Package `ale`

February 14, 2024

**Title**  Interpretable Machine Learning and Statistical Inference with Accumulated Local Effects (ALE)

**Version**  0.3.0

**Description**  Accumulated Local Effects (ALE) were initially developed as a model-agnostic approach for global explanations of the results of black-box machine learning algorithms. ALE has a key advantage over other approaches like partial dependence plots (PDP) and SHapley Additive exPlanations (SHAP): its values represent a clean functional decomposition of the model. As such, ALE values are not affected by the presence or absence of interactions among variables in a mode. Moreover, its computation is relatively rapid. This package rewrites the original code from the `ALEPlot` package for calculating ALE data and it completely reimplements the plotting of ALE values. It also extends the original ALE concept to add bootstrap-based confidence intervals and ALE-based statistics that can be used for statistical inference. For more details, see Okoli, Chit. 2023. “Statistical Inference Using Machine Learning and Classical Techniques Based on Accumulated Local Effects (ALE).” arXiv. <arXiv:2310.09877>. <doi:10.48550/arXiv.2310.09877>.

**License**  GPL-2

**Language**  en-ca

**Encoding**  UTF-8

**RoxygenNote**  7.3.1

**Suggests**  ALEPlot, knitr, mgcv, patchwork, readr, rmarkdown, testthat

(>= 3.0.0)

**VignetteBuilder**  knitr

**Imports**  assertthat, broom, dplyr, ellipsis, furrr, future, ggplot2, ggpubr, glue, grDevices, insight, labeling, progressr, purrr, rlang, stats, stringr, tidyr, univariateML, yaImpute

**Depends**  R (>= 3.5.0)


**BugReports**  https://github.com/tripartio/ale/issues

**Config/testthat/edition**  3

**LazyData**  true

**NeedsCompilation**  no
**Author**  Chitu Okoli [aut, cre] (<https://orcid.org/0000-0001-5574-7572>),  
Dan Apley [cph] (The current code for calculating ALE interaction  
values is copied with few changes from Dan Apley’s ALEPlot package.  
We gratefully acknowledge his open-source contribution. However, he  
was not directly involved in the development of this ale package.)

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**Repository**  CRAN

**Date/Publication**  2024-02-14 00:04:05 UTC

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**R topics documented:**

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**Description**

`ale()` is the central function that manages the creation of ALE data and plots for one-way ALE. For two-way interactions, see `ale_ixn()`. This function calls `ale_core` (a non-exported function) that manages the ALE data and plot creation in detail. For details, see the introductory vignette for this package or the details and examples below.

**Usage**

```r
ale(  
data,  
model,  
x_cols = NULL,  
y_col = NULL,  
...,  
parallel = parallel::detectCores(logical = FALSE) - 1,  
model_packages = as.character(NA),  
output = c("plots", "data", "stats", "conf_regions"),  
pred_fun = function(object, newdata, type = pred_type) {  
  stats::predict(object = object, newdata = newdata, type = type)  
},  
pred_type = "response",
```
p_values = NULL,
p_alpha = c(0.01, 0.05),
x_intervals = 100,
boot_it = 0,
seed = 0,
boot_alpha = 0.05,
boot_centre = "mean",
relative_y = "median",
y_type = NULL,
median_band_pct = c(0.05, 0.5),
rug_sample_size = 500,
min_rug_per_interval = 1,
ale_xs = NULL,
ale_ns = NULL,
compact_plots = FALSE,
silent = FALSE
)

Arguments

data dataframe. Dataset from which to create predictions for the ALE.
model model object. Model for which ALE should be calculated. May be any kind of
R object that can make predictions from data.
x_cols character. Vector of column names from data for which one-way ALE data is to
be calculated (that is, simple ALE without interactions). If not provided, ALE
will be created for all columns in data except y_col.
y_col character length 1. Name of the outcome target label (y) variable. If not pro-
vided, ale() will try to detect it automatically. For non-standard models, y_col
should be provided. For survival models, set y_col to the name of the binary
event column; in that case, pred_type should also be specified.
...
parallel non-negative integer length 1. Number of parallel threads (workers or tasks) for
parallel execution of the function. See details.
model_packages character. Character vector of names of packages that model depends on that
might not be obvious. The (ale) package should be able to automatically rec-
ognize and load most packages that are needed, but with parallel processing
enabled (which is the default), some packages might not be properly loaded.
If you get a strange error message that mentions something somewhere about
'future', try adding the package for your model to this vector, especially if you
see such errors after the progress bars begin displaying (assuming you did not
disable progress bars with silent = TRUE).
output character in c('plots', 'data', 'stats', 'conf_regions'). Vector of types of results
to return. 'plots' will return an ALE plot; 'data' will return the source ALE
data; 'stats' will return ALE statistics. Each option must be listed to return the
specified component. By default, all are returned.
pred_fun, pred_type

function character length 1. pred_fun is a function that returns a vector of predicted values of type pred_type from model on data. See details.

