm(500),50,10)
Y = matrix(rnorm(500),50,10)
X = scale(X, scale = TRUE)
Y = scale(Y, scale = TRUE)
# group factor could be omitted if you don't have any group
group <- rep(c("Ctrl","Treat"), each = 25)
cv <- o2cv(X, Y, 1:2, 1:2, 1:2, group=group, nr_folds = 2, ncores=1)

```

---

|       |                                             |
|-------|---------------------------------------------|
| o2pls | <i>fit O2PLS model with best nc, nx, ny</i> |
|-------|---------------------------------------------|

---

**Description**

fit O2PLS model with best nc, nx, ny

**Usage**

```
o2pls(X, Y, nc, nx, ny, scale = FALSE, center = FALSE)
```

**Arguments**

|        |                                                              |
|--------|--------------------------------------------------------------|
| X      | a Numeric matrix (input)                                     |
| Y      | a Numeric matrix (input)                                     |
| nc     | Integer. Number of joint PLS components.                     |
| nx     | Integer. Number of orthogonal components in X                |
| ny     | Integer. Number of orthogonal components in Y                |
| scale  | boolean values determining if data should be scaled or not   |
| center | boolean values determining if data should be centered or not |

**Value**

An object containing

|          |                       |
|----------|-----------------------|
| Xscore   | Joint X scores        |
| Xloading | Joint X loadings      |
| Yscore   | Joint Y scores        |
| Yloading | Joint Y loadings      |
| TYosc    | Orthogonal X scores   |
| PYosc    | Orthogonal X loadings |
| WYosc    | Orthogonal X weights  |
| UXosc    | Orthogonal Y scores   |
| PXosc    | Orthogonal Y loadings |

|          |                                                                                                                        |
|----------|------------------------------------------------------------------------------------------------------------------------|
| CXosc    | Orthogonal $Y$ weights                                                                                                 |
| BU       | Regression coefficient in $Tt \sim U$                                                                                  |
| BT       | Regression coefficient in $U \sim Tt$                                                                                  |
| Xhat     | Prediction of $X$ with $Y$                                                                                             |
| Yhat     | Prediction of $Y$ with $X$                                                                                             |
| R2Xhat   | Variation of the predicted $X$ as proportion of variation in $X$                                                       |
| R2Yhat   | Variation of the predicted $Y$ as proportion of variation in $Y$                                                       |
| R2X      | Variation of the modeled part in $X$ (defined by Joint + Orthogonal variation) as proportion of total variation in $X$ |
| R2Y      | Variation of the modeled part in $Y$ (defined by Joint + Orthogonal variation) as proportion of total variation in $Y$ |
| R2Xcorr  | Variation of the joint part in $X$                                                                                     |
| R2Ycorr  | Variation of the joint part in $Y$                                                                                     |
| R2Xo     | Variation of the orthogonal part in $X$ as proportion of variation in $X$                                              |
| R2Yo     | Variation of the orthogonal part in $Y$ as proportion of variation in $Y$                                              |
| R2Xp     | Variation in $X$ joint part predicted by $Y$ Joint part                                                                |
| R2Yp     | Variation in $Y$ joint part predicted by $X$ Joint part                                                                |
| varXj    | Variation in each Latent Variable (LV) in $X$ Joint part                                                               |
| varYj    | Variation in each Latent Variable (LV) in $Y$ Joint part                                                               |
| varXorth | Variation in each Latent Variable (LV) in $X$ Orthogonal part                                                          |
| varYorth | Variation in each Latent Variable (LV) in $Y$ Orthogonal part                                                          |
| Exy      | Residuals in $X$                                                                                                       |
| Fxy      | Residuals in $Y$                                                                                                       |

### Author(s)

Kai Guo

### Examples

```
set.seed(123)
X = matrix(rnorm(500), 50, 10)
Y = matrix(rnorm(500), 50, 10)
X = scale(X, scale = TRUE)
Y = scale(Y, scale = TRUE)
fit <- o2pls(X, Y, 1, 2, 2)
summary(fit)
```

---

 o2pls-class

---

*Class "O2pls" This class represents the Annotation information*


---

**Description**

Class "O2pls" This class represents the Annotation information

**Slots**

X a Numeric matrix (input)

Y a Numeric matrix (input)

params paramaters ysed in o2pls analysis

results list of o2pls results

**Author(s)**

Kai Guo

---

 opllda

---

*Orthogonal partial least squares discriminant analysis*


---

**Description**

Computes orthogonal scores partial least squares regressions with the NIPALS algorithm. It return a comprehensive set of pls outputs (e.g. scores and vip).

**Usage**

