Package: ml (via r-universe)

June 2, 2026

Title Supervised Learning with Mandatory Splits and Seeds

Version 1.0.0

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Description Implements the split-fit-evaluate-assess workflow from Hastie, Tibshirani, and Friedman (2009, ISBN:978-0-387-84857-0) ``The Elements of Statistical Learning'', Chapter 7. Provides three-way data splitting with automatic stratification, mandatory seeds for reproducibility, automatic data type handling, and 10 algorithms out of the box. Uses 'Rust' backend for cross-language deterministic splitting. Designed for tabular supervised learning with minimal ceremony. Polyglot parity with the 'Python' 'mlw' package on 'PyPI'.

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SystemRequirements Cargo ('Rust' package manager), rustc (>= 1.56.0, optional)

Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.3

URL https://github.com/epagogy/ml, https://epagogy.ai

BugReports https://github.com/epagogy/ml/issues

Depends R (>= 4.1.0)

Imports cli, rlang, stats, utils, withr

Suggests testthat (>= 3.0.0), xgboost (>= 2.0.0), ranger, rpart, e1071, kknn, glmnet, naivebayes, lightgbm, tm, tibble, knitr, rmarkdown, caret, rsample

Config/testthat/edition 3

VignetteBuilder knitr

Config/pak/sysreqs libclang-dev

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

Date/Publication 2026-04-03 17:52:15 UTC

RemoteUrl https://github.com/epagogy/ml

RemoteRef HEAD

RemoteSha 733303866ecba86ab83fdbd7ef3e7b8d2a24bf1f

RemoteSubdir r

Contents

`ml` *The ml module — all verbs accessed via ml$verb()*

Description

Provides the module-style interface `ml$verb()` as an alternative to the standard `ml_verb()` function style. Both styles are equivalent and call the same underlying implementation.

Usage

```
ml
```

Format

A locked environment with 22 verb entries.

Details

Note: `ml$fit(...)` and `ml_fit(...)` produce identical results.

Examples

```
s <- ml$split(iris, "Species", seed = 42)
model <- ml$fit(s$train, "Species", seed = 42)
ml$evaluate(model, s$valid)
```

ml_algorithms *List available ML algorithms*

Description

Returns a data.frame showing which algorithms support classification and regression, and which require optional packages.

Usage

```
ml_algorithms(task = NULL)
```

Arguments

task	Optional filter: "classification" or "regression"

Value

A data.frame with columns: algorithm, classification, regression, optional_dep, installed

Examples

```
ml_algorithms()
ml_algorithms(task = "classification")
```

ml_assess *Assess model on held-out test data (do once)*

Description

The final exam — separate from `ml_evaluate()` to force a conscious choice. Errors if called more than once on the same model. Use `s$test` (not `s$valid`) for the test data.

Usage

```
ml_assess(model, test)
```

Arguments

model	An `ml_model`
test	Test data.frame (use `s$test`). Specify by name for clarity.

Value

An object of class `ml_evidence` (sealed — not substitutable for `ml_metrics`)

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
verdict <- ml_assess(model, test = s$test)
```

`ml_best` *Get the best model from a leaderboard*

Description

Returns the top-ranked fitted model from screen() or compare(). NULL if no models were stored.

Usage

```
ml_best(lb)
```

Arguments

`lb`	An ml_leaderboard

Value

An ml_model or NULL

Examples

```
s <- ml_split(iris, "Species", seed = 42)
lb <- ml_screen(s, "Species", seed = 42)
best <- ml_best(lb)
predict(best, s$valid)
```

`ml_calibrate` *Calibrate predicted probabilities*

Description

Applies Platt scaling (logistic regression on raw probabilities) to produce better-calibrated class probability estimates. Use validation data for calibration – never training data.

Usage

```
ml_calibrate(model, data = NULL)
```

Arguments

model	An ml_model from ml_fit()
data	A data.frame of calibration data (use validation set)

Details

Binary classification only.

Value

An ml_calibrated_model that behaves like an ml_model but returns calibrated probabilities

Examples

```
s <- ml_split(ml_dataset("cancer"), "target", seed = 42)
model <- ml_fit(s$train, "target", algorithm = "xgboost", seed = 42)
cal <- ml_calibrate(model, data = s$valid)
ml_evaluate(cal, s$valid)
```

---

ml_check *Verify bitwise reproducibility for a given dataset*

Description

Fits the same model twice with the same seed and asserts predictions are identical. Returns a list with passed, algorithm, seed, and message.

Usage

```
ml_check(data, target, algorithm = "random_forest", seed)
```

Arguments

data	A data.frame with features and target
target	Target column name
algorithm	Algorithm to check (default "random_forest")
seed	Random seed

Value

A list with passed (logical), algorithm, seed, message. Supports isTRUE(result$passed) for assertions.

Examples

```
result <- ml_check(iris, "Species", seed = 42)
result$passed
```

`ml_check_data` *Pre-flight data quality checks*

Description

Runs before fit() to catch common data quality issues that silently degrade model performance.

Usage

