Package: NPLStoolbox (via r-universe)

May 28, 2026

Title N-Way Partial Least Squares Modelling of Multi-Way Data

Version 1.1.0.9000

Description Creation and selection of N-way Partial Least Squares (NPLS) models. Selection of the optimal number of components can be done using ncrossreg(). NPLS was originally described by Rasmus Bro, see <doi:10.1002/%28SICI%291099-128X%28199601%2910%3A1%3C47%3A%3AAID-CEM400%3E3.0.CO%3B2-C>.

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Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

Imports dplyr, parafac4microbiome, pracma, rTensor, stats

Depends R (>= 2.10)

LazyData true

Suggests CMTFtoolbox, ggpattern, ggplot2, ggpubr, knitr, readr, rmarkdown, scales, stringr, testthat (>= 3.0.0), tidyr

Config/testthat/edition 3

URL `https://github.com/GRvanderPloeg/NPLStoolbox`, `https://grvanderploeg.com/NPLStoolbox/`

BugReports `https://github.com/GRvanderPloeg/NPLStoolbox/issues`

VignetteBuilder knitr

Config/pak/sysreqs cmake make libicu-dev

Repository https://grvanderploeg.r-universe.dev

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RemoteUrl https://github.com/grvanderploeg/nplstoolbox

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Contents

`Cornejo2025` *Cornejo2025 longitudinal dataset measured in transgender persons*

Description

The Cornejo2025 longitudinal dataset as three-dimensional arrays, with subjects in mode 1, features in mode 2 and time in mode 3.

Usage

```
Cornejo2025
```

Format

'Cornejo2025':
A list object with seven elements:

Tongue_microbiome List object of the tongue longitudinal microbiota data.
Salivary_microbiome List object of the saliva longitudinal microbiota data.
Salivary_cytokines List object of the longitudinal salivary cytokine data.
Salivary_biochemistry List object of the longitudinal salivary biochemistry data.
Circulatory_hormones List object of the longitudinal circulatory hormone data.
Clinical_measurements List object of the longitudinal clinical outcome data.
Subject_metadata Matrix with subject metadata.

Source

TBD

`Jakobsen2025` *Jakobsen2025 longitudinal dataset measured in mother-infant dyads*

Description

The Jakobsen2025 longitudinal dataset as three-dimensional arrays, with subjects in mode 1, features in mode 2 and time in mode 3.

Usage

```
Jakobsen2025
```

Format

'Jakobsen2025':

A list object with seven elements:

faeces List object of the longitudinal infant faecal microbiota data.

milkMicrobiome List object of the longitudinal HM microbiota data.

milkMetabolomics List object of the longitudinal salivary cytokine data.

Source

TBD

`ncrossreg` *Cross-validation of NPLS by classical K-fold CV.*

Description

This function runs ACMTF-R with cross-validation. A deterministic K–fold partition is used: the subjects are split in order into `cvFolds` groups. For each fold the training set consists of the other folds and the test set is the current fold.

Usage

```
ncrossreg(X, y, maxNumComponents = 5, maxIter = 120, cvFolds = dim(X)[1])
```

Arguments

`X`	Centered tensor of independent data
`y`	Centered dependent variable
`maxNumComponents`	Maximum number of components to investigate (default 5).
`maxIter`	Maximum number of iterations (default 100).

`cvFolds`	Number of folds to use in the cross-validation. For example, if `cvFolds` is 5, then the subjects are deterministically partitioned into 5 groups (each CV iteration uses 4/5 for training and 1/5 for testing). Default: equal to the number of subjects (i.e. jack-knifing).

Value

A list with two elements: - **varExp**: a tibble with the variance–explained (for X and Y) per number of components. - **RMSE**: a tibble with the RMSE (computed over the unified CV prediction vector) per number of components.

Examples

```
set.seed(123)
X <- array(rnorm(25 * 5 * 4), dim = c(25, 5, 4))
y <- rnorm(25)  # Random response variable
result = ncrossreg(X, y, cvFolds=2, maxNumComponents=2)
```

`npred` *Predict Y for new data by projecting the data onto the latent space defined by an NPLS model.*

Description

Predict Y for new data by projecting the data onto the latent space defined by an NPLS model.

Usage

```
npred(model, newX)
```

Arguments

`model`	NPLS model
`newX`	New data organized in a matrix of (Inew x J x K) with Inew new subjects

Value

Ypred: vector of the predicted value(s) of Y for the new data

Examples

```
Y = as.numeric(as.factor(Cornejo2025$Tongue$mode1$GenderID))
Ycnt = Y - mean(Y)
model = triPLS1(Cornejo2025$Tongue$data, Ycnt, numComponents=1)
npred(model, Cornejo2025$Tongue$data[1,,])
```

`triPLS1` *Tri-PLS1: three-way PLS regressed onto a y vector*

Description

Tri-PLS1: three-way PLS regressed onto a y vector

Usage

```
triPLS1(X, y, numComponents, tol = 1e-10, maxIter = 100)
```

Arguments

`X`	Centered tensor of independent data
`y`	Centered dependent variable
`numComponents`	Number of components to fit
`tol`	Relative change in loss for the model to converge (default 1e-10).
`maxIter`	Maximum number of iterations (default 100).

Value

Model

Examples

```
set.seed(123)
X <- array(rnorm(100 * 5 * 4), dim = c(100, 5, 4))  # Random tensor (100 samples, 5 vars, 4 vars)
y <- rnorm(100)  # Random response variable
model <- triPLS1(X, y, numComponents = 2)
```

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