Package 'counterfactuals'

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Type Package

```
Title Counterfactual Explanations
Version 0.1.4
Maintainer Susanne Dandl <dandls.datascience@gmail.com>
Description Modular and unified R6-based interface for counterfactual explanation methods.
     The following methods are currently implemented: Burgh-
     mans et al. (2022) <doi:10.48550/arXiv.2104.07411>,
     Dandl et al. (2020) <doi:10.1007/978-3-030-58112-
     1 31> and Wexler et al. (2019) <doi:10.1109/TVCG.2019.2934619>.
     Optional extensions allow these methods to be applied to a variety of models and use cases.
     Once generated, the counterfactuals can be analyzed and visualized by provided functionalities.
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BugReports https://github.com/dandls/counterfactuals/issues
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```

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Counterfactual Method Base class for Counterfactual Explanation Methods

Description

Abstract base class for counterfactual explanation methods.

Inheritance

 $Child\ classes:\ Counterfactual Method Classif,\ Counterfactual Method Regr$

Methods

Public methods:

- CounterfactualMethod\$new()
- CounterfactualMethod\$print()
- CounterfactualMethod\$clone()

Method new(): Creates a new CounterfactualMethod object.

```
Usage:
CounterfactualMethod$new(
  predictor,
  lower = NULL,
  upper = NULL,
  distance_function = NULL)
```

Arguments:

predictor (Predictor)

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

lower (numeric() | NULL)

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

upper (numeric() | NULL)

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

distance_function (character(1) | function())

Either the name of an already implemented distance function (currently 'gower' or 'gower_c') or a function having three arguments: x, y, and data. The function should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method print(): Prints a CounterfactualMethod object. The method calls a (private) \$print_parameters() method which should be implemented by the leaf classes.

Usage:

CounterfactualMethod\$print()

Method clone(): The objects of this class are cloneable with this method.

Usage:

CounterfactualMethod\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

 ${\tt Counterfactual Method Classif}$

Base class for Counterfactual Explanation Methods for Classification Tasks

Description

Abstract base class for counterfactual explanation methods for classification tasks.

CounterfactualMethodClassif can only be initialized for classification tasks. Child classes inherit the (public) \$find_counterfactuals() method, which calls a (private) \$run() method. This \$run() method should be implemented by the child classes and return the counterfactuals as a data.table (preferably) or a data.frame.

Inheritance

Child classes: MOCClassif, WhatIfClassif, NICEClassif

Super class

counterfactuals::CounterfactualMethod -> CounterfactualMethodClassif

Methods

Public methods:

- CounterfactualMethodClassif\$new()
- CounterfactualMethodClassif\$find_counterfactuals()
- CounterfactualMethodClassif\$clone()

Method new(): Creates a new CounterfactualMethodClassif object.

```
Usage:
```

```
CounterfactualMethodClassif$new(
  predictor,
  lower = NULL,
  upper = NULL,
  distance_function = NULL
)
Arguments:
```

predictor (Predictor)

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

```
lower (numeric() | NULL)
```

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric() | NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
distance_function (function() | NULL)
```

A distance function that may be used by the leaf classes. If specified, the function must have three arguments: x, y, and data and return a double matrix with nrow(x) rows and nrow(y) columns.

Method find_counterfactuals(): Runs the counterfactual method and returns the counterfactuals. It searches for counterfactuals that have a predicted probability in the interval desired_prob for the desired_class.

Usage:

```
CounterfactualMethodClassif$find_counterfactuals(
  x_interest,
  desired_class = NULL,
  desired_prob = c(0.5, 1)
)
Arguments:
```

```
x_interest (data.table(1) | data.frame(1))
```

A single row with the observation of interest.

desired_class (character(1) | NULL)

The desired class. If NULL (default) then predictor\$class is taken.

desired_prob (numeric(1) | numeric(2))

The desired predicted probability of the desired_class. It can be a numeric scalar or a vector with two numeric values that specify a probability interval. For hard classification tasks this can be set to 0 or 1, respectively. A scalar is internally converted to an interval.

Returns: A Counterfactuals object containing the results.

Method clone(): The objects of this class are cloneable with this method.

Usage:

CounterfactualMethodClassif\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

CounterfactualMethodRegr

Base class for Counterfactual Explanation Methods for Regression Tasks

Description

Abstract base class for counterfactual explanation methods for regression tasks.

CounterfactualMethodRegr can only be initialized for regression tasks. Child classes inherit the (public) \$find_counterfactuals() method, which calls a (private) \$run() method. This \$run() method should be implemented by the child classes and return the counterfactuals as a data.table (preferably) or a data.frame.

Inheritance

Child classes: MOCRegr, WhatIfRegr, NICERegr

Super class

counterfactuals::CounterfactualMethod -> CounterfactualMethodRegr

Methods

Public methods:

- CounterfactualMethodRegr\$new()
- CounterfactualMethodRegr\$find_counterfactuals()
- CounterfactualMethodRegr\$clone()

Method new(): Creates a new CounterfactualMethodRegr object.

```
Usage:
```

```
CounterfactualMethodRegr$new(
  predictor,
  lower = NULL,
  upper = NULL,
  distance_function = NULL
)
Arguments:
```

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

```
lower (numeric() | NULL)
```

predictor (Predictor)

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric() | NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
distance_function (function() | NULL)
```

A distance function that may be used by the leaf classes. If specified, the function must have three arguments: x, y, and data and return a double matrix with nrow(x) rows and nrow(y) columns.

Method find_counterfactuals(): Runs the counterfactual method and returns the counterfactuals. It searches for counterfactuals that have a predicted outcome in the interval desired_outcome.

Usage:

CounterfactualMethodRegr\$find_counterfactuals(x_interest, desired_outcome)

Arguments:

```
x_interest (data.table(1) | data.frame(1))
A single row with the observation of interest.
```

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desired_outcome (numeric(1) | numeric(2))

The desired predicted outcome. It can be a numeric scal

The desired predicted outcome. It can be a numeric scalar or a vector with two numeric values that specify an outcome interval. A scalar is internally converted to an interval.

Returns: A Counterfactuals object containing the results.

Method clone(): The objects of this class are cloneable with this method.

```
Usage:
```

```
CounterfactualMethodRegr$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Counterfactuals

Counterfactuals Class

Description

A Counterfactuals object should be created by the \$find_counterfactuals method of CounterfactualMethodRegr or CounterfactualMethodClassif. It contains the counterfactuals and has several methods for their evaluation and visualization.

Active bindings

```
desired (list(1)|list(2))
```

A list with the desired properties of the counterfactuals. For regression tasks it has one element desired_outcome (CounterfactualMethodRegr) and for classification tasks two elements desired_class and desired_prob (CounterfactualMethodClassif).

```
data (data.table)
```

The counterfactuals for x_interest.

```
x_interest (data.table(1))
```

A single row with the observation of interest.

```
distance_function (function())
```

The distance function used in the second and fourth evaluation measure. The function must have three arguments: x, y, and data and return a numeric matrix. If set to NULL (default), then Gower distance (Gower 1971) is used.

```
method (character)
```

A single row with the observation of interest.

