Package ‘cvms’

July 14, 2022

Title Cross-Validation for Model Selection

Version 1.3.4

Description Cross-validate one or multiple regression and classification models and get relevant evaluation metrics in a tidy format. Validate the best model on a test set and compare it to a baseline evaluation. Alternatively, evaluate predictions from an external model. Currently supports regression and classification (binary and multiclass). Described in chp. 5 of Jeyaraman, B. P., Olsen, L. R., & Wambugu M. (2019, ISBN: 9781838550134).

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URL https://github.com/ludvigolsen/cvms

BugReports https://github.com/ludvigolsen/cvms/issues

Depends R (>= 3.5)

Imports checkmate (>= 2.0.0),
  data.table (>= 1.12),
  dplyr (>= 0.8.5),
  ggplot2,
  lifecycle,
  lme4 (>= 1.1-23),
  MuMIn (>= 1.43.17),
  parameters (>= 0.15.0),
  plyr,
  pROC (>= 1.16.0),
  purrr,
  rearrr (>= 0.3.0),
  recipes (>= 0.1.13),
  rlang (>= 0.4.7),
  stats,
  stringr,
  tibble (>= 3.0.3),
  tidy (>= 1.1.2),
  utils

Suggests AUC,
  covr (>= 3.3.1),
  e1071 (>= 1.7-2),
  furrr,
  ggimage (>= 0.2.8),
R topics documented:

ggnewscale (>= 0.4.3),
groupdata2 (>= 1.4.1),
knitr,
merDeriv (>= 0.2-4),
nnet (>= 7.3-12),
randomForest (>= 4.6-14),
rmarkdown,
rsvg,
testthat (>= 2.3.2),
xpectr (>= 0.4.1)

VignetteBuilder knitr
RdMacros lifecycle
Encoding UTF-8
LazyData true
RoxygenNote 7.1.2

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Create baseline evaluations

Description

[Maturing]

Create a baseline evaluation of a test set.

In modelling, a baseline is a result that is meaningful to compare the results from our models to. For instance, in classification, we usually want our results to be better than random guessing. E.g. if we have three classes, we can expect an accuracy of 33.33%, as for every observation we have 1/3 chance of guessing the correct class. So our model should achieve a higher accuracy than 33.33% before it is more useful to us than guessing.

While this expected value is often fairly straightforward to find analytically, it only represents what we can expect on average. In reality, it’s possible to get far better results than that by guessing. baseline() (binomial, multinomial) finds the range of likely values by evaluating multiple sets of random predictions and summarizing them with a set of useful descriptors. If random guessing frequently obtains an accuracy of 40%, perhaps our model should have better performance than this, before we declare it better than guessing.

How:

When `family` is binomial: evaluates `n` sets of random predictions against the dependent variable, along with a set of all 0 predictions and a set of all 1 predictions. See also baseline_binomial().

When `family` is multinomial: creates one-vs-all (binomial) baseline evaluations for `n` sets of random predictions against the dependent variable, along with sets of “all class x,y,z,...” predictions. See also baseline_multinomial().

When `family` is gaussian: fits baseline models (y ~ 1) on `n` random subsets of `train_data` and evaluates each model on `test_data`. Also evaluates a model fitted on all rows in `train_data`. See also baseline_gaussian().

Wrapper functions:

Consider using one of the wrappers, as they are simpler to use and understand: baseline_gaussian(), baseline_multinomial(), and baseline_binomial().

Usage

```r
baseline(
  test_data,
  dependent_col,
  family,
  train_data = NULL,
  n = 100,
  metrics = list(),
)```
positive = 2,
cutoff = 0.5,
random_generator_fn = runif,
random_effects = NULL,
min_training_rows = 5,
min_training_rows_left_out = 3,
REML = FALSE,
parallel = FALSE
)

Arguments

test_data data.frame.
dependent_col Name of dependent variable in the supplied test and training sets.
family Name of family. (Character)
    Currently supports "gaussian", "binomial" and "multinomial".
train_data data.frame. Only used when 'family' is "gaussian".
n Number of random samplings to perform. (Default is 100)
    For gaussian: The number of random samplings of 'train_data' to fit baseline models on.
    For binomial and multinomial: The number of sets of random predictions to evaluate.
metrics list for enabling/disabling metrics.
    E.g. list("RMSE" = FALSE) would remove RMSE from the regression results, and
    list("Accuracy" = TRUE) would add the regular Accuracy metric to the classification results. Default values (TRUE/FALSE) will be used for the remaining available metrics.
    You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i. list("all" = FALSE,"RMSE" = TRUE) would return only the RMSE metric.
    The list can be created with gaussian_metrics(), binomial_metrics(), or multinomial_metrics().
    Also accepts the string "all".
positive Level from dependent variable to predict. Either as character (preferable) or level index (1 or 2 - alphabetically).
    E.g. if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".
    Note: For reproducibility, it’s preferable to specify the name directly, as different locales may sort the levels differently.
    Used when calculating confusion matrix metrics and creating ROC curves.
    N.B. Only affects evaluation metrics, not the returned predictions.
    N.B. Binomial only. (Character or Integer)
cutoff Threshold for predicted classes. (Numeric)
    N.B. Binomial only
random_generator_fn Function for generating random numbers when type is "multinomial". The softmax function is applied to the generated numbers to transform them to probabilities.
The first argument must be the number of random numbers to generate, as no other arguments are supplied.

To test the effect of using different functions, see `multiclass_probability_tibble()`.

N.B. **Multinomial only**

random_effects Random effects structure for the Gaussian baseline model. (Character)

E.g. with "(1|ID)", the model becomes "y ~ 1 + (1|ID)".

N.B. **Gaussian only**

min_training_rows Minimum number of rows in the random subsets of `train_data`.

**Gaussian only**. (Integer)

min_training_rows_left_out Minimum number of rows left out of the random subsets of `train_data`.

I.e. a subset will maximally have the size:

\[
\text{max\_rows\_in\_subset} = \text{nrow(`train\_data`)} - \text{min\_training\_rows\_left\_out}.
\]

N.B. **Gaussian only**. (Integer)

REML Whether to use Restricted Maximum Likelihood. (Logical)

N.B. **Gaussian only**. (Integer)

parallel Whether to run the "n" evaluations in parallel. (Logical)

Remember to register a parallel backend first. E.g. with `doParallel::registerDoParallel`.

Details

Packages used:

- **Models:**
  - Gaussian: `stats::lm, lme4::lmer`

- **Results:** Gaussian:
  - r2m: `MuMIn::r.squaredGLMM`
  - r2c: `MuMIn::r.squaredGLMM`
  - AIC: `stats::AIC`
  - AICc: `MuMIn::AICC`
  - BIC: `stats::BIC`

- **Binomial and Multinomial:**
  - ROC and related metrics:
    - Binomial: `pROC::roc`
    - Multinomial: `pROC::multiclass.roc`

Value

list containing:

1. a tibble with summarized results (called `summarized_metrics`)
2. a tibble with random evaluations (`random_evaluations`)
3. a tibble with the summarized class level results (`summarized_class_level_results`) (Multinomial only)
**Gaussian Results:**

The **Summarized Results** tibble contains:
- Average RMSE, MAE, NRMSE(IQR), RRSE, RAE, RMSLE.
- See the additional metrics (disabled by default) at `?gaussian_metrics`.
- The **Measure** column indicates the statistical descriptor used on the evaluations. The row where **Measure == All_rows** is the evaluation when the baseline model is trained on all rows in `train_data`.
- The **Training Rows** column contains the aggregated number of rows used from `train_data` when fitting the baseline models.

The **Random Evaluations** tibble contains:
- The **non-aggregated metrics**.
- A nested tibble with the **predictions** and targets.
- A nested tibble with the **coefficients** of the baseline models.
- Number of **training rows** used when fitting the baseline model on the training set.
- A nested **Process** information object with information about the evaluation.
- Name of **dependent** variable.
- Name of **fixed** effect (bias term only).
- **Random** effects structure (if specified).

**Binomial Results:**

Based on the generated test set predictions, a confusion matrix and ROC curve are used to get the following:
- **ROC**:
  - AUC, Lower CI, and Upper CI
  - Note, that the ROC curve is only computed when AUC is enabled.
- **Confusion Matrix**:
  - Balanced Accuracy, Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, Prevalence, and MCC (Matthews correlation coefficient).

The **Summarized Results** tibble contains:
- The **Measure** column indicates the statistical descriptor used on the evaluations. The row where **Measure == All_0** is the evaluation when all predictions are 0.
- The row where **Measure == All_1** is the evaluation when all predictions are 1.
- The **aggregated metrics**.

The **Random Evaluations** tibble contains:
- The **non-aggregated metrics**.
- A nested tibble with the **predictions** and targets.
- A list of **ROC** curve objects (if computed).
- A nested tibble with the **confusion matrix**. The **Pos_** columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. I.e. the level you wish to predict.
- A nested **Process** information object with information about the evaluation.
- Name of **dependent** variable.
Multinomial Results:

Based on the generated test set predictions, one-vs-all (binomial) evaluations are performed and aggregated to get the same metrics as in the binomial results (excluding MCC, AUC, Lower CI and Upper CI), with the addition of Overall Accuracy and multiclass MCC in the summarized results. It is possible to enable multiclass AUC as well, which has been disabled by default as it is slow to calculate when there's a large set of classes.

Note: we also refer to the one-vs-all evaluations as the class level results.

The Summarized Results tibble contains:
Summary of the random evaluations.

How: First, the one-vs-all binomial evaluations are aggregated by repetition, then, these aggregations are summarized. Besides the metrics from the binomial evaluations (see Binomial Results above), it also includes Overall Accuracy and multiclass MCC.

The Measure column indicates the statistical descriptor used on the evaluations. The Mean, Median, SD, IQR, Max, Min, NAs, and INFs measures describe the Random Evaluations tibble, while the CL_Max, CL_Min, CL_NAs, and CL_INFs describe the Class Level results.

The rows where Measure == All_<<class name>> are the evaluations when all the observations are predicted to be in that class.

The Summarized Class Level Results tibble contains:
The (nested) summarized results for each class, with the same metrics and descriptors as the Summarized Results tibble. Use tidyr::unnest on the tibble to inspect the results.

How: The one-vs-all evaluations are summarized by class.

The rows where Measure == All_0 are the evaluations when none of the observations are predicted to be in that class, while the rows where Measure == All_1 are the evaluations when all of the observations are predicted to be in that class.

The Random Evaluations tibble contains:
The repetition results with the same metrics as the Summarized Results tibble.

How: The one-vs-all evaluations are aggregated by repetition. If a metric contains one or more NAs in the one-vs-all evaluations, it will lead to an NA result for that repetition.

Also includes:
A nested tibble with the one-vs-all binomial evaluations (Class Level Results), including nested Confusion Matrices and the Support column, which is a count of how many observations from the class is in the test set.
A nested tibble with the predictions and targets.
A list of ROC curve objects.
A nested tibble with the multiclass confusion matrix.
A nested Process information object with information about the evaluation.
Name of dependent variable.

Author(s)
Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>
See Also

Other baseline functions: baseline_binomial(), baseline_gaussian(), baseline_multinomial()

Examples

```r
# Attach packages
library(cvms)
library(groupdata2) # partition()
library(dplyr) # %>% arrange()
library(tibble)

# Data is part of cvms
data <- participant.scores

# Set seed for reproducibility
set.seed(1)

# Partition data
partitions <- partition(data, p = 0.7, list_out = TRUE)
train_set <- partitions[[1]]
test_set <- partitions[[2]]

# Create baseline evaluations
# Note: usually n=100 is a good setting

# Gaussian
baseline(
  test_data = test_set, train_data = train_set,
  dependent_col = "score", random_effects = "(1|session)",
  n = 2, family = "gaussian"
)

# Binomial
baseline(
  test_data = test_set, dependent_col = "diagnosis",
  n = 2, family = "binomial"
)

# Multinomial
# Create some data with multiple classes
multiclass_data <- tibble(
  "target" = rep(paste0("class_", 1:5), each = 10)
) %>%
  dplyr::sample_n(35)
baseline(
  test_data = multiclass_data,
  dependent_col = "target",
  n = 4, family = "multinomial"
)

# Parallelize evaluations
# Attach doParallel and register four cores
```
# Uncomment:
# library(doParallel)
# registerDoParallel(4)

# Binomial
baseline(
    test_data = test_set, dependent_col = "diagnosis",
    n = 4, family = "binomial"
    #, parallel = TRUE  # Uncomment
)

# Gaussian
baseline(
    test_data = test_set, train_data = train_set,
    dependent_col = "score", random_effects = "(1|session)",
    n = 4, family = "gaussian"
    #, parallel = TRUE  # Uncomment
)

# Multinomial
(mb <- baseline(
    test_data = multiclass_data,
    dependent_col = "target",
    n = 6, family = "multinomial"
    #, parallel = TRUE  # Uncomment
)))

# Inspect the summarized class level results
# for class_2
mb$summarized_class_level_results %>%
  dplyr::filter(Class == "class_2") %>%
  tidyr::unnest(Results)

# Multinomial with custom random generator function
# that creates very "certain" predictions
# (once softmax is applied)
rcertain <- function(n) {
  (runif(n, min = 1, max = 100)^1.4) / 100
}

baseline(
    test_data = multiclass_data,
    dependent_col = "target",
    n = 6, family = "multinomial",
    random_generator_fn = rcertain
    #, parallel = TRUE  # Uncomment
)
Description

[Maturing]

Create a baseline evaluation of a test set.

In modelling, a baseline is a result that is meaningful to compare the results from our models to. For instance, in classification, we usually want our results to be better than random guessing. E.g. if we have three classes, we can expect an accuracy of 33.33%, as for every observation we have 1/3 chance of guessing the correct class. So our model should achieve a higher accuracy than 33.33% before it is more useful to us than guessing.

While this expected value is often fairly straightforward to find analytically, it only represents what we can expect on average. In reality, it's possible to get far better results than that by guessing. baseline_binomial() finds the range of likely values by evaluating multiple sets of random predictions and summarizing them with a set of useful descriptors. Additionally, it evaluates a set of all 0 predictions and a set of all 1 predictions.

Usage

baseline_binomial(
    test_data, 
    dependent_col, 
    n = 100, 
    metrics = list(), 
    positive = 2, 
    cutoff = 0.5, 
    parallel = FALSE 
)

Arguments

- **test_data** data.frame.
- **dependent_col** Name of dependent variable in the supplied test and training sets.
- **n** The number of sets of random predictions to evaluate. (Default is 100)
- **metrics** list for enabling/disabling metrics. E.g. list("F1" = FALSE) would remove F1 from the results, and list("Accuracy" = TRUE/FALSE) will be used for the remaining available metrics. You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i. list("all" = FALSE,"Accuracy" = TRUE) would return only the Accuracy metric.
  The list can be created with binomial_metrics(). Also accepts the string "all".
- **positive** Level from dependent variable to predict. Either as character (preferable) or level index (1 or 2 - alphabetically).
  E.g. if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".
  **Note:** For reproducibility, it’s preferable to specify the name directly, as different locales may sort the levels differently. Used when calculating confusion matrix metrics and creating ROC curves. N.B. Only affects evaluation metrics, not the returned predictions.
cutoff: Threshold for predicted classes. (Numeric)
parallel: Whether to run the 'n' evaluations in parallel. (Logical)

Remember to register a parallel backend first. E.g. with doParallel::registerDoParallel.

Details
Packages used:
ROC and AUC: pROC::roc

Value
list containing:
1. a tibble with summarized results (called summarized_metrics)
2. a tibble with random evaluations (random Evaluations)

Based on the generated test set predictions, a confusion matrix and ROC curve are used to get the following:
ROC:
AUC, Lower CI, and Upper CI

Note, that the ROC curve is only computed when AUC is enabled.

Confusion Matrix:
Balanced Accuracy, Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, Prevalence, and MCC (Matthews correlation coefficient).

The Summarized Results tibble contains:
The Measure column indicates the statistical descriptor used on the evaluations. The row where Measure == All_0 is the evaluation when all predictions are 0. The row where Measure == All_1 is the evaluation when all predictions are 1.

The aggregated metrics.

The Random Evaluations tibble contains:
The non-aggregated metrics.
A nested tibble with the predictions and targets.
A list of ROC curve objects (if computed).
A nested tibble with the confusion matrix. The Pos_. columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. I.e: the level you wish to predict.

A nested Process information object with information about the evaluation.
Name of dependent variable.

Author(s)
Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>
See Also

Other baseline functions: baseline_gaussian(), baseline_multinomial(), baseline()

Examples

```r
# Attach packages
library(cvms)
library(groupdata2) # partition()
library(dplyr) # %>% arrange()

# Data is part of cvms
data <- participant.scores

# Set seed for reproducibility
set.seed(1)

# Partition data
partitions <- partition(data, p = 0.7, list_out = TRUE)
train_set <- partitions[[1]]
test_set <- partitions[[2]]

# Create baseline evaluations
# Note: usually n=100 is a good setting
baseline_binomial(
  test_data = test_set,
  dependent_col = "diagnosis",
  n = 2
)

# Parallelize evaluations

# Attach doParallel and register four cores
# Uncomment:
# library(doParallel)
# registerDoParallel(4)

# Make sure to uncomment the parallel argument
baseline_binomial(
  test_data = test_set,
  dependent_col = "diagnosis",
  n = 4
  #, parallel = TRUE  # Uncomment
)
```

**baseline_gaussian**

Create baseline evaluations for regression models

**Description**

[Maturing]

Create a baseline evaluation of a test set.
In modelling, a *baseline* is a result that is meaningful to compare the results from our models to. In regression, we want our model to be better than a model without any predictors. If our model does not perform better than such a simple model, it’s unlikely to be useful.

`baseline_gaussian()` fits the intercept-only model (`y ~ 1`) on `n` random subsets of `train_data` and evaluates each model on `test_data`. Additionally, it evaluates a model fitted on all rows in `train_data`.

### Usage

