

# Package ‘PEAXAI’

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**Title** Probabilistic Efficiency Analysis Using Explainable Artificial Intelligence

**Version** 1.0.0

**Description** Provides a probabilistic framework that integrates Data Envelopment Analysis (DEA) (Banker et al., 1984) <[doi:10.1287/mnsc.30.9.1078](https://doi.org/10.1287/mnsc.30.9.1078)> with machine learning classifiers (Kuhn, 2008) <[doi:10.18637/jss.v028.i05](https://doi.org/10.18637/jss.v028.i05)> to estimate both the (in)efficiency status and the probability of efficiency for decision-making units. The approach trains predictive models on DEA-derived efficiency labels (Charnes et al., 1985) <[doi:10.1016/0304-4076\(85\)90133-2](https://doi.org/10.1016/0304-4076(85)90133-2)>, enabling explainable artificial intelligence (XAI) workflows with global and local interpretability tools, including permutation importance (Molnar et al., 2018) <[doi:10.21105/joss.00786](https://doi.org/10.21105/joss.00786)>, Shapley value explanations (Strumbelj & Kononenko, 2014) <[doi:10.1007/s10115-013-0679-x](https://doi.org/10.1007/s10115-013-0679-x)>, and sensitivity analysis (Cortez, 2011) <<https://CRAN.R-project.org/package=rminer>>. The framework also supports probability-threshold peer selection and counterfactual improvement recommendations for benchmarking and policy evaluation. The probabilistic efficiency framework is detailed in González-Moyano et al. (2025) “Probability-based Technical Efficiency Analysis through Machine Learning”, in review for publication.

**License** GPL-3

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convex\_facets

*Create New SMOTE Units to Balance Data combinations of  $m + s$* 

## Description

This function creates new DMUs to address data imbalances. If the majority class is efficient, it generates new inefficient DMUs by worsening the observed units. Conversely, if the majority class is inefficient, it projects inefficient DMUs to the frontier. Finally, a random selection is performed to keep a proportion of 0.65 for the majority class and 0.35 for the minority class.

## Usage

```
convex_facets(data, x, y, RTS = "vrs", balance_data = NULL)
```

**Arguments**

data	A <code>data.frame</code> containing the variables used in the model.
x	Column indexes of the input variables in the data.
y	Column indexes of the output variables in the data.
RTS	Text string or number defining the underlying DEA technology / returns-to-scale assumption (default: "vrs"). Accepted values: 0 / "fdh" Free disposability hull, no convexity assumption. 1 / "vrs" Variable returns to scale, convexity and free disposability. 2 / "drs" Decreasing returns to scale, convexity, down-scaling and free disposability. 3 / "crs" Constant returns to scale, convexity and free disposability. 4 / "irs" Increasing returns to scale (up-scaling, not down-scaling), convexity and free disposability. 5 / "add" Additivity (scaling up and down, but only with integers), and free disposability.
balance_data	A numeric vector indicating the different levels of balance required (e.g., <code>c(0.1, 0.45, 0.6)</code> ).

**Value**

It returns a `data.frame` with the newly created set of DMUs incorporated.

---

data	<i>Simulated efficiency dataset (100 DMUs)</i>
------	--

---

**Description**

Dataset with 100 simulated decision-making units (DMUs) used to illustrate the basic workflow of **PEAXAI** in a simple single-input/single-output setting.

**Usage**

```
data(data)
```

**Format**

A `data.frame` with 100 rows and 3 columns:

**x1** Input of the DMU (e.g., resource use, cost or effort).

**y** Observed output, potentially affected by technical inefficiency.

**yD** Deterministic (theoretical) output on the efficient frontier.

## Details

Each DMU uses one input  $x_1$  to produce an output  $y$ . The variable  $y_D$  represents the theoretical output on the deterministic frontier, that is, the output level that would be observed in the absence of technical inefficiency.