p_values

instructions for calculating p-values and to determine the median band. If NULL (default), no p-values are calculated and median_band_pct is used to determine the median band. To calculate p-values, an object generated by the create_p_funs() function must be provided here. If p_values is set to ‘auto’, this ale() function will try to automatically create the p-values function; this only works with standard R model types. Any error message will be given if p-values cannot be generated. Any other input provided to this argument will result in an error. For more details about creating p-values, see documentation for create_p_funs(). Note that p-values will not be generated if 'stats' are not included as an option in the output argument.

p_alpha

numeric length 2 from 0 to 1. Alpha for "confidence interval" ranges for printing bands around the median for single-variable plots. These are the default values used if p_values are provided. If p_values are not provided, then median_band_pct is used instead. The inner band range will be the median value of y ± p_alpha[2] of the relevant ALE statistic (usually ALE range or normalized ALE range). For plots with a second outer band, its range will be the median ± p_alpha[1]. For example, in the ALE plots, for the default p_alpha = c(0.01, 0.05), the inner band will be the median ± ALE minimum or maximum at p = 0.05 and the outer band will be the median ± ALE minimum or maximum at p = 0.01.

x_intervals

positive integer length 1. Maximum number of intervals on the x-axis for the ALE data for each column in x_cols. The number of intervals that the algorithm generates might eventually be fewer than what the user specifies if the data values for a given x value do not support that many intervals.

boot_it

non-negative integer length 1. Number of bootstrap iterations for the ALE values. If boot_it = 0 (default), then ALE will be calculated on the entire dataset with no bootstrapping.

seed

integer length 1. Random seed. Supply this between runs to assure that identical random ALE data is generated each time

boot_alpha

numeric length 1 from 0 to 1. Alpha for percentile-based confidence interval range for the bootstrap intervals; the bootstrap confidence intervals will be the lowest and highest (1 - 0.05) / 2 percentiles. For example, if boot_alpha = 0.05 (default), the intervals will be from the 2.5 and 97.5 percentiles.

boot_centre

character length 1 in c('mean', 'median'). When bootstrapping, the main estimate for ale_y is considered to be boot_centre. Regardless of the value specified here, both the mean and median will be available.

relative_y

character length 1 in c('median', 'mean', 'zero'). The ale_y values will be adjusted relative to this value. 'median' is the default. 'zero' will maintain the default of ALEPlot::ALEPlot(), which is not shifted.

y_type

character length 1. Datatype of the y (outcome) variable. Must be one of c('binary', 'numeric', 'multinomial', 'ordinal'). Normally determined automatically; only provide for complex non-standard models that require it.
median_band_pct
numeric length 2 from 0 to 1. Alpha for "confidence interval" ranges for printing bands around the median for single-variable plots. These are the default values used if p_values are not provided. If p_values are provided, then median_band_pct is ignored. The inner band range will be the median value of y ± median_band_pct[1]/2. For plots with a second outer band, its range will be the median ± median_band_pct[2]/2. For example, for the default median_band_pct = c(0.05, 0.5), the inner band will be the median ± 2.5% and the outer band will be the median ± 25%.

rug_sample_size, min_rug_per_interval
single non-negative integer length 1. Rug plots are normally down-sampled otherwise they are too slow. rug_sample_size specifies the size of this sample. To prevent down-sampling, set to Inf. To suppress rug plots, set to 0. When down-sampling, the rug plots maintain representativeness of the data by guaranteeing that each of the x_intervals intervals will retain at least min_rug_per_interval elements; usually set to just 1 or 2.

ale_xs, ale_ns
list of ale_x and ale_n vectors. If provided, these vectors will be used to set the intervals of the ALE x axis for each variable. By default (NULL), the function automatically calculates the ale_x intervals. ale_xs is normally used in advanced analyses where the ale_x intervals from a previous analysis are reused for subsequent analyses (for example, for full model bootstrapping; see the model_bootstrap() function).

compact_plots
logical length 1, default FALSE. When output includes 'plots', the returned ggplot objects each include the environments of the plots. This lets the user modify the plots with all the flexibility of ggplot, but it can result in very large return objects (sometimes even hundreds of megabytes large). To compact the plots to their bare minimum, set compact_plots = TRUE. However, returned plots will not be easily modifiable, so this should only be used if you do not want to subsequently modify the plots.

silent
logical length 1, default FALSE. If TRUE, do not display any non-essential messages during execution (such as progress bars). Regardless, any warnings and errors will always display. See details for how to enable progress bars.

Details

ale_core.R
Core functions for the ale package: ale, ale_ixn, and ale_core

Value

list with the following elements:

- data: a list whose elements, named by each requested x variable, are each a tibble with the following columns:
  - ale_x: the values of each of the ALE x intervals or categories.
  - ale_n: the number of rows of data in each ale_x interval or category.
– ale_y: the ALE function value calculated for that interval or category. For bootstrapped
ALE, this is the same as ale_y_mean by default or ale_y_median if the boot_centre
= 'median' argument is specified. Regardless, both ale_y_mean and ale_y_median are
returned as columns here.
– ale_y_lo, ale_y_hi: the lower and upper confidence intervals, respectively, for the
bootstrapped ale_y value. Note: regardless what options are requested in the output
argument, this data element is always returned.