```r
baseline_gaussian(
  test_data,  # data.frame.
  train_data,  # data.frame.
  dependent_col,  # Name of dependent variable in the supplied test and training sets.
  n = 100,  # The number of random samplings of `train_data` to fit baseline models on. (Default is 100)
  metrics = list(),  # list for enabling/disabling metrics.
  random_effects = NULL,  # Random effects structure for the baseline model. (Character)
  min_training_rows = 5,  # Minimum number of rows in the random subsets of `train_data`.
  min_training_rows_left_out = 3,  # Minimum number of rows left out of the random subsets of `train_data`. I.e. a subset will maximally have the size: `max_rows_in_subset = nrow(`train_data`) - `min_training_rows_left_out`.
  REML = FALSE,  # Whether to use Restricted Maximum Likelihood. (Logical)
  parallel = FALSE  # Whether to run the `n` evaluations in parallel. (Logical)
)
```

### Arguments

- `test_data` data.frame.
- `train_data` data.frame.
- `dependent_col` Name of dependent variable in the supplied test and training sets.
- `n` The number of random samplings of `train_data` to fit baseline models on. (Default is 100)
- `metrics` list for enabling/disabling metrics.
  - E.g. `list("RMSE" = FALSE)` would remove RMSE from the results, and `list("TAE" = TRUE)` would add the Total Absolute Error metric to the results. Default values (TRUE/FALSE) will be used for the remaining available metrics.
  - You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i. `list("all" = FALSE,"RMSE" = TRUE)` would return only the RMSE metric.
  - The list can be created with `gaussian_metrics()`.
  - Also accepts the string "all".
- `random_effects` Random effects structure for the baseline model. (Character)
  - E.g. with "(1|ID)", the model becomes "y ~ 1 + (1|ID)".
- `min_training_rows` Minimum number of rows in the random subsets of `train_data`.
- `min_training_rows_left_out` Minimum number of rows left out of the random subsets of `train_data`. I.e. a subset will maximally have the size: `max_rows_in_subset = nrow(`train_data`) - `min_training_rows_left_out`.
- `REML` Whether to use Restricted Maximum Likelihood. (Logical)
- `parallel` Whether to run the `n` evaluations in parallel. (Logical)

Remember to register a parallel backend first. E.g. with `doParallel::registerDoParallel`. 

Details

Packages used:

Models:
stats::lm, lme4::lmer

Results:
\texttt{r2m} : MuMIn::\texttt{r.squaredGLMM} \\
\texttt{r2c} : MuMIn::\texttt{r.squaredGLMM} \\
\texttt{AIC} : stats::\texttt{AIC} \\
\texttt{AICc} : MuMIn::\texttt{AICc} \\
\texttt{BIC} : stats::\texttt{BIC}

Value

list containing:

1. a \texttt{tibble} with summarized results (called \texttt{summarized_metrics})
2. a \texttt{tibble} with random evaluations (\texttt{random_evaluations})

The \textbf{Summarized Results} \texttt{tibble} contains:

Average RMSE, MAE, NRMSE(IQR), RRSE, RAE, RMSLE.

See the additional metrics (disabled by default) at \texttt{?gaussian_metrics}.

The \textbf{Measure} column indicates the statistical descriptor used on the evaluations. The row where \texttt{Measure} == \texttt{All\_rows} is the evaluation when the baseline model is trained on all rows in `\texttt{train\_data}`.

The \textbf{Training Rows} column contains the aggregated number of rows used from `\texttt{train\_data}`, when fitting the baseline models.

The \textbf{Random Evaluations} \texttt{tibble} contains:

The \textbf{non-aggregated metrics}.

A nested \texttt{tibble} with the \textbf{predictions} and targets.

A nested \texttt{tibble} with the \textbf{coefficients} of the baseline models.

Number of \textbf{training rows} used when fitting the baseline model on the training set.

A nested \textbf{Process} information object with information about the evaluation.

Name of \textbf{dependent} variable.

Name of \textbf{fixed} effect (bias term only).

\textbf{Random} effects structure (if specified).

Author(s)

Ludvig Renbo Olsen, \texttt{<r-pkgs@ludvigolsen.dk>}

See Also

Other baseline functions: \texttt{baseline\_binomial()}, \texttt{baseline\_multinomial()}, \texttt{baseline()}

Examples

# Attach packages
library(cvms)
library(groupdata2) # partition()
library(dplyr) # %>% arrange()

# Data is part of cvms
data <- participant.scores

# Set seed for reproducibility
set.seed(1)

# Partition data
partitions <- partition(data, p = 0.7, list_out = TRUE)
train_set <- partitions[[1]]
test_set <- partitions[[2]]

# Create baseline evaluations
# Note: usually n=100 is a good setting
baseline_gaussian(
  test_data = test_set,
  train_data = train_set,
  dependent_col = "score",
  random_effects = "(1|session)",
  n = 2
)

# Parallelize evaluations

# Attach doParallel and register four cores
# Uncomment:
# library(doParallel)
# registerDoParallel(4)

# Make sure to uncomment the parallel argument
baseline_gaussian(
  test_data = test_set,
  train_data = train_set,
  dependent_col = "score",
  random_effects = "(1|session)",
  n = 4
  #, parallel = TRUE  # Uncomment
)

baseline_multinomial

Create baseline evaluations

Description

[Maturing]
Create a baseline evaluation of a test set.
In modelling, a baseline is a result that is meaningful to compare the results from our models to. For instance, in classification, we usually want our results to be better than random guessing. E.g. if we have three classes, we can expect an accuracy of 33.33%, as for every observation we have 1/3 chance of guessing the correct class. So our model should achieve a higher accuracy than 33.33% before it is more useful to us than guessing.

While this expected value is often fairly straightforward to find analytically, it only represents what we can expect on average. In reality, it’s possible to get far better results than that by guessing. baseline_multinomial() finds the range of likely values by evaluating multiple sets of random predictions and summarizing them with a set of useful descriptors.

Technically, it creates one-vs-all (binomial) baseline evaluations for the \(n\) sets of random predictions and summarizes them. Additionally, sets of "all class x,y,z,..." predictions are evaluated.

Usage

```r
baseline_multinomial(
  test_data, dependent_col, 
n = 100, metrics = list(),
  random_generator_fn = runif, parallel = FALSE
)
```

Arguments

test_data data.frame.

dependent_col Name of dependent variable in the supplied test and training sets.
n The number of sets of random predictions to evaluate. (Default is 100)
metrics list for enabling/disabling metrics.
E.g. list("F1" = FALSE) would remove F1 from the results, and list("Accuracy" = TRUE) would add the regular Accuracy metric to the results. Default values (TRUE/FALSE) will be used for the remaining available metrics.

You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i. list("all" = FALSE,"Accuracy" = TRUE) would return only the Accuracy metric.

The list can be created with multinomial_metrics().
Also accepts the string "all".

random_generator_fn Function for generating random numbers. The softmax function is applied to the generated numbers to transform them to probabilities.
The first argument must be the number of random numbers to generate, as no other arguments are supplied.

To test the effect of using different functions, see multiclass_probability_tibble().

parallel Whether to run the \(n\) evaluations in parallel. (Logical)
Remember to register a parallel backend first. E.g. with doParallel::registerDoParallel.

Details

Packages used:
Multiclass ROC curve and AUC: pROC::multiclass.roc
Value list containing:

1. a tibble with summarized results (called `summarized_metrics`)
2. a tibble with random evaluations (`random_evaluations`)
3. a tibble with the summarized class level results (`summarized_class_level_results`)

Macro metrics:
Based on the generated predictions, one-vs-all (binomial) evaluations are performed and aggregated to get the following macro metrics:

Balanced Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, and Prevalence.

In general, the metrics mentioned in `binomial_metrics()` can be enabled as macro metrics (excluding MCC, AUC, Lower CI, Upper CI, and the AIC/AICc/BIC metrics). These metrics also has a weighted average version.

N.B. we also refer to the one-vs-all evaluations as the class level results.

Multiclass metrics:
In addition, the Overall Accuracy and multiclass MCC metrics are computed. Multiclass AUC can be enabled but is slow to calculate with many classes.

The Summarized Results tibble contains:
Summary of the random evaluations.

How: The one-vs-all binomial evaluations are aggregated by repetition and summarized. Besides the metrics from the binomial evaluations, it also includes Overall Accuracy and multiclass MCC.

The Measure column indicates the statistical descriptor used on the evaluations. The Mean, Median, SD, IQR, Max, Min, NAs, and INFs measures describe the Random Evaluations tibble, while the CL_Max, CL_Min, CL_NAs, and CL_INFs describe the Class Level results.

The rows where Measure == All_<class name>> are the evaluations when all the observations are predicted to be in that class.

The Summarized Class Level Results tibble contains:
The (nested) summarized results for each class, with the same metrics and descriptors as the Summarized Results tibble. Use `tidyr::unnest` on the tibble to inspect the results.

How: The one-vs-all evaluations are summarized by class.

The rows where Measure == All_0 are the evaluations when none of the observations are predicted to be in that class, while the rows where Measure == All_1 are the evaluations when all of the observations are predicted to be in that class.

The Random Evaluations tibble contains:
The repetition results with the same metrics as the Summarized Results tibble.

How: The one-vs-all evaluations are aggregated by repetition. If a metric contains one or more NAs in the one-vs-all evaluations, it will lead to an NA result for that repetition.

Also includes:
baseline_multinomial

A nested tibble with the one-vs-all binomial evaluations (Class Level Results), including nested Confusion Matrices and the Support column, which is a count of how many observations from the class is in the test set.

A nested tibble with the predictions and targets.

A list of ROC curve objects.

A nested tibble with the multiclass confusion matrix.

A nested Process information object with information about the evaluation.

Name of dependent variable.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other baseline functions: baseline_binomial(), baseline_gaussian(), baseline()

Examples

```r
# Attach packages
library(cvms)
library(groupdata2) # partition()
library(dplyr) # %>% arrange()
library(tibble)

# Data is part of cvms
data <- participant.scores

# Set seed for reproducibility
set.seed(1)

# Partition data
partitions <- partition(data, p = 0.7, list_out = TRUE)
train_set <- partitions[[1]]
test_set <- partitions[[2]]

# Create baseline evaluations
# Note: usually n=100 is a good setting

# Create some data with multiple classes
multiclass_data <- tibble(
  "target" = rep(paste0("class_", 1:5), each = 10)
) %>%
dplyr::sample_n(35)

baseline_multinomial(
  test_data = multiclass_data,
  dependent_col = "target",
  n = 4
)

# Parallelize evaluations

# Attach doParallel and register four cores
```
# Uncomment:
# library(doParallel)
# registerDoParallel(4)

# Make sure to uncomment the parallel argument
mb <- baseline_multinomial(
  test_data = multiclass_data,
  dependent_col = "target",
  n = 6
  #, parallel = TRUE  # Uncomment

)

# Inspect the summarized class level results
# for class_2
mb$summarized_class_level_results %>%
  dplyr::filter(Class == "class_2") %>%
  tidyr::unnest(Results)

# Multinomial with custom random generator function
# that creates very "certain" predictions
# (once softmax is applied)
rcertain <- function(n) {
  (runif(n, min = 1, max = 100)^1.4) / 100
}

# Make sure to uncomment the parallel argument
baseline_multinomial(
  test_data = multiclass_data,
  dependent_col = "target",
  n = 6,
  random_generator_fn = rcertain
  #, parallel = TRUE  # Uncomment

)

---

**binomial_metrics**  
Select metrics for binomial evaluation

**Description**

[Experimental]
Enable/disable metrics for binomial evaluation. Can be supplied to the `metrics` argument in many of the `cvms` functions.

Note: Some functions may have slightly different defaults than the ones supplied here.

**Usage**

```r
binomial_metrics(
  all = NULL,
  balanced_accuracy = NULL,
  accuracy = NULL,
  f1 = NULL,
```

```r
element
```
sensitivity = NULL,
specificity = NULL,
pos_pred_value = NULL,
neg_pred_value = NULL,
auc = NULL,
lower_ci = NULL,
upper_ci = NULL,
kappa = NULL,
mcc = NULL,
detection_rate = NULL,
detection_prevalence = NULL,
prevalence = NULL,
false_neg_rate = NULL,
false_pos_rate = NULL,
false_discovery_rate = NULL,
false_omission_rate = NULL,
threat_score = NULL,
aic = NULL,
aicc = NULL,
bic = NULL
)

Arguments

all  Enable/disable all arguments at once. (Logical)
    Specifying other metrics will overwrite this, why you can use (all = FALSE, accuracy = TRUE) to get only the Accuracy metric.

balanced_accuracy  Balanced Accuracy (Default: TRUE)
accuracy  Accuracy (Default: FALSE)
f1  F1 (Default: TRUE)
sensitivity  Sensitivity (Default: TRUE)
specificity  Specificity (Default: TRUE)
pos_pred_value  Pos Pred Value (Default: TRUE)
neg_pred_value  Neg Pred Value (Default: TRUE)
auc  AUC (Default: TRUE)
lower_ci  Lower CI (Default: TRUE)
upper_ci  Upper CI (Default: TRUE)
kappa  Kappa (Default: TRUE)
mcc  MCC (Default: TRUE)
detection_rate  Detection Rate (Default: TRUE)
detection_prevalence  Detection Prevalence (Default: TRUE)
prevalence  Prevalence (Default: TRUE)
false_neg_rate  False Neg Rate (Default: FALSE)
false_pos_rate  False Pos Rate (Default: FALSE)
false_discovery_rate  False Discovery Rate (Default: FALSE)
**combine_predictors**

Generate model formulas by combining predictors

---

### Description

[Maturing]

Create model formulas with every combination of your fixed effects, along with the dependent variable and random effects. 259,358 formulas have been precomputed with two- and three-way interactions for up to 8 fixed effects, with up to 5 included effects per formula. Uses the + and * operators, so lower order interactions are automatically included.

### Usage

```r
combine_predictors(
  dependent,
  fixed_effects,
  random_effects = NULL,
  max_fixed_effects = 5,
  max_interaction_size = 3,
  max_effect_frequency = NULL
)
```
**Arguments**

- **dependent**  
  Name of dependent variable. (Character)

- **fixed_effects**  
  List of fixed effects. (Character)  
  Max. limit of 8 effects **when interactions are included!**  
  A fixed effect name cannot contain: white spaces, "*" or "+".  
  Effects in sublists will be interchanged. This can be useful, when we have multiple versions of a predictor (e.g. \( x1 \) and \( \log(x1) \)) that we do not wish to have in the same formula.  
  Example of interchangeable effects:  
  \[
  \text{list}\left( \text{list}("x1","\log_x1"),"x2","x3" \right)
  \]

- **random_effects**  
  The random effects structure. (Character)  
  Is appended to the model formulas.

- **max_fixed_effects**  
  Maximum number of fixed effects in a model formula. (Integer)  
  Max. limit of 5 **when interactions are included!**

- **max_interaction_size**  
  Maximum number of effects in an interaction. (Integer)  
  Max. limit of 3.  
  Use this to limit the n-way interactions allowed. 0 or 1 excludes interactions all together.  
  A model formula can contain multiple interactions.

- **max_effect_frequency**  
  Maximum number of times an effect is included in a formula string.

**Value**

List of model formulas.  
E.g.:  
\[
\text{c("y \sim x1 + (1|z)"","y \sim x2 + (1|z)"","y \sim x1 + x2 + (1|z)"","y \sim x1 \times x2 + (1|z)")}
\]

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

**Examples**

```r
# Attach packages
library(cvms)

# Create effect names
dependent <- "y"
fixed_effects <- c("a", "b", "c")
random_effects <- "(1|e)"

# Create model formulas
combine_predictors(
  dependent, fixed_effects,
  random_effects
)
```
```r
# Create effect names with interchangeable effects in sublists
defined_effects <- list("a", list("b", "log_b"), "c")

# Create model formulas
combine_predictors(
  dependent, defined_effects, 
  random_effects
)
```

**compatible.formula.terms**

Compatible formula terms

**Description**

162,660 pairs of compatible terms for building model formulas with up to 15 fixed effects.

**Format**

A data frame with 162,660 rows and 5 variables:

- **left** term, fixed effect or interaction, with fixed effects separated by "*"
- **right** term, fixed effect or interaction, with fixed effects separated by "*"
- **max_interaction_size** maximum interaction size in the two terms, up to 3
- **num_effects** number of unique fixed effects in the two terms, up to 5
- **min_num_fixed_effects** minimum number of fixed effects required to use a formula with the two terms, i.e. the index in the alphabet of the last of the alphabetically ordered effects (letters) in the two terms, so 4 if left == "A" and right == "D"

**Details**

A term is either a fixed effect or an interaction between fixed effects (up to three-way), where the effects are separated by the "*" operator.

Two terms are compatible if they are not redundant, meaning that both add a fixed effect to the formula. E.g. as the interaction "x1 * x2 * x3" expands to "x1 + x2 + x3 + x1 * x2 + x1 * x3 + x2 * x3 + x1 * x2 * x3", the higher order interaction makes these "sub terms" redundant. Note: All terms are compatible with NA.

Effects are represented by the first fifteen capital letters.

Used to generate the model formulas for `combine_predictors`.

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>
confusion_matrix

Description

[Experimental]

Creates a confusion matrix from targets and predictions. Calculates associated metrics.

Multiclass results are based on one-vs-all evaluations. Both regular averaging and weighted averaging are available. Also calculates the Overall Accuracy.

Note: In most cases you should use `evaluate()` instead. It has additional metrics and works in magrittr pipes (e.g. `%>%`) and with `dplyr::group_by()`. `confusion_matrix()` is more lightweight and may be preferred in programming when you don’t need the extra stuff in `evaluate()`.

Usage