```
ml_check_data(data, target, severity = "warn")
```

Arguments

`data`	A data.frame
`target`	Target column name
`severity`	"warn" (default) or "error". If "error", raises on any issue.

Details

Checks performed:

- NaN in target (silently dropped by split)
- Inf in features
- ID columns (100\
- Zero-variance features (constant columns)
- High-null columns (>50\
- Severe class imbalance (<5\
- Duplicate rows (>10\
- Feature redundancy (|r| > 0.95)

Value

A list with `warnings`, `errors`, `has_issues`, `passed`. Supports `isTRUE(result$passed)` for assertions.

Examples

```
report <- ml_check_data(iris, "Species")
report$passed
```

ml_compare *Compare pre-fitted models on the same data*

Description

Evaluates multiple fitted models on the same dataset without re-fitting. All models must share the same target column and task.

Usage

```
ml_compare(models, data, sort_by = "auto")
```

Arguments

models	A list of ml_model objects (or ml_tuning_result, auto-unwrapped)
data	A data.frame containing the target column
sort_by	"auto" or a metric name string

Value

An object of class ml_leaderboard (data.frame with formatted print)

Examples

```
s <- ml_split(iris, "Species", seed = 42)
m1 <- ml_fit(s$train, "Species", algorithm = "logistic", seed = 42)
m2 <- ml_fit(s$train, "Species", algorithm = "random_forest", seed = 42)
ml_compare(list(m1, m2), s$valid)
```

ml_config *Configure ml package settings*

Description

Set global configuration for the ml package. Currently supports guards to control partition enforcement.

Usage

```
ml_config(guards = NULL)
```

Arguments

guards	Character: "strict" (default) enforces split provenance — all verbs reject data not produced by ml_split(). "off" disables guards for exploration/education.

Value

Invisibly returns the previous settings as a list.

Examples

```
ml_config(guards = "off")    # disable guards
ml_config(guards = "strict") # re-enable (default)
```

---

ml_cv *Create k-fold cross-validation from a split*

Description

Takes an existing `ml_split_result` and creates k-fold rotations within its dev partition (train + valid). The test partition stays sealed on the original split for `ml_assess()`.

Usage

```
ml_cv(s, target, folds = 5L, seed = NULL, stratify = TRUE)
```

Arguments

`s`	An `ml_split_result` from `ml_split()`
`target`	Target column name (string)
`folds`	Number of folds (default 5)
`seed`	Random seed for fold assignment
`stratify`	Logical. Stratify folds by target for classification (default TRUE)

Details

Two primitives, strict separation of concerns: `ml_split()` creates the three-way boundary, `ml_cv()` creates rotations within that boundary.

Value

An `ml_cv_result` that `ml_fit()` accepts directly. The original split's `$test` remains available via `s$test` for `ml_assess()`.

Examples

```
s <- ml_split(iris, "Species", seed = 42)
c <- ml_cv(s, "Species", folds = 5, seed = 42)
model <- ml_fit(c, "Species", seed = 42)
model$scores_
```

`ml_cv_group` *Create group-aware cross-validation from a split*

Description

No group appears in both train and validation within any fold. Prevents leakage from repeated measurements (patients, stores, sensors).

Usage

```
ml_cv_group(s, target, groups, folds = 5L, seed = NULL)
```

Arguments

`s`	An `ml_split_result` from `ml_split()` or `ml_split_group()`
`target`	Target column name (string)
`groups`	Column name identifying groups
`folds`	Number of folds (default 5)
`seed`	Random seed for group assignment

Value

An `ml_cv_result` with group-aware folds

Examples

```
df <- data.frame(pid = rep(1:20, each = 5), x = rnorm(100), y = sample(0:1, 100, TRUE))
s <- ml_split(df, "y", seed = 42)
c <- ml_cv_group(s, "y", groups = "pid", folds = 5, seed = 42)
```

`ml_cv_temporal` *Create temporal cross-validation from a split*

Description

Expanding-window CV for time series. Data must already be sorted chronologically (use `ml_split_temporal()` first).

Usage

```
ml_cv_temporal(
  s,
  target,
  folds = 5L,
  embargo = 0L,
  window = "expanding",
  window_size = NULL
)
```

Arguments

s	An ml_split_result from ml_split_temporal()
target	Target column name (string)
folds	Number of folds (default 5)
embargo	Integer. Number of rows to skip between train end and valid start (gap to prevent temporal leakage from autocorrelation). Default 0. Must be >= 0.
window	"expanding" (default, all prior rows as train) or "sliding" (fixed-size training window). When "sliding", window_size must also be supplied.
window_size	Integer. Required when window = "sliding". Number of rows in each training window.

Value

An ml_cv_result with expanding-window folds

Examples

```
df <- data.frame(date = 1:100, x = rnorm(100), y = sample(0:1, 100, TRUE))
s <- ml_split_temporal(df, "y", time = "date")
c <- ml_cv_temporal(s, "y", folds = 5)
# With embargo to prevent autocorrelation leakage:
c2 <- ml_cv_temporal(s, "y", folds = 5, embargo = 5L)
```

---

ml_dataset *Load a built-in dataset*

Description

Returns one of the built-in datasets. Useful for experimenting with the ml API before applying it to your own data.

Usage