Methods

Public methods:

- Counterfactuals\$new()
- Counterfactuals\$evaluate()
- Counterfactuals\$evaluate_set()
- Counterfactuals\$predict()
- Counterfactuals\$subset_to_valid()
- Counterfactuals\$revert_subset_to_valid()
- Counterfactuals\$plot_parallel()
- Counterfactuals\$plot_freq_of_feature_changes()
- Counterfactuals\$get_freq_of_feature_changes()
- Counterfactuals\$plot_surface()
- Counterfactuals\$print()
- Counterfactuals\$clone()

Method new(): Creates a new Counterfactuals object. This method should only be called by the \$find_counterfactuals methods of CounterfactualMethodRegr and CounterfactualMethodClassif.

```
Usage:
Counterfactuals$new(
  cfactuals,
  predictor,
  x_interest,
  param_set,
  desired,
  method = NULL
Arguments:
cfactuals (data.table)
   The counterfactuals. Must have the same column names and types as predictor$data$X.
predictor (Predictor)
   The object (created with iml::Predictor$new()) holding the machine learning model and
   the data.
x_interest (data.table(1) | data.frame(1))
   A single row with the observation of interest.
param_set (ParamSet)
   A ParamSet based on the features of predictor$data$X.
desired (list(1)|list(2))
   A list with the desired properties of the counterfactuals. It should have one element
   desired_outcome for regression tasks (CounterfactualMethodRegr) and two elements desired_class
   and desired_prob for classification tasks (CounterfactualMethodClassif).
method (character)
   Name of the method with which counterfactuals were generated. Default is NULL which
   means that no name is provided.
```

Method evaluate(): Evaluates the counterfactuals. It returns the counterfactuals together with the evaluation measures.

```
Usage:
Counterfactuals$evaluate(
  measures = c("dist_x_interest", "dist_target", "no_changed", "dist_train",
    "minimality"),
  show_diff = FALSE,
  k = 1L
  weights = NULL
)
Arguments:
```

The name of one or more evaluation measures. The following measures are available:

- dist_x_interest: The distance of a counterfactual to x_interest measured by Gower's dissimilarity measure (Gower 1971).
- dist_target: The absolute distance of the prediction for a counterfactual to the interval desired_outcome (regression tasks) or desired_prob (classification tasks).
- no_changed: The number of feature changes w.r.t. x_interest.

measures (character)

• dist_train: The (weighted) distance to the k nearest training data points measured by Gower's dissimilarity measure (Gower 1971).

• minimality: The number of changed features that each could be set to the value of x_interest while keeping the desired prediction value.

```
show_diff (logical(1))
```

Should the counterfactuals be displayed as their differences to x_interest? Default is FALSE. If set to TRUE, positive values for numeric features indicate an increase compared to the feature value in x_interest, negative values indicate a decrease. For factors, the feature value is displayed if it differs from x_interest; NA means "no difference" in both cases.

```
k (integerish(1))
```

How many nearest training points should be considered for computing the dist_train measure? Default is 1L.

```
weights (numeric(k) | NULL)
```

How should the k nearest training points be weighted when computing the dist_train measure? If NULL (default) then all k points are weighted equally. If a numeric vector of length k is given, the i-th element specifies the weight of the i-th closest data point.

Method evaluate_set(): Evaluates a set of counterfactuals. It returns the evaluation measures.

Usage:

```
Counterfactuals$evaluate_set(
  measures = c("diversity", "no_nondom", "frac_nondom", "hypervolume"),
  nadir = NULL
)
```

Arguments:

measures (character)

The name of one or more evaluation measures. The following measures are available:

- diversity: Diversity of returned counterfactuals in the feature space
- no_nondom: Number of counterfactuals that are not dominated by other counterfactuals.
- frac_nondom: Fraction of counterfactuals that are not dominated by other counterfactuals
- hypervolume: Hypervolume of the induced Pareto front

```
nadir (numeric)
```

Max objective values to calculate dominated hypervolume. Only considered, if hypervolume is one of the measures. May be a scalar, in which case it is used for all four objectives, or a vector of length 4. Default is NULL, meaning the nadir point by Dandl et al. (2020) is used: (min distance between prediction of x_interest to desired_prob/_outcome, 1, number of features, 1).

Method predict(): Returns the predictions for the counterfactuals.

Usage:

```
Counterfactuals$predict()
```

Method subset_to_valid(): Subset data to those meeting the desired prediction, Process could be reverted using revert_subset_to_valid().

Usage:

```
Counterfactuals$subset_to_valid()
```

Method revert_subset_to_valid(): Subset data to those meeting the desired prediction, Process could be reverted using revert_subset_to_valid().

Usage:

```
Counterfactuals$revert_subset_to_valid()
```

Method plot_parallel(): Plots a parallel plot that connects the (scaled) feature values of each counterfactual and highlights x_interest in blue.

```
Usage:
```

```
Counterfactuals$plot_parallel(
  feature_names = NULL,
  row_ids = NULL,
  digits_min_max = 2L
)
```

Arguments:

feature_names (character | NULL)

The names of the (numeric) features to display. If NULL (default) all features are displayed. row_ids (integerish|NULL)

The row ids of the counterfactuals to display. If NULL (default) all counterfactuals are displayed.

digits_min_max Maximum number of digits for the minimum and maximum features values. Default is 2L.

Method plot_freq_of_feature_changes(): Plots a bar chart with the frequency of feature changes across all counterfactuals.

```
Usage:
```

```
Counterfactuals$plot_freq_of_feature_changes(subset_zero = FALSE)
```

Arguments:

```
subset_zero (logical(1))
```

Should unchanged features be excluded from the plot? Default is FALSE.

Method get_freq_of_feature_changes(): Returns the frequency of feature changes across all counterfactuals.

Usage:

```
Counterfactuals$get_freq_of_feature_changes(subset_zero = FALSE)
```

Arguments:

```
subset_zero (logical(1))
```

Should unchanged features be excluded? Default is FALSE.

Returns: A (named) numeric vector with the frequency of feature changes.

Method plot_surface(): Creates a surface plot for two features. x_interest is represented as a white dot and all counterfactuals that differ from x_interest **only** in the two selected features are represented as black dots. The tick marks next to the axes show the marginal distribution of the observed data (predictor\$data\$X).

The exact plot type depends on the selected feature types and number of features:

dist_to_interval 11

```
• 2 numeric features: surface plot
```

- 2 non-numeric features: heatmap
- 1 numeric or non-numeric feature: line graph

Usage:

```
Counterfactuals$plot_surface(feature_names, grid_size = 250L)
```

Arguments:

```
feature_names (character(2))
```

The names of the features to plot.

```
grid_size (integerish(1))
```

The grid size of the plot. It is ignored in case of two non-numeric features. Default is 250L.

Method print(): Prints the Counterfactuals object.

Usage:

Counterfactuals\$print()

Method clone(): The objects of this class are cloneable with this method.

Usage:

Counterfactuals\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

References

Gower, J. C. (1971), "A general coefficient of similarity and some of its properties". Biometrics, 27, 623–637.

dist_to_interval

Computes the (absolute, pairwise) distance between the vector elements and an interval

Description

Computes the (absolute, pairwise) distance between the vector elements and an interval

Usage

```
dist_to_interval(x, interval)
```

Arguments

An interval.

12 make_param_set

eval	(11	STA	nc	e

Evaluates a distance function and checks for correct output format

Description

This function serves as an evaluation wrapper for some distance function. It checks that the output of distance_function is a numeric matrix with nrow(x) rows and nrow(y) columns as expected.

Usage

```
eval_distance(distance_function, x, y, data = NULL)
```

Arguments

distance_function

(function())

A distance function to evaluate.

x (data.frame() | numeric())

A matrix or a data frame containing variables that should be used in the compu-

tation of the distance.

y (data.frame() | numeric())

A matrix or a data frame containing variables that should be used in the compu-

tation of the distance.

data (data.frame()|NULL)

A data frame or data table containing the entire data set. This can be used to

compute statistics used in the computation of the distance, e.g., standard devia-

tion or range.

make_param_set

Creates a ParamSet for the features of a data.table.