```
opllda(X, Y, nc, scale = FALSE, center = TRUE, maxiter = 100, tol = 1e-05)
```

**Arguments**

|         |                                                                                             |
|---------|---------------------------------------------------------------------------------------------|
| X       | a O2pls object or a matrix of predictor variables.                                          |
| Y       | a single vector indicate the group                                                          |
| nc      | the number of pls components (the one joint components + number of orthogonal components ). |
| scale   | logical indicating whether X must be scaled (suggest TRUE).                                 |
| center  | boolean values determining if data should be centered or not                                |
| maxiter | maximum number of iterations.                                                               |
| tol     | limit for convergence of the algorithm in the nipals algorithm.                             |

**Value**

a list containing the following elements:

- `nc` the number of components used (one joint components + number of orthogonal components)
- `scores` a matrix of scores corresponding to the observations in `X`, The components retrieved correspond to the ones optimized or specified.
- `Xloadings` a matrix of loadings corresponding to the explanatory variables. The components retrieved correspond to the ones optimized or specified.
- `Yloadings` a matrix of partial least squares loadings corresponding to `Y`
- `vip` the VIP matrix.
- `xvar` a matrix indicating the standard deviation of each component (`sd`), the variance explained by each single component (`explained_var`) and the cumulative explained variance (`cumulative_explained_var`). These values are computed based on the data used to create the projection matrices.
- `projection_matrix` the matrix of projection matrix
- `weight` a matrix of partial least squares ("pls") weights.

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(50),10,5)
Y <- matrix(rnorm(50),10,5)
fit <- o2pls(X,Y,2,1,1)
yy <- rep(c(0,1),5)
fit0 <- oplstda(fit,yy,2)
```

---

plot.O2pls

*Score or loading plot for the O2PLS results*

---

**Description**

Score or loading plot for the O2PLS results

**Usage**

```
## S3 method for class 'O2pls'
plot(
  x,
  type = "score",
  var = "Xjoint",
  group = NULL,
  ind = c(1, 2),
```

```

    color = NULL,
    top = 20,
    ellipse = TRUE,
    order = FALSE,
    pt.size = 3,
    label = TRUE,
    label.size = 4,
    repel = TRUE,
    rotation = FALSE,
    ...
  )

```

### Arguments

|            |                                                            |
|------------|------------------------------------------------------------|
| x          | an O2pls object                                            |
| type       | score or loading                                           |
| var        | specify Xjoint                                             |
| group      | color used for score plot                                  |
| ind        | which components to be used for score plot or loading plot |
| color      | color used for score or loading plot                       |
| top        | the number of largest loading value to plot                |
| ellipse    | TRUE/FALSE                                                 |
| order      | order by the value or not                                  |
| pt.size    | point size                                                 |
| label      | plot label or not (TRUE/FALSE)                             |
| label.size | label size                                                 |
| repel      | use ggrepel to show the label or not                       |
| rotation   | flip the figure or not (TRUE/FALSE)                        |
| ...        | For consistency                                            |

### Value

a ggplot2 object

### Author(s)

Kai Guo

### Examples

```

X <- matrix(rnorm(50),10,5)
Y <- matrix(rnorm(50),10,5)
fit <- o2pls(X,Y,2,1,1)
plot(fit, type="score")

```

---

|              |                                                         |
|--------------|---------------------------------------------------------|
| plot.o2plsda | <i>Score, VIP or loading plot for the O2PLS results</i> |
|--------------|---------------------------------------------------------|

---

### Description

Score, VIP or loading plot for the O2PLS results

### Usage

```
## S3 method for class 'o2plsda'
plot(
  x,
  type = "score",
  group = NULL,
  ind = c(1, 2),
  color = NULL,
  top = 20,
  ellipse = TRUE,
  order = FALSE,
  pt.size = 3,
  label = TRUE,
  label.size = 4,
  repel = FALSE,
  rotation = FALSE,
  ...
)
```