```
ml_dataset(name)
```

Arguments

name	Dataset name (string)

Details

Available datasets: "iris", "wine", "cancer", "diabetes", "houses", "churn", "fraud"

Value

A data.frame

Examples

```
churn <- ml_dataset("churn")
head(churn)
```

`ml_drift` *Detect data drift between reference and new data*

Description

Compares a reference dataset (typically training data) to new data using per-feature statistical tests or adversarial validation.

Usage

```
ml_drift(
  reference,
  new,
  method = "statistical",
  threshold = 0.05,
  exclude = NULL,
  target = NULL,
  seed = NULL,
  algorithm = "random_forest"
)
```

Arguments

`reference`	A data.frame — reference dataset (typically training data)
`new`	A data.frame — new data to compare against the reference
`method`	Detection method: "statistical" (default) or "adversarial"
`threshold`	p-value threshold for statistical method (default 0.05)
`exclude`	Character vector of column names to skip (e.g., ID columns)
`target`	Target column name — automatically excluded from drift analysis
`seed`	Random seed (required for method = "adversarial")
`algorithm`	Algorithm for adversarial classifier: "random_forest" (default) or "xgboost"

Details

Statistical method (default): per-feature distribution tests with no labels required.

- Numeric features: Kolmogorov-Smirnov two-sample test
- Categorical features: Chi-squared test on value counts

Adversarial method: trains a binary classifier to distinguish reference from new data. AUC near 0.5 means similar distributions; AUC near 1.0 means very different distributions.

- `$train_scores`: per-row probability of "looks like new data" for reference rows. Use `sort(result$train_scores, decreasing = TRUE)[1:n]` to select validation rows that mirror the new distribution.
- `$features`: most discriminative features (temporal leakage candidates)

Pair with `ml_shelf()` for complete monitoring: drift() detects input distribution shift (label-free), shelf() detects performance degradation (requires labels).

Value

An object of class `ml_drift_result` with:

- `$shifted`: TRUE if drift detected
- `$features`: named numeric — p-values (statistical) or importances (adversarial)
- `$features_shifted`: character vector of drifted feature names
- `$severity`: "none", "low", "medium", or "high"
- $auc: adversarial mode only — classifier AUC
- `$train_scores`: adversarial mode only — per-row reference probabilities

Examples

```
s    <- ml_split(iris, "Species", seed = 42)
# Simulate drift by perturbing test data
new  <- s$test
new$Sepal.Length <- new$Sepal.Length + 2
result <- ml_drift(reference = s$train, new = new, target = "Species")
result$shifted
result$features_shifted
```

`ml_embed` *Embed texts into numeric features*

Description

Fits a text vectorizer on training texts and returns an embedder object that stores the vocabulary for consistent transform at prediction time.

Usage

```
ml_embed(texts, method = "tfidf", max_features = 100L)
```

Arguments

`texts`	A character vector of texts to embed
`method`	Embedding method. Currently only "tfidf" is supported.
`max_features`	Maximum vocabulary size (number of TF-IDF features). Default 100.

Details

Currently supports TF-IDF ('tm' package). SBERT and neural methods are planned for future gates.

Value

An object of class `ml_embedder` with:

- `$vectors`: data.frame of TF-IDF features (n_texts x max_features)
- `$method`: the method used
- `$vocab_size`: number of features generated
- `$transform(new_texts)`: apply stored vocabulary to new texts

Examples

```
if (requireNamespace("tm", quietly = TRUE)) {
  texts <- c("good product", "bad service", "great value", "poor quality")
  emb <- ml_embed(texts, method = "tfidf", max_features = 20)
  emb$vocab_size
  nrow(emb$vectors)

  # Transform new texts using the fitted vocabulary
  new_texts <- c("excellent quality", "terrible service")
  new_vecs <- emb$transform(new_texts)
}
```

`ml_enough` *Learning curve analysis — do you need more data?*

Description

Trains at increasing data sizes and reports train vs validation performance at each step. Answers: is the model still learning (more data helps), or saturated (more data unlikely to help)?

Usage

```
ml_enough(s, target, seed = NULL, algorithm = "auto", steps = 8L, cv = 3L)
```

Arguments

`s`	An `ml_split_result` from `ml_split()`
`target`	Target column name
`seed`	Random seed (optional in R; auto-generated if NULL)
`algorithm`	Algorithm to use (default `"auto"`). Any algorithm supported by `ml_fit()`.
`steps`	Integer >= 2. Number of data-size steps to evaluate, evenly spaced from ~10%% to 100%% of training data. Default 8.
`cv`	Integer >= 2. Number of cross-validation folds for validation score at each step. Default 3.

Value

An `ml_enough_result` with fields:

- `$saturated` — logical, TRUE if curve plateaus (< 1%% gain in last half)
- `$curve` — data.frame: n_samples, train_score, val_score
- `$metric` — metric name used
- `$n_current` — total training rows in the full dataset
- `$recommendation` — human-readable action

Examples