Description

Creates a ParamSet for the columns of dt. Depending on the class of a column, a different Domain is created:

```
• double: p_dbl()
```

• integer: p_int()

• character: p_fct() (with unique values as levels)

• factor: p_fct() (with factor levels as levels)

Usage

```
make_param_set(dt, lower = NULL, upper = NULL)
```

Arguments

dt (data.table())

The data for the ParamSet.

lower (numeric() | NULL)

Vector of minimum values for numeric features. If not NULL, it should be named with the corresponding feature names. If NULL (default) lower is taken

for each numeric feature as its minimum value in dt.

upper (numeric() | NULL)

Vector of maximum values for numeric features. If not NULL, it should be named with the corresponding feature names. If NULL (default) upper is taken

for each numeric feature as its maximum value in dt.

Value

A ParamSet for the features of dt.

MOCClassif	MOC (Multi-Objective Counterfactual Explanations) for Classification Tasks
------------	--

Description

MOC (Dandl et. al 2020) solves a multi-objective optimization problem to find counterfactuals. The four objectives to minimize are:

- dist_target: Distance to desired_prob (classification tasks) or desired_prob (regression tasks).
- 2. dist_x_interest: Dissimilarity to x_interest measured by Gower's dissimilarity measure (Gower 1971).
- 3. no_changed: Number of feature changes.
- 4. dist_train: (Weighted) sum of dissimilarities to the k nearest data points in predictor\$data\$X.

For optimization, it uses the NSGA II algorithm (Deb et. al 2002) with mixed integer evolutionary strategies (Li et al. 2013) and some tailored adjustments for the counterfactual search (Dandl et al. 2020). Default values for the hyperparameters are based on Dandl et al. 2020.

Details

Several population initialization strategies are available:

- 1. random: Feature values of new individuals are sampled from the feature value ranges in predictor\$data\$X. Some features values are randomly reset to their initial value in x_interest.
- 2. sd: Like random, except that the sample ranges of numerical features are limited to one standard deviation from their initial value in x_interest.

3. icecurve: As in random, feature values are sampled from the feature value ranges in predictor\$data\$X. Then, however, features are reset with probabilities relative to their importance: the higher the importance of a feature, the higher the probability that its values differ from its value in x_interest. The feature importance is measured using ICE curves (Goldstein et al. 2015).

4. traindata: Contrary to the other strategies, feature values are drawn from (non-dominated) data points in predictor\$data\$X; if not enough non-dominated data points are available, remaining individuals are initialized by random sampling. Subsequently, some features values are randomly reset to their initial value in x_interest (as for random).

If use_conditional_mutator is set to TRUE, a conditional mutator samples feature values from the conditional distribution given the other feature values with the help of transformation trees (Hothorn and Zeileis 2017). For details see Dandl et al. 2020.

Super classes

```
counterfactuals::CounterfactualMethod -> counterfactuals::CounterfactualMethodClassif
-> MOCClassif
```

Active bindings

```
optimizer (OptimInstanceMultiCrit)
The object used for optimization.
```

Methods

Public methods:

- MOCClassif\$new()
- MOCClassif\$plot_statistics()
- MOCClassif\$get_dominated_hv()
- MOCClassif\$plot_search()
- MOCClassif\$clone()

Method new(): Create a new MOCClassif object.

```
Usage:
MOCClassif$new(
   predictor,
   epsilon = NULL,
   fixed_features = NULL,
   max_changed = NULL,
   mu = 20L,
   termination_crit = "gens",
   n_generations = 175L,
   p_rec = 0.71,
   p_rec_gen = 0.62,
   p_mut = 0.73,
   p_mut_gen = 0.5,
   p_mut_use_orig = 0.4,
   k = 1L,
```

```
weights = NULL,
  lower = NULL,
  upper = NULL,
  init_strategy = "icecurve",
  use_conditional_mutator = FALSE,
  quiet = FALSE,
  distance_function = "gower"
Arguments:
predictor (Predictor)
    The object (created with iml::Predictor$new()) holding the machine learning model and
    the data.
epsilon (numeric(1) | NULL)
    If not NULL, candidates whose prediction for the desired_class is farther away from the
    interval desired_prob than epsilon are penalized. NULL (default) means no penalization.
fixed_features (character() | NULL)
    Names of features that are not allowed to be changed. NULL (default) allows all features to
    be changed.
max_changed (integerish(1) | NULL)
    Maximum number of feature changes. NULL (default) allows any number of changes.
mu (integerish(1))
    The population size. Default is 20L.
termination_crit (character(1)|NULL)
    Termination criterion, currently, two criterions are implemented: "gens" (default), which
    stops after n_generations generations, and "genstag", which stops after the hypervolume
    did not improve for n_generations generations (the total number of generations is limited
    to 500).
n_generations (integerish(1))
    The number of generations. Default is 175L.
p_rec (numeric(1))
    Probability with which an individual is selected for recombination. Default is 0.71.
p_rec_gen (numeric(1))
    Probability with which a feature/gene is selected for recombination. Default is \emptyset.62.
p_mut (numeric(1))
    Probability with which an individual is selected for mutation. Default is 0.73.
p_mut_gen (numeric(1))
    Probability with which a feature/gene is selected for mutation. Default is 0.5.
p_mut_use_orig (numeric(1))
    Probability with which a feature/gene is reset to its original value in x_interest after
    mutation. Default is 0.4.
k (integerish(1))
    The number of data points to use for the forth objective. Default is 1L.
weights (numeric(1) | numeric(k) | NULL)
    The weights used to compute the weighted sum of dissimilarities for the forth objective. It
    is either a single value or a vector of length k. If it has length k, the i-th element specifies
    the weight of the i-th closest data point. The values should sum up to 1. NULL (default)
```

means all data points are weighted equally.

```
lower (numeric() | NULL)
```

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric() | NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
init_strategy (character(1))
```

The population initialization strategy. Can be icecurve (default), random, sd or traindata. For more information, see the Details section.

```
use_conditional_mutator (logical(1))
```

Should a conditional mutator be used? The conditional mutator generates plausible feature values based on the values of the other feature. Default is FALSE.

```
quiet (logical(1))
```

Should information about the optimization status be hidden? Default is FALSE.

```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function to be used in the second and fourth objective. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method plot_statistics(): Plots the evolution of the mean and minimum objective values together with the dominated hypervolume over the generations. All values for a generation are computed based on all non-dominated individuals that emerged until that generation.

```
Usage:
```

```
MOCClassif$plot_statistics(centered_obj = TRUE)
```

Arguments:

```
centered_obj (logical(1))
```

Should the objective values be centered? If set to FALSE, each objective value is visualized in a separate plot, since they (usually) have different scales. If set to TRUE (default), they are visualized in a single plot.

Method get_dominated_hv(): Calculates the dominated hypervolume of each generation.

Usage:

```
MOCClassif$get_dominated_hv()
```

Returns: A data. table with the dominated hypervolume of each generation.

Method plot_search(): Visualizes two selected objective values of all emerged individuals in a scatter plot.

```
Usage:
```

```
MOCClassif$plot_search(objectives = c("dist_target", "dist_x_interest"))
```

Arguments:

```
objectives (character(2))
```

The two objectives to be shown in the plot. Possible values are "dist_target", "dist_x_interest, "no changed", and "dist_train".