The dataset is purely simulated and is intended for examples and vignettes. It contains 100 DMUs with heterogeneous input levels and corresponding output levels. The observed output  $y$  can be interpreted as  $y \leq y_D$ , where the gap between  $y_D$  and  $y$  reflects technical inefficiency (plus possible noise, depending on how the data were generated).

## Source

Simulated data generated by the authors for illustrative purposes.

## Examples

```
data(data)
str(data)
summary(data)

if (requireNamespace("ggplot2", quietly = TRUE)) {
  ggplot2::ggplot(data, ggplot2::aes(x = x1)) +
    ggplot2::geom_point(ggplot2::aes(y = y), alpha = 0.6) +
    ggplot2::geom_line(ggplot2::aes(y = yD), color = "red") +
    ggplot2::labs(
      x = "Input x1",
      y = "Output",
      title = "Simulated DMUs and theoretical frontier"
    ) +
    ggplot2::theme_minimal()
}
```

---

find\_beta\_maxmin

*Search Range for Directional Efficiency Parameter ( $\beta$ )*

---

## Description

Estimates, for each observation, the minimum and maximum feasible values of the directional distance parameter  $\beta$  used in projection-based efficiency analysis. This function is an internal step of [PEAXAI\\_targets](#), providing the initial search bounds for the iterative determination of efficiency targets.

## Usage

```
find_beta_maxmin(
  data,
  x,
  y,
```

```

    final_model,
    calibration_model,
    efficiency_thresholds,
    n_expand,
    vector_gx,
    vector_gy,
    max_y,
    min_x
)

```

### Arguments

<code>data</code>	A <code>data.frame</code> or <code>matrix</code> containing input and output variables.
<code>x</code>	A numeric vector with the column indexes of input variables in <code>data</code> .
<code>y</code>	A numeric vector with the column indexes of output variables in <code>data</code> .
<code>final_model</code>	A fitted <b>caret</b> model of class "train" that supports <code>predict(type = "prob")</code> and returns a probability column for the efficient class.
<code>calibration_model</code>	A model to calibrate.
<code>efficiency_thresholds</code>	A numeric vector of probability levels in (0,1). Its minimum and maximum values delimit the target interval used to bracket $\beta$ .
<code>n_expand</code>	Integer. Increment step size applied to $\beta$ at each iteration.
<code>vector_gx</code>	A numeric vector or <code>data.frame</code> with directional changes for inputs (typically negative direction), usually built inside <code>PEAXAI_targets</code> .
<code>vector_gy</code>	A numeric vector or <code>data.frame</code> with directional changes for outputs (positive direction).
<code>max_y</code>	Numeric. Upper-limit multiplier for output expansion relative to observed maxima.
<code>min_x</code>	Numeric. Lower-limit multiplier for input contraction relative to observed minima.

### Details

For each DMU, the function expands outputs and contracts inputs along the specified direction until the predicted probability of efficiency (from `final_model`) reaches the maximum in `efficiency_thresholds` or feasible domain limits. The resulting interval  $[\beta_{\min}, \beta_{\max}]$  is then used by `PEAXAI_targets` to refine projections via grid search.

### Value

A `data.frame` with two numeric columns:

- `min` Minimum feasible value of  $\beta$  for each observation.
- `max` Maximum feasible value of  $\beta$  for each observation.

**See Also**

[PEAXAI\\_targets](#) (efficiency projections based on  $\beta$ ); [train](#) (model training with class probabilities).

---

firms

*Spanish Food Industry Firms Dataset*

---

**Description**

Dataset containing information on food industry companies located in Spain, used to illustrate efficiency analysis within the **PEAXAI** package. The dataset reflects the institutional and market heterogeneity that shapes firm-level efficiency across Spain's 17 autonomous communities.