```
s <- ml_split(iris, "Species", seed = 42)
result <- ml_enough(s, "Species", seed = 42)
result$recommendation
```

`ml_evaluate` *Evaluate model on validation data (iterate freely)*

Description

The practice exam — call as many times as needed. For the one-time final grade on held-out test data, use `ml_assess()`.

Usage

```
ml_evaluate(model, data)
```

Arguments

`model`	An `ml_model` or `ml_tuning_result`
`data`	A data.frame containing the target column

Value

An object of class `ml_metrics` (named numeric vector with print method)

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
metrics <- ml_evaluate(model, s$valid)
metrics[["accuracy"]]
```

ml_explain *Explain model via feature importance*

Description

Returns a data frame of feature importances, normalized to sum to 1.0, sorted descending. Uses tree-based impurity importance for 'xgboost' and 'random_forest', absolute coefficients for 'logistic', 'linear', and 'elastic_net'. Not supported for 'svm' or 'knn'.

Usage

```
ml_explain(model)
```

Arguments

model	An ml_model or ml_tuning_result

Value

An object of class ml_explanation (a data.frame with columns feature and importance; custom print shows a bar chart)

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", algorithm = "random_forest", seed = 42)
ml_explain(model)
```

ml_fit *Fit a machine learning model*

Description

Trains a model using cross-validation (if data is an ml_split_result with folds) or holdout (if data is a data.frame). Automatically detects task type, handles encoding, and records metadata for reproducibility.

Usage

```
ml_fit(
  data,
  target,
  algorithm = "auto",
  seed = NULL,
  task = "auto",
  balance = FALSE,
```

```
  engine = "auto",
  ...
)
```

Arguments

data	A data.frame, ml_split_result, or ml_split_result with folds
target	Target column name (string)
algorithm	"auto" (default), "xgboost", "random_forest", "svm", "knn", "logistic", "linear", "naive_bayes", "elastic_net"
seed	Random seed. NULL (default) auto-generates and stores for reproducibility.
task	"auto", "classification", or "regression"
balance	Logical. If TRUE, applies class-weight balancing for imbalanced classification problems. Ignored for regression. Default: FALSE.
engine	Backend engine: "auto" (Rust if available, else CRAN packages), "ml" (Rust required), or "r" (CRAN packages only). Default: "auto".
...	Additional hyperparameters passed to the engine (e.g., max_depth = 6, num.trees = 200)

Details

Formula interfaces are not supported. Pass the data frame and target column name as a string. Unordered factors use one-hot encoding for linear models and ordinal encoding for tree-based models. Ordered factors always use ordinal encoding.

Value

An object of class ml_model

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
model$algorithm
```

---

ml_leak *Detect potential data leakage*

Description

Analyzes feature-target relationships before modeling. Runs pure data introspection – no model fitting.

Usage

```
ml_leak(data, target)
```

Arguments

data	A data.frame or ml_split_result
target	Target column name

Details

Checks performed:

1. Feature-target correlation (Pearson |r|, numeric features)
2. High-cardinality ID columns
3. Target name in feature names
4. Duplicate rows between train and test (SplitResult only)

Value

A list with clean (logical), n_warnings, checks (list of check results), suspects (list of suspect features). Class ml_leak_report.

Examples

```
s <- ml_split(iris, "Species", seed = 42)
report <- ml_leak(s, "Species")
report$clean
```

---

ml_load *Load a model from disk*

Description

Load a model from disk

Usage

```
ml_load(path)
```

Arguments

path	Path to a .mlr file saved with ml_save()

Value

An ml_model or ml_tuning_result

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
path <- file.path(tempdir(), "iris_model.mlr")
ml_save(model, path)
loaded <- ml_load(path)
loaded$algorithm
```

`ml_optimize` *Optimize decision threshold for binary classification*

Description

Sweeps thresholds from `min_threshold` to 0.95 in two phases (coarse 0.05 steps, then fine 0.005 steps around the coarse best) and returns a copy of the model with a tuned threshold. Subsequent `ml_predict()` calls apply this threshold to positive-class probability instead of 0.5.

Usage

```
ml_optimize(model, data, metric = "f1", min_threshold = "auto")
```

Arguments

`model`	An `ml_model` or `ml_tuning_result` (binary classification only).
`data`	A data.frame containing the target column used as true labels.
`metric`	Character. Optimisation objective: `"f1"`, `"accuracy"`, `"precision"`, or `"recall"`. Ranking metrics (`"roc_auc"`, `"log_loss"`) are rejected because they are threshold-independent.
`min_threshold`	Lower bound of the sweep. `"auto"` (default) computes `max(0.001, 1 / n_positives)` — the minimum meaningful threshold for imbalanced data. Pass a numeric value to override.

Value

An `ml_optimize_result` (also an `ml_model`). The threshold is baked in — every `ml_predict()` call uses it automatically. Inspect with `result$threshold`. The original model is unchanged.

Examples

