

Package ‘missPLS’

April 30, 2026

Type Package

Title Methods and Reproducible Workflows for Partial Least Squares with Missing Data

Version 0.2.1

Date 2026-04-07

Depends R (>= 4.1.0)

Imports mice, plsRglm, stats, utils, VIM

Suggests bcv, knitr, mlbench, plsdo, rmarkdown, testthat (>= 3.0.0)

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Description Methods-first tooling for reproducing and extending the partial least squares regression studies on incomplete data described in Nengsih et al. (2019) <[doi:10.1515/sagmb-2018-0059](https://doi.org/10.1515/sagmb-2018-0059)>. The package provides simulation helpers, missingness generators, imputation wrappers, component-selection utilities, real-data diagnostics, and reproducible study orchestration for Nonlinear Iterative Partial Least Squares (NIPALS)-Partial Least Squares (PLS) workflows.

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Encoding UTF-8

LazyData true

VignetteBuilder knitr

Config/testthat/edition 3

RoxygenNote 7.3.3

URL <https://fbertran.github.io/missPLS/>,
<https://github.com/fbertran/missPLS>

BugReports <https://github.com/fbertran/missPLS/issues>

NeedsCompilation no

Repository CRAN

Date/Publication 2026-04-30 07:50:09 UTC

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add_missingness	<i>Add missing values to a predictor matrix</i>
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Description

Create MCAR or MAR missingness on the predictor matrix x . Missingness is generated column-wise so that each predictor receives approximately the same missing-data proportion, matching the simulation strategy used in the original work.

Usage

```
add_missingness(
  x,
  y,
  mechanism = c("MCAR", "MAR"),
  missing_prop,
  seed = NULL,
  mar_y_bias = 0.8
)
```

Arguments

<code>x</code>	Predictor matrix or data frame.
<code>y</code>	Numeric response vector.
<code>mechanism</code>	Missingness mechanism: "MCAR" or "MAR".
<code>missing_prop</code>	Missing-data proportion as a fraction (0.05) or a percentage (5).
<code>seed</code>	Optional random seed. If supplied, it is used only for this call.
<code>mar_y_bias</code>	Proportion of missing values assigned to the upper half of the observed y values under the MAR mechanism.

Value

A list with components `x_incomplete`, `missing_mask`, `missing_prop`, `mechanism`, and `seed`.

Examples

```
sim <- simulate_pls_data(n = 20, p = 10, true_ncomp = 2, seed = 1)
miss <- add_missingness(sim$x, sim$y, mechanism = "MCAR", missing_prop = 10, seed = 2)
mean(is.na(miss$x_incomplete))
```

bromhexine

Bromhexine dataset

Description

Bromhexine in pharmaceutical syrup used in the article and thesis.

Usage

```
bromhexine
```

Format

A `misspls_dataset` list with components:

name Dataset name.

x A numeric 23 × 64 predictor matrix.

y A numeric response vector of length 23.

data A data frame with response `y` and predictors `x1` to `x64`.

source A short source reference.

preprocessing Dataset preprocessing notes.

notes Additional study notes.

Source

Goicoechea and Olivieri (1999a), calibration and test files bundled in `extra_docs/pls_data`.

diagnose_real_data *Diagnose a real dataset*

Description

Compute correlation summaries and VIF-style diagnostics for a packaged real dataset.

Usage

```
diagnose_real_data(dataset, cor_threshold = 0.7)
```

Arguments

`dataset` A packaged dataset name or `misspls_dataset` object.
`cor_threshold` Absolute-correlation threshold used when reporting predictor pairs and predictor-response associations.

Value

A list with correlation and VIF summaries.

Examples

```
diag_bromhexine <- diagnose_real_data("bromhexine")  
names(diag_bromhexine)
```

impute_pls_data *Impute a predictor matrix*

Description

Apply one of the imputation strategies used in the article and thesis.