### Arguments

|            |                                                            |
|------------|------------------------------------------------------------|
| x          | an o2plsda object                                          |
| type       | score, vip or loading                                      |
| group      | color used for score plot                                  |
| ind        | which components to be used for score plot or loading plot |
| color      | color used for score or loading plot                       |
| top        | the number of largest loading value to plot                |
| ellipse    | TRUE/FALSE                                                 |
| order      | order by the value or not                                  |
| pt.size    | point size                                                 |
| label      | plot label or not (TRUE/FALSE)                             |
| label.size | label size                                                 |
| repel      | use ggrepel to show the label or not                       |
| rotation   | flip the figure or not (TRUE/FALSE)                        |
| ...        | For consistency                                            |

**Value**

a ggplot2 object

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(50),10,5)
Y <- matrix(rnorm(50),10,5)
fit <- o2pls(X,Y,2,1,1)
yy <- rep(c(0,1),5)
fit0 <- oplstda(fit,yy,2)
plot(fit0, type="score", group = factor(yy))
```

---

plot.plsda

*Score, VIP or loading plot for the plsda results*

---

**Description**

Score, VIP or loading plot for the plsda results

**Usage**

```
## S3 method for class 'plsda'
plot(
  x,
  type = "score",
  group = NULL,
  ind = c(1, 2),
  color = NULL,
  top = 20,
  ellipse = TRUE,
  order = FALSE,
  pt.size = 3,
  label = TRUE,
  label.size = 4,
  repel = FALSE,
  rotation = FALSE,
  ...
)
```

**Arguments**

|            |                                                            |
|------------|------------------------------------------------------------|
| x          | an plsda object                                            |
| type       | score, vip or loading                                      |
| group      | color used for score plot                                  |
| ind        | which components to be used for score plot or loading plot |
| color      | color used for score or loading plot                       |
| top        | the number of largest loading value to plot                |
| ellipse    | TRUE/FALSE                                                 |
| order      | order by the value or not                                  |
| pt.size    | point size                                                 |
| label      | plot label or not (TRUE/FALSE)                             |
| label.size | label size                                                 |
| repel      | use ggrepel to show the label or not                       |
| rotation   | flip the figure or not (TRUE/FALSE)                        |
| ...        | For consistency                                            |

**Value**

a ggplot2 object

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),each=5)
fit0 <- plsda(X,Y,2)
plot(fit0, type = "score", group = factor(Y))
```

---

plsda

*Partial least squares discriminant analysis*

---

**Description**

Perform a PLS discriminant analysis

**Usage**

```
plsda(X, Y, nc, scale = TRUE, center = TRUE, cv = TRUE, nr_folds = 5)
```

**Arguments**

|          |                                                                                             |
|----------|---------------------------------------------------------------------------------------------|
| X        | a matrix of predictor variables.                                                            |
| Y        | a single vector indicate the group                                                          |
| nc       | the number of pls components (the one joint components + number of orthogonal components ). |
| scale    | logical indicating whether X must be scaled (suggest TRUE).                                 |
| center   | logical indicating whether X must be centered (suggest TRUE).                               |
| cv       | logical indicating whether cross-validation will be performed or not (suggest TRUE).        |
| nr_folds | nr_folds Integer to indicate the folds for cross validation.                                |

**Value**

a list containing the following elements:

- nc the number of components used(one joint components + number of orthogonal components
- scores a matrix of scores corresponding to the observations in X, The components retrieved correspond to the ones optimized or specified.
- Xloadings a matrix of loadings corresponding to the explanatory variables. The components retrieved correspond to the ones optimized or specified.
- vip the VIP matrix.
- xvar variance explained of X by each single component.
- R2Y variance explained of Y by each single component.
- PRESS The residual sum of squares for the samples which were not used to fit the model
- Q2 quality of cross-validation

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),each=5)
fit <- plsda(X,Y,2)
```

---

`print.o2pls`*Print the summary of O2PLS results.*

---

**Description**

Print the summary of O2PLS results.

**Usage**

```
## S3 method for class 'o2pls'  
print(x, ...)
```

**Arguments**

|                  |                 |
|------------------|-----------------|
| <code>x</code>   | An O2pls object |
| <code>...</code> | For consistency |

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(50),10,5)  
Y <- matrix(rnorm(50),10,5)  
object <- o2pls(X,Y,1,1,1)  
print(object)
```

---

`print.plsda`*Print the summary of plsda results.*

---

**Description**

Print the summary of plsda results.

