Package: pharmax.ml (via r-universe)

May 27, 2026

Title R-Native Machine Learning Helpers for Pharmacometrics

Version 0.3.0.9000

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Description R-native machine learning helpers for exploratory pharmacometric workflows. Includes covariate screening, conformal prediction intervals, explainability helpers, data quality checks, ensemble summaries, synthetic benchmarks, calibration summaries, and bounded evidence summaries.

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URL https://github.com/pharmax-org/pharmax, https://pharmax-org.github.io/pharmax

BugReports https://github.com/pharmax-org/pharmax/issues

Depends R (>= 4.1.0)

Imports cli (>= 3.6.0), dplyr (>= 1.1.0), ggplot2 (>= 3.5.0), glmnet (>= 4.1), purrr, ranger (>= 0.16.0), rlang (>= 1.1.0), stats, tibble

Suggests testthat (>= 3.0.0), withr, knitr, rmarkdown

Config/testthat/edition 3

VignetteBuilder knitr

Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.3

Repository https://pharmax-org.r-universe.dev

Date/Publication 2026-05-27 07:41:18 UTC

RemoteUrl https://github.com/pharmax-org/pharmax

RemoteRef HEAD

RemoteSha ec769714bbb5ce973aed6b7020fdbac45f81df95

RemoteSubdir packages/pharmax.ml

Contents

`plot.pharmax_conformal_calibration`
Plot conformal calibration intervals

Description

Plot conformal calibration intervals

Usage

```
## S3 method for class 'pharmax_conformal_calibration'
plot(x, ...)
```

Arguments

`x`	A `pharmax_conformal_calibration` object.
`...`	Unused.

Value

A ggplot2 object.

plot.pharmax_covariate *Plot covariate screening results*

Description

Plot covariate screening results

Usage

```
## S3 method for class 'pharmax_covariate'
plot(x, ...)
```

Arguments

x	A pharmax_covariate object.
...	Unused.

Value

A ggplot2 object.

px_benchmark_covariate *Benchmark covariate screening on synthetic scenarios*

Description

Benchmark covariate screening on synthetic scenarios

Usage

```
px_benchmark_covariate(
  scenarios = c("known_signal", "no_signal", "correlated", "missingness"),
  replicates = 5L,
  n = 120L,
  method = "auto",
  n_top = 5L,
  seed = 2026L
)
```

Arguments

scenarios	Scenario names passed to px_simulate_covariates().
replicates	Number of replicates per scenario.
n	Number of rows per replicate.
method	Screening method passed to px_covariate().
n_top	Number of top covariates to retain.
seed	Random seed.

Value

A pharmax_covariate_benchmark object.

---

px_bootstrap_uq *Bootstrap prediction uncertainty*

Description

Bootstrap prediction uncertainty

Usage

```
px_bootstrap_uq(truth, prediction, n_boot = 200L, alpha = 0.1, seed = 42L)
```

Arguments

truth	Observed outcomes.
prediction	Point predictions.
n_boot	Number of bootstrap replicates.
alpha	Miscoverage rate.
seed	Random seed.

Value

A pharmax_bootstrap_uq object.

`px_calibrate_conformal` *Calibrate conformal interval coverage*

Description

Calibrate conformal interval coverage

Usage

```
px_calibrate_conformal(truth, lower, upper, prediction = NULL, alpha = NULL)
```

Arguments

`truth`	Observed values.
`lower`	Lower interval bounds.
`upper`	Upper interval bounds.
`prediction`	Optional point predictions.
`alpha`	Optional target miscoverage rate.

Value

A `pharmax_conformal_calibration` object.

`px_conformal` *Conformal prediction intervals*

Description

Conformal prediction intervals

Usage

```
px_conformal(
  truth,
  prediction,
  new_prediction,
  alpha = 0.1,
  method = c("split", "cross", "jackknife_plus")
)
```

Arguments

`truth`	Observed values in the calibration set.
`prediction`	Predicted values in the calibration set.
`new_prediction`	Predicted values for new observations.
`alpha`	Miscoverage rate.
`method`	Conformal method. `"split"` is fully implemented; `"cross"` and `"jackknife_plus"` return conservative split-style intervals in this public proof slice.