• stats: if stats are requested in the output argument (as is the default), returns a list. If
not requested, returns NULL. The returned list provides ALE statistics of the data element
duplicated and presented from various perspectives in the following elements:
  – by_term: a list named by each requested x variable, each of whose elements is a tibble
    with the following columns:
    * statistic: the ALE statistic specified in the row (see the by_statistic element
      below).
    * estimate: the bootstrapped mean or median of the statistic, depending on the
      boot_centre argument to the ale() function. Regardless, both mean and median
      are returned as columns here.
    * conf.low, conf.high: the lower and upper confidence intervals, respectively, for
      the bootstrapped estimate.
  – by_statistic: list named by each of the following ALE statistics: aled, aler_min,
    aler_max, naled, naler_min, naler_max. See vignette('ale-statistics') for de-
    tails.
  – estimate: a tibble whose data consists of the estimate values from the by_term element
    above. The columns are term (the variable name) and the statistic for which the estimate
    is given: aled, aler_min, aler_max, naled, naler_min, naler_max.
  – effects_plot: a ggplot object which is the ALE effects plot for all the x variables.

• plots: if plots are requested in the output argument (as is the default), returns a list whose
  elements, named by each requested x variable, are each a ggplot object of the ALE y values
  plotted against the x variable intervals. If plots is not included in output, this element is
  NULL.

• conf_regions: if conf_regions are requested in the output argument (as is the default),
  returns a list. If not requested, returns NULL. The returned list provides summaries of the con-
  fidence regions of the relevant ALE statistics of the data element. The list has the following
  elements:
  – by_term: a list named by each requested x variable, each of whose elements is a tibble
    with the relevant data for the confidence regions. (See vignette('ale-statistics')
    for details about confidence regions.)
  – significant: a tibble that summarizes the by_term to only show confidence regions
    that are statistically significant. Its columns are those from by_term plus a term column
    to specify which x variable is indicated by the respective row.
  – sig_criterion: a length-one character vector that reports which values were used to
determine statistical significance: if p_values was provided to the ale() function, it will
    be used; otherwise, median_band_pct will be used.

• Various values echoed from the original call to the ale() function, provided to document the
  key elements used to calculate the ALE data, statistics, and plots: y_col, x_cols, boot_it,
seed, boot_alpha, boot_centre, relative_y, y_type, median_band_pct, rug_sample_size. These are either the values provided by the user or used by default if the user did not change them.

- **y_summary**: summary statistics of y values used for the ALE calculation. These statistics are based on the actual values of y_col unless if y_type is a probability or other value that is constrained in the [0, 1] range. In that case, y_summary is based on the predicted values of y_col by applying model to the data. y_summary is a named numeric vector. Most of the elements are the percentile of the y values. E.g., the ’5%’ element is the 5th percentile of y values. The following elements have special meanings:
  - The first element is named either p or q and its value is always 0. The value is not used; only the name of the element is meaningful. p means that the following special y_summary elements are based on the provided p_values object. q means that quantiles were calculated based on median_band_pct because p_values was not provided.
  - min, mean, max: the minimum, mean, and maximum y values, respectively. Note that the median is 50%, the 50th percentile.
  - med_lo_2, med_lo, med_hi, med_hi_2: med_lo and med_hi are the inner lower and upper confidence intervals of y values with respect to the median (50%); med_lo_2 and med_hi_2 are the outer confidence intervals. See the documentation for the p_alpha and median_band_pct arguments to understand how these are determined.

**Custom predict function**

The calculation of ALE requires modifying several values of the original data. Thus, ale() needs direct access to a predict function that work on model. By default, ale() uses a generic default predict function of the form predict(object, newdata, type) with the default prediction type of ‘response’. If, however, the desired prediction values are not generated with that format, the user must specify what they want. Most of the time, the only modification needed is to change the prediction type to some other value by setting the pred_type argument (e.g., to ‘prob’ to generated classification probabilities). But if the desired predictions need a different function signature, then the user must create a custom prediction function and pass it to pred_fun. The requirements for this custom function are:

- It must take three required arguments and nothing else:
  - object: a model
  - newdata: a dataframe or compatible table type
  - type: a string; it should usually be specified as type = pred_type These argument names are according to the R convention for the generic stats::predict function.
- It must return a vector of numeric values as the prediction.

You can see an example below of a custom prediction function.

**Note**: survival models probably do not need a custom prediction function but y_col must be set to the name of the binary event column and pred_type must be set to the desired prediction type.