**Usage**

```
data(firms)
```

**Format**

A data.frame with 917 rows and 6 columns:

**total\_assets** Total assets (millions of euros).

**employees** Number of employees.

**fixed\_assets** Tangible fixed assets (millions of euros).

**personnel\_expenses** Personnel expenses (millions of euros).

**operating\_income** Operating income (millions of euros).

**autonomous\_community** Autonomous community where the firm operates.

**Details**

The dataset includes 917 food industry firms with more than 50 employees, collected from the *SABI* database for the year 2023. Each observation corresponds to a single company. Variables reflect both operational and financial dimensions relevant for productivity and efficiency assessment.

The output variable is:

- **operating\_income** — Operating income (in millions of euros), measuring revenues generated from core business activities.

The input variables are:

- **total\_assets** — Total assets (millions of euros), representing resources employed.
- **employees** — Number of employees, indicating workforce size (only firms with more than 50 workers are included).
- **fixed\_assets** — Tangible fixed assets (millions of euros), such as buildings and machinery.
- **personnel\_expenses** — Personnel expenses (millions of euros), including salaries, benefits, and training.

The variable `autonomous_community` identifies the territorial location of each firm within Spain.

The sample displays substantial dispersion across variables, encompassing both small and large firms. This heterogeneity affects measures of central tendency—mean and median values differ considerably—thus providing a realistic challenge for efficiency and explainability analyses.

### Source

SABI (Sistema de Análisis de Balances Ibéricos) database, 2023. Firms with more than 50 employees in the Spanish food industry.

### Examples

```
data(firms)
str(firms)
summary(firms)

if (requireNamespace("ggplot2", quietly = TRUE)) {
  ggplot2::ggplot(firms, ggplot2::aes(x = employees, y = operating_income)) +
    ggplot2::geom_point(alpha = 0.6) +
    ggplot2::labs(
      x = "Number of employees",
      y = "Operating income (millions of euros)",
      title = "Spanish Food Industry Firms (2023)"
    ) +
    ggplot2::theme_minimal() +
    ggplot2::theme(
      plot.title = ggplot2::element_text(face = "bold"),
      axis.line = ggplot2::element_line(color = "black"),
      axis.ticks = ggplot2::element_line(color = "black"),
      panel.grid.minor = ggplot2::element_blank()
    )
}
```

---

get\_SMOTE\_DMUs

*Create New SMOTE Units to Balance Data combinations of  $m + s$*

---

### Description

This function creates new DMUs to address data imbalances. If the majority class is efficient, it generates new inefficient DMUs by worsening the observed units. Conversely, if the majority class is inefficient, it projects inefficient DMUs to the frontier. Finally, a random selection is performed to keep a proportion of 0.65 for the majority class and 0.35 for the minority class.

### Usage

```
get_SMOTE_DMUs(data, facets, x, y, RTS = "vrs", balance_data = NULL, seed)
```

**Arguments**

data	A list of data.frames, where each element represents a dataset with labeled data.
facets	A list where each element represents a subgroup containing index combinations that generate efficient units.
x	Column indexes of the input variables in the data.
y	Column indexes of the output variables in the data.
RTS	Text string or number defining the underlying DEA technology / returns-to-scale assumption (default: "vrs"). Accepted values: 0 / "fdh" Free disposability hull, no convexity assumption. 1 / "vrs" Variable returns to scale, convexity and free disposability. 2 / "drs" Decreasing returns to scale, convexity, down-scaling and free disposability. 3 / "crs" Constant returns to scale, convexity and free disposability. 4 / "irs" Increasing returns to scale (up-scaling, not down-scaling), convexity and free disposability. 5 / "add" Additivity (scaling up and down, but only with integers), and free disposability.
balance_data	A numeric vector indicating the different levels of balance required (e.g., c(0.1, 0.45, 0.6)).
seed	Integer. Seed for reproducibility.

**Value**

A list where each element corresponds to a balance level, containing a single data.frame with the real and synthetic DMUs, correctly labeled.