```r
confusion_matrix(
  targets, predictions,
  metrics = list(),
  positive = 2,
  c_levels = NULL,
  do_one_vs_all = TRUE,
  parallel = FALSE
)
```

Arguments

- **targets**: vector with true classes. Either numeric or character.
- **predictions**: vector with predicted classes. Either numeric or character.
- **metrics**: list for enabling/disabling metrics. E.g. `list("Accuracy" = TRUE)` would add the regular accuracy metric, while `list("F1" = FALSE)` would remove the F1 metric. Default values (TRUE/FALSE) will be used for the remaining available metrics.

  You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why for instance `list("all" = FALSE,"Accuracy" = TRUE)` would return only the Accuracy metric.

  The list can be created with `binomial_metrics()` or `multinomial_metrics()`. Also accepts the string "all".

- **positive**: Level from `targets` to predict. Either as character (preferable) or level index (1 or 2 - alphabetically). (Two-class only)

  E.g. if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".

  Note: For reproducibility, it’s preferable to specify the name directly, as different locales may sort the levels differently.
confusion_matrix

c_levels  vector with categorical levels in the targets. Should have same type as `targets`.
    If NULL, they are inferred from `targets`.
    N.B. the levels are sorted alphabetically. When `positive` is numeric (i.e. an index), it therefore still refers to the index of the alphabetically sorted levels.

do_one_vs_all  Whether to perform one-vs-all evaluations when working with more than 2 classes (multiclass).
    If you are only interested in the confusion matrix, this allows you to skip most of the metric calculations.

parallel  Whether to perform the one-vs-all evaluations in parallel. (Logical)
    N.B. This only makes sense when you have a lot of classes or a very large dataset.
    Remember to register a parallel backend first. E.g. with doParallel::registerDoParallel.

Details

The following formulas are used for calculating the metrics:

Sensitivity = TP / (TP + FN)
Specificity = TN / (TN + FP)
Pos Pred Value = TP / (TP + FP)
Neg Pred Value = TN / (TN + FN)
Balanced Accuracy = (Sensitivity + Specificity) / 2
Accuracy = (TP + TN) / (TP + TN + FP + FN)
Overall Accuracy = Correct / (Correct + Incorrect)
F1 = 2 * Pos Pred Value * Sensitivity / (Pos Pred Value + Sensitivity)
MCC = ((TP * TN) - (FP * FN)) / sqrt((TP + FP) * (TP + FN) * (TN + FP) * (TN + FN))
Note for MCC: Formula is for the binary case. When the denominator is 0, we set it to 1 to avoid NaN. See the metrics vignette for the multiclass version.
Detection Rate = TP / (TP + FN + TN + FP)
Detection Prevalence = (TP + FP) / (TP + FN + TN + FP)
Threat Score = TP / (TP + FN + FP)
False Neg Rate = 1 - Sensitivity
False Pos Rate = 1 - Specificity
False Discovery Rate = 1 - Pos Pred Value
False Omission Rate = 1 - Neg Pred Value
For Kappa the counts (TP, TN, FP, FN) are normalized to percentages (summing to 1). Then the following is calculated:

p_observed = TP + TN
p_expected = (TN + FP) * (TN + FN) + (FN + TP) * (FP + TP)
Kappa = (p_observed - p_expected) / (1 - p_expected)
Value
tibble with:
Nested **confusion matrix** (tidied version)
Nested confusion matrix (**table**)
The Positive Class.
Multiclass only: Nested **Class Level Results** with the two-class metrics, the nested confusion matrices, and the **Support** metric, which is a count of the class in the target column and is used for the weighted average metrics.
The following metrics are available (see `metrics`):

**Two classes or more:**

<table>
<thead>
<tr>
<th>Metric</th>
<th>Name</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>Balanced Accuracy</td>
<td>&quot;Balanced Accuracy&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Accuracy</td>
<td>&quot;Accuracy&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>F1</td>
<td>&quot;F1&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Sensitivity</td>
<td>&quot;Sensitivity&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Specificity</td>
<td>&quot;Specificity&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Positive Predictive Value</td>
<td>&quot;Pos Pred Value&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Negative Predictive Value</td>
<td>&quot;Neg Pred Value&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Kappa</td>
<td>&quot;Kappa&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Matthews Correlation Coefficient</td>
<td>&quot;MCC&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Detection Rate</td>
<td>&quot;Detection Rate&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Detection Prevalence</td>
<td>&quot;Detection Prevalence&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Prevalence</td>
<td>&quot;Prevalence&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>False Negative Rate</td>
<td>&quot;False Neg Rate&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>False Positive Rate</td>
<td>&quot;False Pos Rate&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>False Discovery Rate</td>
<td>&quot;False Discovery Rate&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>False Omission Rate</td>
<td>&quot;False Omission Rate&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>Threat Score</td>
<td>&quot;Threat Score&quot;</td>
<td>Disabled</td>
</tr>
</tbody>
</table>

The **Name** column refers to the name used in the package. This is the name in the output and when enabling/disabling in `metrics`.

**Three classes or more:**
The metrics mentioned above (excluding MCC) has a weighted average version (disabled by default; weighted by the **Support**).
In order to enable a weighted metric, prefix the metric name with "Weighted " when specifying `metrics`.
E.g. `metrics = list("Weighted Accuracy" = TRUE)`.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Name</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall Accuracy</td>
<td>&quot;Overall Accuracy&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Weighted *</td>
<td>&quot;Weighted *&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>Multiclass MCC</td>
<td>&quot;MCC&quot;</td>
<td>Enabled</td>
</tr>
</tbody>
</table>
cross_validate

Cross-validate regression models for model selection

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other evaluation functions: `binomial_metrics()`, `evaluate_residuals()`, `evaluate()`, `gaussian_metrics()`, `multinomial_metrics()`

Examples

```r
# Attach cvms
library(cvms)

# Two classes

# Create targets and predictions
targets <- c(0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1)
predictions <- c(1, 1, 0, 0, 0, 1, 1, 1, 0, 1, 0, 0)

# Create confusion matrix with default metrics
cm <- confusion_matrix(targets, predictions)

# Enable weighted accuracy

# Create confusion matrix with weighted accuracy enabled
cm <- confusion_matrix(targets, predictions, 
  metrics = list("Weighted Accuracy" = TRUE))
```

**Description**

[Stable]

Cross-validate one or multiple linear or logistic regression models at once. Perform repeated cross-validation. Returns results in a tibble for easy comparison, reporting and further analysis.

See `cross_validate_fn()` for use with custom model functions.

**Usage**

```r
cross_validate(
  data,  
  formulas,  
  family,  
  fold_cols = ".folds",  
  control = NULL,  
  REML = FALSE,  
  cutoff = 0.5,  
  positive = 2,  
  metrics = list(),  
  preprocessing = NULL,  
  rm_nc = FALSE,  
  parallel = FALSE,  
  verbose = FALSE,  
  link = deprecated(),  
  models = deprecated(),  
  model_verbose = deprecated()
)
```

**Arguments**

- `data` `data.frame`. Must include one or more grouping factors for identifying folds - as made with `groupdata2::fold()`.
- `formulas` Model formulas as strings. (Character) E.g. `c("y~x","y~z")`. Can contain random effects. E.g. `c("y~x+(1|r)","y~z+(1|r)")`.
- `family` Name of the family. (Character) Currently supports "gaussian" for linear regression with `lm()` / `lme4::lmer()` and "binomial" for binary classification with `glm()` / `lme4::glmer()`.
  See `cross_validate_fn()` for use with other model functions.
- `fold_cols` Name(s) of grouping factor(s) for identifying folds. (Character) Include names of multiple grouping factors for repeated cross-validation.
- `control` Construct control structures for mixed model fitting (with `lme4::lmer()` or `lme4::glmer()`). See `lme4::lmerControl` and `lme4::glmerControl`. N.B. Ignored if fitting `lm()` or `glm()` models.
- `REML` Restricted Maximum Likelihood. (Logical)
- `cutoff` Threshold for predicted classes. (Numeric) N.B. **Binomial models only**
**positive**
Level from dependent variable to predict. Either as character (preferable) or level index (1 or 2 - alphabetically).
E.g. if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".

**Note:** For reproducibility, it’s preferable to specify the name directly, as different locales may sort the levels differently.

Used when calculating confusion matrix metrics and creating ROC curves.
The Positive Class column in the output can be used to verify this setting.
N.B. Only affects evaluation metrics, not the model training or returned predictions.

**metrics**
list for enabling/disabling metrics.
E.g. list("RMSE" = FALSE) would remove RMSE from the results, and list("Accuracy" = TRUE) would add the regular Accuracy metric to the classification results. Default values (TRUE/FALSE) will be used for the remaining available metrics.
You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why list("all" = FALSE, "RMSE" = TRUE) would return only the RMSE metric.
The list can be created with gaussian_metrics() or binomial_metrics(). Also accepts the string "all".

**preprocessing**
Name of preprocessing to apply.
Available preprocessings are:

- "standardize" Centers and scales the numeric predictors.
- "range" Normalizes the numeric predictors to the 0-1 range. Values outside the min/max range in the test fold are truncated to 0/1.
- "scale" Scales the numeric predictors to have a standard deviation of one.
- "center" Centers the numeric predictors to have a mean of zero.

The preprocessing parameters (mean, SD, etc.) are extracted from the training folds and applied to both the training folds and the test fold. They are returned in the Preprocess column for inspection.
N.B. The preprocessings should not affect the results to a noticeable degree, although "range" might due to the truncation.

**rm_nc**
Remove non-converged models from output. (Logical)

**parallel**
Whether to cross-validate the list of models in parallel. (Logical)
Remember to register a parallel backend first. E.g. with doParallel::registerDoParallel.

**verbose**
Whether to message process information like the number of model instances to fit and which model function was applied. (Logical)

**link, models, model_verbose**
Deprecated.

**Details**
Packages used:

**Models:**
Gaussian: `stats::lm, lme4::lmer`

Binomial: `stats::glm, lme4::glmer`

**Results:**

**Shared:**
- AIC: `stats::AIC`
- AICc: `MuMIn::AICc`
- BIC: `stats::BIC`

**Gaussian:**
- `r2m`: `MuMIn::r.squaredGLMM`
- `r2c`: `MuMIn::r.squaredGLMM`

**Binomial:**
- ROC and AUC: `pROC::roc`

**Value**

A tibble with results for each model.

**Shared across families:** A nested tibble with **coefficients** of the models from all iterations.
- Number of *total folds*.
- Number of *fold columns*.
- Count of **convergence warnings**. Consider discarding models that did not converge on all iterations. Note: you might still see results, but these should be taken with a grain of salt!
- Count of **other warnings**. These are warnings without keywords such as "convergence".
- Count of **Singular Fit messages**. See `lme4::isSingular` for more information.

A nested tibble with the **warnings and messages** caught for each model.

A nested **Process** information object with information about the evaluation.
- Name of **dependent** variable.
- Names of **fixed** effects.
- Names of **random** effects, if any.

A nested tibble with **preprocessing** parameters, if any.

---

**Gaussian Results:**

Average RMSE, MAE, NRMSE(IQR), RRSE, RAE, RMSLE, AIC, AICc, and BIC of all the iterations*, omitting potential NAs from non-converged iterations. Note that the Information Criterion metrics (AIC, AICc, and BIC) are also averages.

See the additional metrics (disabled by default) at `?gaussian_metrics`.

A nested tibble with the **predictions** and targets.

A nested tibble with the non-averaged **results** from all iterations.

* In repeated cross-validation, the metrics are first averaged for each fold column (repetition) and then averaged again.
Binomial Results:

Based on the collected predictions from the test folds*, a confusion matrix and a ROC curve are created to get the following:

ROC:
AUC, Lower CI, and Upper CI

Confusion Matrix:
Balanced Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, Prevalence, and MCC (Matthews correlation coefficient).

See the additional metrics (disabled by default) at ?binomial_metrics.
Also includes:
A nested tibble with predictions, predicted classes (depends on cutoff), and the targets. Note, that the predictions are not necessarily of the specified positive class, but of the model’s positive class (second level of dependent variable, alphabetically).

The pROC::roc ROC curve object(s).
A nested tibble with the confusion matrix/matrices. The Pos_column tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. I.e. the level you wish to predict.
A nested tibble with the results from all fold columns.
The name of the Positive Class.

* In repeated cross-validation, an evaluation is made per fold column (repetition) and averaged.

Author(s)

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See Also

Other validation functions: cross_validate_fn(), validate_fn(), validate()

Examples

# Attach packages
library(cvms)
library(groupdata2) # fold()
library(dplyr) # %>% arrange()

# Data is part of cvms
data <- participant.scores

# Set seed for reproducibility
set.seed(7)

# Fold data
data <- fold(
data,
k = 4,
cat_col = "diagnosis",
id_col = "participant"
### Gaussian Cross-validation

```r
# Cross-validate a single model

cross_validate(
  data,
  formulas = "score~diagnosis",
  family = "gaussian",
  REML = FALSE
)
```

### Binomial Cross-validation

```r
# Binomial

cross_validate(
  data,
  formulas = "diagnosis~score",
  family = "binomial"
)
```

### Multiple Models Cross-validation

```r
# Cross-validate multiple models

formulas <- c(
  "score~diagnosis+(1|session)",
  "score~age+(1|session)"
)

cross_validate(
  data,
  formulas = formulas,
  family = "gaussian",
  REML = FALSE
)
```

### Parallel Cross-validation

```r
# Use parallelization

# Attach doParallel and register four cores
# Uncomment:
# library(doParallel)
# registerDoParallel(4)

# Cross-validate a list of model formulas in parallel
# Make sure to uncomment the parallel argument

cross_validate(
  data,
  formulas = formulas,
  family = "gaussian",
  #, parallel = TRUE  # Uncomment
)
```
Cross-validate custom model functions for model selection

Description

[Experimental]
Cross-validate your model function with one or multiple model formulas at once. Perform repeated cross-validation. Preprocess the train/test split within the cross-validation. Perform hyperparameter tuning with grid search. Returns results in a tibble for easy comparison, reporting and further analysis.

Compared to \texttt{cross_validate()}\texttt{()}, this function allows you supply a custom model function, a predict function, a preprocess function and the hyperparameter values to cross-validate.

Supports regression and classification (binary and multiclass). See `type`.

Note that some metrics may not be computable for some types of model objects.

Usage

\begin{verbatim}
cross_validate_fn(
  data,
  formulas,
  type,
  model_fn,
  predict_fn,
  preprocess_fn = NULL,
  preprocess_once = FALSE,
  hyperparameters = NULL,
  fold_cols = ".folds",
  cutoff = 0.5,
  positive = 2,
  metrics = list(),
  rm_nc = FALSE,
  parallel = FALSE,
  verbose = TRUE
)
\end{verbatim}

Arguments

- **data**: data.frame.
  Must include one or more grouping factors for identifying folds - as made with \texttt{groupdata2::fold()}.
- **formulas**: Model formulas as strings. (Character)
  Will be converted to \texttt{formula} objects before being passed to `model_fn`.
  E.g. \texttt{c("y~x","y~z")}.
  Can contain random effects.
  E.g. \texttt{c("y~x+(1|r)","y~z+(1|r)")}.
- **type**: Type of evaluation to perform:
  "gaussian" for regression (like linear regression).
  "binomial" for binary classification.
  "multinomial" for multiclass classification.
cross_validate_fn

model_fn
Model function that returns a fitted model object. Will usually wrap an existing model function like e1071::svm or nnet::multinom.
Must have the following function arguments:
function(train_data, formula, hyperparameters)

predict_fn
Function for predicting the targets in the test folds/sets using the fitted model object. Will usually wrap stats::predict(), but doesn’t have to.
Must have the following function arguments:
function(test_data, model, formula, hyperparameters, train_data)
Must return predictions in the following formats, depending on `type`:

**Binomial:** vector or one-column matrix/data.frame with probabilities (0-1) of the second class, alphabetically. E.g.:
c(0.3, 0.5, 0.1, 0.5)

**Gaussian:** vector or one-column matrix/data.frame with the predicted value. E.g.:
c(3.7, 0.9, 1.2, 7.3)

**Multinomial:** data.frame with one column per class containing probabilities of the class. Column names should be identical to how the class names are written in the target column. E.g.:

<table>
<thead>
<tr>
<th>class_1</th>
<th>class_2</th>
<th>class_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.269</td>
<td>0.528</td>
<td>0.203</td>
</tr>
<tr>
<td>0.368</td>
<td>0.322</td>
<td>0.310</td>
</tr>
<tr>
<td>0.375</td>
<td>0.371</td>
<td>0.254</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

preprocess_fn
Function for preprocessing the training and test sets. Can, for instance, be used to standardize both the training and test sets with the scaling and centering parameters from the training set.
Must have the following function arguments:
function(train_data, test_data, formula, hyperparameters)
Must return a list with the preprocessed `train_data` and `test_data`. It may also contain a tibble with the parameters used in preprocessing:
list("train" = train_data,
"test" = test_data,
"parameters" = preprocess_parameters)
Additional elements in the returned list will be ignored.
The optional parameters tibble will be included in the output. It could have the following format:

<table>
<thead>
<tr>
<th>Measure</th>
<th>var_1</th>
<th>var_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>37.921</td>
<td>88.231</td>
</tr>
<tr>
<td>SD</td>
<td>12.4</td>
<td>5.986</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

N.B. When `preprocess_once` is FALSE, the current formula and hyperparameters will be provided. Otherwise, these arguments will be NULL.
cross_validate_fn

preprocess_once

Whether to apply the preprocessing once (ignoring the formula and hyperparameters arguments in `preprocess_fn`) or for every model separately. (Logical)

When preprocessing does not depend on the current formula or hyperparameters, we can do the preprocessing of each train/test split once, to save time. This **may require holding a lot more data in memory** though, why it is not the default setting.

hyperparameters

Either a named list with hyperparameter values to combine in a grid or a data.frame with one row per hyperparameter combination.

**Named list for grid search:** Add ".n" to sample the combinations. Can be the number of combinations to use, or a percentage between 0 and 1.

**E.g.**

```r
list(".n" = 10,# sample 10 combinations
     "lrn_rate" = c(0.1,0.01,0.001),
     "h_layers" = c(10,100,1000),
     "drop_out" = runif(5,0.3,0.7))
```

data.frame with specific hyperparameter combinations: One row per combination to test.

**E.g.**

```
lrn_rate  h_layers  drop_out
0.1       10        0.65
0.1       1000      0.65
0.01      1000      0.63
...       ...       ...
```

fold_cols

Name(s) of grouping factor(s) for identifying folds. (Character)

Include names of multiple grouping factors for repeated cross-validation.

cutoff

Threshold for predicted classes. (Numeric)

**N.B. Binomial models only**

positive

Level from dependent variable to predict. Either as character (**preferable**) or level index (1 or 2 - alphabetically).

**E.g.** if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".

**Note:** For reproducibility, it’s preferable to specify the name directly, as different locales may sort the levels differently.

Used when calculating confusion matrix metrics and creating ROC curves.

The Positive Class column in the output can be used to verify this setting.

**N.B. Only affects evaluation metrics, not the model training or returned predictions.**

**N.B. Binomial models only.**

metrics

list for enabling/disabling metrics.

**E.g.** `list("RMSE" = FALSE)` would remove RMSE from the regression results, and `list("Accuracy" = TRUE)` would add the regular Accuracy metric to the classification results. Default values (TRUE/FALSE) will be used for the remaining available metrics.
You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i. list("all" = FALSE,"RMSE" = TRUE) would return only the RMSE metric.

The list can be created with gaussian_metrics(), binomial_metrics(), or multinomial_metrics().

Also accepts the string "all".

You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i. list("all" = FALSE,"RMSE" = TRUE) would return only the RMSE metric.

The list can be created with gaussian_metrics(), binomial_metrics(), or multinomial_metrics().

Also accepts the string "all".

```
rm_nc
```

Remove non-converged models from output. (Logical)

```
parallel
```

Whether to cross-validate the list of models in parallel. (Logical)

Remember to register a parallel backend first. E.g. with doParallel::registerDoParallel.