**ALE statistics**

For details about the ALE-based statistics (ALED, ALER, NALED, and NALER), see vignette(‘ale-statistics’).
Parallel processing

Parallel processing using the \{furrr\} library is enabled by default. By default, it will use all the available physical CPU cores (minus the core being used for the current R session) with the setting `parallel = parallel::detectCores(logical = FALSE) - 1`. Note that only physical cores are used (not logical cores or "hyperthreading") because machine learning can only take advantage of the floating point processors on physical cores, which are absent from logical cores. Trying to use logical cores will not speed up processing and might actually slow it down with useless data transfer. If you will dedicate the entire computer to running this function (and you don’t mind everything else running very slow while it runs), you may use all cores by setting `parallel = parallel::detectCores(logical = FALSE)`. To disable parallel processing, set `parallel = 0`.

Progress bars

Progress bars are implemented with the \{progressr\} package, which lets the user fully control progress bars. To disable progress bars, set `silent = TRUE`. The first time a function is called in the \{ale\} package that requires progress bars, it checks if the user has activated the necessary \{progressr\} settings. If not, the \{ale\} package automatically enables \{progressr\} progress bars with the \cli\ handler and prints a message notifying the user.

If you like the default progress bars and you want to make them permanent, then you can add the following lines of code to your \.Rprofile\ configuration file and they will become your defaults for every R session; you will not see the message again:

```r
progressr::handlers(global = TRUE)
progressr::handlers('cli')
```

For more details on formatting progress bars to your liking, see the introduction to the \{progressr\} package.

References


Examples

```r
set.seed(0)
diamonds_sample <- ggplot2::diamonds[sample(nrow(ggplot2::diamonds), 1000), ]

# Create a GAM model with flexible curves to predict diamond price
# Smooth all numeric variables and include all other variables
gam_diamonds <- mgcv::gam(
  price ~ s(carat) + s(depth) + s(table) + s(x) + s(y) + s(z) +
  cut + color + clarity,
  data = diamonds_sample
)
summary(gam_diamonds)
```
# Simple ALE without bootstrapping
ale_gam_diamonds <- ale(
    diamonds_sample, gam_diamonds,
    parallel = 2 # CRAN limit (delete this line on your own computer)
)

# Plot the ALE data
ale_gam_diamonds$plots |> patchwork::wrap_plots()

# Bootstrapped ALE
# This can be slow, since bootstrapping runs the algorithm boot_it times

# Create ALE with 100 bootstrap samples
ale_gam_diamonds_boot <- ale(
    diamonds_sample, gam_diamonds, boot_it = 100,
    parallel = 2 # CRAN limit (delete this line on your own computer)
)

# Bootstrapped ALEs print with confidence intervals
ale_gam_diamonds_boot$plots |> patchwork::wrap_plots()

# If the predict function you want is non-standard, you may define a
# custom predict function. It must return a single numeric vector.
custom_predict <- function(object, newdata, type = pred_type) {
    predict(object, newdata, type = type, se.fit = TRUE)$fit
}

ale_gam_diamonds_custom <- ale(
    diamonds_sample, gam_diamonds,
    pred_fun = custom_predict, pred_type = 'link',
    parallel = 2 # CRAN limit (delete this line on your own computer)
)

# Plot the ALE data
ale_gam_diamonds_custom$plots |> patchwork::wrap_plots()
Description

This is the central function that manages the creation of ALE data and plots for two-way ALE interactions. For simple one-way ALE, see `ale()`. See documentation there for functionality shared between both functions.

For details, see the introductory vignette for this package or the details and examples below.

For the plots, `n_y_quant` is the number of quantiles into which to divide the predicted variable (y). The middle quantiles are grouped specially:

- The middle quantile is the first confidence interval of `median_band_pct` (`median_band_pct[1]`) around the median. This middle quantile is special because it generally represents no meaningful interaction.
- The quantiles above and below the middle are extended from the borders of the middle quantile to the regular borders of the other quantiles.

There will always be an odd number of quantiles: the special middle quantile plus an equal number of quantiles on each side of it. If `n_y_quant` is even, then a middle quantile will be added to it. If `n_y_quant` is odd, then the number specified will be used, including the middle quantile.

Usage

```r
ale_ixn(
  data,
  model,
  x1_cols = NULL,
  x2_cols = NULL,
  y_col = NULL,
  ...,  
  parallel = parallel::detectCores(logical = FALSE) - 1,
  model_packages = as.character(NA),
  output = c("plots", "data"),
  pred_fun = function(object, newdata, type = pred_type) {
    stats::predict(object =
      object, newdata = newdata, type = type)
  },
  pred_type = "response",
  x_intervals = 100,
  relative_y = "median",
  y_type = NULL,
  median_band_pct = c(0.05, 0.5),
  rug_sample_size = 500,
  min_rug_per_interval = 1,
  ale_xs = NULL,
  n_x1_int = 20,
  n_x2_int = 20,
  n_y_quant = 10,
  compact_plots = FALSE,
  silent = FALSE
)
```
Arguments

data See documentation for ale()
model See documentation for ale()

x1_cols, x2_cols character. Vectors of column names from data for which two-way interaction
ALE data is to be calculated. ALE data will be calculated for each x1 column
interacting with each x2 column. x1_cols can be of any standard datatype (logical, factor, or numeric) but x2_cols can only be numeric. If ixn is TRUE, then
both values must be provided.