Value

A tibble with predictions and conformal interval bounds.

`px_covariate` *ML covariate screening*

Description

Screens covariates against pharmacometric parameter columns using R-native methods.

Usage

```
px_covariate(
  data,
  covariates = NULL,
  parameters = NULL,
  method = c("auto", "rf", "elastic_net", "lasso", "aalasso", "cor"),
  n_top = 10L,
  seed = 42L
)
```

Arguments

`data`	Data frame containing parameter and covariate columns.
`covariates`	Covariate column names. Auto-detects `COV_` columns when `NULL`.
`parameters`	Parameter column names. Auto-detects `ETA_`, `EBE_`, or `PARAM_`.
`method`	One of `"auto"`, `"rf"`, `"elastic_net"`, `"lasso"`, `"aalasso"`, or `"cor"`.
`n_top`	Number of top covariates per parameter.
`seed`	Random seed.

Value

A `pharmax_covariate` object.

px_data_quality *Assess ML data quality*

Description

Assess ML data quality

Usage

```
px_data_quality(
  data,
  impute = c("none", "median", "knn", "rf"),
  outlier = c("none", "iqr", "isolation"),
  reduce = c("none", "pca"),
  cluster = FALSE
)
```

Arguments

`data`	Data frame.
`impute`	Imputation strategy: `"none"`, `"median"`, `"knn"`, or `"rf"`.
`outlier`	Outlier strategy: `"none"`, `"iqr"`, or `"isolation"`.
`reduce`	Dimensionality reduction: `"none"` or `"pca"`.
`cluster`	Whether to add a simple cluster summary.

Value

A list with cleaned data and quality summaries.

px_ensemble *Ensemble predictions*

Description

Ensemble predictions

Usage

```
px_ensemble(
  ...,
  weights = NULL,
  newdata = NULL,
  method = c("average", "weighted", "stacking")
)
```

Arguments

...	Numeric prediction vectors or a data frame of predictions.
weights	Optional numeric weights.
newdata	Optional data used when inputs are fitted models.
method	Ensemble method: "average", "weighted", or "stacking".

Value

Numeric vector of ensemble predictions with a pharmax_ensemble class.

---

px_explain *Explain a fitted model with permutation importance*

Description

Explain a fitted model with permutation importance

Usage

```
px_explain(
  model,
  data,
  truth = NULL,
  metric = c("rmse"),
  method = c("permutation", "pdp", "ice"),
  seed = 42L
)
```

Arguments

model	Fitted model with a predict() method.
data	Data frame of predictors.
truth	Observed outcome.
metric	Loss metric, currently "rmse".
method	Explanation method: "permutation", "pdp", or "ice".
seed	Random seed.

Value

Tibble of feature importance values.

px_ml_report *Create an ML decision-support report object*

Description

Create an ML decision-support report object

Usage

```
px_ml_report(
  screen,
  quality = NULL,
  calibration = NULL,
  benchmark = NULL,
  context = list()
)
```

Arguments

screen	A pharmax_covariate object.
quality	Optional pharmax_data_quality object.
calibration	Optional pharmax_conformal_calibration object.
benchmark	Optional pharmax_covariate_benchmark object.
context	Optional named list describing the context of use.

Value

A pharmax_ml_report object.

px_simulate_covariates *Simulate synthetic covariate benchmark data*

Description

Simulate synthetic covariate benchmark data

Usage

```
px_simulate_covariates(
  n = 120L,
  scenario = c("known_signal", "no_signal", "correlated", "missingness"),
  seed = 2026L,
  signal = 0.75,
  noise = 0.3
)
```

Arguments

n	Number of rows.
scenario	Scenario: "known_signal", "no_signal", "correlated", or "missingness".
seed	Random seed.
signal	Signal strength for known-signal scenarios.
noise	Residual noise standard deviation.

Value

A data frame with COV_ covariates and ETA_ parameters.

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