```
verbose
```

Whether to message process information like the number of model instances to fit. (Logical)

Details

Packages used:

```
Results:
```

```
Shared:
```

```
AIC : stats::AIC
```

```
AICc : MuMIn::AICc
```

```
BIC : stats::BIC
```

```
Gaussian:
```

```
r2m : MuMIn::r.squaredGLMM
```

```
r2c : MuMIn::r.squaredGLMM
```

```
Binomial and Multinomial:
```

```
ROC and related metrics:
```

```
Binomial: pROC::roc
```

```
Multinomial: pROC::multiclass.roc
```

Value

```
tibble with results for each model.
```

N.B. The Fold column in the nested tibbles contains the test fold in that train/test split.

```
Shared across families:
```

```
A nested tibble with coefficients of the models from all iterations. The coefficients are extracted from the model object with parameters::model_parameters() or coef() (with some restrictions on the output). If these attempts fail, a default coefficients tibble filled with NAs is returned.
```

```
Nested tibble with the used preprocessing parameters, if a passed preprocess_fn returns the parameters in a tibble.
```

```
Number of total folds.
```

```
Number of fold columns.
```

Count of convergence warnings, using a limited set of keywords (e.g. "convergence"). If a convergence warning does not contain one of these keywords, it will be counted with other warnings. Consider discarding models that did not converge on all iterations. Note: you might still see results, but these should be taken with a grain of salt!

```
Nested tibble with the warnings and messages caught for each model.
```

```
A nested Process information object with information about the evaluation.
```

```
N.B. The Fold column in the nested tibbles contains the test fold in that train/test split.
```

```
Shared across families:
```

```
A nested tibble with coefficients of the models from all iterations. The coefficients are extracted from the model object with parameters::model_parameters() or coef() (with some restrictions on the output). If these attempts fail, a default coefficients tibble filled with NAs is returned.
```

```
Nested tibble with the used preprocessing parameters, if a passed preprocess_fn returns the parameters in a tibble.
```

```
Number of total folds.
```

```
Number of fold columns.
```

Count of convergence warnings, using a limited set of keywords (e.g. "convergence"). If a convergence warning does not contain one of these keywords, it will be counted with other warnings. Consider discarding models that did not converge on all iterations. Note: you might still see results, but these should be taken with a grain of salt!

```
Nested tibble with the warnings and messages caught for each model.
```

```
A nested Process information object with information about the evaluation.
```
Name of **dependent** variable.
Names of **fixed** effects.
Names of **random** effects, if any.

---

**Gaussian Results:**

Average RMSE, MAE, NRMSE(IQR), RRSE, RAE, RMSLE of all the iterations*, **omitting potential NAs from non-converged iterations.**

See the additional metrics (disabled by default) at `?gaussian_metrics`.

A nested tibble with the **predictions** and targets.

A nested tibble with the non-averaged **results** from all iterations.

* In repeated cross-validation, the metrics are first averaged for each fold column (repetition) and then averaged again.

---

**Binomial Results:**

Based on the **collected** predictions from the test folds*, a confusion matrix and a ROC curve are created to get the following:

**ROC:**
AUC, Lower CI, and Upper CI

**Confusion Matrix:**
Balanced Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, Prevalence, and MCC (Matthews correlation coefficient).

See the additional metrics (disabled by default) at `?binomial_metrics`.

Also includes:

A nested tibble with **predictions**, predicted classes (depends on cutoff), and the targets. Note, that the predictions are **not necessarily** of the specified positive class, but of the model's positive class (second level of dependent variable, alphabetically).

The `pROC::roc` ROC curve object(s).

A nested tibble with the **confusion matrix/matrices**. The Pos_ columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. I.e. the level you wish to predict.

A nested tibble with the **results** from all fold columns.

The name of the **Positive Class**.

* In repeated cross-validation, an evaluation is made per fold column (repetition) and averaged.

---

**Multinomial Results:**

For each class, a **one-vs-all** binomial evaluation is performed. This creates a **Class Level Results** tibble containing the same metrics as the binomial results described above (excluding MCC, AUC, Lower CI and Upper CI), along with a count of the class in the target column (Support). These metrics are used to calculate the macro metrics. The nested class level results tibble is also included in the output tibble, and could be reported along with the macro and overall metrics.
cross_validate_fn

The output tibble contains the macro and overall metrics. The metrics that share their name with the metrics in the nested class level results tibble are averages of those metrics (note: does not remove NAs before averaging). In addition to these, it also includes the Overall Accuracy and the multiclass MCC.

Other available metrics (disabled by default, see metrics): Accuracy, multiclass AUC, Weighted Balanced Accuracy, Weighted Accuracy, Weighted F1, Weighted Sensitivity, Weighted Specificity, Weighted Pos Pred Value, Weighted Neg Pred Value, Weighted Kappa, Weighted Detection Rate, Weighted Detection Prevalence, and Weighted Prevalence.

Note that the "Weighted" average metrics are weighted by the Support.

Also includes:
- A nested tibble with the predictions, predicted classes, and targets.
- A list of ROC curve objects when AUC is enabled.
- A nested tibble with the multiclass Confusion Matrix.

Class Level Results

Besides the binomial evaluation metrics and the Support, the nested class level results tibble also contains a nested tibble with the Confusion Matrix from the one-vs-all evaluation. The Pos_ columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. In our case, 1 is the current class and 0 represents all the other classes together.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other validation functions: cross_validate(), validate_fn(), validate()

Examples

```r
# Attach packages
library(cvms)
library(groupdata2) # fold()
library(dplyr) # %>% arrange() mutate()

# Note: More examples of custom functions can be found at:
# model_fn: model_functions()
# predict_fn: predict_functions()
# preprocess_fn: preprocess_functions()

# Data is part of cvms
data <- participant.scores

# Set seed for reproducibility
set.seed(7)

# Fold data
data <- fold(
  data,
  k = 4,
  cat_col = "diagnosis",
  id_col = "participant"
) %>%
```
mutate(diagnosis = as.factor(diagnosis)) %>%
  arrange(.folds)

# Cross-validate multiple formulas

formulas_gaussian <- c(
  "score ~ diagnosis",
  "score ~ age"
)
formulas_binomial <- c(
  "diagnosis ~ score",
  "diagnosis ~ age"
)

# Gaussian

# Create model function that returns a fitted model object
lm_model_fn <- function(train_data, formula, hyperparameters) {
  lm(formula = formula, data = train_data)
}

# Create predict function that returns the predictions
lm_predict_fn <- function(test_data, model, formula,
                           hyperparameters, train_data) {
  stats::predict(
    object = model,
    newdata = test_data,
    type = "response",
    allow.new.levels = TRUE
  )
}

# Cross-validate the model function
cross_validate_fn(
  data,
  formulas = formulas_gaussian,
  type = "gaussian",
  model_fn = lm_model_fn,
  predict_fn = lm_predict_fn,
  fold_cols = ".folds"
)

# Binomial

# Create model function that returns a fitted model object
glm_model_fn <- function(train_data, formula, hyperparameters) {
  glm(formula = formula, data = train_data, family = "binomial")
}

# Create predict function that returns the predictions
glm_predict_fn <- function(test_data, model, formula,
                            hyperparameters, train_data) {
  stats::predict(  
    object = model,
    newdata = test_data,
    type = "response",
    allow.new.levels = TRUE
  )
}
40
cross_validate_fn

object = model,
newdata = test_data,
type = "response",
allow.new.levels = TRUE
)
}

# Cross-validate the model function
cross_validate_fn(
data,
formulas = formulas_binomial,
type = "binomial",
model_fn = glm_model_fn,
predict_fn = glm_predict_fn,
fold_cols = ".folds"
)

# Support Vector Machine (svm)
# with hyperparameter tuning

# Create model function that returns a fitted model object
# We use the hyperparameters arg to pass in the kernel and cost values
svm_model_fn <- function(train_data, formula, hyperparameters) {
  # Expected hyperparameters:
  # - kernel
  # - cost
  if (!"kernel" %in% names(hyperparameters))
    stop("hyperparameters must include 'kernel'")
  if (!"cost" %in% names(hyperparameters))
    stop("hyperparameters must include 'cost'")
  e1071::svm(
    formula = formula,
data = train_data,
    kernel = hyperparameters["kernel"],
    cost = hyperparameters["cost"],
    scale = FALSE,
    type = "C-classification",
    probability = TRUE
  )
}

# Create predict function that returns the predictions
svm_predict_fn <- function(test_data, model, formula,
                           hyperparameters, train_data) {
predictions <- stats::predict(
  object = model,
  newdata = test_data,
  allow.new.levels = TRUE,
  probability = TRUE
)

# Extract probabilities
probabilities <- dplyr::as_tibble(
# Cross-validate the model function

cv <- cross_validate_fn(data,
    formulas = formulas_binomial,
    type = "binomial",
    model_fn = svm_model_fn,
    predict_fn = svm_predict_fn,
    hyperparameters = svm_hparams,
    fold_cols = ".folds"
)

cv

# The `HParams` column has the nested hyperparameter values

cv %>%
    select(Dependent, Fixed, HParams, `Balanced Accuracy`, F1, AUC, MCC) %>%
    tidyr::unnest(cols = "HParams") %>%
    arrange(desc("Balanced Accuracy"), desc(F1))

# Use parallelization
# The below examples show the speed gains when running in parallel
#
# Attach doParallel and register four cores
# Uncomment:
# library(doParallel)
# registerDoParallel(4)

# Specify hyperparameters such that we will cross-validate 20 models

hparams <- list(
    "kernel" = c("linear", "radial"),
    "cost" = 1:5
)

# Cross-validate a list of 20 models in parallel
# Make sure to uncomment the parallel argument

system.time({
    cross_validate_fn(
        data,
        formulas = formulas_binomial,
        type = "binomial",
        model_fn = svm_model_fn,
        predict_fn = svm_predict_fn,
        hyperparameters = hparams,
        fold_cols = ".folds"
    )
})
formulas = formulas_gaussian, 
  type = "gaussian", 
  model_fn = svm_model_fn, 
  predict_fn = svm_predict_fn, 
  hyperparameters = hparams, 
  fold_cols = ".folds" 
  #, parallel = TRUE  # Uncomment 
})
})

# Cross-validate a list of 20 models sequentially
system.time(
  cross_validate_fn(
    data,
    formulas = formulas_gaussian, 
    type = "gaussian", 
    model_fn = svm_model_fn, 
    predict_fn = svm_predict_fn, 
    hyperparameters = hparams, 
    fold_cols = ".folds" 
    #, parallel = TRUE  # Uncomment 
  )
)  
)

---

**cvms**

*cvms: A package for cross-validating regression and classification models*

**Description**

Perform (repeated) cross-validation on a list of model formulas. Validate the best model on a validation set. Perform baseline evaluations on your test set. Generate model formulas by combining your fixed effects. Evaluate predictions from an external model.

**Details**

Returns results in a tibble for easy comparison, reporting and further analysis.

The main functions are: `cross_validate()`, `cross_validate_fn()`, `validate()`, `validate_fn()`, `baseline()`, and `evaluate()`.

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>
evaluate

Evaluate your model’s performance

Description

[Maturing]
Evaluate your model’s predictions on a set of evaluation metrics.
Create ID-aggregated evaluations by multiple methods.
Currently supports regression and classification (binary and multiclass). See `type`.

Usage

```r
evaluate(
  data,
  target_col,
  prediction_cols,
  type,
  id_col = NULL,
  id_method = "mean",
  apply_softmax = FALSE,
  cutoff = 0.5,
  positive = 2,
  metrics = list(),
  include_predictions = TRUE,
  parallel = FALSE,
  models = deprecated()
)
```

Arguments

data data.frame with predictions, targets and (optionally) an ID column. Can be grouped with `group_by`.

Multinomial: When `type` is "multinomial", the predictions can be passed in one of two formats.

Probabilities (Preferable):
One column per class with the probability of that class. The columns should have the name of their class, as they are named in the target column. E.g.:

<table>
<thead>
<tr>
<th>class_1</th>
<th>class_2</th>
<th>class_3</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.269</td>
<td>0.528</td>
<td>0.203</td>
<td>class_2</td>
</tr>
<tr>
<td>0.368</td>
<td>0.322</td>
<td>0.310</td>
<td>class_3</td>
</tr>
<tr>
<td>0.375</td>
<td>0.371</td>
<td>0.254</td>
<td>class_2</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

Classes:
A single column of type character with the predicted classes. E.g.:

<table>
<thead>
<tr>
<th>prediction</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>class_2</td>
<td>class_2</td>
</tr>
<tr>
<td>class_1</td>
<td>class_3</td>
</tr>
</tbody>
</table>
Binomial: When `type` is "binomial", the predictions can be passed in one of two formats.

Probabilities (Preferable): One column with the probability of class being the second class alphabetically (1 if classes are 0 and 1). E.g.:

<table>
<thead>
<tr>
<th>prediction</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.769</td>
<td>1</td>
</tr>
<tr>
<td>0.368</td>
<td>1</td>
</tr>
<tr>
<td>0.375</td>
<td>0</td>
</tr>
</tbody>
</table>

Note: At the alphabetical ordering of the class labels, they are of type character, why e.g. 100 would come before 7.

Classes: A single column of type character with the predicted classes. E.g.:

<table>
<thead>
<tr>
<th>prediction</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>class_0</td>
<td>class_1</td>
</tr>
<tr>
<td>class_1</td>
<td>class_1</td>
</tr>
<tr>
<td>class_1</td>
<td>class_0</td>
</tr>
</tbody>
</table>

Note: The prediction column will be converted to the probability 0.0 for the first class alphabetically and 1.0 for the second class alphabetically.

Gaussian: When `type` is "gaussian", the predictions should be passed as one column with the predicted values. E.g.:

<table>
<thead>
<tr>
<th>prediction</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>28.9</td>
<td>30.2</td>
</tr>
<tr>
<td>33.2</td>
<td>27.1</td>
</tr>
<tr>
<td>23.4</td>
<td>21.3</td>
</tr>
</tbody>
</table>

N.B. Current methods assume that the target class/value is constant within the IDs.

N.B. When aggregating by ID, some metrics may be disabled.
evaluate

id_method Method to use when aggregating predictions by ID. Either "mean" or "majority". When `type` is gaussian, only the "mean" method is available.

mean: The average prediction (value or probability) is calculated per ID and evaluated. This method assumes that the target class/value is constant within the IDs.

majority: The most predicted class per ID is found and evaluated. In case of a tie, the winning classes share the probability (e.g. P = 0.5 each when two majority classes). This method assumes that the target class/value is constant within the IDs.

apply_softmax Whether to apply the softmax function to the prediction columns when `type` is "multinomial".

N.B. Multinomial models only.

cutoff Threshold for predicted classes. (Numeric)

N.B. Binomial models only.

positive Level from dependent variable to predict. Either as character (preferable) or level index (1 or 2 - alphabetically).

E.g. if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".

Note: For reproducibility, it’s preferable to specify the name directly, as different locales may sort the levels differently.

Used when calculating confusion matrix metrics and creating ROC curves.
The Positive Class column in the output can be used to verify this setting.

N.B. Only affects the evaluation metrics.

N.B. Binomial models only.

metrics list for enabling/disabling metrics.

E.g. list("RMSE" = FALSE) would remove RMSE from the regression results, and list("Accuracy" = TRUE) would add the regular Accuracy metric to the classification results. Default values (TRUE/FALSE) will be used for the remaining available metrics.

You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i.

list("all" = FALSE, "RMSE" = TRUE) would return only the RMSE metric.
The list can be created with gaussian_metrics(), binomial_metrics(), or multinomial_metrics().

Also accepts the string "all".

include_predictions Whether to include the predictions in the output as a nested tibble. (Logical)

parallel Whether to run evaluations in parallel, when `data` is grouped with `group_by`.

models Deprecated.

Details

Packages used:

**Binomial and Multinomial:**

ROC and AUC:

Binomial: pROC::roc

Multinomial: pROC::multiclass.roc
Gaussian Results:

tibble containing the following metrics by default:
Average RMSE, MAE, NRMSE(IQR), RRSE, RAE, RMSLE.
See the additional metrics (disabled by default) at \texttt{gaussian_metrics}.
Also includes:
A nested tibble with the Predictions and targets.
A nested Process information object with information about the evaluation.

Binomial Results:

tibble with the following evaluation metrics, based on a confusion matrix and a ROC curve
fitted to the predictions:
Confusion Matrix:
Balanced Accuracy, Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, Prevalence, and MCC (Matthews correlation coefficient).
ROC:
AUC, Lower CI, and Upper CI
Note, that the ROC curve is only computed if AUC is enabled. See metrics.
Also includes:
A nested tibble with the predictions and targets.
A list of ROC curve objects (if computed).
A nested tibble with the confusion matrix. The Pos_ columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. I.e. the level you wish to predict.
A nested Process information object with information about the evaluation.

Multinomial Results:

For each class, a one-vs-all binomial evaluation is performed. This creates a Class Level Results
tibble containing the same metrics as the binomial results described above (excluding Accuracy, MCC, AUC, Lower CI and Upper CI), along with a count of the class in the target column (Support).
These metrics are used to calculate the macro metrics. The nested class level results tibble is also
included in the output tibble, and could be reported along with the macro and overall metrics.
The output tibble contains the macro and overall metrics. The metrics that share their name with
the metrics in the nested class level results tibble are averages of those metrics (note: does not
remove NAs before averaging). In addition to these, it also includes the Overall Accuracy and
the multiclass MCC.
Other available metrics (disabled by default, see metrics): Accuracy, multiclass AUC, Weighted
Balanced Accuracy, Weighted Accuracy, Weighted F1, Weighted Sensitivity, Weighted Sensitivity,
Weighted Specificity, Weighted Pos Pred Value, Weighted Neg Pred Value, Weighted Kappa,
Weighted Detection Rate, Weighted Detection Prevalence, and Weighted Prevalence.
Note that the "Weighted" average metrics are weighted by the `Support`.
When having a large set of classes, consider keeping `AUC` disabled.

Also includes:

- A nested tibble with the **Predictions** and targets.
- A list of **ROC** curve objects when `AUC` is enabled.
- A nested tibble with the multiclass **Confusion Matrix**.
- A nested **Process** information object with information about the evaluation.

**Class Level Results:**

Besides the binomial evaluation metrics and the `Support`, the nested class level results tibble also contains a nested tibble with the **Confusion Matrix** from the one-vs-all evaluation. The `Pos_` columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. In our case, 1 is the current class and 0 represents all the other classes together.

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

**See Also**

Other evaluation functions: `binomial_metrics()`, `confusion_matrix()`, `evaluate_residuals()`, `gaussian_metrics()`, `multinomial_metrics()`

**Examples**