```
s     <- ml_split(iris[iris$Species != "virginica", ], "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
opt   <- ml_optimize(model, data = s$valid, metric = "f1")
opt$threshold
```

`ml_plot` *Visual diagnostics for a fitted model*

Description

Produces diagnostic plots using base R graphics. No extra packages required.

Usage

```
ml_plot(model, data = NULL, kind = "importance", ...)
```

Arguments

`model`	An `ml_model` from `ml_fit()`
`data`	A data.frame for computing predictions (required for all except `"importance"`)
`kind`	Plot type. One of `"importance"`, `"roc"`, `"confusion"`, `"residual"`, `"calibration"`. Default: `"importance"`.
`...`	Passed to the underlying base R plot call

Details

Available kinds:

- `"importance"` — feature importance bar chart
- `"roc"` — ROC curve (classification)
- `"confusion"` — confusion matrix heatmap (classification)
- `"residual"` — residuals vs fitted (regression)
- `"calibration"` — predicted vs actual probabilities (classification)

Value

Invisibly returns NULL (called for its side effect)

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", algorithm = "random_forest", seed = 42)
ml_plot(model, kind = "importance")
ml_plot(model, data = s$valid, kind = "confusion")
```

ml_predict *Predict from a fitted model (ml_predict style)*

Description

Alias for `predict(model, newdata = ...)`. Matches Python `ml.predict()`.

Usage

```
ml_predict(model, new_data)
```

Arguments

`model`	An `ml_model` or `ml_tuning_result`
`new_data`	A data.frame with the same features used for training

Value

A vector of predicted class labels (classification) or numeric values (regression).

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
preds <- ml_predict(model, s$valid)
head(preds)
```

ml_predict_proba *Predict class probabilities*

Description

Predict class probabilities

Usage

```
ml_predict_proba(model, new_data)
```

Arguments

`model`	An `ml_model` object (classification only)
`new_data`	A data.frame with the same features used for training

Value

A data.frame with one column per class. Values are probabilities summing to 1.0 per row. Column names are the original class labels.

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", algorithm = "random_forest", seed = 42)
probs <- ml_predict_proba(model, s$valid)
head(probs)
```

`ml_prepare` *Prepare data for ML: encode, impute, and scale*

Description

Grammar primitive #2: DataFrame -> PreparedData.

Usage

```
ml_prepare(data, target, algorithm = "auto", task = "auto")
```

Arguments

`data`	A data.frame including the target column.
`target`	Name of the target column (string).
`algorithm`	Algorithm hint for encoding strategy: "auto", "random_forest", "logistic", etc. Tree-based algorithms use ordinal encoding; linear algorithms use one-hot encoding for low-cardinality categoricals.
`task`	"classification", "regression", or "auto" (detected from target).

Details

In the default workflow, `ml_fit()` calls preparation internally per fold. Use `ml_prepare()` explicitly when you need manual control: inspect the preprocessing state, apply the same encoding to external data, or chain preparation with fitting.

Value

An `ml_prepared_data` object with:

- `$data` — transformed data.frame (all-numeric, ready for ml_fit)
- `$state` — NormState list; use .transform(state, X) on new data
- `$target` — target column name
- `$task` — detected or provided task type

Examples

```
df <- data.frame(x1 = rnorm(50), x2 = rnorm(50), y = rnorm(50))
s <- ml_split(df, "y", seed = 42)
p <- ml_prepare(s$train, "y")
p$task       # "classification" or "regression"
p$data       # encoded feature matrix
```

`ml_profile` *Profile data before modeling*

Description

Computes per-column statistics and emits warnings for common data quality issues: missing values, constant columns, high cardinality, imbalanced targets, and near-collinear features.

Usage

```
ml_profile(data, target = NULL)
```

Arguments

`data`	A data.frame (also accepts tibble or data.table)
`target`	Optional target column name (enables task detection + distribution stats)

Value

An object of class `ml_profile_result` (list with formatted print)

Examples

```
ml_profile(iris, "Species")
```

`ml_quick` *One-call workflow: split + screen + fit + evaluate*

Description

The fastest path from raw data to a trained, evaluated model. Screens logistic, random_forest, and xgboost, picks the best, fits on training data, and evaluates on validation.

Usage

```
ml_quick(data, target, seed)
```

Arguments

data	A data.frame with features and target
target	Target column name
seed	Random seed

Value

A list with model (ml_model), metrics (ml_metrics), and split (ml_split_result).

Examples

```
result <- ml_quick(iris, "Species", seed = 42)
result$model
result$metrics
```

---

ml_report *Generate an HTML training report*

Description

Produces a self-contained HTML report with model metadata, evaluation metrics, and feature importances. Open in any browser.