Usage

```
impute_pls_data(  
  x,  
  method = c("mice", "knn", "svd"),  
  seed = NULL,  
  m,  
  k = 15L,  
  svd_rank = 10L,  
  svd_maxiter = 1000L  
)
```

Arguments

<code>x</code>	Incomplete predictor matrix or data frame.
<code>method</code>	Imputation method: "mice", "knn", or "svd".
<code>seed</code>	Optional random seed forwarded to stochastic imputers when supported.
<code>m</code>	Number of imputations for method = "mice". By default this is set to the missing-data percentage rounded to the nearest integer.
<code>k</code>	Number of neighbours for method = "knn".
<code>svd_rank</code>	Target rank for method = "svd".
<code>svd_maxiter</code>	Maximum number of iterations for the fallback SVD routine.

Value

A `misspls_imputation` object.

Examples

```
sim <- simulate_pls_data(n = 20, p = 10, true_ncomp = 2, seed = 1)
miss <- add_missingness(sim$x, sim$y, mechanism = "MCAR", missing_prop = 10, seed = 2)
imp <- impute_pls_data(miss$x_incomplete, method = "knn", seed = 3)
length(imp$datasets)
```

octane	<i>Octane dataset</i>
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Description

Octane in gasoline from NIR data used in the article and thesis.

Usage

```
octane
```

Format

A `misspls_dataset` list with components:

name Dataset name.

x A numeric 68 x 493 predictor matrix.

y A numeric response vector of length 68.

data A data frame with response `y` and predictors `x1` to `x493`.

source A short source reference.

preprocessing Dataset preprocessing notes.

notes Additional study notes.

Source

Goicoechea and Olivieri (2003), calibration and test files bundled in `extra_docs/pls_data`.

ozone_complete	<i>Complete-case ozone dataset</i>
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Description

Los Angeles ozone pollution complete-case dataset used in the article and thesis.

Usage

ozone_complete

Format

A `misspls_dataset` list with components:

name Dataset name.

x A numeric 203 x 12 predictor matrix.

y A numeric response vector of length 203.

data A data frame with response `y` and predictors `x1` to `x12`.

source A short source reference.

preprocessing Dataset preprocessing notes.

notes Additional study notes.

Source

`m1bench::Ozone`, restricted to the 203 complete observations used in the published analysis.

run_real_data_study	<i>Run a real-data study</i>
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Description

Run a real-data study

Usage

```
run_real_data_study(
  dataset,
  seed = NULL,
  missing_props = seq(5, 50, 5),
  mechanisms = c("MCAR", "MAR"),
  reps = 1L,
  baseline_reps = 100L,
  max_ncomp = 12L,
```

```

criteria = c("Q2-L00", "Q2-10fold", "AIC", "AIC-DoF", "BIC", "BIC-DoF"),
incomplete_methods = c("nipals_standard", "nipals_adaptative"),
imputation_methods = c("mice", "knn", "svd"),
folds = 10L,
mar_y_bias = 0.8
)

```

Arguments

dataset	A packaged dataset name or <code>misspls_dataset</code> object.
seed	Optional base random seed.
missing_props	Missing-data proportions as fractions or percentages.
mechanisms	Missing-data mechanisms.
reps	Number of replicate missingness draws for each mechanism and proportion.
baseline_reps	Number of repeated complete-data Q2-10fold selections used to determine t^{**} .
max_ncomp	Maximum number of extracted components.
criteria	Criteria evaluated on incomplete and imputed data.
incomplete_methods	Incomplete-data NIPALS workflows.
imputation_methods	Imputation methods.
folds	Number of folds used by "Q2-10fold".
mar_y_bias	MAR bias parameter passed to <code>add_missingness()</code> .

Value

A data frame with one row per study run.

run_simulation_study *Run a simulation study*

Description

Run the simulation workflows used in the article and thesis.