**Usage**

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

**Arguments**

|                  |                 |
|------------------|-----------------|
| <code>x</code>   | An plsda object |
| <code>...</code> | For consistency |

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),each=5)
fit <- plsda(X,Y,2)
print(fit)
```

scores

*Extract the scores from an O2PLS fit***Description**

This function extracts score matrices from an O2PLS fit

**Usage**

```
scores(x, ...)
```

**Arguments**

|     |                       |
|-----|-----------------------|
| x   | Object of class O2pls |
| ... | For consistency       |

**Value**

Scores matrix

scores.O2pls

*Extract the scores from an O2PLS fit***Description**

This function extracts scores parameters from an O2PLS fit

**Usage**

```
## S3 method for class 'O2pls'
scores(x, score = c("Xjoint", "Yjoint", "Xorth", "Yorth"), ...)
```

**Arguments**

|       |                                                                   |
|-------|-------------------------------------------------------------------|
| x     | Object of class O2pls                                             |
| score | the scores matrix for one of "Xjoint", "Yjoint", "Xorth", "Yorth" |
| ...   | Other arguments                                                   |

**Value**

score matrix

---

|                |                                                     |
|----------------|-----------------------------------------------------|
| scores.o2plsda | <i>Extract the scores from an O2PLS DA analysis</i> |
|----------------|-----------------------------------------------------|

---

**Description**

Extract the scores from an O2PLS DA analysis

**Usage**

```
## S3 method for class 'o2plsda'  
scores(x, ...)
```

**Arguments**

x                    Object of class o2plsda  
...                  Other arguments

**Value**

score matrix

**Author(s)**

Kai Guo

---

|              |                                          |
|--------------|------------------------------------------|
| scores.plsda | <i>Extract the scores PLSDA analysis</i> |
|--------------|------------------------------------------|

---

**Description**

Extract the scores PLSDA analysis

**Usage**

```
## S3 method for class 'plsda'  
scores(x, ...)
```

**Arguments**

x                    Object of class plsda  
...                  Other arguments

**Value**

score matrix

**Author(s)**

Kai Guo

---

summary.o2pls

*Summary of an O2PLS object*

---

**Description**

Summary of an O2PLS object

**Usage**

```
## S3 method for class 'O2pls'  
summary(object, ...)
```

**Arguments**

|        |                 |
|--------|-----------------|
| object | a O2pls object  |
| ...    | For consistency |

**Value**

Detail of O2PLS results

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(50),10,5)  
Y <- matrix(rnorm(50),10,5)  
object <- o2pls(X,Y,1,1,1)  
summary(object)
```

---

|               |                                   |
|---------------|-----------------------------------|
| summary.plsda | <i>Summary of an plsda object</i> |
|---------------|-----------------------------------|

---

**Description**

Summary of an plsda object

**Usage**

```
## S3 method for class 'plsda'
summary(object, ...)
```

**Arguments**

|        |                 |
|--------|-----------------|
| object | a plsda object  |
| ...    | For consistency |

**Value**

Detail of plsda results

**Author(s)**

Kai Guo

**Examples**

```
X <- matrix(rnorm(500),10,50)
Y <- rep(c("a","b"),each=5)
fit <- plsda(X,Y,2)
summary(fit)
```

---

|     |                                                        |
|-----|--------------------------------------------------------|
| vip | <i>Extract the VIP values from the O2PLS-DA object</i> |
|-----|--------------------------------------------------------|

---

**Description**

Extract the VIP values from the O2PLS-DA object

**Usage**

```
vip(x)
```

**Arguments**

|   |                                    |
|---|------------------------------------|
| x | the o2plsda object or plsda object |
|---|------------------------------------|

*vip*

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**Value**

a data frame

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