Usage

```
ml_report(model, data = NULL, path = "model_report.html")
```

Arguments

model	An ml_model from ml_fit()
data	A data.frame for computing metrics (use validation data)
path	Output file path. Default: "model_report.html"

Value

The path to the saved report (invisibly)

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", algorithm = "random_forest", seed = 42)
tmp <- tempfile(fileext = ".html")
ml_report(model, data = s$valid, path = tmp)
unlink(tmp)
```

ml_save *Save a model to disk*

Description

Saves an `ml_model` or `ml_tuning_result` to a `.mlr` file using `saveRDS` with a version wrapper.

Usage

```
ml_save(model, path)
```

Arguments

`model`	An `ml_model` or `ml_tuning_result`
`path`	File path (recommended extension: `.mlr`)

Value

The normalized path, invisibly.

Security

`ml_load()` uses `readRDS()` internally, which can execute arbitrary R code during deserialization. Never load `.mlr` files from untrusted sources.

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
path <- file.path(tempdir(), "iris_model.mlr")
ml_save(model, path)
loaded <- ml_load(path)
```

ml_screen *Screen all algorithms on your data*

Description

Fits every available algorithm on the training data and ranks by validation performance. Use this to identify promising candidates before tuning.

Usage

```
ml_screen(
  data,
  target,
  algorithms = NULL,
  seed = NULL,
  sort_by = "auto",
  time_budget = NULL,
  keep_models = TRUE,
  ...
)
```

Arguments

data	An ml_split_result (NOT a raw data.frame — split first to prevent overfitting)
target	Target column name
algorithms	Character vector of algorithm names, or NULL for all available
seed	Random seed. NULL auto-generates.
sort_by	"auto" (roc_auc for binary clf, f1_macro for multiclass, rmse for regression), or a metric name string
time_budget	Maximum seconds for entire screen. Stops between algorithms (not mid-fit) when budget exceeded. NULL (default) = no limit.
keep_models	If FALSE, discard fitted models after scoring to save memory. ml_best() will return NULL. Default TRUE.
...	Additional arguments passed to ml_fit()

Details

Multiple comparison bias: Selecting the best from N algorithms on the same validation set produces optimistic estimates. The winning algorithm benefits from selection bias. Use ml_validate() on held-out test data for trustworthy comparisons.

For imbalanced data, consider sort_by = "f1" — the default roc_auc can hide failures on minority classes.

Value

An object of class ml_leaderboard (data.frame with formatted print)

Examples

```
s <- ml_split(iris, "Species", seed = 42)
lb <- ml_screen(s, "Species", seed = 42)
lb
```

`ml_shelf` *Check if a model is past its shelf life*

Description

Evaluates the model on new labeled data and compares performance to the model's original training metrics. Requires ground truth labels.

Usage

```
ml_shelf(model, new, target, tolerance = 0.05)
```

Arguments

`model`	An `ml_model` or `ml_tuning_result` with `$scores_` populated (i.e., trained with `ml_fit(cv_result, target)`)
`new`	A data.frame — new labeled dataset including the target column
`target`	Name of the target column in `new`
`tolerance`	Allowed degradation per metric (default 0.05 = 5pp). Any key metric degrading beyond tolerance marks the model as stale.

Details

Run this when outcome labels become available (e.g., daily/weekly batch scoring, then wait for outcomes). Pair with `ml_drift()` for complete monitoring:

- `ml_drift()`: input distribution shift (label-free, run always)
- `ml_shelf()`: performance degradation (needs labels, run periodically)

Requires `model$scores_` from a cross-validated fit. If the model was trained on a holdout split (no CV), `scores_` will be NULL and shelf() raises a model_error.

Value

An object of class `ml_shelf_result` with:

- `$fresh`: TRUE if model performance is within tolerance
- `$stale`: inverse of fresh
- `$metrics_then`: original training metrics (from model$scores_)
- `$metrics_now`: current metrics on new data
- `$degradation`: per-metric delta (negative = worse for higher-is-better)
- `$recommendation`: human-readable guidance

Examples

```
cv    <- ml_split(iris, "Species", seed = 42, folds = 3)
model <- ml_fit(cv, "Species", algorithm = "logistic", seed = 42)
# Simulate a new labeled batch
new_batch <- iris[sample(nrow(iris), 30), ]
result <- ml_shelf(model, new = new_batch, target = "Species")
result$fresh
result$degradation
```

`ml_split` *Split data into train/valid/test partitions or cross-validation folds*

Description

Three-way split is the default (60/20/20), following Hastie, Tibshirani, and Friedman (2009, ISBN:978-0-387-84857-0) Chapter 7. Automatically stratifies for classification.

Usage

```
ml_split(
  data,
  target = NULL,
  seed = NULL,
  ratio = c(0.6, 0.2, 0.2),
  folds = NULL,
  stratify = TRUE,
  task = "auto",
  time = NULL,
  groups = NULL
)
```

Arguments

`data`	A data.frame (also accepts tibble or data.table)
`target`	Target column name (enables stratification + task detection)
`seed`	Random seed. NULL (default) auto-generates and stores for reproducibility. Pass an integer for reproducible splits.
`ratio`	Numeric vector of length 3: c(train, valid, test). Must sum to 1.0.
`folds`	Integer for k-fold CV (e.g., `folds = 5`). Overrides ratio.
`stratify`	Logical. Auto-stratify for classification targets (default TRUE).
`task`	"auto", "classification", or "regression". Override task detection.
`time`	Column name for temporal/chronological split. Data is sorted by this column, and the time column is dropped from output. Deterministic (seed is ignored). Cannot combine with `groups`.
`groups`	Column name for group-aware split. No group appears in both train and validation/test. Cannot combine with `time`.