Method clone(): The objects of this class are cloneable with this method.

```
Usage:
MOCClassif$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

References

Dandl, S., Molnar, C., Binder, M., and Bischl, B. (2020). "Multi-Objective Counterfactual Explanations". In: Parallel Problem Solving from Nature – PPSN XVI, edited by Thomas Bäck, Mike Preuss, André Deutz, Hao Wang, Carola Doerr, Michael Emmerich, and Heike Trautmann, 448–469, Cham, Springer International Publishing, doi:10.1007/9783030581121_31.

Deb, K., Pratap, A., Agarwal, S., & Meyarivan, T. A. M. T. (2002). "A fast and elitist multiobjective genetic algorithm: NSGA-II". IEEE transactions on evolutionary computation, 6(2), 182-197.

Goldstein, A., Kapelner, A., Bleich, J., and Pitkin, E. (2015). "Peeking Inside the Black Box: Visualizing Statistical Learning with Plots of Individual Conditional Expectation". Journal of Computational and Graphical Statistics 24 (1): 44–65. doi:10.1080/10618600.2014.907095.

Gower, J. C. (1971). A general coefficient of similarity and some of its properties. Biometrics, 27, 623–637.

Hothorn, T., Zeileis, A. (2017), "Transformation Forests". Technical Report, arXiv 1701.02110.

Li, Rui, L., Emmerich, M. T. M., Eggermont, J. Bäck, T., Schütz, M., Dijkstra, J., Reiber, J. H. C. (2013). "Mixed Integer Evolution Strategies for Parameter Optimization." Evolutionary Computation 21 (1): 29–64. doi:10.1162/EVCO_a_00059.

Examples

```
if (require("randomForest")) {
    # Train a model
    rf = randomForest(Species ~ ., data = iris)
    # Create a predictor object
    predictor = iml::Predictor$new(rf, type = "prob")
    # Find counterfactuals for x_interest
    moc_classif = MOCClassif$new(predictor, n_generations = 15L, quiet = TRUE)

    cfactuals = moc_classif$find_counterfactuals(
        x_interest = iris[150L, ], desired_class = "versicolor", desired_prob = c(0.5, 1)
    )
    # Print the counterfactuals
    cfactuals$data
    # Plot evolution of hypervolume and mean and minimum objective values
    moc_classif$plot_statistics()
}
```

MOCRegr	MOC (Multi-Objective Counterfactual Explanations) for Regression Tasks
	Tasks

Description

MOC (Dandl et. al 2020) solves a multi-objective optimization problem to find counterfactuals. The four objectives to minimize are:

- 1. dist_target: Distance to desired_prob (classification tasks) or desired_prob (regression tasks).
- 2. dist_x_interest: Dissimilarity to x_interest measured by Gower's dissimilarity measure (Gower 1971).
- 3. no_changed: Number of feature changes.
- 4. dist_train: (Weighted) sum of dissimilarities to the k nearest data points in predictor\$data\$X.

For optimization, it uses the NSGA II algorithm (Deb et. al 2002) with mixed integer evolutionary strategies (Li et al. 2013) and some tailored adjustments for the counterfactual search (Dandl et al. 2020). Default values for the hyperparameters are based on Dandl et al. 2020.

Details

Several population initialization strategies are available:

- 1. random: Feature values of new individuals are sampled from the feature value ranges in predictor\$data\$X. Some features values are randomly reset to their initial value in x_interest.
- sd: Like random, except that the sample ranges of numerical features are limited to one standard deviation from their initial value in x_interest.
- 3. icecurve: As in random, feature values are sampled from the feature value ranges in predictor\$data\$X. Then, however, features are reset with probabilities relative to their importance: the higher the importance of a feature, the higher the probability that its values differ from its value in x_interest. The feature importance is measured using ICE curves (Goldstein et al. 2015).
- 4. traindata: Contrary to the other strategies, feature values are drawn from (non-dominated) data points in predictor\$data\$X; if not enough non-dominated data points are available, remaining individuals are initialized by random sampling. Subsequently, some features values are randomly reset to their initial value in x_interest (as for random).

If use_conditional_mutator is set to TRUE, a conditional mutator samples feature values from the conditional distribution given the other feature values with the help of transformation trees (Hothorn and Zeileis 2017). For details see Dandl et al. 2020.

Super classes

counterfactuals:: Counterfactual Method -> counterfactuals:: Counterfactual Method Regr -> MOCRegr

Active bindings

```
optimizer (OptimInstanceMultiCrit)
    The object used for optimization.
```

Methods

```
Public methods:
```

```
• MOCRegr$new()
```

- MOCRegr\$plot_statistics()
- MOCRegr\$get_dominated_hv()
- MOCRegr\$plot_search()
- MOCRegr\$clone()

Method new(): Create a new MOCRegr object.

```
Usage:
MOCRegr$new(
  predictor,
  epsilon = NULL,
  fixed_features = NULL,
 max_changed = NULL,
  mu = 20L
  termination_crit = "gens",
  n_{generations} = 175L,
  p_{rec} = 0.71,
  p_rec_gen = 0.62,
  p_mut = 0.73,
  p_mut_gen = 0.5,
  p_mut_use_orig = 0.4,
  k = 1L
  weights = NULL,
  lower = NULL,
  upper = NULL,
  init_strategy = "icecurve",
  use_conditional_mutator = FALSE,
  quiet = FALSE,
  distance_function = "gower"
)
Arguments:
predictor (Predictor)
   The object (created with iml::Predictor$new()) holding the machine learning model and
   the data.
```

epsilon (numeric(1) | NULL)

If not NULL, candidates whose prediction is farther away from the interval desired_outcome than epsilon are penalized. NULL (default) means no penalization.

```
fixed_features (character() | NULL)
```

Names of features that are not allowed to be changed. NULL (default) allows all features to be changed.

```
max_changed (integerish(1) | NULL)
```

Maximum number of feature changes. NULL (default) allows any number of changes.

mu (integerish(1))

The population size. Default is 20L.

```
termination_crit (character(1)|NULL)
```

Termination criterion, currently, two criterions are implemented: "gens" (default), which stops after n_generations generations, and "genstag", which stops after the hypervolume did not improve for n_generations generations (the total number of generations is limited to 500).

```
n_generations (integerish(1))
```

The number of generations. Default is 175L.

```
p_rec (numeric(1))
```

Probability with which an individual is selected for recombination. Default is 0.71.

```
p_rec_gen (numeric(1))
```

Probability with which a feature/gene is selected for recombination. Default is 0.62.

```
p_mut (numeric(1))
```

Probability with which an individual is selected for mutation. Default is 0.73.

```
p_mut_gen (numeric(1))
```

Probability with which a feature/gene is selected for mutation. Default is 0.5.

```
p_mut_use_orig (numeric(1))
```

Probability with which a feature/gene is reset to its original value in x_interest after mutation. Default is 0.4.

```
k (integerish(1))
```

The number of data points to use for the forth objective. Default is 1L.

```
weights (numeric(1) | numeric(k) | NULL)
```

The weights used to compute the weighted sum of dissimilarities for the forth objective. It is either a single value or a vector of length k. If it has length k, the i-th element specifies the weight of the i-th closest data point. The values should sum up to 1. NULL (default) means all data points are weighted equally.