y_col See documentation for ale()
...
not used. Inserted to require explicit naming of subsequent arguments.

parallel See documentation for ale()
model_packages See documentation for ale()
output See documentation for ale()
pred_fun, pred_type See documentation for ale()
x_intervals See documentation for ale()
relative_y See documentation for ale()
y_type See documentation for ale()
median_band_pct See documentation for ale()
rug_sample_size, min_rug_per_interval See documentation for ale()
ale-xs See documentation for ale()
n_x1_int, n_x2_int positive scalar integer. Number of intervals for the x1 or x2 axes respectively
for interaction plot. These values are ignored if x1 or x2 are not numeric (i.e, if
they are logical or factors).
n_y_quant positive scalar integer. Number of intervals over which the range of y values is
divided for the colour bands of the interaction plot. See details.

compact_plots See documentation for ale()
silent See documentation for ale()

Value

list of ALE interaction data tibbles and plots. The list has two levels of depth:

- The first level is named by the x1 variables.
- Within each x1 variable list, the second level is named by the x2 variables.
- Within each x1-x2 list element, the data or plot is returned as requested in the output argument.
Examples

```r
set.seed(0)
diamonds_sample <- ggplot2::diamonds[sample(nrow(ggplot2::diamonds), 1000), ]

# Create a GAM model with flexible curves to predict diamond price
# Smooth all numeric variables and include all other variables
gam_diamonds <- mgcv::gam(
  formula = price ~ s(carat) + s(depth) + s(table) + s(x) + s(y) + s(z) +
           cut + color + clarity,
  data = diamonds_sample
)
summary(gam_diamonds)

# ALE two-way interactions
ale_ixn_gam_diamonds <- ale_ixn(
  diamonds_sample, gam_diamonds,
  parallel = 2  # CRAN limit (delete this line on your own computer)
)

# Print interaction plots
ale_ixn_gam_diamonds$plots |> 
  purrr::walk(.x1) {
    # plot all x2 plots in each .x1 element
    patchwork::wrap_plots(.x1) |> 
    print()
  }
```

---

census

<table>
<thead>
<tr>
<th>Census Income</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>census</strong></td>
</tr>
</tbody>
</table>

Description

Census data that indicates, among other details, if the respondent’s income exceeds $50,000 per year. Also known as “Adult” dataset.

Usage

```r
census
```

Format

A tibble with 32,561 rows and 15 columns:

- **higher_income** TRUE if income > $50,000
create_p_funs

**age** continuous


**fnlwgt** continuous. "A proxy for the demographic background of the people: 'People with similar demographic characteristics should have similar weights'" For more details, see https://www.openml.org/search?type=data&id=1590.

**education** Bachelors, Some-college, 11th, HS-grad, Prof-school, Assoc-acdm, Assoc-voc, 9th, 7th-8th, 12th, Masters, 1st-4th, 10th, Doctorate, 5th-6th, Preschool

**education_num** continuous

**marital_status** Married-civ-spouse, Divorced, Never-married, Separated, Widowed, Married-spouse-absent, Married-AF-spouse


**relationship** Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried

**race** White, Asian-Pac-Islander, Amer-Indian-Eskimo, Other, Black

**sex** Female, Male

**capital_gain** continuous

**capital_loss** continuous

**hours_per_week** continuous

**native_country** United-States, Cambodia, England, Puerto-Rico, Canada, Germany, Outlying-US(Guam-USVI-etc), India, Japan, Greece, South, China, Cuba, Iran, Honduras, Philippines, Italy, Poland, Jamaica, Vietnam, Mexico, Portugal, Ireland, France, Dominican-Republic, Laos, Ecuador, Taiwan, Haiti, Columbia, Hungary, Guatemala, Nicaragua, Scotland, Thailand, Yugoslavia, El-Salvador, Trinidad&Tobago, Peru, Hong, Holland-Netherlands

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**Source**


---

**create_p_funs**

Create a p-value functions object that can be used to generate p-values

**Description**

Calculating p-values is not trivial for ALE statistics because ALE is non-parametric and model-agnostic. Because ALE is non-parametric (that is, it does not assume any particular distribution of data), the a1e package generates p-values by calculating ALE for many random variables; this makes the procedure somewhat slow. For this reason, they are not calculated by default; they must be explicitly requested. Because the a1e package is model-agnostic (that is, it works with any kind of R model), the a1e() function cannot always automatically manipulate the model object to create
create_p_funs

the p-values. It can only do so for models that follow the standard R statistical modelling conven-
tions, which includes almost all built-in R algorithms (like `stats::lm()` and `stats::glm()` and
many widely used statistics packages (like mgcv and survival), but which excludes most machine
learning algorithms (like tidymodels and caret). For non-standard algorithms, the user needs to
do a little work to help the ale function correctly manipulate its model object:

- The full model call must be passed as a character string in the argument 'random_model_call_string',
  with two slight modifications as follows.
- In the formula that specifies the model, you must add a variable named 'random_variable'.
  This corresponds to the random variables that create_p_funs() will use to estimate p-values.
- The dataset on which the model is trained must be named 'rand_data'. This corresponds to
  the modified datasets that will be used to train the random variables.