```r
# Attach packages
library(cvms)
library(dplyr)

# Load data
data <- participant.scores

# Fit models
gaussian_model <- lm(age ~ diagnosis, data = data)
binomial_model <- glm(diagnosis ~ score, data = data)

# Add predictions
data["gaussian_predictions"] <- predict(gaussian_model, data, type = "response",
allow.new.levels = TRUE
)
data["binomial_predictions"] <- predict(binomial_model, data, allow.new.levels = TRUE
)

# Gaussian evaluation
evaluate(
  data = data, target_col = "age",
prediction_cols = "gaussian_predictions",
type = "gaussian"
)

# Binomial evaluation
```
evaluate(
    data = data, target_col = "diagnosis",
    prediction_cols = "binomial_predictions",
    type = "binomial"
  )

# Multinomial

# Create a tibble with predicted probabilities and targets
data_mc <- multiclass_probability_tibble(
    num_classes = 3, num_observations = 45,
    apply_softmax = TRUE, FUN = runif,
    class_name = "class_",
    add_targets = TRUE
  )

class_names <- paste0("class_", 1:3)

# Multinomial evaluation
evaluate(
    data = data_mc, target_col = "Target",
    prediction_cols = class_names,
    type = "multinomial"
  )

# ID evaluation

# Gaussian ID evaluation
# Note that 'age' is the same for all observations
# of a participant
evaluate(
    data = data, target_col = "age",
    prediction_cols = "gaussian_predictions",
    id_col = "participant",
    type = "gaussian"
  )

# Binomial ID evaluation
evaluate(
    data = data, target_col = "diagnosis",
    prediction_cols = "binomial_predictions",
    id_col = "participant",
    id_method = "mean", # alternatively: "majority"
    type = "binomial"
  )

# Multinomial ID evaluation

# Add IDs and new targets (must be constant within IDs)
data_mc[["Target"]]<- NULL
data_mc[["ID"]]<- rep(1:9, each = 5)
id_classes <- tibble::tibble(  "ID" = 1:9,
    "class_1" = runif(45),
    "class_2" = runif(45),
    "class_3" = runif(45)
  )

evaluate(
    data = data, target_col = "class_1",
    prediction_cols = "class_1",
    id_col = "ID",
    id_method = "majority",
    type = "multinomial"
  )
"Target" = sample(x = class_names, size = 9, replace = TRUE)
)

data_mc <- data_mc %>%
dplyr::left_join(id_classes, by = "ID")

# Perform ID evaluation
evaluate(
  data = data_mc, target_col = "Target",
  prediction_cols = class_names,
  id_col = "ID",
  id_method = "mean",  # alternatively: "majority"
  type = "multinomial"
)

# Training and evaluating a multinomial model with nnet

# Create a data frame with some predictors and a target column
class_names <- paste0("class_", 1:4)
data_for_nnet <- multiclass_probability_tibble(
  num_classes = 3,  # Here, number of predictors
  num_observations = 30,
  apply_softmax = FALSE,
  FUN = rnorm,
  class_name = "predictor_"
) %>%
dplyr::mutate(Target = sample(
  class_names,
  size = 30,
  replace = TRUE
))

# Train multinomial model using the nnet package
mn_model <- nnet::multinom(  
  "Target ~ predictor_1 + predictor_2 + predictor_3",
  data = data_for_nnet
)

# Predict the targets in the dataset
# (we would usually use a test set instead)
predictions <- predict(
  mn_model,
  data_for_nnet,
  type = "probs"
) %>%
dplyr::as_tibble()

# Add the targets
predictions[["Target"]]<- data_for_nnet[["Target"]]

# Evaluate predictions
evaluate(
  data = predictions,
  target_col = "Target",
  prediction_cols = class_names,
  type = "multinomial"
)
evaluate_residuals

Evaluate residuals from a regression task

Description

[Experimental]
Calculates a large set of error metrics from regression residuals.

Note: In most cases you should use evaluate() instead. It works in magrittr pipes (e.g. %>%) and with dplyr::group_by(). evaluate_residuals() is more lightweight and may be preferred in programming when you don’t need the extra stuff in evaluate().

Usage

evaluate_residuals(data, target_col, prediction_col, metrics = list())

Arguments

data data.frame with predictions and targets.

target_col Name of the column with the true values in `data`.

prediction_col Name of column with the predicted values in `data`.

metrics list for enabling/disabling metrics.
E.g. list("RMSE" = FALSE) would disable RMSE. Default values (TRUE/FALSE) will be used for the remaining available metrics.
You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why for instance list("all" = FALSE,"RMSE" = TRUE) would return only the RMSE metric.
The list can be created with gaussian_metrics(). Also accepts the string "all".

Details

The metric formulas are listed in 'The Available Metrics' vignette.

Value

tibble data.frame with the calculated metrics.
The following metrics are available (see `metrics`):

<table>
<thead>
<tr>
<th>Metric</th>
<th>Name</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Absolute Error</td>
<td>&quot;MAE&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Root Mean Square Error</td>
<td>&quot;RMSE&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Normalized RMSE (by target range)</td>
<td>&quot;NRMSE(RNG)&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>Normalized RMSE (by target IQR)</td>
<td>&quot;NRMSE(IQR)&quot;</td>
<td>Enabled</td>
</tr>
<tr>
<td>Normalized RMSE (by target STD)</td>
<td>&quot;NRMSE(STD)&quot;</td>
<td>Disabled</td>
</tr>
<tr>
<td>Normalized RMSE (by target mean)</td>
<td>&quot;NRMSE(AVG)&quot;</td>
<td>Disabled</td>
</tr>
</tbody>
</table>
Relative Squared Error "RSE" Disabled
Root Relative Squared Error "RRSE" Enabled
Relative Absolute Error "RAE" Enabled
Root Mean Squared Log Error "RMSLE" Enabled
Mean Absolute Log Error "MALE" Disabled
Mean Absolute Percentage Error "MAPE" Disabled
Mean Squared Error "MSE" Disabled
Total Absolute Error "TAE" Disabled
Total Squared Error "TSE" Disabled

The **Name** column refers to the name used in the package. This is the name in the output and when enabling/disabling in `metrics`.

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

**See Also**

Other evaluation functions: `binomial_metrics()`, `confusion_matrix()`, `evaluate()`, `gaussian_metrics()`, `multinomial_metrics()`

**Examples**

``` r
# Attach packages
library(cvms)

data <- data.frame(
  "targets" = rnorm(100, 14.7, 3.6),
  "predictions" = rnorm(100, 13.2, 4.6)
)

evaluate_residuals(
  data = data,
  target_col = "targets",
  prediction_col = "predictions"
)
```

---

**Description**

[Experimental]

Creates a list of font settings for plotting with cvms plotting functions.

NOTE: This is very experimental and will likely change.
Usage

```r
font(
  size = NULL,
  color = NULL,
  alpha = NULL,
  nudge_x = NULL,
  nudge_y = NULL,
  angle = NULL,
  family = NULL,
  fontface = NULL,
  hjust = NULL,
  vjust = NULL,
  lineheight = NULL,
  digits = NULL,
  prefix = NULL,
  suffix = NULL
)
```

Arguments

- `size`, `color`, `alpha`, `nudge_x`, `nudge_y`, `angle`, `family`, `fontface`, `hjust`, `vjust`, `lineheight`
  - As passed to `ggplot2::geom_text`.
- `digits` - Number of digits to round to. If negative, no rounding will take place.
- `prefix` - A string prefix.
- `suffix` - A string suffix.

Value

List of settings.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

- Other plotting functions: `plot_confusion_matrix()`, `plot_metric_density()`, `plot_probabilities_ecdf()`, `plot_probabilities()`, `sum_tile_settings()`

---

**gaussian_metrics**

*Select metrics for Gaussian evaluation*

Description

[Experimental]

Enable/disable metrics for Gaussian evaluation. Can be supplied to the `metrics` argument in many of the cvms functions.

Note: Some functions may have slightly different defaults than the ones supplied here.
gaussian_metrics

Usage

gaussian_metrics(
    all = NULL,
    rmse = NULL,
    mae = NULL,
    nrmse_rng = NULL,
    nrmse_iqr = NULL,
    nrmse_std = NULL,
    nrmse_avg = NULL,
    rae = NULL,
    rse = NULL,
    rrse = NULL,
    rmsle = NULL,
    male = NULL,
    mape = NULL,
    mse = NULL,
    tae = NULL,
    tse = NULL,
    r2m = NULL,
    r2c = NULL,
    aic = NULL,
    aicc = NULL,
    bic = NULL
)

Arguments

all Enable/disable all arguments at once. (Logical)
    Specifying other metrics will overwrite this, why you can use (all = FALSE, rmse = TRUE) to get only the RMSE metric.

rmse RMSE. (Default: TRUE)
    Root Mean Square Error.

mae MAE. (Default: TRUE)
    Mean Absolute Error.

nrmse_rng NRMSE(RNG). (Default: FALSE)
    Normalized Root Mean Square Error (by target range).

nrmse_iqr NRMSE(IQR). (Default: TRUE)
    Normalized Root Mean Square Error (by target interquartile range).

nrmse_std NRMSE(STD). (Default: FALSE)
    Normalized Root Mean Square Error (by target standard deviation).

nrmse_avg NRMSE(AVG). (Default: FALSE)
    Normalized Root Mean Square Error (by target mean).

rae RAE. (Default: TRUE)
    Relative Absolute Error.

rse RSE. (Default: FALSE)
    Relative Squared Error.

rrse RRSE. (Default: TRUE)
    Root Relative Squared Error.
gaussian_metrics

rmsle RMSLE. (Default: TRUE)
Root Mean Square Log Error.

male MALE. (Default: FALSE)
Mean Absolute Log Error.

mape MAPE. (Default: FALSE)
Mean Absolute Percentage Error.

mse MSE. (Default: FALSE)
Mean Square Error.

tae TAE. (Default: FALSE)
Total Absolute Error

tse TSE. (Default: FALSE)
Total Squared Error.

r2m r2m. (Default: FALSE)
Marginal R-squared.

r2c r2c. (Default: FALSE)
Conditional R-squared.

aic AIC. (Default: FALSE)
Akaike Information Criterion.

aicc AICc. (Default: FALSE)
Corrected Akaike Information Criterion.

bic BIC. (Default: FALSE)
Bayesian Information Criterion.

Author(s)
Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also
Other evaluation functions: binomial_metrics(), confusion_matrix(), evaluate_residuals(), evaluate(), multinomial_metrics()

Examples

# Attach packages
library(cvms)

# Enable only RMSE
gaussian_metrics(all = FALSE, rmse = TRUE)

# Enable all but RMSE
gaussian_metrics(all = TRUE, rmse = FALSE)

# Disable RMSE
.gaussian_metrics(rmse = FALSE)
Examples of model functions

Description

[Experimental]
Examples of model functions that can be used in `cross_validate_fn()`. They can either be used directly or be starting points.

The `update_hyperparameters()` function updates the list of hyperparameters with default values for missing hyperparameters. You can also specify required hyperparameters.

Usage

`model_functions(name)`

Arguments

name

Name of model to get model function for, as it appears in the following list:

<table>
<thead>
<tr>
<th>Name</th>
<th>Function</th>
<th>Hyperparameters (default)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;lm&quot;</td>
<td><code>stats::lm()</code></td>
<td></td>
</tr>
<tr>
<td>&quot;lmer&quot;</td>
<td><code>lme4::lmer()</code></td>
<td>REML (FALSE)</td>
</tr>
<tr>
<td>&quot;glm_binomial&quot;</td>
<td><code>stats::glm()</code></td>
<td></td>
</tr>
<tr>
<td>&quot;glmer_binomial&quot;</td>
<td><code>lme4::glmer()</code></td>
<td></td>
</tr>
<tr>
<td>&quot;svm_gaussian&quot;</td>
<td><code>e1071::svm()</code></td>
<td>kernel (&quot;radial&quot;), cost (1)</td>
</tr>
<tr>
<td>&quot;svm_binomial&quot;</td>
<td><code>e1071::svm()</code></td>
<td>kernel (&quot;radial&quot;), cost (1)</td>
</tr>
<tr>
<td>&quot;svm_multinomial&quot;</td>
<td><code>e1071::svm()</code></td>
<td>kernel (&quot;radial&quot;), cost (1)</td>
</tr>
<tr>
<td>&quot;naive_bayes&quot;</td>
<td><code>e1071::naiveBayes()</code></td>
<td>laplace (0)</td>
</tr>
</tbody>
</table>

Value

A function with the following form:

```r
function(train_data, formula, hyperparameters) {
  # Return fitted model object
}
```

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other example functions: `predict_functions()`, `preprocess_functions()`, `update_hyperparameters()`
most_challenging

Find the data points that were hardest to predict

Description

[Experimental] Finds the data points that, overall, were the most challenging to predict, based on a prediction metric.

Usage

```r
most_challenging(
  data,
  type,
  obs_id_col = "Observation",
  target_col = "Target",
  prediction_cols = ifelse(type == "gaussian", "Prediction", "Predicted Class"),
  threshold = 0.15,
  threshold_is = "percentage",
  metric = NULL,
  cutoff = 0.5
)
```

Arguments

data: data.frame with predictions, targets and observation IDs. Can be grouped by `dplyr::group_by()`.

Predictions can be passed as values, predicted classes or predicted probabilities:

**N.B.** Adds `.Machine$double.eps` to all probabilities to avoid `log(0)`.

**Multinomial:** When `type` is "multinomial", the predictions can be passed in one of two formats.

*Probabilities (Preferable):*

One column per class with the probability of that class. The columns should have the name of their class, as they are named in the target column. E.g.:

```
class_1   class_2   class_3   target
0.269      0.528    0.203    class_2
0.368      0.322    0.310    class_3
0.375      0.371    0.254    class_2
...        ...      ...      ...
```

*Classes:*

A single column of type character with the predicted classes. E.g.:

```
prediction   target
class_2      class_2
class_1      class_3
class_1      class_2
...          ...
```

**Binomial:** When `type` is "binomial", the predictions can be passed in
one of two formats.

**Probabilities (Preferable):** One column with the probability of class being the second class alphabetically ("dog" if classes are "cat" and "dog"). E.g.:

<table>
<thead>
<tr>
<th>prediction</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.769</td>
<td>&quot;dog&quot;</td>
</tr>
<tr>
<td>0.368</td>
<td>&quot;dog&quot;</td>
</tr>
<tr>
<td>0.375</td>
<td>&quot;cat&quot;</td>
</tr>
</tbody>
</table>

Note: At the alphabetical ordering of the class labels, they are of type character, why e.g. 100 would come before 7.

**Classes:**
A single column of type character with the predicted classes. E.g.:

<table>
<thead>
<tr>
<th>prediction</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>class_0</td>
<td>class_1</td>
</tr>
<tr>
<td>class_1</td>
<td>class_1</td>
</tr>
<tr>
<td>class_1</td>
<td>class_0</td>
</tr>
</tbody>
</table>

**Gaussian:** When `type` is "gaussian", the predictions should be passed as one column with the predicted values. E.g.:

<table>
<thead>
<tr>
<th>prediction</th>
<th>target</th>
</tr>
</thead>
<tbody>
<tr>
<td>28.9</td>
<td>30.2</td>
</tr>
<tr>
<td>33.2</td>
<td>27.1</td>
</tr>
<tr>
<td>23.4</td>
<td>21.3</td>
</tr>
</tbody>
</table>

**type**
Type of task used to get the predictions:
"gaussian" for regression (like linear regression).
"binomial" for binary classification.
"multinomial" for multiclass classification.

**obs_id_col**
Name of column with observation IDs. This will be used to aggregate the performance of each observation.

**target_col**
Name of column with the true classes/values in `data`.

**prediction_cols**
Name(s) of column(s) with the predictions.

**threshold**
Threshold to filter observations by. Depends on `type` and `threshold_is`.
The threshold can either be a **percentage** or a **score**. For percentages, a lower threshold returns fewer observations. For scores, this depends on `type`.

**Gaussian:**

- **threshold_is** "percentage": (Approximate) percentage of the observations with the largest root mean square errors to return.
- **threshold_is** "score": Observations with a root mean square error larger than or equal to the threshold will be returned.

**Binomial, Multinomial:**
threshold_is "percentage": (Approximate) percentage of the observations to return with:
MAE, Cross Entropy: Highest error scores.
Accuracy: Lowest accuracies

threshold_is "score": MAE, Cross Entropy: Observations with an error score above or equal to the threshold will be returned.
Accuracy: Observations with an accuracy below or equal to the threshold will be returned.

threshold_is Either "score" or "percentage". See `threshold`.

metric The metric to use. If NULL, the default metric depends on the format of the prediction columns.

Binomial, Multinomial: "Accuracy", "MAE" or "Cross Entropy".
When one prediction column with predicted classes is passed, the default is "Accuracy". In this configuration, the other metrics are not calculated.
When one or more prediction columns with predicted probabilities are passed, the default is "MAE". This is the Mean Absolute Error of the probability of the target class.

Gaussian: Ignored. Always uses "RMSE".

cutoff Threshold for predicted classes. (Numeric)
N.B. Binomial only.

Value
data.frame with the most challenging observations and their metrics.
`>=' / `<=' denotes the threshold as score.

Author(s)
Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

Examples

```r
# Attach packages
library(cvms)
library(dplyr)

## Multinomial

# Find the most challenging data points (per classifier)
# in the predicted.musicians dataset
# which resembles the "Predictions" tibble from the evaluation results

# Passing predicted probabilities
# Observations with 30% highest MAE scores
most_challenging(
predicted.musicians,
obs_id_col = "ID",
prediction_cols = c("A", "B", "C", "D"),
type = "multinomial",

```
```
threshold = 0.30
)

# Observations with 25% highest Cross Entropy scores
most_challenging(
    predicted.musicians,
    obs_id_col = "ID",
    prediction_cols = c("A", "B", "C", "D"),
    type = "multinomial",
    threshold = 0.25,
    metric = "Cross Entropy"
)

# Passing predicted classes
# Observations with 30% lowest Accuracy scores
most_challenging(
    predicted.musicians,
    obs_id_col = "ID",
    prediction_cols = "Predicted Class",
    type = "multinomial",
    threshold = 0.30
)

# The 40% lowest-scoring on accuracy per classifier
predicted.musicians %>%
  dplyr::group_by(Classifier) %>%
  most_challenging(
    obs_id_col = "ID",
    prediction_cols = "Predicted Class",
    type = "multinomial",
    threshold = 0.40
)

# Accuracy scores below 0.05
most_challenging(
    predicted.musicians,
    obs_id_col = "ID",
    type = "multinomial",
    threshold = 0.05,
    threshold_is = "score"
)

##
## Binomial
##

# Subset the predicted.musicians
binom_data <- predicted.musicians %>%
  dplyr::filter(Target %in% c("A", "B")) %>%
  dplyr::rename(Prediction = B)

# Passing probabilities
# Observations with 30% highest MAE
most_challenging(
    binom_data,
    obs_id_col = "ID",
    type = "binomial",
    threshold = 0.30)

most_challenging
predictions_cols = "Prediction",
threshold = 0.30
)

# Observations with 30% highest Cross Entropy
most_challenging(
  binom_data,
  obs_id_col = "ID",
  type = "binomial",
  predictions_cols = "Prediction",
  threshold = 0.30,
  metric = "Cross Entropy"
)

# Observations with 30% lowest Accuracy scores
most_challenging(
  binom_data,
  obs_id_col = "ID",
  type = "binomial",
  predictions_cols = "Predicted Class",
  threshold = 0.30
)

## Gaussian

set.seed(1)
df <- data.frame(
  "Observation" = rep(1:10, n = 3),
  "Target" = rnorm(n = 30, mean = 25, sd = 5),
  "Prediction" = rnorm(n = 30, mean = 27, sd = 7)
)

# The 20% highest RMSE scores
most_challenging(
  df,
  type = "gaussian",
  threshold = 0.2
)

# RMSE scores above 9
most_challenging(
  df,
  type = "gaussian",
  threshold = 9,
  threshold_is = "score"
)

### Generate a multiclass probability tibble
multiclass_probability_tibble

Description

[Maturing]
Generate a tibble with random numbers containing one column per specified class. When the softmax function is applied, the numbers become probabilities that sum to 1 row-wise. Optionally, add columns with targets and predicted classes.