```
lower (numeric() | NULL)
```

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric() | NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
init_strategy (character(1))
```

The population initialization strategy. Can be icecurve (default), random, sd or traindata. For more information, see the Details section.

```
use_conditional_mutator (logical(1))
```

Should a conditional mutator be used? The conditional mutator generates plausible feature values based on the values of the other feature. Default is FALSE.

```
quiet (logical(1))
```

Should information about the optimization status be hidden? Default is FALSE.

```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function to be used in the second and fourth objective. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method plot_statistics(): Plots the evolution of the mean and minimum objective values together with the dominated hypervolume over the generations. All values for a generation are computed based on all non-dominated individuals that emerged until that generation.

Usage:

```
MOCRegr$plot_statistics(centered_obj = TRUE)
```

Arguments:

```
centered_obj (logical(1))
```

Should the objective values be centered? If set to FALSE, each objective value is visualized in a separate plot, since they (usually) have different scales. If set to TRUE (default), they are visualized in a single plot.

Method get_dominated_hv(): Calculates the dominated hypervolume of each generation.

Usage:

MOCRegr\$get_dominated_hv()

Returns: A data. table with the dominated hypervolume of each generation.

Method plot_search(): Visualizes two selected objective values of all emerged individuals in a scatter plot.

Usage:

```
MOCRegr$plot_search(objectives = c("dist_target", "dist_x_interest"))
```

Arguments:

```
objectives (character(2))
```

The two objectives to be shown in the plot. Possible values are "dist_target", "dist_x_interest, "no_changed", and "dist_train".

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
MOCRegr$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

References

Dandl, S., Molnar, C., Binder, M., and Bischl, B. (2020). "Multi-Objective Counterfactual Explanations". In: Parallel Problem Solving from Nature – PPSN XVI, edited by Thomas Bäck, Mike Preuss, André Deutz, Hao Wang, Carola Doerr, Michael Emmerich, and Heike Trautmann, 448–469, Cham, Springer International Publishing, doi:10.1007/9783030581121_31.

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Deb, K., Pratap, A., Agarwal, S., & Meyarivan, T. A. M. T. (2002). "A fast and elitist multiobjective genetic algorithm: NSGA-II". IEEE transactions on evolutionary computation, 6(2), 182-197.

Goldstein, A., Kapelner, A., Bleich, J., and Pitkin, E. (2015). "Peeking Inside the Black Box: Visualizing Statistical Learning with Plots of Individual Conditional Expectation". Journal of Computational and Graphical Statistics 24 (1): 44–65. doi:10.1080/10618600.2014.907095.

Gower, J. C. (1971). A general coefficient of similarity and some of its properties. Biometrics, 27, 623–637.

Hothorn, T., Zeileis, A. (2017), "Transformation Forests". Technical Report, arXiv 1701.02110.

Li, Rui, L., Emmerich, M. T. M., Eggermont, J. Bäck, T., Schütz, M., Dijkstra, J., Reiber, J. H. C. (2013). "Mixed Integer Evolution Strategies for Parameter Optimization." Evolutionary Computation 21 (1): 29–64. doi:10.1162/EVCO_a_00059.

Examples

```
if (require("randomForest")) {
    # Train a model
    rf = randomForest(mpg ~ ., data = mtcars)
    # Create a predictor object
    predictor = iml::Predictor$new(rf)
    # Find counterfactuals for x_interest

moc_regr = MOCRegr$new(predictor, n_generations = 15L, quiet = TRUE)
    cfactuals = moc_regr$find_counterfactuals(x_interest = mtcars[1L, ], desired_outcome = c(22, 26))
    # Print the counterfactuals
    cfactuals$data
    # Plot evolution of hypervolume and mean and minimum objective values
    moc_regr$plot_statistics()
}
```

NICEClassif

NICE (Nearest Instance Counterfactual Explanations) for Classification Tasks

Description

NICE (Brughmans and Martens 2021) searches for counterfactuals by iteratively replacing feature values of x_interest with the corresponding value of its most similar (optionally correctly classified) instance x_nn.

Details

NICE starts the counterfactual search for $x_{interest}$ by finding its most similar (optionally) correctly classified neighbor x_{int} .

In the first iteration, NICE creates new instances by replacing a different feature value of x_interest with the corresponding value of x_nn in each new instance. Thus, if x_nn differs from x_interest

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in d features, d new instances are created.

Then, the reward values for the created instances are computed with the chosen reward function. Available reward functions are sparsity, proximity, and plausibility.

In the second iteration, NICE creates d-1 new instances by replacing a different feature value of the highest reward instance of the previous iteration with the corresponding value of x_interest, and so on.

If finish_early = TRUE, the algorithm terminates when the predicted desired_class probability for the highest reward instance is in the interval desired_prob; if finish_early = FALSE, the algorithm continues until x_nn is recreated.

Once the algorithm terminated, it depends on return_multiple which instances are returned as counterfactuals: if return_multiple = FALSE, then only the highest reward instance in the last iteration is returned as counterfactual; if return_multiple = TRUE, then all instances (of all iterations) whose predicted desired_class probability is in the interval desired_prob are returned as counterfactuals.

If finish_early = FALSE and return_multiple = FALSE, then x_nn is returned as single counter-factual.

This NICE implementation corresponds to the original version of Brughmans and Martens (2021) when return_multiple = FALSE, finish_early = TRUE, and x_n_c = TRUE.

Super classes

```
counterfactuals::CounterfactualMethod-> counterfactuals::CounterfactualMethodClassif
-> NICEClassif
```

Active bindings

```
x_nn (logical(1))
     The most similar (optionally) correctly classified instance of x_interest.
archive (list())
```

A list that stores the history of the algorithm run. For each algorithm iteration, it has one element containing a data. table, which stores all created instances of this iteration together with their reward values and their predictions.

Methods

Public methods:

- NICEClassif\$new()
- NICEClassif\$clone()

Method new(): Create a new NICEClassif object.

```
Usage:
NICEClassif$new(
  predictor,
  optimization = "sparsity",
  x_nn_correct = TRUE,
  return_multiple = FALSE,
  finish_early = TRUE,
```

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```
distance_function = "gower"
)
Arguments:
predictor (Predictor)
```

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

```
optimization (character(1))
```

The reward function to optimize. Can be sparsity (default), proximity or plausibility. x_n (default), proximity or plausibility.

Should only *correctly* classified data points in predictor\$data\$X be considered for the most similar instance search? Default is TRUE.

```
return_multiple (logical(1))
```

Should multiple counterfactuals be returned? If TRUE, the algorithm returns all created instances whose desired_class prediction is in the interval desired_prob. For more information, see the Details section.

```
finish_early (logical(1))
```

Should the algorithm terminate after an iteration in which the desired_class prediction for the highest reward instance is in the interval desired_prob. If FALSE, the algorithm continues until x_n is recreated.

```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function used to compute the distances between x_i therest and the training data points for finding x_n n. If optimization is set to proximity, the distance function is also used for calculating the distance between candidates and x_i therest. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function is allowed as input. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with x rows and maximum x row(y) columns.

Method clone(): The objects of this class are cloneable with this method.

```
Usage:
NICEClassif$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

References

Brughmans, D., & Martens, D. (2021). NICE: An Algorithm for Nearest Instance Counterfactual Explanations. arXiv 2104.07411 v2.

Gower, J. C. (1971), "A general coefficient of similarity and some of its properties". Biometrics, 27, 623–637.