See the example below for how this is implemented.

Usage

create_p_funs(
  data,
  model,
  ...,
  parallel = parallel::detectCores(logical = FALSE) - 1,
  model_packages = as.character(NA),
  random_model_call_string = NULL,
  random_model_call_string_vars = character(),
  y_col = NULL,
  pred_fun = function(object, newdata, type = pred_type) {
    stats::predict(object =
      object, newdata = newdata, type = type)
  },
  pred_type = "response",
  rand_it = 1000,
  silent = FALSE,
  .testing_mode = FALSE
)

Arguments

data See documentation for ale()
model See documentation for ale()
... not used. Inserted to require explicit naming of subsequent arguments.
parallel See documentation for ale()
model_packages See documentation for ale()
random_model_call_string

character string. If NULL, create_p_funs() tries to automatically detect and
construct the call for p-values. If it cannot, the function will fail early. In that
case, a character string of the full call for the model must be provided that in-
cludes the random variable. See details.
create_p_funs

random_model_call_string_vars
See documentation for model_call_string_vars in model_bootstrap(); the operation is very similar.

y_col
See documentation for ale()
pred_fun, pred_type
See documentation for ale().
rand_it
non-negative integer length 1. Number of times that the model should be re-trained with a new random variable. The default of 1000 should give reasonably stable p-values. It can be reduced as low as 100 for faster test runs.
silent
See documentation for ale()
.testing_mode logical. Internal use only.

Value

The return value is a list of class c('p_funs', 'ale', 'list') with an ale_version attribute whose value is the version of the ale package used to create the object. See examples for an illustration of how to inspect this list. Its elements are:

- value_to_p: a list of functions named for each each available ALE statistic. Each function signature is function(x) where x is a numeric. The function returns the p-value (minimum 0; maximum 1) for the respective statistic based on the random variable analysis. For an input x that returns p, its interpretation is that p% of random variables obtained the same or higher statistic value. For example, to get the p-value of a NALED of 4.2, enter p_funs$value_to_p(4.2). A return value of 0.03 means that only 3% of random variables obtained a NALED greater than or equal to 4.2.

- p_to_random_value: a list of functions named value_to_p. These are the inverse functions of value_to_p. The signature is function(p) where p is a numeric from 0 to 1. The function returns the numeric value of the random variable statistic that would yield the provided p-value. For an input p that returns x, its interpretation is that p% of random variables obtained the same or higher statistic value. For example, to get the random variable ALED for the 0.05 p-value, enter p_funs$p_to_random_value(0.05). A return value of 102 means that only 5% of random variables obtained an ALED greater than or equal to 102.

- rand_stats: a tibble whose rows are each of the rand_it iterations of the random variable analysis and whose columns are the ALE statistics obtained for each random variable.

- residuals: the actual y_col values from data minus the predicted values from the model (without random variables) on the data. residual_distribution: the closest estimated distribution for the residuals as determined by univariateML::rml(). This is the distribution used to generate all the random variables.

Approach to calculating p-values

The ale package takes a literal frequentist approach to the calculation of p-values. That is, it literally retrains the model 1000 times, each time modifying it by adding a distinct random variable to the model. (The number of iterations is customizable with the rand_it argument.) The ALEs and ALE statistics are calculated for each random variable. The percentiles of the distribution of these random-variable ALEs are then used to determine p-values for non-random variables. Thus, p-values are interpreted as the frequency of random variable ALE statistics that exceed the value of ALE statistic of the actual variable in question. The specific steps are as follows:
create_p_funs

- The residuals of the original model trained on the training data are calculated (residuals are the actual y target value minus the predicted values).
- The closest distribution of the residuals is detected with `univariateML::model_select()`.
- 1000 new models are trained by generating a random variable each time with `univariateML::rml()` and then training a new model with that random variable added.
- The ALEs and ALE statistics are calculated for each random variable.
- For each ALE statistic, the empirical cumulative distribution function (from `stats::ecdf()`) is used to create a function to determine p-values according to the distribution of the random variables’ ALE statistics.