Usage

```r
multiclass_probability_tibble(
  num_classes,
  num_observations,
  apply_softmax = TRUE,
  FUN = runif,
  class_name = "class_",
  add_predicted_classes = FALSE,
  add_targets = FALSE
)
```

Arguments

- `num_classes` The number of classes. Also the number of columns in the tibble.
- `num_observations` The number of observations. Also the number of rows in the tibble.
- `apply_softmax` Whether to apply the softmax function row-wise. This will transform the numbers to probabilities that sum to 1 row-wise.
- `FUN` Function for generating random numbers. The first argument must be the number of random numbers to generate, as no other arguments are supplied.
- `class_name` The prefix for the column names. The column index is appended.
- `add_predicted_classes` Whether to add a column with the predicted classes. (Logical) The class with the highest value is the predicted class.
- `add_targets` Whether to add a column with randomly selected target classes. (Logical)

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

Examples

```r
# Attach cvms
library(cvms)

# Create a tibble with 5 classes and 10 observations
# Apply softmax to make sure the probabilities sum to 1
multiclass_probability_tibble(
  num_classes = 5,
  num_observations = 10,
  apply_softmax = TRUE
)

# Using the rnorm function to generate the random numbers
multiclass_probability_tibble(
  num_classes = 10,
  num_observations = 100,
  apply_softmax = TRUE,
  FUN = rnorm
)
```
multinomial_metrics

Select metrics for multinomial evaluation

**Description**

[Experimental]

Enable/disable metrics for multinomial evaluation. Can be supplied to the `metrics` argument in many of the `cvms` functions.

Note: Some functions may have slightly different defaults than the ones supplied here.

**Usage**

```r
multinomial_metrics(
  all = NULL,
  overall_accuracy = NULL,
  balanced_accuracy = NULL,
  w_balanced_accuracy = NULL,
  accuracy = NULL,
  w_accuracy = NULL,
  f1 = NULL,
  w_f1 = NULL,
  sensitivity = NULL,
  w_sensitivity = NULL,
  specificity = NULL,
)```
multinomial_metrics

w_specificity = NULL,
pos_pred_value = NULL,
w_pos_pred_value = NULL,
neg_pred_value = NULL,
w_neg_pred_value = NULL,
auc = NULL,
kappa = NULL,
w_kappa = NULL,
mcc = NULL,
detection_rate = NULL,
w_detection_rate = NULL,
detection_prevalence = NULL,
w_detection_prevalence = NULL,
prevalence = NULL,
w_prevalence = NULL,
false_neg_rate = NULL,
w_false_neg_rate = NULL,
false_pos_rate = NULL,
w_false_pos_rate = NULL,
false_discovery_rate = NULL,
w_false_discovery_rate = NULL,
false_omission_rate = NULL,
w_false_omission_rate = NULL,
threat_score = NULL,
w_threat_score = NULL,
aic = NULL,
aicc = NULL,
bic = NULL
)

Arguments

all Enable/disable all arguments at once. (Logical)
Specifying other metrics will overwrite this, why you can use (all = FALSE, accuracy = TRUE) to get only the Accuracy metric.

overall_accuracy Overall Accuracy (Default: TRUE)
balanced_accuracy Balanced Accuracy (Default: TRUE)
w_balanced_accuracy Weighted Balanced Accuracy (Default: FALSE)
accuracy Accuracy (Default: FALSE)
w_accuracy Weighted Accuracy (Default: FALSE)
f1 F1 (Default: TRUE)
w_f1 Weighted F1 (Default: FALSE)
sensitivity Sensitivity (Default: TRUE)
w_sensitivity Weighted Sensitivity (Default: FALSE)
specificity Specificity (Default: TRUE)
w_specificity Weighted Specificity (Default: FALSE)
multinomial_metrics

pos_pred_value  Pos Pred Value (Default: TRUE)
w_pos_pred_value  Weighted Pos Pred Value (Default: FALSE)

neg_pred_value  Neg Pred Value (Default: TRUE)
w_neg_pred_value  Weighted Neg Pred Value (Default: FALSE)
auc  AUC (Default: FALSE)
kappa  Kappa (Default: TRUE)
w_kappa  Weighted Kappa (Default: FALSE)
mcc  MCC (Default: TRUE)
Multiclass Matthews Correlation Coefficient.
detection_rate  Detection Rate (Default: TRUE)
w_detection_rate  Weighted Detection Rate (Default: FALSE)
detection_prevalence  Detection Prevalence (Default: TRUE)
w_detection_prevalence  Weighted Detection Prevalence (Default: FALSE)
prevalence  Prevalence (Default: TRUE)
w_prevalence  Weighted Prevalence (Default: FALSE)
false_neg_rate  False Neg Rate (Default: FALSE)
w_false_neg_rate  Weighted False Neg Rate (Default: FALSE)
false_pos_rate  False Pos Rate (Default: FALSE)
w_false_pos_rate  Weighted False Pos Rate (Default: FALSE)
false_discovery_rate  False Discovery Rate (Default: FALSE)
w_false_discovery_rate  Weighted False Discovery Rate (Default: FALSE)
false_omission_rate  False Omission Rate (Default: FALSE)
w_false_omission_rate  Weighted False Omission Rate (Default: FALSE)
threat_score  Threat Score (Default: FALSE)
w_threat_score  Weighted Threat Score (Default: FALSE)
aic  AIC (Default: FALSE)
aiic  AICc (Default: FALSE)
bic  BIC (Default: FALSE)

Author(s)
Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also
Other evaluation functions: binomial_metrics(), confusion_matrix(), evaluate_residuals(), evaluate(), gaussian_metrics()
Examples

```r
# Attach packages
library(cvms)

# Enable only Balanced Accuracy
multinomial_metrics(all = FALSE, balanced_accuracy = TRUE)

# Enable all but Balanced Accuracy
multinomial_metrics(all = TRUE, balanced_accuracy = FALSE)

# Disable Balanced Accuracy
multinomial_metrics(balanced_accuracy = FALSE)
```

Description

Made-up data on 60 musicians in 4 groups for multiclass classification.

Format

A data frame with 60 rows and 9 variables:

- **ID**: Musician identifier, 60 levels
- **Age**: Age of the musician. Between 17 and 66 years.
- **Class**: The class of the musician. One of "A", "B", "C", and "D".
- **Height**: Height of the musician. Between 146 and 196 centimeters.
- **Drums**: Whether the musician plays drums. 0 = No, 1 = Yes.
- **Bass**: Whether the musician plays bass. 0 = No, 1 = Yes.
- **Guitar**: Whether the musician plays guitar. 0 = No, 1 = Yes.
- **Keys**: Whether the musician plays keys. 0 = No, 1 = Yes.
- **Vocals**: Whether the musician sings. 0 = No, 1 = Yes.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

predicted.musicians
participant.scores  Participant scores

Description

Made-up experiment data with 10 participants and two diagnoses. Test scores for 3 sessions per participant, where participants improve their scores each session.

Format

A data.frame with 30 rows and 5 variables:

- **participant**: participant identifier, 10 levels
- **age**: age of the participant, in years
- **diagnosis**: diagnosis of the participant, either 1 or 0
- **score**: test score of the participant, on a 0-100 scale
- **session**: testing session identifier, 1 to 3

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

plot_confusion_matrix  Plot a confusion matrix

Description

[Experimental]

Creates a `ggplot2` object representing a confusion matrix with counts, overall percentages, row percentages and column percentages. An extra row and column with sum tiles and the total count can be added.

The confusion matrix can be created with `evaluate()`. See `Examples`.

While this function is intended to be very flexible (hence the large number of arguments), the defaults should work in most cases for most users. See the `Examples`.

Usage

```r
plot_confusion_matrix(
  conf_matrix,
  target_col = "Target",
  prediction_col = "Prediction",
  counts_col = "N",
  class_order = NULL,
  add_sums = FALSE,
  add_counts = TRUE,
  add_normalized = TRUE,
  add_row_percentages = TRUE,
)```
### Arguments

- **conf_matrix**: Confusion matrix tibble with each combination of targets and predictions along with their counts. E.g. for a binary classification:

<table>
<thead>
<tr>
<th>Target</th>
<th>Prediction</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>class_1</td>
<td>class_1</td>
<td>5</td>
</tr>
<tr>
<td>class_1</td>
<td>class_2</td>
<td>9</td>
</tr>
<tr>
<td>class_2</td>
<td>class_1</td>
<td>3</td>
</tr>
<tr>
<td>class_2</td>
<td>class_2</td>
<td>2</td>
</tr>
</tbody>
</table>

As created with the various evaluation functions in cvms, like `evaluate()`.

**Note**: If you supply the results from `evaluate()` or `confusion_matrix()` directly, the confusion matrix tibble is extracted automatically, if possible.

- **target_col**: Name of column with target levels.
- **prediction_col**: Name of column with prediction levels.
- **counts_col**: Name of column with a count for each combination of the target and prediction levels.
- **class_order**: Names of the classes in `conf_matrix` in the desired order. When `NULL`, the classes are ordered alphabetically.
- **add_sums**: Add tiles with the row/column sums. Also adds a total count tile. (Logical)

The appearance of these tiles can be specified in `sums_settings`.

**Note**: Adding the sum tiles with a palette requires the `ggnewscale` package.
add_counts Add the counts to the middle of the tiles. (Logical)
add_normalized Normalize the counts to percentages and add to the middle of the tiles. (Logical)
add_row_percentages Add the row percentages, i.e. how big a part of its row the tile makes up. (Logical)
By default, the row percentage is placed to the right of the tile, rotated 90 degrees.
add_col_percentages Add the column percentages, i.e. how big a part of its column the tile makes up. (Logical)
By default, the row percentage is placed at the bottom of the tile.
diag_percentages_only Whether to only have row and column percentages in the diagonal tiles. (Logical)
rm_zero_percentages Whether to remove row and column percentages when the count is 0. (Logical)
rm_zero_text Whether to remove counts and normalized percentages when the count is 0. (Logical)
add_zero_shading Add image of skewed lines to zero-tiles. (Logical)
Note: Adding the zero-shading requires the rsvg and ggimage packages.
add_arrows Add the arrows to the row and col percentages. (Logical)
Note: Adding the arrows requires the rsvg and ggimage packages.
counts_on_top Switch the counts and normalized counts, such that the counts are on top. (Logical)
palette Color scheme. Passed directly to `palette` in ggplot2::scale_fill_distiller.
Try these palettes: "Greens", "Oranges", "Greys", "Purples", "Reds", as well as the default "Blues".
intensity_by The measure that should control the color intensity of the tiles. Either `counts` or `normalized`. For the latter, the color limits become 0-100, why the intensities can better be compared across plots.
theme_fn The ggplot2 theme function to apply.
place_x_axis_above Move the x-axis text to the top and reverse the levels such that the "correct" diagonal goes from top left to bottom right. (Logical)
rotate_y_text Whether to rotate the y-axis text to be vertical instead of horizontal. (Logical)
digits Number of digits to round to (percentages only). Set to a negative number for no rounding.
Can be set for each font individually via the font_* arguments.
font_counts list of font settings for the counts. Can be provided with font().
font_normalized list of font settings for the normalized counts. Can be provided with font().
font_row_percentages list of font settings for the row percentages. Can be provided with font().
font_col_percentages list of font settings for the column percentages. Can be provided with font().
plot_confusion_matrix

arrow_size  
Size of arrow icons. (Numeric)

Is divided by $\sqrt{\text{row(conf_matrix)}}$ and passed on to ggimage::geom_icon().

arrow_nudge_from_text  
Distance from the percentage text to the arrow. (Numeric)

tile_border_color  
Color of the tile borders. Passed as ‘colour’ to ggplot2::geom_tile.

tile_border_size  
Size of the tile borders. Passed as ‘size’ to ggplot2::geom_tile.

tile_border_linetype  
Linetype for the tile borders. Passed as ‘linetype’ to ggplot2::geom_tile.

sums_settings  
A list of settings for the appearance of the sum tiles. Can be provided with sum_tile_settings().

darkness  
How dark the darkest colors should be, between 0 and 1, where 1 is darkest. Technically, a lower value increases the upper limit in ggplot2::scale_fill_distiller.

Details

Inspired by Antoine Sachet’s answer at https://stackoverflow.com/a/53612391/11832955

Value

A ggplot2 object representing a confusion matrix. Color intensity depends on either the counts (default) or the overall percentages.

By default, each tile has the normalized count (overall percentage) and count in the middle, the column percentage at the bottom, and the row percentage to the right and rotated 90 degrees.

In the “correct” diagonal (upper left to bottom right, by default), the column percentages are the class-level sensitivity scores, while the row percentages are the class-level positive predictive values.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other plotting functions: font(), plot_metric_density(), plot_probabilities_ecdf(), plot_probabilities(), sum_tile_settings()

Examples

# Attach cvms
library(cvms)
library(ggplot2)

# Two classes

# Create targets and predictions data frame
data <- data.frame(
)

plot_confusion_matrix

stringsAsFactors = FALSE

# Evaluate predictions and create confusion matrix
eval <- evaluate(
  data = data,
  target_col = "target",
  prediction_cols = "prediction",
  type = "binomial"
)

# Inspect confusion matrix tibble
eval[['Confusion Matrix']][[1]]

# Plot confusion matrix
# Supply confusion matrix tibble directly
plot_confusion_matrix(eval[['Confusion Matrix']][[1]])
# Plot first confusion matrix in evaluate() output
plot_confusion_matrix(eval)

# Add sum tiles
plot_confusion_matrix(eval, add_sums = TRUE)

# Three (or more) classes

# Create targets and predictions data frame
data <- data.frame(
  stringsAsFactors = FALSE
)

# Evaluate predictions and create confusion matrix
eval <- evaluate(
  data = data,
  target_col = "target",
  prediction_cols = "prediction",
  type = "multinomial"
)

# Inspect confusion matrix tibble
eval[['Confusion Matrix']][[1]]

# Plot confusion matrix
# Supply confusion matrix tibble directly
plot_confusion_matrix(eval[['Confusion Matrix']][[1]])
# Plot first confusion matrix in evaluate() output
plot_confusion_matrix(eval)

# Add sum tiles
plot_confusion_matrix(eval, add_sums = TRUE)

# Counts only
plot_confusion_matrix(  
eval[['Confusion Matrix']][[1]],

plot_metric_density

```
add_normalized = FALSE,
add_row_percentages = FALSE,
add_col_percentages = FALSE
```

# Change color palette to green
# Change theme to `theme_light`
```
plot_confusion_matrix(
  eval[['Confusion Matrix']][[1]],
  palette = "Greens",
  theme_fn = ggplot2::theme_light
)
```

# The output is a ggplot2 object
# that you can add layers to
# Here we change the axis labels
```
plot_confusion_matrix(eval[['Confusion Matrix']][[1]]) +
ggplot2::labs(x = "True", y = "Guess")
```

---

**plot_metric_density**  

*Density plot for a metric*

**Description**

*Experimental*  

Creates a ggplot2 object with a density plot for one of the columns in the passed data.frame(s).

Note: In its current form, it is mainly intended as a quick way to visualize the results from cross-validations and baselines (random evaluations). It may change significantly in future versions.

**Usage**

```
plot_metric_density(
  results = NULL,
  baseline = NULL,
  metric = "",
  fill = c("darkblue", "lightblue"),
  alpha = 0.6,
  theme_fn = ggplot2::theme_minimal,
  xlim = NULL
)
```

**Arguments**

- **results**: data.frame with a metric column to create density plot for.  
  To only plot the baseline, set to NULL.
- **baseline**: data.frame with the random evaluations from `baseline()`. Should contain a column for the metric.  
  To only plot the results, set to NULL.
- **metric**: Name of the metric column in `results` to plot. (Character)
plot_metric_density

fill          Colors of the plotted distributions. The first color is for the `baseline`, the second for the `results`.
alpha         Transparency of the distribution (0 - 1).
theme_fn      The ggplot2 theme function to apply.
xlim          Limits for the x-axis. Can be set to NULL. E.g. c(0,1).

Value

A ggplot2 object with the density of a metric, possibly split in 'Results' and 'Baseline'.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other plotting functions: font(), plot_confusion_matrix(), plot_probabilities_ecdf(), plot_probabilities(), sum_tile_settings()

Examples

```r
# Attach packages
library(cvms)
library(dplyr)

# We will use the musicians and predicted.musicians datasets
musicians
predicted.musicians

# Set seed
set.seed(42)

# Create baseline for targets
bsl <- baseline_multinomial(  
  test_data = musicians,
  dependent_col = "Class",
  n = 20 # Normally 100
)

# Evaluate predictions grouped by classifier and fold column
eval <- predicted.musicians %>%
  dplyr::group_by(Classifier, "Fold Column") %>%
  evaluate(  
    target_col = "Target",
    prediction_cols = c("A", "B", "C", "D"),
    type = "multinomial"
  )

# Plot density of the Overall Accuracy metric
plot_metric_density(  
  results = eval,
  baseline = bsl$random_evaluations,
  metric = "Overall Accuracy",
)```

```r
precomputed.formulas

xlim = c(0,1)
)

# The bulk of classifier results are much better than
# the baseline results

precomputed.formulas  Precomputed formulas

Description

Fixed effect combinations for model formulas with/without two- and three-way interactions. Up to eight fixed effects in total with up to five fixed effects per formula.