Examples

```
if (require("randomForest")) {
    # Train a model
    rf = randomForest(Species ~ ., data = iris)
```

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```
# Create a predictor object
predictor = iml::Predictor$new(rf, type = "prob")
# Find counterfactuals
nice_classif = NICEClassif$new(predictor)
cfactuals = nice_classif$find_counterfactuals(
    x_interest = iris[150L, ], desired_class = "versicolor", desired_prob = c(0.5, 1)
)
# Print the results
cfactuals$data
# Print archive
nice_classif$archive
}
```

NICERegr

NICE (Nearest Instance Counterfactual Explanations) for Regression Tasks

Description

NICE (Brughmans and Martens 2021) searches for counterfactuals by iteratively replacing feature values of x_interest with the corresponding value of its most similar (optionally correctly predicted) instance x_nn. While the original method is only applicable to classification tasks (see NICEClassif), this implementation extend it to regression tasks.

Details

NICE starts the counterfactual search for x_interest by finding its most similar (optionally) correctly predicted neighbor x_nn with(in) the desired prediction (range). Correctly predicted means that the prediction of x_nn is less than a user-specified margin_correct away from the true outcome of x_nn. This is designed to mimic the search for x_nn for regression tasks. If no x_nn satisfies this constraint, a warning is returned that no counterfactual could be found.

In the first iteration, NICE creates new instances by replacing a different feature value of x_interest with the corresponding value of x_nn in each new instance. Thus, if x_nn differs from x_interest in d features, d new instances are created.

Then, the reward values for the created instances are computed with the chosen reward function. Available reward functions are sparsity, proximity, and plausibility.

In the second iteration, NICE creates d-1 new instances by replacing a different feature value of the highest reward instance of the previous iteration with the corresponding value of x_interest, and so on.

If finish_early = TRUE, the algorithm terminates when the predicted outcome for the highest reward instance is in the interval desired_outcome; if finish_early = FALSE, the algorithm continues until x_nn is recreated.

Once the algorithm terminated, it depends on return_multiple which instances are returned as counterfactuals: if return_multiple = FALSE, then only the highest reward instance in the last iteration is returned as counterfactual; if return_multiple = TRUE, then all instances (of all iterations) whose predicted outcome is in the interval desired_outcome are returned as counterfactuals.

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If finish_early = FALSE and return_multiple = FALSE, then x_nn is returned as single counterfactual.

The function computes the dissimilarities using Gower's dissimilarity measure (Gower 1971).

Super classes

```
counterfactuals:: Counterfactual Method -> counterfactuals:: Counterfactual Method Regr-> NICERegr
```

Active bindings

```
x_nn (logical(1))
The most similar (optionally) correctly classified instance of x_interest.

archive (list())
```

A list that stores the history of the algorithm run. For each algorithm iteration, it has one element containing a data.table, which stores all created instances of this iteration together with their reward values and their predictions.

Methods

Public methods:

- NICERegr\$new()
- NICERegr\$clone()

Method new(): Create a new NICERegr object.

```
Usage:
NICERegr$new(
    predictor,
    optimization = "sparsity",
    x_nn_correct = TRUE,
    margin_correct = NULL,
    return_multiple = FALSE,
    finish_early = TRUE,
    distance_function = "gower"
)
Arguments:
predictor (Predictor)
```

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

```
optimization (character(1))
```

The reward function to optimize. Can be sparsity (default), proximity or plausibility. x_n (default), proximity or plausibility.

Should only *correctly* classified data points in predictor\$data\$X be considered for the most similar instance search? Default is TRUE.

```
margin_correct (numeric(1) | NULL)
```

The accepted margin for considering a prediction as "correct". Ignored if $x_n_c = FALSE$. If NULL, the accepted margin is set to half the median absolute distance between the true and predicted outcomes in the data (predictor\$data).

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```
return_multiple (logical(1))
```

Should multiple counterfactuals be returned? If TRUE, the algorithm returns all created instances whose prediction is in the interval desired_outcome. For more information, see the Details section.

```
finish_early (logical(1))
```

Should the algorithm terminate after an iteration in which the prediction for the highest reward instance is in the interval desired_outcome. If FALSE, the algorithm continues until x_nn is recreated.

```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function used to compute the distances between x_interest and the training data points for finding x_nn. If optimization is set to proximity, the distance function is also used for calculating the distance between candidates and x_interest. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function is allowed as input. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method clone(): The objects of this class are cloneable with this method.

```
Usage:
NICERegr$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

References

Brughmans, D., & Martens, D. (2021). NICE: An Algorithm for Nearest Instance Counterfactual Explanations. arXiv 2104.07411 v2.

Gower, J. C. (1971), "A general coefficient of similarity and some of its properties". Biometrics, 27, 623–637.

Examples

```
if (require("randomForest")) {
    set.seed(123456)
# Train a model
    rf = randomForest(mpg ~ ., data = mtcars)
# Create a predictor object
    predictor = iml::Predictor$new(rf)
# Find counterfactuals
    nice_regr = NICERegr$new(predictor)
    cfactuals = nice_regr$find_counterfactuals(
        x_interest = mtcars[1L, ], desired_outcome = c(22, 26)
)
# Print the results
    cfactuals$data
# Print archive
    nice_regr$archive
}
```

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RandomSearchClassif Random Search for Classification Tasks

Description

RandomSearch randomly samples a population of candidates and returns non-dominated candidates w.r.t to the objectives of MOC (Dandl et. al 2020) as counterfactuals. RandomSearch is equivalent to MOC with zero generations and the random initialization strategy.

The four objectives of MOC (Dandl et. al 2020) to are:

- 1. Distance to desired_prob (classification tasks) or desired_prob (regression tasks).
- 2. Dissimilarity to x_interest measured by Gower's dissimilarity measure (Gower 1971).
- 3. Number of feature changes.
- 4. (Weighted) sum of dissimilarities to the k nearest data points in predictor\$data\$X.

Details

RandomSearch is typically used as a baseline in benchmark comparisons with MOC. The total number of samples drawn is mu * n_generations. Using separate parameters mu and n_generations is only required to make certain statistics comparable with MOC (e.g. the evolution of the dominated hypervolume).

Super classes

counterfactuals::CounterfactualMethod-> counterfactuals::CounterfactualMethodClassif
-> RandomSearchClassif

Active bindings

optimizer (OptimInstanceMultiCrit)
The object used for optimization.

Methods

Public methods:

- RandomSearchClassif\$new()
- RandomSearchClassif\$plot_statistics()
- RandomSearchClassif\$get_dominated_hv()
- RandomSearchClassif\$plot_search()
- RandomSearchClassif\$clone()

Method new(): Create a new RandomSearchClassif object.

Usage:

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```
RandomSearchClassif$new(
  predictor,
  fixed_features = NULL,
  max_changed = NULL,
  mu = 20L
  n_{generations} = 175L,
  p_use_orig = 0.5,
  k = 1L
  weights = NULL,
  lower = NULL,
  upper = NULL,
  distance_function = "gower"
Arguments:
```

predictor (Predictor)

The object (created with iml::Predictor\$new()) holding the machine learning model and

```
fixed_features (character() | NULL)
```

Names of features that are not allowed to be changed. NULL (default) allows all features to be changed.

```
max_changed (integerish(1) | NULL)
```

Maximum number of feature changes. NULL (default) allows any number of changes.

```
mu (integerish(1))
```

The population size. Default is 20L. The total number of random samples is set to mu * n_generations. See the Details for further details.

```
n_generations (integerish(1))
```

The number of generations. Default is 175L. The total number of random samples is set to mu * n_generations. See the Details section for further details.

```
p_use_orig (numeric(1))
```

Probability with which a feature/gene is reset to its original value in x_interest after random sampling. Default is 0.5.

```
k (integerish(1))
```

The number of data points to use for the forth objective. Default is 1L.

```
weights (numeric(1) | numeric(k) | NULL)
```

The weights used to compute the weighted sum of dissimilarities for the forth objective. It is either a single value or a vector of length k. If it has length k, the i-th element specifies the weight of the i-th closest data point. The values should sum up to 1. NULL (default) means all data points are weighted equally.