---

label_efficiency	<i>Data preprocessing and efficiency labeling with Additive DEA</i>
------------------	---

---

**Description**

Labels each DMU (Decision Making Unit) as efficient or not using the Additive DEA model, optionally after basic data preprocessing. The resulting factor class\_efficiency has levels c("not\_efficient", "efficient") where "efficient" is the positive class for downstream modeling.

**Usage**

```
label_efficiency(data, REF = data, x, y, RTS = "vrs")
```

**Arguments**

data	A data.frame or matrix containing all variables.
REF	Optional reference set of inputs that defines the technology (defaults to the columns indicated by x in data). Must have the same number of rows as data.
x	Integer vector with column indices of input variables in data.
y	Integer vector with column indices of output variables in data.
RTS	Character or integer specifying the DEA technology / returns-to-scale assumption (default: "vrs"). Accepted values: 0 / "fdh" Free disposability hull (no convexity). 1 / "vrs" Variable returns to scale (convexity + free disposability). 2 / "drs" Decreasing returns to scale (convexity, down-scaling, free disposability). 3 / "crs" Constant returns to scale (convexity + free disposability). 4 / "irs" Increasing returns to scale (up-scaling only, convexity + free disposability). 5 / "add" Additivity (integer up/down scaling) with free disposability.

**Details**

Internally relies on [dea.add](#) to compute Additive DEA scores and derive the binary efficiency label.

**Value**

A data.frame equal to data (retaining all input x and output y columns) plus a new factor column `class_efficiency` with levels `c("not_efficient", "efficient")`.

**See Also**

[dea.add](#)

**Examples**

```
# Example (assuming columns 1:2 are inputs and 3 is output):
# out <- my_fun(data = df, x = 1:2, y = 3, RTS = "vrs")
# table(out$class_efficiency)
```

**Description**

Trains one or multiple classification algorithms to identify Pareto-efficient decision-making units (DMUs). It jointly searches model hyperparameters and the class-balancing level (synthetic samples via SMOTE) using k-fold cross-validation or a train/validation/test split, selecting the configuration that maximizes the specified metric(s). Returns, for each technique, the best fitted model together with training summaries, performance metrics, and the selected balancing level.

**Usage**

```
PEAXAI_fitting(
  data,
  x,
  y,
  RTS = "vrs",
  imbalance_rate = NULL,
  trControl,
  methods,
  metric_priority = "Balanced_Accuracy",
  calibration_method = NULL,
  hold_out = NULL,
  seed = NULL,
  verbose = TRUE
)
```

**Arguments**

<code>data</code>	A data.frame or matrix containing the variables in the model.
<code>x</code>	Integer vector with column indices of input variables in data.
<code>y</code>	Integer vector with column indices of output variables in data.
<code>RTS</code>	Text string or number defining the underlying DEA technology / returns-to-scale assumption (default: "vrs"). Accepted values: 0 / "fdh" Free disposability hull, no convexity assumption. 1 / "vrs" Variable returns to scale, convexity and free disposability. 2 / "drs" Decreasing returns to scale, convexity, down-scaling and free disposability. 3 / "crs" Constant returns to scale, convexity and free disposability. 4 / "irs" Increasing returns to scale (up-scaling, not down-scaling), convexity and free disposability. 5 / "add" Additivity (scaling up and down, but only with integers), and free disposability.
<code>imbalance_rate</code>	Optional target(s) for class balance via SMOTE. If NULL, no synthetic balancing is performed.
<code>trControl</code>	A caret::trainControl-like list that specifies the resampling strategy; recognized values for \$method include "cv", "test_set", and "none". See <b>caret</b> documentation.
<code>methods</code>	A list of selected machine learning models and their hyperparameters.
<code>metric_priority</code>	A string specifying the summary metric for classification to select the optimal model. Default includes "Balanced_Accuracy" due to (normally) unbalanced data.
<code>calibration_method</code>	Character string specifying the probability calibration method applied to the fitted classifier. Supported options are:

	"none" No probability calibration is applied; raw classifier probabilities are returned.
	"platt" Platt scaling, which fits a logistic regression model mapping raw scores to calibrated probabilities. Suitable for relatively small samples and parametric probability adjustment.
	"isotonic" Isotonic regression, a non-parametric monotonic calibration method that adapts flexibly to the empirical score-probability relationship. Recommended for larger samples where sufficient calibration data are available.
	Calibration is performed using validation data whenever resampling is enabled.
hold_out	Numeric proportion in (0,1) for validation split (default NULL). If NULL, training and validation use the same data.
seed	Integer. Seed for reproducibility.
verbose	Logical; if TRUE, prints progress messages (default FALSE).

### Value

A "PEAXAI" (list) with the best technique, best fitted models and their performance and the results by fold.

### Examples

```
data("firms", package = "PEAXAI")

data <- subset(
  firms,
  autonomous_community == "Comunidad Valenciana"
)

trControl <- list(
  method = "cv",
  number = 3
)

# glm method
methods <- list(
  "glm" = list(
    weights = "dinamic"
  )
)

models <- PEAXAI_fitting(
  data = data,
  x = c(1:4),
  y = 5,
  RTS = "vrs",
  imbalance_rate = NULL,
  methods = methods,
  trControl = trControl,
  metric_priority = c("Balanced_Accuracy", "Precision"),
  calibration_method = "platt",
```

```

    seed = 1,
    verbose = FALSE
  )

```

---

PEAXAI\_global\_importance

*Global feature importance for efficiency classifiers*

---

## Description

Computes **global feature importance** for a fitted classification model that separates Pareto-efficient DMUs, using one of three XAI backends:

- "SA" — Sensitivity Analysis via **rminer**.
- "SHAP" — Model-agnostic SHAP approximations via **fastshap**.
- "PI" — Permutation Importance via **iml**.

You can evaluate the model on either the training domain (`background = "train"`) or the real-world domain (`background = "real"`) and compute importance on a chosen target set (`"train"` or `"real"`). Importances are returned normalized to sum to 1.

## Usage

```

PEAXAI_global_importance(
  data,
  x,
  y,
  final_model,
  background = "train",
  target = "train",
  importance_method
)

```

## Arguments

<code>data</code>	A <code>data.frame</code> (or <code>matrix</code> ) with predictors and outcomes. The function will internally reorder columns to <code>c(x, y)</code> .
<code>x</code>	Integer or character vector with the columns used as <b>inputs</b> (predictors).
<code>y</code>	Integer or character vector with the columns used as <b>outputs</b> (targets used to define <code>class_efficiency</code> in training; not included in <code>X</code> when explaining).
<code>final_model</code>	A fitted model. If it is a base- <code>glm</code> binomial, probabilities are obtained with <code>type = "response"</code> ; otherwise the function expects <code>predict(type = "prob")</code> with a column named <code>"efficient"</code> .
<code>background</code>	Character, <code>"train"</code> (default) or <code>"real"</code> . Background data define the distribution used for the reference model behaviour.

**target** Character, "train" (default) or "real". Dataset on which importance is computed.

**importance\_method** A named list (or data.frame-like) with the backend and its args:

- name** One of "SA", "SHAP", "PI".
- method (SA)** One of "1D-SA", "sens", "DSA", "MSA", "CSA", "GSA".
- measures (SA)** e.g. "AAD", "gradient", "variance", "range".
- levels (SA)** Discretization levels used by `rminer::Importance`.
- baseline (SA)** Baseline value for SA, if applicable.
- nsim (SHAP)** Number of Monte Carlo samples for `fastshap::explain`.
- n.repetitions (PI)** Number of permutations per feature for `iml::FeatureImp`.

### Details

Internally, the function builds background/target sets with `xai_prepare_sets()`. For glm models, the positive class is assumed to be the **second level** ("efficient") and probabilities are extracted with `type = "response"`. For other models (e.g., **caret**), `predict(type = "prob")[, "efficient"]` is used.