Value

An ml_split_result. Access $train, $valid, $test, $dev (train + valid). When folds is set, also $folds (CV on dev).

Examples

```
s <- ml_split(iris, "Species", seed = 42)
nrow(s$train)
nrow(s$dev)
```

---

ml_split_group *Split data with group non-overlap — no group leaks across partitions*

Description

Domain specialization of ml_split() for clinical trials, repeated measures, and any data where observations are nested within groups (patients, subjects, hospitals). No group appears in more than one partition.

Usage

```
ml_split_group(
  data,
  target = NULL,
  groups,
  seed = NULL,
  ratio = c(0.6, 0.2, 0.2),
  folds = NULL,
  stratify = TRUE,
  task = "auto"
)
```

Arguments

data	A data.frame
target	Target column name (optional, enables stratification)
groups	Column name identifying groups
seed	Random seed for reproducibility
ratio	Numeric vector c(train, valid, test). Must sum to 1.0.
folds	Integer for group CV. When set, ignores ratio.
stratify	Logical. Stratify by target within groups (default TRUE).
task	"auto", "classification", or "regression"

Details

Also covers Leave-Source-Out CV: when groups represent data sources (hospitals, devices), this produces deployment-realistic evaluation.

Value

An `ml_split_result`. When `folds` is set, includes `$folds` and `$test`.

Examples

```
df <- data.frame(pid = rep(1:10, each = 5), x = rnorm(50), y = sample(0:1, 50, TRUE))
s <- ml_split_group(df, "y", groups = "pid", seed = 42)
nrow(s$train)
```

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ml_split_temporal *Split data chronologically — no future leakage*

Description

Domain specialization of `ml_split()` for time series and forecasting. Data is sorted by the `time` column and partitioned by position. Deterministic: seed is ignored (chronological order is the only order).

Usage

```
ml_split_temporal(
  data,
  target = NULL,
  time,
  ratio = c(0.6, 0.2, 0.2),
  folds = NULL,
  task = "auto"
)
```

Arguments

`data`	A data.frame
`target`	Target column name (optional, enables task detection)
`time`	Column name containing timestamps or orderable values. Used for sorting, then dropped from output partitions.
`ratio`	Numeric vector c(train, valid, test). Must sum to 1.0.
`folds`	Integer for temporal CV (expanding window). When set, ignores ratio.
`task`	"auto", "classification", or "regression"

Value

An `ml_split_result`. When `folds` is set, includes `$folds` and `$test`.

Examples

```
df <- data.frame(date = 1:100, x = rnorm(100), y = sample(0:1, 100, TRUE))
s <- ml_split_temporal(df, "y", time = "date")
nrow(s$train)
```

`ml_stack` *Ensemble stacking*

Description

Trains a stacking ensemble with out-of-fold meta-features. Base models generate out-of-fold predictions, which are used to train a meta-learner.

Usage

```
ml_stack(data, target, models = NULL, meta = NULL, cv_folds = 5L, seed = NULL)
```

Arguments

`data`	A data.frame with features and target
`target`	Target column name
`models`	Character vector of base algorithm names, or NULL for defaults
`meta`	Meta-learner algorithm. Default: "logistic" (classification) or "linear" (regression)
`cv_folds`	Number of CV folds for generating out-of-fold predictions
`seed`	Random seed

Details

Note: This function uses global normalization (not per-fold), because the stacking CV is internal to the meta-learner training. This is the one exception to the per-fold normalization rule.

Value

An `ml_model` with `$is_stacked = TRUE`

Examples

```
s <- ml_split(iris, "Species", seed = 42)
stacked <- ml_stack(s$train, "Species", seed = 42)
predict(stacked, s$valid)
```

`ml_tune` *Tune hyperparameters via random or grid search*

Description

Tune hyperparameters via random or grid search

Usage

```
ml_tune(
  data,
  target,
  model = NULL,
  algorithm = NULL,
  n_trials = 20L,
  cv_folds = 3L,
  method = "random",
  seed = NULL,
  params = NULL
)
```

Arguments

`data`	A data.frame or `ml_split_result`
`target`	Target column name
`model`	An `ml_model` object (to clone algorithm from), or NULL
`algorithm`	Algorithm name (if model is NULL)
`n_trials`	Number of random search trials (default 20)
`cv_folds`	Number of CV folds per trial (default 3)
`method`	"random" (default) or "grid"
`seed`	Random seed
`params`	Named list of parameter ranges (overrides defaults). For numeric ranges, provide a 2-element numeric vector c(min, max). For discrete, provide a character/integer vector.

Value

An object of class `ml_tuning_result`

Examples

```
s <- ml_split(iris, "Species", seed = 42)
tuned <- ml_tune(s$train, "Species", algorithm = "xgboost", n_trials = 5, seed = 42)
tuned$best_params_
```

`ml_validate` *Validate model against rules and/or baseline*

Description

Three modes: (1) absolute rules, (2) regression prevention vs baseline, (3) combined. Returns a structured result with pass/fail and diagnostics.