```
lower (numeric() | NULL)
```

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric() | NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

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```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function to be used in the second and fourth objective. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method plot_statistics(): Plots the evolution of the mean and minimum objective values together with the dominated hypervolume over the generations. All values for a generation are computed based on all non-dominated individuals that emerged until that generation. The randomly drawn samples are therefore split into n_generations folds of size mu. This function mimics MOCs plot_statistics() method. See the Details section for further information.

Usage:

```
RandomSearchClassif$plot_statistics(centered_obj = TRUE)
```

Arguments:

```
centered_obj (logical(1))
```

Should the objective values be centered? If set to FALSE, each objective value is visualized in a separate plot, since they (usually) have different scales. If set to TRUE (default), they are visualized in a single plot.

Method get_dominated_hv(): Calculates the dominated hypervolume of each generation. The randomly drawn samples are therefore split into n_generations folds of size mu. This function mimics MOCs get_dominated_hv() method. See the Details section for further information.

Usage:

RandomSearchClassif\$get_dominated_hv()

Returns: A data.table with the dominated hypervolume of each generation.

Method plot_search(): Visualizes two selected objective values of all emerged individuals in a scatter plot. The randomly drawn samples are therefore split into n_generations folds of size mu. This function mimics MOCs plot_search() method. See the Details section for further information.

```
Usage:
RandomSearchClassif$plot_search(
  objectives = c("dist_target", "dist_x_interest")
)
Arguments:
```

objectives (character(2))

The two objectives to be shown in the plot. Possible values are "dist_target", "dist_x_interest,"

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
RandomSearchClassif$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

"no_changed", and "dist_train".

References

Dandl, S., Molnar, C., Binder, M., and Bischl, B. (2020). "Multi-Objective Counterfactual Explanations". In: Parallel Problem Solving from Nature – PPSN XVI, edited by Thomas Bäck, Mike Preuss, André Deutz, Hao Wang, Carola Doerr, Michael Emmerich, and Heike Trautmann, 448–469, Cham, Springer International Publishing, doi:10.1007/9783030581121_31.

Deb, K., Pratap, A., Agarwal, S., & Meyarivan, T. A. M. T. (2002). "A fast and elitist multiobjective genetic algorithm: NSGA-II". IEEE transactions on evolutionary computation, 6(2), 182-197.

Goldstein, A., Kapelner, A., Bleich, J., and Pitkin, E. (2015). "Peeking Inside the Black Box: Visualizing Statistical Learning with Plots of Individual Conditional Expectation". Journal of Computational and Graphical Statistics 24 (1): 44–65. doi:10.1080/10618600.2014.907095.

Gower, J. C. (1971). A general coefficient of similarity and some of its properties. Biometrics, 27, 623–637.

Li, Rui, L., Emmerich, M. T. M., Eggermont, J. Bäck, T., Schütz, M., Dijkstra, J., Reiber, J. H. C. (2013). "Mixed Integer Evolution Strategies for Parameter Optimization." Evolutionary Computation 21 (1): 29–64. doi:10.1162/EVCO_a_00059.

Examples

```
if (require("randomForest")) {
    # Train a model
    rf = randomForest(Species ~ ., data = iris)
    # Create a predictor object
    predictor = iml::Predictor$new(rf, type = "prob")
# Find counterfactuals for x_interest
    rs_classif = RandomSearchClassif$new(predictor, n_generations = 30L)
    cfactuals = rs_classif$find_counterfactuals(
        x_interest = iris[150L, ], desired_class = "versicolor", desired_prob = c(0.5, 1)
    )
    # Print the counterfactuals
    cfactuals$data
# Plot evolution of hypervolume and mean and minimum objective values
    rs_classif$plot_statistics()
}
```

RandomSearchRegr

Random Search for Regression Tasks

Description

RandomSearch randomly samples a population of candidates and returns non-dominated candidates w.r.t to the objectives of MOC (Dandl et. al 2020) as counterfactuals. RandomSearch is equivalent to MOC with zero generations and the random initialization strategy.

The four objectives of MOC (Dandl et. al 2020) to are:

1. Distance to desired_prob (classification tasks) or desired_prob (regression tasks).

- 2. Dissimilarity to x_interest measured by Gower's dissimilarity measure (Gower 1971).
- 3. Number of feature changes.
- 4. (Weighted) sum of dissimilarities to the k nearest data points in predictor\$data\$X.

Details

RandomSearch is typically used as a baseline in benchmark comparisons with MOC. The total number of samples drawn is mu * n_generations. Using separate parameters mu and n_generations is only required to make certain statistics comparable with MOC (e.g. the evolution of the dominated hypervolume).

Super classes

```
counterfactuals:: Counterfactual Method -> counterfactuals:: Counterfactual Method Regr -> Random Search Regr \\
```

Active bindings

```
optimizer (OptimInstanceMultiCrit)
The object used for optimization.
```

Methods

Public methods:

- RandomSearchRegr\$new()
- RandomSearchRegr\$plot_statistics()
- RandomSearchRegr\$get_dominated_hv()
- RandomSearchRegr\$plot_search()
- RandomSearchRegr\$clone()

Method new(): Create a new RandomSearchRegr object.

Usage:

Arguments:

```
RandomSearchRegr$new(
   predictor,
   fixed_features = NULL,
   max_changed = NULL,
   mu = 20L,
   n_generations = 175L,
   p_use_orig = 0.5,
   k = 1L,
   weights = NULL,
   lower = NULL,
   upper = NULL,
   distance_function = "gower"
)
```

predictor (Predictor)

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

fixed_features (character() | NULL)

Names of features that are not allowed to be changed. NULL (default) allows all features to be changed.

```
max_changed (integerish(1) | NULL)
```

Maximum number of feature changes. NULL (default) allows any number of changes.

mu (integerish(1))

The population size. Default is 20L. The total number of random samples is set to $mu * n_generations$. See the Details section for further details.

```
n_generations (integerish(1))
```

The number of generations. Default is 175L. The total number of random samples is set to $mu * n_generations$. See the Details section for further details.

```
p_use_orig (numeric(1))
```

Probability with which a feature/gene is reset to its original value in x_i nterest after random sampling. Default is 0.5.

k (integerish(1))

The number of data points to use for the forth objective. Default is 1L.

```
weights (numeric(1) | numeric(k) | NULL)
```

The weights used to compute the weighted sum of dissimilarities for the forth objective. It is either a single value or a vector of length k. If it has length k, the i-th element specifies the weight of the i-th closest data point. The values should sum up to 1. NULL (default) means all data points are weighted equally.

```
lower (numeric() | NULL)
```

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric()|NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function to be used in the second and fourth objective. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method plot_statistics(): Plots the evolution of the mean and minimum objective values together with the dominated hypervolume over the generations. All values for a generation are computed based on all non-dominated individuals that emerged until that generation. The randomly drawn samples are therefore split into n_generations folds of size mu. This function mimics MOCs plot_statistics() method. See the Details section for further information.