Format

A data.frame with 259,358 rows and 5 variables:

- **formula_** combination of fixed effects, separated by "+" and "*
- **max_interaction_size** maximum interaction size in the formula, up to 3
- **max_effect_frequency** maximum count of an effect in the formula, e.g. the 3 A's in "A + B + A * C + A * D"
- **num_effects** number of unique effects included in the formula
- **min_num_fixed_effects** minimum number of fixed effects required to use the formula, i.e. the index in the alphabet of the last of the alphabetically ordered effects (letters) in the formula, so 4 for the formula: "A + B + D"

Details

Effects are represented by the first eight capital letters.

Used by `combine_predictors`.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

predicted.musicians  Predicted musician groups

Description

Predictions by 3 classifiers of the 4 classes in the `musicians` dataset. Obtained with 5-fold stratified cross-validation (3 repetitions). The three classifiers were fit using `nnet::multinom`, `randomForest::randomForest`, and `e1071::svm`. 
Format

A data.frame with 540 rows and 10 variables:

- **Classifier**: The applied classifier. One of "nnet_multinom", "randomForest", and "e1071_svm".
- **Fold Column**: The fold column name. Each is a unique 5-fold split. One of ".folds_1", ".folds_2", and ".folds_3".
- **Fold**: The fold. 1 to 5.
- **ID**: Musician identifier, 60 levels.
- **Target**: The actual class of the musician. One of "A", "B", "C", and "D".
- **A**: The probability of class "A".
- **B**: The probability of class "B".
- **C**: The probability of class "C".
- **D**: The probability of class "D".
- **Predicted Class**: The predicted class. The argmax of the four probability columns.

Details

Used formula: "Class ~ Height + Age + Drums + Bass + Guitar + Keys + Vocals"

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

musicians

Examples

```r
# Attach packages
library(cvms)
library(dplyr)

# Evaluate each fold column
predicted.musicians %>%
  dplyr::group_by(Classifier, `Fold Column`) %>%
  evaluate(target_col = "Target",
            prediction_cols = c("A", "B", "C", "D"),
            type = "multinomial")

# Overall ID evaluation
# I.e. if we average all 9 sets of predictions,
# how well did we predict the targets?
overall_id_eval <- predicted.musicians %>%
  evaluate(target_col = "Target",
            prediction_cols = c("A", "B", "C", "D"),
            type = "multinomial",
            id_col = "ID")
overall_id_eval

# Plot the confusion matrix
plot_confusion_matrix(overall_id_eval$'Confusion Matrix'[1])
```
predict_functions

Examples of predict fn functions

Description

[Experimental]
Examples of predict functions that can be used in cross_validate_fn(). They can either be used directly or be starting points.

Usage

predict_functions(name)

Arguments

name 
Name of model to get predict function for, as it appears in the following table.

The Model HParams column lists hyperparameters used in the respective model function.

<table>
<thead>
<tr>
<th>Name</th>
<th>Function</th>
<th>Model HParams</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;lm&quot;</td>
<td>stats::lm()</td>
<td></td>
</tr>
<tr>
<td>&quot;lmer&quot;</td>
<td>lme4::lmer()</td>
<td></td>
</tr>
<tr>
<td>&quot;glm_binomial&quot;</td>
<td>stats::glm()</td>
<td>family = &quot;binomial&quot;</td>
</tr>
<tr>
<td>&quot;glmer_binomial&quot;</td>
<td>lme4::glmer()</td>
<td>family = &quot;binomial&quot;</td>
</tr>
<tr>
<td>&quot;svm_gaussian&quot;</td>
<td>e1071::svm()</td>
<td>type = &quot;eps-regression&quot;</td>
</tr>
<tr>
<td>&quot;svm_binomial&quot;</td>
<td>e1071::svm()</td>
<td>type = &quot;C-classification&quot;, probability = TRUE</td>
</tr>
<tr>
<td>&quot;svm_multinomial&quot;</td>
<td>e1071::svm()</td>
<td>type = &quot;C-classification&quot;, probability = TRUE</td>
</tr>
<tr>
<td>&quot;naive_bayes&quot;</td>
<td>e1071::naiveBayes()</td>
<td></td>
</tr>
<tr>
<td>&quot;nnet_multinom&quot;</td>
<td>nnet::multinom()</td>
<td></td>
</tr>
<tr>
<td>&quot;nnet_gaussian&quot;</td>
<td>nnet::nnet()</td>
<td></td>
</tr>
<tr>
<td>&quot;nnet_binomial&quot;</td>
<td>nnet::nnet()</td>
<td>linout = TRUE</td>
</tr>
<tr>
<td>&quot;randomForest_gaussian&quot;</td>
<td>randomForest::randomForest()</td>
<td></td>
</tr>
<tr>
<td>&quot;randomForest_binomial&quot;</td>
<td>randomForest::randomForest()</td>
<td></td>
</tr>
<tr>
<td>&quot;randomForest_multinomial&quot;</td>
<td>randomForest::randomForest()</td>
<td></td>
</tr>
</tbody>
</table>

Value

A function with the following form:

```r
function(test_data,model,formula,hyperparameters,train_data) {
  # Use model to predict test_data
  # Return predictions
}
```

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other example functions: model_functions(), preprocess_functions(), update_hyperparameters()
Description

[Experimental]
Examples of preprocess functions that can be used in `cross_validate_fn()` and `validate_fn()`. They can either be used directly or be starting points.

The examples use `recipes`, but you can also use `caret::preProcess()` or similar functions.

In these examples, the preprocessing will only affect the numeric predictors.

You may prefer to hardcode a formula like "y ~ ." (where y is your dependent variable) as that will allow you to set `preprocess_one` to `TRUE` in `cross_validate_fn()` and `validate_fn()` and save time.

Usage

`preprocess_functions(name)`

Arguments

- `name` Name of preprocessing function as it appears in the following list:

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;standardize&quot;</td>
<td>Centers and scales the numeric predictors</td>
</tr>
<tr>
<td>&quot;range&quot;</td>
<td>Normalizes the numeric predictors to the 0-1 range</td>
</tr>
<tr>
<td>&quot;scale&quot;</td>
<td>Scales the numeric predictors to have a standard deviation of one</td>
</tr>
<tr>
<td>&quot;center&quot;</td>
<td>Centers the numeric predictors to have a mean of zero</td>
</tr>
<tr>
<td>&quot;warn&quot;</td>
<td>Identity function that throws a warning and a message</td>
</tr>
</tbody>
</table>

Value

A function with the following form:

```r
function(train_data, test_data, formula, hyperparameters) {
  # Preprocess train_data and test_data
  # Return a list with the preprocessed datasets
  # and optionally a data frame with preprocessing parameters
  list(
    "train" = train_data,
    "test" = test_data,
    "parameters" = tidy_parameters
  )
}
```

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>
See Also
Other example functions: model_functions(), predict_functions(), update_hyperparameters()

Description

[Experimental]
Classes for storing process information from prediction evaluations.
Used internally.

Usage

process_info_binomial(
  data,
  target_col,
  prediction_cols,
  id_col,
  cat_levels,
  positive,
  cutoff,
  locale = NULL
)

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

## S3 method for class 'process_info_binomial'
as.character(x, ...)

process_info_multinomial(
  data,
  target_col,
  prediction_cols,
  pred_class_col,
  id_col,
  cat_levels,
  apply_softmax,
  locale = NULL
)

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

## S3 method for class 'process_info_multinomial'
as.character(x, ...)

process_info_gaussian(data, target_col, prediction_cols, id_col, locale = NULL)
reconstruct_formulas

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

## S3 method for class 'process_info_gaussian'
as.character(x, ...)

### Arguments

data  Data frame.
target_col  Name of target column.
prediction_cols  Names of prediction columns.
id_col  Name of ID column.
cat_levels  Categorical levels (classes).
positive  Name of the positive class.
cutoff  The cutoff used to get class predictions from probabilities.
locale  The locale when performing the evaluation. Relevant when any sorting has been performed.
x  a process info object used to select a method.
...  further arguments passed to or from other methods.
pred_class_col  Name of predicted classes column.
apply_softmax  Whether softmax has been applied.

### Value

List with relevant information.

### Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

---

**Description**

[Maturing]

In the (cross-)validation results from functions like `cross_validate()`, the model formulas have been split into the columns Dependent, Fixed and Random. Quickly reconstruct the model formulas from these columns.

**Usage**

`reconstruct_formulas(results, topn = NULL)`
**Arguments**

- `results` : data.frame with results from `cross_validate()` or `validate()` (tbl). Must contain at least the columns "Dependent" and "Fixed". For random effects, the "Random" column should be included.

- `topn` : Number of top rows to return. Simply applies `head()` to the results tibble.

**Value**

- list of model formulas.

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

---

**Description**

[Experimental]

Select the columns that define the models, such as the formula terms and hyperparameters.

If an expected column is not in the `results` tibble, it is simply ignored.

**Usage**

```r
select_definitions(results, unnest_hparams = TRUE, additional_includes = NULL)
```

**Arguments**

- `results` : Results tibble. E.g. from `cross_validate()` or `evaluate()`.

- `unnest_hparams` : Whether to unnest the `HParams` column. (Logical)

- `additional_includes` : Names of additional columns to select. (Character)

**Value**

- The model definition columns from the results tibble.

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>
select_metrics  Select columns with evaluation metrics and model definitions

Description

[Maturing]
When reporting results, we might not want all the nested tibbles and process information columns. This function selects the evaluation metrics and model formulas only. If an expected column is not in the `results` tibble, it is simply ignored.

Usage

```r
select_metrics(results, include_definitions = TRUE, additional_includes = NULL)
```

Arguments

- `results`: Results tibble. E.g. from `cross_validate()` or `evaluate()`.
- `include_definitions`: Whether to include the Dependent, Fixed and (possibly) Random and HParams columns. (Logical)
- `additional_includes`: Names of additional columns to select. (Character)

Value

The results tibble with only the metric and model definition columns.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

simplify_formula  Simplify formula with inline functions

Description

[Experimental]
Extracts all variables from a formula object and creates a new formula with all predictor variables added together without the inline functions.

E.g.:
\[ y \sim x \ast z + \log(a) + (1 \mid b) \]
becomes
\[ y \sim x + z + a + b. \]

This is useful when passing a formula to `recipes::recipe()` for preprocessing a dataset, as used in the `preprocess_functions()`.
*summarize_metrics*

**Usage**

```r
simplify_formula(formula, data = NULL, string_out = FALSE)
```

**Arguments**

- **formula**
  
  Formula object.

  If a string is passed, it will be converted with `as.formula()`.

  When a side only contains a NULL, it is kept. Otherwise NULLs are removed.

  An intercept (1) will only be kept if there are no variables on that side of the formula.

- **data**
  
  data.frame. Used to extract variables when the formula contains a ".".

- **string_out**
  
  Whether to return as a string. (Logical)

**Author(s)**

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

**Examples**

```r
# Attach cvms
library(cvms)

# Create formula
f1 <- "y ~ x*z + log(a) + (1|b)"

# Simplify formula (as string)
simplify_formula(f1)

# Simplify formula (as formula)
simplify_formula(as.formula(f1))
```

---

*summarize_metrics*    
**Summarize metrics with common descriptors**

**Description**

*Experimental*

Summarizes all numeric columns. Counts the NAs and Inf in the columns.

**Usage**

```r
summarize_metrics(data, cols = NULL, na.rm = TRUE, inf.rm = TRUE)
```

**Arguments**

- **data**
  
  data.frame with numeric columns to summarize.

- **cols**
  
  Names of columns to summarize. Non-numeric columns are ignored. (Character)

- **na.rm**
  
  Whether to remove NAs before summarizing. (Logical)

- **inf.rm**
  
  Whether to remove Inf in the columns. (Logical)
sum_tile_settings

Value

tibble where each row is a descriptor of the column.
The Measure column contains the name of the descriptor.
The NAs row is a count of the NAs in the column.
The INFs row is a count of the Inf s in the column.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

Examples

# Attach packages
library(cvms)
library(dplyr)

df <- data.frame("a" = c("a", "a", "a", "b", "b", "b", "c", "c", "c"),
    "b" = c(0.8, 0.6, 0.3, 0.2, 0.4, 0.5, 0.8, 0.1, 0.5),
    "c" = c(0.2, 0.3, 0.4, 0.6, 0.5, 0.8, 0.1, 0.8, 0.3))

# Summarize all numeric columns
summarize_metrics(df)

# Summarize column "b"
summarize_metrics(df, cols = "b")

sum_tile_settings

Create a list of settings for the sum tiles in plot_confusion_matrix()

Description

[Experimental]

Creates a list of settings for plotting the column/row sums in plot_confusion_matrix().
The 'tc_' in the arguments refers to the total count tile.
NOTE: This is very experimental and will likely change.

Usage

sum_tile_settings(
    palette = NULL,
    label = NULL,
    tile_fill = NULL,
    font_color = NULL,
    tile_border_color = NULL,
    tile_border_size = NULL,
    tile_border_linetype = NULL,
    tc_tile_fill = NULL,
    tc_font_color = NULL,
    tc_tile_border_color = NULL,
    tc_tile_border_size = NULL,
    tc_tile_border_linetype = NULL
)
Arguments

palette  Color scheme to use for sum tiles. Should be different from the `palette` used for the regular tiles. Passed directly to `palette` in `ggplot2::scale_fill_distiller`. Try these palettes: "Greens", "Oranges", "Greys", "Purples", "Reds", and "Blues". Note: When `tile_fill` is specified, the `palette` is ignored.

label  The label to use for the sum column and the sum row.

tc_tile_fill, tile_fill  Specific background color for the tiles. Passed as `fill` to `ggplot2::geom_tile`. If specified, the `palette` is ignored.

tc_font_color, font_color  Color of the text in the tiles with the column and row sums.

tc_tile_border_color, tile_border_color  Color of the tile borders. Passed as `colour` to `ggplot2::geom_tile`.

tc_tile_border_size, tile_border_size  Size of the tile borders. Passed as `size` to `ggplot2::geom_tile`.

tc_tile_border_linetype, tile_border_linetype  Linetype for the tile borders. Passed as `linetype` to `ggplot2::geom_tile`.

Value

List of settings.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other plotting functions: `font()`, `plot_confusion_matrix()`, `plot_metric_density()`, `plot_probabilities_ecdf()`, `plot_probabilities()`

Description

[Experimental]

1. Checks if the required hyperparameters are present and throws an error when it is not the case.
2. Inserts the missing hyperparameters with the supplied default values.

For managing hyperparameters in custom model functions for `cross_validate_fn()` or `validate_fn()`.

Usage

`update_hyperparameters(..., hyperparameters, .required = NULL)`
update_hyperparameters

Arguments

... Default values for missing hyperparameters. E.g.:

    kernel = "linear", cost = 10

hyperparameters list of hyperparameters as supplied to cross_validate_fn(). Can also be a single-row data.frame.

.required Names of required hyperparameters. If any of these are not present in the hyperparameters, an error is thrown.

Value

A named list with the updated hyperparameters.

Author(s)

Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also

Other example functions: model_functions(), predict_functions(), preprocess_functions()

Examples

# Attach packages
library(cvms)

# Create a list of hyperparameters
hparams <- list(
    "kernel" = "radial",
    "scale" = TRUE
)

# Update hyperparameters with defaults
# Only 'cost' is changed as it's missing
update_hyperparameters(
    cost = 10,
    kernel = "linear",
    "scale" = FALSE,
    hyperparameters = hparams
)

# 'cost' is required
# throws error
xpectr::capture_side_effects(
    update_hyperparameters(
        kernel = "linear",
        "scale" = FALSE,
        hyperparameters = hparams,
        .required = "cost"
    )
)
validate

Validate regression models on a test set

Description

[Stable]
Train linear or logistic regression models on a training set and validate it by predicting a test/validation set. Returns results in a tibble for easy reporting, along with the trained models.

See validate_fn() for use with custom model functions.

Usage

validate(
  train_data, # data.frame.
  formulas, # Model formulas as strings. (Character)
  family, # E.g. c("y~x","y~z").
  test_data = NULL, # Can contain random effects.
  partitions_col = ".partitions", # E.g. c("y~x+(1|r)","y~z+(1|r)").
  control = NULL, # Name of the family. (Character)
  REML = FALSE, # Currently supports "gaussian" for linear regression with lm() / lme4::lmer() and "binomial" for binary classification with glm() / lme4::glmer().
  cutoff = 0.5, # See cross_validate_fn() for use with other model functions.
  positive = 2, #
  metrics = list(), #
  preprocessing = NULL, #
  err_nc = FALSE, #
  rm_nc = FALSE, #
  parallel = FALSE, #
  verbose = FALSE, #
  link = deprecated(), #
  models = deprecated(), #
  model_verbose = deprecated() #
)

Arguments

train_data data.frame.
Can contain a grouping factor for identifying partitions - as made with groupdata2::partition(). See `partitions_col`.

formulas Model formulas as strings. (Character)
E.g. c("y~x","y~z").
Can contain random effects.
E.g. c("y~x+(1|r)","y~z+(1|r)").

family Name of the family. (Character)
Currently supports "gaussian" for linear regression with lm() / lme4::lmer() and "binomial" for binary classification with glm() / lme4::glmer(). See cross_validate_fn() for use with other model functions.

test_data data.frame. If specifying `partitions_col`, this can be NULL.
partitions_col Name of grouping factor for identifying partitions. (Character)

Rows with the value 1 in `partitions_col` are used as training set and rows with the value 2 are used as test set.

N.B. Only used if `test_data` is NULL.

control Construct control structures for mixed model fitting (with `lme4::lmer()` or `lme4::glmer()`). See `lme4::lmerControl` and `lme4::glmerControl`.

N.B. Ignored if fitting `lm()` or `glm()` models.

REML Restricted Maximum Likelihood. (Logical)

cutoff Threshold for predicted classes. (Numeric)

N.B. Binomial models only

positive Level from dependent variable to predict. Either as character (preferable) or level index (1 or 2 - alphabetically).

E.g. if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".

Note: For reproducibility, it's preferable to specify the name directly, as different locales may sort the levels differently.

Used when calculating confusion matrix metrics and creating ROC curves.

The Positive Class column in the output can be used to verify this setting.