### Value

A named numeric vector (or 1-row data.frame) of normalized importances, with names matching the predictor columns; the values sum to 1.

### See Also

[explain](#), [FeatureImp](#), [Importance](#)

### Examples

```
data("firms", package = "PEAXAI")

data <- subset(
  firms,
  autonomous_community == "Comunidad Valenciana"
)

x <- 1:4
y <- 5
RTS <- "vrs"
imbalance_rate <- NULL

trControl <- list(
  method = "cv",
  number = 3
)

# glm method
methods <- list(
  "glm" = list(
```

```

        weights = "dinamic"
      )
    )

metric_priority <- c("Balanced_Accuracy", "ROC_AUC")

models <- PEAXAI_fitting(
  data = data, x = x, y = y, RTS = RTS,
  imbalance_rate = imbalance_rate,
  methods = methods,
  trControl = trControl,
  metric_priority = metric_priority,
  seed = 1,
  verbose = FALSE
)

final_model <- models[["best_model_fit"]][["glm"]]

imp <- PEAXAI_global_importance(
  data = data, x = x, y = y,
  final_model = final_model,
  background = "real", target = "real",
  importance_method = list(name = "PI", n.repetitions = 5)
)

head(imp)

```

---

PEAXAI\_peer

*Identify Benchmark Peers Based on Estimated Efficiency Probabilities*


---

## Description

Identifies peer units (i.e., reference benchmarks) for each decision-making unit (DMU) based on predicted probabilities of technical efficiency. Given a fitted classification model that estimates the probability of being efficient, the function selects, for each DMU, its nearest efficient peer according to Euclidean or weighted distances. Multiple efficiency thresholds can be specified to assess different levels of benchmarking stringency.

## Usage

```

PEAXAI_peer(
  data,
  x,
  y,
  final_model,
  calibration_model = NULL,
  efficiency_thresholds,

```

```

    targets,
    weighted = FALSE,
    relative_importance = NULL
  )

```

### Arguments

<code>data</code>	A data frame or matrix containing input and output variables used in the efficiency model.
<code>x</code>	Integer vector indicating the column indices of input variables in data.
<code>y</code>	Integer vector indicating the column indices of output variables in data.
<code>final_model</code>	A fitted classification model used to estimate efficiency probabilities. Supported classes: "train" (from <b>caret</b> ) or "glm" (binomial).
<code>calibration_model</code>	Optional probability-calibration model applied to the raw predicted probabilities from <code>final_model</code> (e.g., Platt scaling or isotonic regression). If provided, calibrated probabilities are used for ranking and threshold-based decisions. Set to NULL to use uncalibrated predictions.
<code>efficiency_thresholds</code>	Numeric vector indicating the minimum probability values required to consider a DMU as efficient.
<code>targets</code>	A named list containing, for each efficiency threshold, the corresponding
<code>weighted</code>	Logical. If TRUE, peers are selected using weighted Euclidean distances based on variable importance. If FALSE (default), unweighted distances are used.
<code>relative_importance</code>	Optional named numeric vector indicating the relative importance of each input/output variable (used when <code>weighted = TRUE</code> ).

### Details

This function enables probabilistic peer identification under uncertainty, supporting flexible definitions of efficiency based on thresholds over estimated probabilities. When `weighted = TRUE`, variable weights (e.g., derived from feature importance) modulate the peer selection process, allowing for context-aware benchmarking.

### Value

A named list of matrices. Each element corresponds to an efficiency threshold and contains, for each DMU, the index of the closest efficient peer. If `weighted = FALSE`, the list contains unweighted peers. If `weighted = TRUE`, the list contains weighted peers.