```
Usage:
```

RandomSearchRegr\$plot_statistics(centered_obj = TRUE)

```
Arguments:
```

```
centered_obj (logical(1))
```

Should the objective values be centered? If set to FALSE, each objective value is visualized in a separate plot, since they (usually) have different scales. If set to TRUE (default), they are visualized in a single plot.

Method get_dominated_hv(): Calculates the dominated hypervolume of each generation. The randomly drawn samples are therefore split into n_generations folds of size mu. This function mimics MOCs get_dominated_hv() method. See the Details section for further information.

Usage:

RandomSearchRegr\$get_dominated_hv()

Returns: A data. table with the dominated hypervolume of each generation.

Method plot_search(): Visualizes two selected objective values of all emerged individuals in a scatter plot. The randomly drawn samples are therefore split into n_generations folds of size mu. This function mimics MOCs plot_search() method. See the Details section for further information.

Usage:

RandomSearchRegr\$plot_search(objectives = c("dist_target", "dist_x_interest"))

Arguments:

objectives (character(2))

The two objectives to be shown in the plot. Possible values are "dist_target", "dist_x_interest, "no_changed", and "dist_train".

Method clone(): The objects of this class are cloneable with this method.

Usage:

RandomSearchRegr\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

References

Dandl, S., Molnar, C., Binder, M., and Bischl, B. (2020). "Multi-Objective Counterfactual Explanations". In: Parallel Problem Solving from Nature – PPSN XVI, edited by Thomas Bäck, Mike Preuss, André Deutz, Hao Wang, Carola Doerr, Michael Emmerich, and Heike Trautmann, 448–469, Cham, Springer International Publishing, doi:10.1007/9783030581121_31.

Deb, K., Pratap, A., Agarwal, S., & Meyarivan, T. A. M. T. (2002). "A fast and elitist multiobjective genetic algorithm: NSGA-II". IEEE transactions on evolutionary computation, 6(2), 182-197.

Goldstein, A., Kapelner, A., Bleich, J., and Pitkin, E. (2015). "Peeking Inside the Black Box: Visualizing Statistical Learning with Plots of Individual Conditional Expectation". Journal of Computational and Graphical Statistics 24 (1): 44–65. doi:10.1080/10618600.2014.907095.

Gower, J. C. (1971). A general coefficient of similarity and some of its properties. Biometrics, 27, 623–637.

Li, Rui, L., Emmerich, M. T. M., Eggermont, J. Bäck, T., Schütz, M., Dijkstra, J., Reiber, J. H. C. (2013). "Mixed Integer Evolution Strategies for Parameter Optimization." Evolutionary Computation 21 (1): 29–64. doi:10.1162/EVCO_a_00059.

smallest_n_indices 35

Examples

```
if (require("randomForest")) {
    # Train a model
    rf = randomForest(mpg ~ ., data = mtcars)
    # Create a predictor object
    predictor = iml::Predictor$new(rf)
    # Find counterfactuals for x_interest
    rs_regr = RandomSearchRegr$new(predictor, n_generations = 30L)
    cfactuals = rs_regr$find_counterfactuals(x_interest = mtcars[1L, ], desired_outcome = c(22, 26))
    # Print the counterfactuals
    cfactuals$data
    # Plot evolution of hypervolume and mean and minimum objective values
    rs_regr$plot_statistics()
}
```

 $smallest_n_indices$

Returns the indices of the n smallest elements in a vector

Description

Returns the indices of the n smallest elements in a vector

Usage

```
smallest_n_indices(x, n = 1L)
```

Arguments

x (numeric())
A numeric vector.

n (numeric(1))
A integer indicating how many elements should be returned

WhatIfClassif

WhatIf for Classification Tasks

Description

WhatIf returns the n_counterfactual most similar observations to x_interest from observations in predictor\$data\$X whose prediction for the desired_class is in the desired_prob interval.

Details

By default, the dissimilarities are computed using Gower's dissimilarity measure (Gower 1971). Only observations whose features values lie between the corresponding values in lower and upper are considered counterfactual candidates.

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Super classes

```
counterfactuals::CounterfactualMethod-> counterfactuals::CounterfactualMethodClassif
-> WhatIfClassif
```

Methods

Public methods:

- WhatIfClassif\$new()
- WhatIfClassif\$clone()

Method new(): Create a new WhatIfClassif object.

```
Usage:
WhatIfClassif$new(
   predictor,
   n_counterfactuals = 1L,
   lower = NULL,
   upper = NULL,
   distance_function = "gower"
)
Arguments:
predictor (Predictor)
```

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

```
n_counterfactuals (integerish(1))
```

The number of counterfactuals to return. Default is 1L.

```
lower (numeric() | NULL)
```

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric() | NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function used to compute the distances between x_interest and the training data points for finding x_nn. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method clone(): The objects of this class are cloneable with this method.

```
Usage:
WhatIfClassif$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

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References

Gower, J. C. (1971), "A general coefficient of similarity and some of its properties". Biometrics, 27, 623–637.

Wexler, J., Pushkarna, M., Bolukbasi, T., Wattenberg, M., Viégas, F., & Wilson, J. (2019). The what-if tool: Interactive probing of machine learning models. IEEE transactions on visualization and computer graphics, 26(1), 56–65.

Examples

```
if (require("randomForest")) {
    # Train a model
    rf = randomForest(Species ~ ., data = iris)
    # Create a predictor object
    predictor = iml::Predictor$new(rf, type = "prob")
# Find counterfactuals for x_interest
    wi_classif = WhatIfClassif$new(predictor, n_counterfactuals = 5L)
    cfactuals = wi_classif$find_counterfactuals(
        x_interest = iris[150L, ], desired_class = "versicolor", desired_prob = c(0.5, 1)
    )
    # Print the results
    cfactuals$data
}
```

WhatIfRegr

WhatIf for Regression Tasks

Description

What If returns the n_counterfactual most similar observations to x_interest from observations in predictor 4x = 1 whose prediction is in the desired_outcome interval.

Details

Only observations whose features values lie between the corresponding values in lower and upper are considered counterfactual candidates.

Super classes

```
counterfactuals:: Counterfactual Method -> counterfactuals:: Counterfactual Method Regressian -> What If Regressian Reg
```

Methods

Public methods:

- WhatIfRegr\$new()
- WhatIfRegr\$clone()

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Method new(): Create a new WhatIfRegr object.

```
Usage:
WhatIfRegr$new(
   predictor,
   n_counterfactuals = 1L,
   lower = NULL,
   upper = NULL,
   distance_function = "gower"
)
Arguments:
predictor (Predictor)
```

The object (created with iml::Predictor\$new()) holding the machine learning model and the data.

```
n_counterfactuals (integerish(1))
```

The number of counterfactuals to return Default is 1L.

```
lower (numeric() | NULL)
```

Vector of minimum values for numeric features. If NULL (default), the element for each numeric feature in lower is taken as its minimum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
upper (numeric() | NULL)
```

Vector of maximum values for numeric features. If NULL (default), the element for each numeric feature in upper is taken as its maximum value in predictor\$data\$X. If not NULL, it should be named with the corresponding feature names.

```
distance_function (function() | 'gower' | 'gower_c')
```

The distance function used to compute the distances between x_interest and the training data points for finding x_nn. Either the name of an already implemented distance function ('gower' or 'gower_c') or a function. If set to 'gower' (default), then Gower's distance (Gower 1971) is used; if set to 'gower_c', a C-based more efficient version of Gower's distance is used. A function must have three arguments x, y, and data and should return a double matrix with nrow(x) rows and maximum nrow(y) columns.

Method clone(): The objects of this class are cloneable with this method.

```
Usage:
WhatIfRegr$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

References

Gower, J. C. (1971), "A general coefficient of similarity and some of its properties". Biometrics, 27, 623–637.

Wexler, J., Pushkarna, M., Bolukbasi, T., Wattenberg, M., Viégas, F., & Wilson, J. (2019). The what-if tool: Interactive probing of machine learning models. IEEE transactions on visualization and computer graphics, 26(1), 56–65.

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Examples

```
if (require("randomForest")) {
    set.seed(123456)
    # Train a model
    rf = randomForest(mpg ~ ., data = mtcars)
    # Create a predictor object
    predictor = iml::Predictor$new(rf)
    # Find counterfactuals for x_interest
    wi_regr = WhatIfRegr$new(predictor, n_counterfactuals = 5L)
    cfactuals = wi_regr$find_counterfactuals(
        x_interest = mtcars[1L, ], desired_outcome = c(22, 26)
)
    # Print the results
    cfactuals
}
```

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