References


Examples

```r
# Sample 1000 rows from the ggplot2::diamonds dataset (for a simple example)
set.seed(0)
diamonds_sample <- ggplot2::diamonds[sample(nrow(ggplot2::diamonds), 1000), ]

# Create a GAM model with flexible curves to predict diamond price
# Smooth all numeric variables and include all other variables
gam_diamonds <- mgcv::gam(
  price ~ s(carat) + s(depth) + s(table) + s(x) + s(y) + s(z) +
  cut + color + clarity,
  data = diamonds_sample
)
summary(gam_diamonds)

# Create p-value functions
pf_diamonds <- create_p_funs(
  diamonds_sample,
  gam_diamonds,
  # only 100 iterations for a quick demo; but usually should remain at 1000
  rand_it = 100,
)

# Examine the structure of the returned object
str(pf_diamonds)
# In RStudio: View(pf_diamonds)

# Calculate ALEs with p-values
ale_gam_diamonds <- ale(
  diamonds_sample,
  gam_diamonds,
  p_values = pf_diamonds
)

# Plot the ALE data. The horizontal bands in the plots use the p-values.
```
ale_gam_diamonds$plots |> 
  patchwork::wrap_plots()

# For non-standard models that give errors with the default settings, 
# you can use 'random_model_call_string' to specify a model for the estimation 
# of p-values from random variables as in this example. 
# See details above for an explanation.
pf_diamonds <- create_p_funs(
  diamonds_sample,
  gam_diamonds,
  random_model_call_string = 'mgcv::gam(
    price ~ s(carat) + s(depth) + s(table) + s(x) + s(y) + s(z) +
    cut + color + clarity + random_variable,
    data = rand_data
  )',
  # only 100 iterations for a quick demo; but usually should remain at 1000
  rand_it = 100,
)

model_bootstrap

model_bootstrap <- function(data, model, 
  ...,
  model_call_string = NULL,
  model_call_string_vars = character(),
  parallel = parallel::detectCores(logical = FALSE) - 1,
  model_packages = as.character(NA),
  boot_it = 100,
  seed = 0,
  boot_alpha = 0.05,
  boot_centre = "mean",
  output = c("ale", "model_stats", "model_coefs"),
  ale_options = list(),
  tidy_options = list(),
  glance_options = list(),
)
compact_plots = FALSE,
silent = FALSE
)

Arguments

data dataframe. Dataset that will be bootstrapped.
model See documentation for ale()
... not used. Inserted to require explicit naming of subsequent arguments.
model_call_string character string. If NULL, model_bootstrap() tries to automatically detect and construct the call for bootstrapped datasets. If it cannot, the function will fail early. In that case, a character string of the full call for the model must be provided that includes boot_data as the data argument for the call. See examples.
model_call_string_vars character. Character vector of names of variables included in model_call_string that are not columns in data. If any such variables exist, they must be specified here or else parallel processing will produce an error. If parallelization is disabled with parallel = 0, then this is not a concern.
parallel See documentation for ale()
model_packages See documentation for ale()
boot_it integer from 0 to Inf. Number of bootstrap iterations. If boot_it = 0, then the model is run as normal once on the full data with no bootstrapping.
seed integer. Random seed. Supply this between runs to assure identical bootstrap samples are generated each time on the same data.
boot_alpha numeric. The confidence level for the bootstrap confidence intervals is 1 - boot_alpha. For example, the default 0.05 will give a 95% confidence interval, that is, from the 2.5% to the 97.5% percentile.
boot_centre See See documentation for ale()
output character vector. Which types of bootstraps to calculate and return:
• 'ale': Calculate and return bootstrapped ALE data and plot.
• 'model_stats': Calculate and return bootstrapped overall model statistics.
• 'model_coefs': Calculate and return bootstrapped model coefficients.
• 'boot_data': Return full data for all bootstrap iterations. This data will always be calculated because it is needed for the bootstrap averages. By default, it is not returned except if included in this output argument.
ale_options, tidy_options, glance_options list of named arguments. Arguments to pass to the ale(), broom::tidy(), or broom::glance() functions, respectively, beyond (or overriding) the defaults. In particular, to obtain p-values for ALE statistics, see the details.
compact_plots See documentation for ale()
silent See documentation for ale()
Details

No modelling results, with or without ALE, should be considered reliable without being bootstrapped. For large datasets, normally the model provided to `ale()` is the final deployment model that has been validated and evaluated on training and testing on subsets; that is why `ale()` is calculated on the full dataset. However, when a dataset is too small to be subdivided into training and test sets for a standard machine learning process, then the entire model should be bootstrapped. That is, multiple models should be trained, one on each bootstrap sample. The reliable results are the average results of all the bootstrap models, however many there are. For details, see the vignette on small datasets or the details and examples below.

`model_bootstrap()` automatically carries out full-model bootstrapping suitable for small datasets. Specifically, it:

- Creates multiple bootstrap samples (default 100; the user can specify any number);
- Creates a model on each bootstrap sample;
- Calculates model overall statistics, variable coefficients, and ALE values for each model on each bootstrap sample;
- Calculates the mean, median, and lower and upper confidence intervals for each of those values across all bootstrap samples.