Usage

```
ml_validate(model, test, rules = NULL, baseline = NULL, tolerance = 0)
```

Arguments

`model`	An `ml_model`
`test`	Test data.frame (use `s$test`)
`rules`	Named list of threshold strings, e.g. `list(accuracy = ">0.85", roc_auc = ">=0.90")`
`baseline`	An `ml_model` — previous model to check for regressions
`tolerance`	Numeric. Allowed absolute degradation (0.02 = 2pp slack). Default 0.0.

Details

Tolerance is absolute (not relative): a tolerance of 0.02 means 2 percentage points of allowed degradation, applied uniformly across all metrics.

Value

An object of class `ml_validate_result`

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
gate <- ml_validate(model, test = s$test, rules = list(accuracy = ">0.80"))
gate$passed
```

ml_verify *Verify provenance integrity of a model*

Description

Checks provenance chain: split parameters -> training fingerprint -> assess ceremony status. Catches accidental self-deception (load-assess loops, test-set shopping) rather than adversarial tampering.

Usage

```
ml_verify(model)
```

Arguments

model	An ml_model, ml_tuning_result, or path to .mlr file

Value

A list with status ("verified"/"unverified"/"warning"), checks, provenance, and assess_count.

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
report <- ml_verify(model)
report$status
```

predict.ml_model *Predict from a fitted model*

Description

Predict from a fitted model

Predict from an ml_model

Usage

```
## S3 method for class 'ml_model'
predict(object, newdata, proba = FALSE, ...)

## S3 method for class 'ml_model'
predict(object, newdata, proba = FALSE, ...)
```

Arguments

object	An ml_model object
newdata	A data.frame
proba	Logical. If TRUE, returns class probabilities (classification only)
...	Ignored

Value

A vector of predicted class labels (classification) or numeric values (regression). If proba = TRUE, returns a data.frame with one column per class; values are probabilities summing to 1.0 per row.

Predicted labels (classification) or numeric values (regression). If proba = TRUE, a data.frame of probabilities.

Examples

```
s <- ml_split(iris, "Species", seed = 42)
model <- ml_fit(s$train, "Species", seed = 42)
preds <- predict(model, newdata = s$valid)
head(preds)
```

---

predict.ml_tuning_result

Predict from best model in a tuning result

Description

Predict from best model in a tuning result

Usage

```
## S3 method for class 'ml_tuning_result'
predict(object, newdata, ...)
```

Arguments

object	An ml_tuning_result
newdata	A data.frame
...	Passed to predict.ml_model

Value

Predictions

print.ml_cv_result *Print ml_cv_result*

Description

Print ml_cv_result

Usage

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

Arguments

x	An ml_cv_result object
...	Ignored

Value

The object x, invisibly.

print.ml_drift_result *Print ml_drift_result*

Description

Print ml_drift_result

Usage

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

Arguments

x	An ml_drift_result object
...	Ignored

Value

The object x, invisibly.

print.ml_embedder *Print ml_embedder*

Description

Print ml_embedder

Usage

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

Arguments

x	An ml_embedder object
...	Ignored

Value

The object x, invisibly.

print.ml_evidence *Print ml_evidence*

Description

Print ml_evidence

Usage

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

Arguments

x	An ml_evidence object
...	Ignored

Value

The object x, invisibly.

print.ml_explanation *Print ml_explanation*

Description

Print ml_explanation

Usage

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

Arguments

x	An ml_explanation object
...	Ignored

Value

The object x, invisibly.

print.ml_leaderboard *Print ml_leaderboard*

Description

Print ml_leaderboard

Usage

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

Arguments

x	An ml_leaderboard object
...	Ignored

Value

The object x, invisibly.

print.ml_metrics *Print ml_metrics*

Description

Print ml_metrics

Usage

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

Arguments

x	An ml_metrics object
...	Ignored

Value

The object x, invisibly.

print.ml_model *Print an ml_model*

Description

Print an ml_model

Usage

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

Arguments

x	An ml_model object
...	Ignored

Value

The object x, invisibly.

print.ml_profile_result *Print ml_profile_result*

Description

Print ml_profile_result

Usage

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

Arguments

x	An ml_profile_result object
...	Ignored

Value

The object x, invisibly.

print.ml_shelf_result *Print ml_shelf_result*

Description

Print ml_shelf_result

Usage

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

Arguments

x	An ml_shelf_result object
...	Ignored

Value

The object x, invisibly.

print.ml_split_result *Print an ml_split_result*

Description

Print an ml_split_result

Usage

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

Arguments

x	An ml_split_result object
...	Ignored

Value

The object x, invisibly.

print.ml_tuning_result *Print an ml_tuning_result*

Description

Print an ml_tuning_result

Usage

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

Arguments

x	An ml_tuning_result object
...	Ignored

Value

The object x, invisibly.

`print.ml_validate_result` *Print ml_validate_result*

Description

Print ml_validate_result

Usage

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

Arguments

`x`	An ml_validate_result object
`...`	Ignored

Value

The object `x`, invisibly.

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