Usage

```

run_simulation_study(
  dimensions = list(c(500L, 100L), c(500L, 20L), c(100L, 20L), c(80L, 25L), c(60L, 33L),
    c(40L, 50L), c(20L, 100L)),
  true_ncomp = c(2L, 4L, 6L),
  missing_props = seq(5, 50, 5),
  mechanisms = c("MCAR", "MAR"),
  reps = 1L,

```

```

seed = NULL,
max_ncomp = 8L,
criteria = c("Q2-L00", "Q2-10fold", "AIC", "AIC-DoF", "BIC", "BIC-DoF"),
incomplete_methods = c("nipals_standard", "nipals_adaptative"),
imputation_methods = c("mice", "knn", "svd"),
folds = 10L,
mar_y_bias = 0.8
)

```

Arguments

dimensions	List of (n, p) integer pairs.
true_ncomp	Vector of true component counts.
missing_props	Missing-data proportions as fractions or percentages.
mechanisms	Missing-data mechanisms.
reps	Number of replicates.
seed	Optional base random seed.
max_ncomp	Maximum number of extracted components.
criteria	Criteria evaluated on complete and imputed data.
incomplete_methods	Incomplete-data NIPALS workflows.
imputation_methods	Imputation methods.
folds	Number of folds used by "Q2-10fold".
mar_y_bias	MAR bias parameter passed to add_missingness() .

Value

A data frame with one row per study run.

select_ncomp	<i>Select the number of PLS components</i>
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Description

Select the number of components for complete, imputed, or incomplete-data PLS workflows.

Usage

```

select_ncomp(
  x,
  y,
  method = c("complete", "nipals_standard", "nipals_adaptative"),
  criterion = c("Q2-L00", "Q2-10fold", "AIC", "AIC-DoF", "BIC", "BIC-DoF"),

```

```

    max_ncomp,
    seed = NULL,
    folds = 10L,
    threshold = 0.0975
  )

```

Arguments

x	Predictor matrix, dataset object, or <code>misspls_imputation</code> object.
y	Numeric response vector. This may be omitted when x already contains a response.
method	Selection workflow: "complete", "nipals_standard", or "nipals_adaptative".
criterion	Selection criterion: "Q2-L00", "Q2-10fold", "AIC", "AIC-DoF", "BIC", or "BIC-DoF".
max_ncomp	Maximum number of components to consider.
seed	Optional random seed used by the cross-validation and imputation aggregation steps.
folds	Number of cross-validation folds used by "Q2-10fold".
threshold	Threshold applied to Q2 criteria.

Value

A one-row data frame describing the selected component count.

Examples

```

sim <- simulate_pls_data(n = 25, p = 10, true_ncomp = 2, seed = 1)
select_ncomp(sim$x, sim$y, method = "complete", criterion = "AIC", max_ncomp = 4, seed = 2)

```

simulate_pls_data	<i>Simulate PLS data</i>
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Description

Simulate a univariate-response PLS dataset using the Li et al.-style generator available in `plsRglm`.

Usage

```
simulate_pls_data(n, p, true_ncomp, seed = NULL, model = "li2002")
```

Arguments

n	Number of observations.
p	Number of predictors.
true_ncomp	True number of latent components.
seed	Optional random seed. If supplied, it is used only for this call.
model	Simulation model. Only "li2002" is currently supported.

Value

A list with components `x`, `y`, `data`, `true_ncomp`, `seed`, and `model`.

Examples

```
sim <- simulate_pls_data(n = 20, p = 10, true_ncomp = 2, seed = 42)
str(sim)
```

`summarize_simulation_study`

Summarize simulation or real-data study results

Description

Summarize simulation or real-data study results

Usage

```
summarize_simulation_study(results)
```

Arguments

`results` A results data frame returned by `run_simulation_study()` or `run_real_data_study()`.

Value

A grouped summary data frame.

Examples

```
sim_results <- run_simulation_study(
  dimensions = list(c(30, 12)),
  true_ncomp = 2,
  missing_props = numeric(0),
  mechanisms = character(0),
  reps = 2,
  seed = 1
)
summarize_simulation_study(sim_results)
```

tetracycline	<i>Tetracycline dataset</i>
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Description

Tetracycline in serum used in the article and thesis.

Usage

```
tetracycline
```

Format

A `misspls_dataset` list with components:

name Dataset name.

x A numeric 107×101 predictor matrix.

y A numeric response vector of length 107.

data A data frame with response `y` and predictors `x1` to `x101`.

source A short source reference.

preprocessing Dataset preprocessing notes.

notes Additional study notes.

Source

Goicoechea and Olivieri (1999b), calibration and test files bundled in `extra_docs/pls_data`.

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