N.B. Only affects evaluation metrics, not the model training or returned predictions.

N.B. Binomial models only.

metrics list for enabling/disabling metrics.

E.g. list("RMSE" = FALSE) would remove RMSE from the results, and list("Accuracy" = TRUE) would add the regular Accuracy metric to the classification results. Default values (TRUE/FALSE) will be used for the remaining available metrics.

You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why list("all" = FALSE, "RMSE" = TRUE) would return only the RMSE metric.

The list can be created with `gaussian_metrics()` or `binomial_metrics()`.

Also accepts the string "all".

preprocessing Name of preprocessing to apply.

Available preprocessings are:

- "standardize": Centers and scales the numeric predictors.
- "range": Normalizes the numeric predictors to the 0-1 range. Values outside the min/max range in the test fold are truncated to 0 or 1.
- "scale": Scales the numeric predictors to have a standard deviation of one.
- "center": Centers the numeric predictors to have a mean of zero.

The preprocessing parameters (mean, SD, etc.) are extracted from the training folds and applied to both the training folds and the test fold. They are returned in the Preprocess column for inspection.

N.B. The preprocessings should not affect the results to a noticeable degree, although "range" might due to the truncation.

err_nc Whether to raise an error if a model does not converge. (Logical)

rm_nc Remove non-converged models from output. (Logical)
validate

parallel Whether to validate the list of models in parallel. (Logical)
Remember to register a parallel backend first. E.g. with doParallel::registerDoParallel.

verbose Whether to message process information like the number of model instances to
fit and which model function was applied. (Logical)

link, models, model_verbose
Depreciated.

Details

Packages used:

**Models:**
- Gaussian: stats::lm, lme4::lmer
- Binomial: stats::glm, lme4::glmer

**Results:**
- Shared:
  - AIC: stats::AIC
  - AICC: MuMIn::AICC
  - BIC: stats::BIC
- Gaussian:
  - r2m: MuMIn::r.squaredGLMM
  - r2c: MuMIn::r.squaredGLMM
- Binomial:
  - ROC and AUC: pROC::roc

**Value**

tibble with the results and model objects.

Shared across families:
A nested tibble with coefficients of the models from all iterations.
Count of convergence warnings. Consider discarding models that did not converge.
Count of other warnings. These are warnings without keywords such as "convergence".
Count of Singular Fit messages. See lme4::isSingular for more information.
Nested tibble with the warnings and messages caught for each model.
Specified family.
Nested model objects.
Name of dependent variable.
Names of fixed effects.
Names of random effects, if any.
Nested tibble with preprocessing parameters, if any.

Gaussian Results:

RMSE, MAE, NRMSE (IQR), RRSE, RAE, RMSLE, AIC, AICC, and BIC.
See the additional metrics (disabled by default) at ?gaussian_metrics.
A nested tibble with the predictions and targets.
Binomial Results:

Based on predictions of the test set, a confusion matrix and ROC curve are used to get the following:

ROC:
AUC, Lower CI, and Upper CI.

Confusion Matrix:
Balanced Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, Prevalence, and MCC (Matthews correlation coefficient).

See the additional metrics (disabled by default) at ?binomial_metrics.

Also includes:
A nested tibble with predictions, predicted classes (depends on cutoff), and the targets. Note, that the predictions are not necessarily of the specified positive class, but of the model’s positive class (second level of dependent variable, alphabetically).

The pROC::roc ROC curve object(s).
A nested tibble with the confusion matrix/matrices. The Pos_columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. I.e. the level you wish to predict.

The name of the Positive Class.

Author(s)
Ludvig Renbo Olsen, <r-pkgs@ludvigolsen.dk>

See Also
Other validation functions: cross_validate_fn(), cross_validate(), validate_fn()

Examples

# Attach packages
library(cvms)
library(groupdata2) # partition()
library(dplyr) # %>% arrange()

# Data is part of cvms
data <- participant.scores

# Set seed for reproducibility
set.seed(7)

# Partition data
# Keep as single data frame
# We could also have fed validate() separate train and test sets.
data_partitioned <- partition(
data, p = 0.7,
cat_col = "diagnosis",
id_col = "participant",
lst_out = FALSE)
validate_fn

Validate a custom model function on a test set

Description

[Experimental]
validate_fn

Fit your model function on a training set and validate it by predicting a test/validation set. Validate different hyperparameter combinations and formulas at once. Preprocess the train/test split. Returns results and fitted models in a tibble for easy reporting and further analysis.

Compared to validate(), this function allows you supply a custom model function, a predict function, a preprocess function and the hyperparameter values to validate.

Supports regression and classification (binary and multiclass). See `type`.

Note that some metrics may not be computable for some types of model objects.

Usage

```r
validate_fn(
  train_data,
  formulas,
  type,
  model_fn,
  predict_fn,
  test_data = NULL,
  preprocess_fn = NULL,
  preprocess_once = FALSE,
  hyperparameters = NULL,
  partitions_col = ".partitions",
  cutoff = 0.5,
  positive = 2,
  metrics = list(),
  rm_nc = FALSE,
  parallel = FALSE,
  verbose = TRUE
)
```

Arguments

- `train_data` data.frame. Can contain a grouping factor for identifying partitions - as made with `groupdata2::partition()`. See `partitions_col`.
- `formulas` Model formulas as strings. (Character) Will be converted to `formula` objects before being passed to `model_fn`. E.g. `c("y~x","y~z")`. Can contain random effects. E.g. `c("y-x+(1|r)","y-z+(1|r)").`
- `type` Type of evaluation to perform: "gaussian" for regression (like linear regression). "binomial" for binary classification. "multinomial" for multiclass classification.
- `model_fn` Model function that returns a fitted model object. Will usually wrap an existing model function like `e1071::svm` or `nnet::multinom`. Must have the following function arguments: `function(train_data,formula,
  hyperparameters)`
predict_fn

Function for predicting the targets in the test folds/sets using the fitted model object. Will usually wrap stats::predict(), but doesn’t have to.

Must have the following function arguments:

function(test_data, model, formula, hyperparameters, train_data)

Must return predictions in the following formats, depending on `type`:

**Binomial:** vector or one-column matrix/data.frame with probabilities (0-1) of the second class, alphabetically. E.g.:

c(0.3, 0.5, 0.1, 0.5)

**Gaussian:** vector or one-column matrix/data.frame with the predicted value. E.g.:

c(3.7, 0.9, 1.2, 7.3)

**Multinomial:** data.frame with one column per class containing probabilities of the class. Column names should be identical to how the class names are written in the target column. E.g.:

class_1  class_2  class_3
0.269 0.528 0.203
0.368 0.322 0.310
0.375 0.371 0.254
...
...
...

test_data

data.frame. If specifying `partitions_col`, this can be NULL.

preprocess_fn

Function for preprocessing the training and test sets.

Can, for instance, be used to standardize both the training and test sets with the scaling and centering parameters from the training set.

Must have the following function arguments:

function(train_data, test_data, formula, hyperparameters)

Must return a list with the preprocessed `train_data` and `test_data`. It may also contain a tibble with the parameters used in preprocessing:

list("train" = train_data,
    "test" = test_data,
    "parameters" = preprocess_parameters)

Additional elements in the returned list will be ignored.

The optional parameters tibble will be included in the output. It could have the following format:

<table>
<thead>
<tr>
<th>Measure</th>
<th>var_1</th>
<th>var_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>37.921</td>
<td>88.231</td>
</tr>
<tr>
<td>SD</td>
<td>12.4</td>
<td>5.986</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

N.B. When `preprocess_once` is FALSE, the current formula and hyperparameters will be provided. Otherwise, these arguments will be NULL.

preprocess_once

Whether to apply the preprocessing once (ignoring the formula and hyperparameters arguments in `preprocess_fn`) or for every model separately. (Logical)
When preprocessing does not depend on the current formula or hyperparameters, we can do the preprocessing of each train/test split once, to save time. This **may require holding a lot more data in memory** though, why it is not the default setting.

**hyperparameters**

Either a named list with hyperparameter values to combine in a grid or a data.frame with one row per hyperparameter combination.

**Named list for grid search:** Add ".n" to sample the combinations. Can be the number of combinations to use, or a percentage between 0 and 1.

E.g.
```r
list(".n" = 10,# sample 10 combinations
     "lrn_rate" = c(0.1,0.01,0.001),
     "h_layers" = c(10,100,1000),
     "drop_out" = runif(5,0.3,0.7))
```

**data.frame with specific hyperparameter combinations:** One row per combination to test.

E.g.
```
     lrn_rate  h_layers  drop_out
     0.1       10       0.65
     0.1      1000      0.65
     0.01     1000      0.63
     ...    ...        ...
```

**partitions_col** Name of grouping factor for identifying partitions. (Character)

Rows with the value 1 in `partitions_col` are used as training set and rows with the value 2 are used as test set.

*N.B. Only used if `test_data` is NULL.*

**cutoff** Threshold for predicted classes. (Numeric)

*NB. Binomial models only*

**positive** Level from dependent variable to predict. Either as character (preferable) or level index (1 or 2 - alphabetically).

E.g. if we have the levels "cat" and "dog" and we want "dog" to be the positive class, we can either provide "dog" or 2, as alphabetically, "dog" comes after "cat".

**Note:** For reproducibility, it’s preferable to specify the name directly, as different locales may sort the levels differently.

Used when calculating confusion matrix metrics and creating ROC curves.

The Positive Class column in the output can be used to verify this setting.

*N.B. Only affects evaluation metrics, not the model training or returned predictions.*

*NB. Binomial models only.*

**metrics**

list for enabling/disabling metrics.

E.g. list("RMSE" = FALSE) would remove RMSE from the regression results, and list("Accuracy" = TRUE) would add the regular Accuracy metric to the classification results. Default values (TRUE/FALSE) will be used for the remaining available metrics.

You can enable/disable all metrics at once by including "all" = TRUE/FALSE in the list. This is done prior to enabling/disabling individual metrics, why f.i. list("all" = FALSE, "RMSE" = TRUE) would return only the RMSE metric.
The list can be created with `gaussian_metrics()`, `binomial_metrics()`, or `multinomial_metrics()`. Also accepts the string "all".

- **rm_nc**: Remove non-converged models from output. (Logical)
- **parallel**: Whether to cross-validate the list of models in parallel. (Logical)
  Remember to register a parallel backend first. E.g. with `doParallel::registerDoParallel`.
- **verbose**: Whether to message process information like the number of model instances to fit. (Logical)

### Details

Packaged used:

**Results:**

- **Shared:**
  - AIC: `stats::AIC`
  - AICC: `MuMIn::AICc`
  - BIC: `stats::BIC`

- **Gaussian:**
  - r2m: `MuMIn::r.squaredGLMM`
  - r2e: `MuMIn::r.squaredGLMM`

- **Binomial and Multinomial:**
  - ROC and related metrics:
    - Binomial: `pROC::roc`
    - Multinomial: `pROC::multiclass.roc`

**Value**

tibble with the results and model objects.

**Shared across families:**

A nested tibble with **coefficients** of the models. The coefficients are extracted from the model object with `parameters::model_parameters()` or `coef()` (with some restrictions on the output). If these attempts fail, a default coefficients tibble filled with NAs is returned.

Nested tibble with the used **preprocessing parameters**, if a passed `preprocess_fn` returns the parameters in a tibble.

Count of **convergence warnings**, using a limited set of keywords (e.g. "convergence"). If a convergence warning does not contain one of these keywords, it will be counted with **other warnings**. Consider discarding models that did not converge on all iterations. Note: you might still see results, but these should be taken with a grain of salt!

Nested tibble with the **warnings and messages** caught for each model.

Specified **family**.

Nested **model** objects.

Name of **dependent** variable.

Names of **fixed** effects.

Names of **random** effects, if any.
Gaussian Results:

RMSE, MAE, NRMSE (IQR), RRSE, RAE, and RMSLE.
See the additional metrics (disabled by default) at ?gaussian_metrics.
A nested tibble with the predictions and targets.

Binomial Results:

Based on predictions of the test set, a confusion matrix and a ROC curve are created to get the following:

ROC:
AUC, Lower CI, and Upper CI
Confusion Matrix:
Balanced Accuracy, F1, Sensitivity, Specificity, Positive Predictive Value, Negative Predictive Value, Kappa, Detection Rate, Detection Prevalence, Prevalence, and MCC (Matthews correlation coefficient).
See the additional metrics (disabled by default) at ?binomial_metrics.
Also includes:
A nested tibble with predictions, predicted classes (depends on cutoff), and the targets. Note, that the predictions are not necessarily of the specified positive class, but of the model’s positive class (second level of dependent variable, alphabetically).
The `pROC::roc` ROC curve object(s).
A nested tibble with the confusion matrix/matrices. The Pos_ columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the "positive" class. I.e. the level you wish to predict.
The name of the Positive Class.

Multinomial Results:

For each class, a one-vs-all binomial evaluation is performed. This creates a Class Level Results tibble containing the same metrics as the binomial results described above (excluding MCC, AUC, Lower CI and Upper CI), along with a count of the class in the target column (Support). These metrics are used to calculate the macro metrics. The nested class level results tibble is also included in the output tibble, and could be reported along with the macro and overall metrics.
The output tibble contains the macro and overall metrics. The metrics that share their name with the metrics in the nested class level results tibble are averages of those metrics (note: does not remove NAs before averaging). In addition to these, it also includes the Overall Accuracy and the multiclass MCC.
Other available metrics (disabled by default, see metrics): Accuracy, multiclass AUC, Weighted Balanced Accuracy, Weighted Accuracy, Weighted F1, Weighted Sensitivity, Weighted Specificity, Weighted Pos Pred Value, Weighted Neg Pred Value, Weighted Kappa, Weighted Detection Rate, Weighted Detection Prevalence, and Weighted Prevalence.
Note that the “Weighted” average metrics are weighted by the Support.
Also includes:
A nested tibble with the predictions, predicted classes, and targets.
A list of ROC curve objects when AUC is enabled.
A nested tibble with the multiclass Confusion Matrix.

Class Level Results
Besides the binomial evaluation metrics and the Support, the nested class level results tibble also contains a nested tibble with the Confusion Matrix from the one-vs-all evaluation. The Pos_ columns tells you whether a row is a True Positive (TP), True Negative (TN), False Positive (FP), or False Negative (FN), depending on which level is the “positive” class. In our case, 1 is the current class and 0 represents all the other classes together.

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See Also
Other validation functions: cross_validate_fn(), cross_validate(), validate()

Examples

```r
# Attach packages
library(cvms)
library(groupdata2) # fold()
library(dplyr) # %>% arrange() mutate()

# Note: More examples of custom functions can be found at:
# model_fn: model_functions()
# predict_fn: predict_functions()
# preprocess_fn: preprocess_functions()

# Data is part of cvms
data <- participant.scores

data <- participant.scores

# Set seed for reproducibility
set.seed(7)

# Fold data
data <- partition(
  data,
p = 0.8,
cat_col = "diagnosis",
id_col = "participant",
list_out = FALSE
) %>%
  mutate(diagnosis = as.factor(diagnosis)) %>%
  arrange(.partitions)

# Formulas to validate
formula_gaussian <- "score ~ diagnosis"
formula_binomial <- "diagnosis ~ score"

# Gaussian

# Create model function that returns a fitted model object
```
lm_model_fn <- function(train_data, formula, hyperparameters) {
  lm(formula = formula, data = train_data)
}

# Create predict function that returns the predictions
lm_predict_fn <- function(test_data, model, formula, hyperparameters, train_data) {
  stats::predict(
    object = model,
    newdata = test_data,
    type = "response",
    allow.new.levels = TRUE
  )
}

# Validate the model function
v <- validate_fn(
  data,
  formulas = formula_gaussian,
  type = "gaussian",
  model_fn = lm_model_fn,
  predict_fn = lm_predict_fn,
  partitions_col = ".partitions"
)

v

# Extract model object
v$Model[[1]]

# Binomial

# Create model function that returns a fitted model object
glm_model_fn <- function(train_data, formula, hyperparameters) {
  glm(formula = formula, data = train_data, family = "binomial")
}

# Create predict function that returns the predictions
glm_predict_fn <- function(test_data, model, formula, hyperparameters, train_data) {
  stats::predict(
    object = model,
    newdata = test_data,
    type = "response",
    allow.new.levels = TRUE
  )
}

# Validate the model function
validate_fn(
  data,
  formulas = formula_binomial,
  type = "binomial",
  model_fn = glm_model_fn,
  predict_fn = glm_predict_fn,
partitions_col = ".partitions"
)

#
# Support Vector Machine (svm)
# with known hyperparameters
#
# Create model function that returns a fitted model object
# We use the hyperparameters arg to pass in the kernel and cost values
# These will usually have been found with cross_validate_fn()
svm_model_fn <- function(train_data, formula, hyperparameters) {
  # Expected hyperparameters:
  #  - kernel
  #  - cost
  if (!"kernel" %in% names(hyperparameters))
    stop("hyperparameters' must include 'kernel'"
  if (!"cost" %in% names(hyperparameters))
    stop("hyperparameters' must include 'cost'"

  e1071::svm(
    formula = formula,
    data = train_data,
    kernel = hyperparameters["kernel"],
    cost = hyperparameters["cost"],
    scale = FALSE,
    type = "C-classification",
    probability = TRUE
  )
)

# Create predict function that returns the predictions
svm_predict_fn <- function(test_data, model, formula,
                            hyperparameters, train_data) {
  predictions <- stats::predict(
    object = model,
    newdata = test_data,
    allow.new.levels = TRUE,
    probability = TRUE
  )

  # Extract probabilities
  probabilities <- dplyr::as_tibble(
    attr(predictions, "probabilities")
  )

  # Return second column
  probabilities[[2]]
}

# Specify hyperparameters to use
# We found these in the examples in ?cross_validate_fn()
svm_hparams <- list(
  "kernel" = "linear",
  "cost" = 10
)
# Validate the model function
validate_fn(
    data,
    formulas = formula_binomial,
    type = "binomial",
    model_fn = svm_model_fn,
    predict_fn = svm_predict_fn,
    hyperparameters = svm_hparams,
    partitions_col = ".partitions"
)

<table>
<thead>
<tr>
<th>wines</th>
<th>Wine varieties</th>
</tr>
</thead>
</table>

**Description**
A list of wine varieties in an approximately Zipfian distribution, ordered by descending frequencies.

**Format**
A data.frame with 368 rows and 1 variable:

**Variety** Wine variety, 10 levels

**Details**
Based on the wine-reviews (v4) kaggle dataset by Zack Thoutt: https://www.kaggle.com/zynicide/wine-reviews

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