P-values The `broom::tidy()` summary statistics will provide p-values as normal, but the situation is somewhat complicated with p-values for ALE statistics. The challenge is that the procedure for obtaining their p-values is very slow: it involves retraining the model 1000 times. Thus, it is not efficient to calculate p-values on every execution of model_bootstrap(). Although the `ale()` function provides an 'auto' option for creating p-values, that option is disabled in model_bootstrap() because it would be far too slow; it would involve retraining the model 1000 times the number of bootstrap iterations. Rather, you must first create a p-values function object using the procedure described in `help(create_p_funs)`. If the name of your p-values object is `p_funs`, you can then request p-values each time you run `model_bootstrap()` by passing it the argument `ale_options = list(p_values = p_funs)`.

Value

list with tibbles of the following elements (depending on values requested in the output argument):

- model_stats: bootstrapped results from `broom::glance()`
- model_coefs: bootstrapped results from `broom::tidy()`
- ale: bootstrapped ALE results
  - data: ALE data (see `ale()` for details about the format)
  - stats: ALE statistics. The same data is duplicated with different views that might be variously useful. The column
    * by_term: statistic, estimate, conf.low, median, mean, conf.high. ("term" means variable name.) The column names are compatible with the `broom` package. The confidence intervals are based on the `ale()` function defaults; they can be changed with the `ale_options` argument. The estimate is the median or the mean, depending on the `boot_centre` argument.
    * by_statistic: term, estimate, conf.low, median, mean, conf.high.
* estimate: term, then one column per statistic. Provided with the default estimate. This
  view does not present confidence intervals.
- plots: ALE plots (see `ale()` for details about the format)
  - `boot_data`: full bootstrap data (not returned by default)
  - `other values`: the `boot_it`, `seed`, `boot_alpha`, and `boot_centre` arguments that were origi-
    nally passed are returned for reference.

References


Examples

```r
# attitude dataset
attitude

## ALE for general additive models (GAM)
## GAM is tweaked to work on the small dataset.
gam_attitude <- mgcv::gam(rating ~ complaints + privileges + s(learning) +
                           raises + s(critical) + advance,
                           data = attitude)
summary(gam_attitude)

# Full model bootstrapping
# Only 4 bootstrap iterations for a rapid example; default is 100
# Increase value of boot_it for more realistic results
mb_gam <- model_bootstrap(
  attitude,
  gam_attitude,
  boot_it = 4,
  parallel = 2 # CRAN limit (delete this line on your own computer)
)

# If the model is not standard, supply `model_call_string` with
# 'data = boot_data' in the string (not as a direct argument to [model_bootstrap()])
m_gam <- model_bootstrap(
  attitude,
  gam_attitude,
  model_call_string = 'mgcv::gam(
                           rating ~ complaints + privileges + s(learning) +
                           raises + s(critical) + advance,
                           data = boot_data
                      )',
  boot_it = 4,
  parallel = 2 # CRAN limit (delete this line on your own computer)
)

# Model statistics and coefficients
```


```r
mb_gam$model_stats
mb_gam$model_coefs

# Plot ALE
mb_gam$ale$plots |> 
  patchwork::wrap_plots()
```

---

**var_cars**

*Multi-variable transformation of the mtcars dataset.*

---

**Description**

This is a transformation of the *mtcars* dataset from R to produce a small dataset with each of the fundamental datatypes: logical, factor, ordered, integer, and double. Most of the transformations are obvious, but two are noteworthy:

- For the unordered factor, the country of the car manufacturer is obtained based on the row names of *mtcars*. This *var_cars* version does not have row names.
- For the ordered factor, gears 3, 4, and 5 are encoded as 'three', 'four', and 'five', respectively. The text labels make it explicit that the variable is ordinal, yet the number names make the order crystal clear.

Here is the original description of the *mtcars* dataset:

The data was extracted from the 1974 *Motor Trend* US magazine, and comprises fuel consumption and 10 aspects of automobile design and performance for 32 automobiles (1973–74 models).

**Usage**

`var_cars`

**Format**

A tibble with 32 observations on 12 variables.

- **mpg** double: Miles/(US) gallon
- **cyl** integer: Number of cylinders
- **disp** double: Displacement (cu.in.)
- **hp** double: Gross horsepower
- **drat** double: Rear axle ratio
- **wt** double: Weight (1000 lbs)
- **qsec** double: 1/4 mile time
vs  logical: Engine (0 = V-shaped, 1 = straight)
am  logical: Transmission (0 = automatic, 1 = manual)
gear ordered: Number of forward gears
carb integer: Number of carburetors
country factor: Country of car manufacturer

Note
Henderson and Velleman (1981) comment in a footnote to Table 1: 'Hocking (original transcriber)'s noncrucial coding of the Mazda’s rotary engine as a straight six-cylinder engine and the Porsche’s flat engine as a V engine, as well as the inclusion of the diesel Mercedes 240D, have been retained to enable direct comparisons to be made with previous analyses.’

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