### Examples

```

data("firms", package = "PEAXAI")

data <- subset(
  firms,
  autonomous_community == "Comunidad Valenciana"
)

```

```

)

x <- 1:4
y <- 5
RTS <- "vrs"
imbalance_rate <- NULL

trControl <- list(
  method = "cv",
  number = 3
)

# glm method
methods <- list(
  "glm" = list(
    weights = "dinamic"
  )
)

metric_priority <- c("Balanced_Accuracy", "ROC_AUC")

models <- PEAXAI_fitting(
  data = data, x = x, y = y, RTS = RTS,
  imbalance_rate = imbalance_rate,
  methods = methods,
  trControl = trControl,
  metric_priority = metric_priority,
  verbose = FALSE,
  seed = 1
)

final_model <- models[["best_model_fit"]][["glm"]]

relative_importance <- PEAXAI_global_importance(
  data = data, x = x, y = y,
  final_model = final_model,
  background = "real", target = "real",
  importance_method = list(name = "PI", n.repetitions = 5)
)

efficiency_thresholds <- seq(0.75, 0.95, 0.1)

directional_vector <- list(relative_importance = relative_importance,
  scope = "global", baseline = "mean")

targets <- PEAXAI_targets(data = data, x = x, y = y, final_model = final_model,
  efficiency_thresholds = efficiency_thresholds, directional_vector = directional_vector,
  n_expand = 0.5, n_grid = 50, max_y = 2, min_x = 1)

peers <- PEAXAI_peer(data = data, x = x, y = y, final_model = final_model,
  efficiency_thresholds = efficiency_thresholds, targets = targets, weighted = FALSE)

```

---

PEAXAI\_predict      *Predict Probability of Efficiency Using a Fitted Model*

---

### Description

Predicts probabilities for new decision-making units (DMUs) using a fitted **caret** classification model. If `calibration_model` is provided, the raw classifier probabilities are post-processed to obtain calibrated probability estimates (e.g., Platt scaling via logistic regression or isotonic calibration via a monotone mapping).

### Usage

```
PEAXAI_predict(data, x, y, final_model, calibration_model = NULL)
```

### Arguments

<code>data</code>	A <code>data.frame</code> or matrix containing the variables used for prediction.
<code>x</code>	Integer vector indicating the column indices of input variables in <code>data</code> .
<code>y</code>	Integer vector indicating the column indices of output variables in <code>data</code> .
<code>final_model</code>	A fitted <b>caret</b> model provided by <code>PEAXAI_fitting()</code> .
<code>calibration_model</code>	Optional calibration object returned by <code>PEAXAI_fitting()</code> . If <code>NULL</code> , raw probabilities are returned. If <code>calibration_model\$method == "glm.fit"</code> , Platt scaling is applied by predicting <code>type = "response"</code> from a logistic regression using the raw score <code>s</code> . Otherwise, an isotonic calibration function is retrieved via <code>calibration_model[[final_model\$method]]</code> and applied to the raw probabilities.

### Value

A numeric vector of predicted probabilities (raw or calibrated), one per row of data.

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PEAXAI\_ranking      *Generate Efficiency Rankings Based on Probabilistic Classification*

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### Description

Produces efficiency rankings of decision-making units (DMUs) according to the probabilities estimated by a fitted classification model. Two ranking modes are supported:

- "predicted": ranks DMUs solely by their predicted probability of being efficient.
- "attainable": ranks DMUs hierarchically according to: (1) the attainable (target) efficiency probability, (2) the size of the improvement parameter  $\beta$  (smaller is better), and (3) the predicted efficiency probability (higher is better).

This allows to integrate both predictive and counterfactual (attainable) information into the efficiency ranking.

**Usage**

```
PEAXAI_ranking(
  data,
  x,
  y,
  final_model,
  calibration_model = NULL,
  efficiency_thresholds,
  targets = NULL,
  rank_basis
)
```

**Arguments**

<code>data</code>	A data.frame or matrix containing the input and output variables.
<code>x</code>	Integer vector specifying the column indices of input variables in <code>data</code> .
<code>y</code>	Integer vector specifying the column indices of output variables in <code>data</code> .
<code>final_model</code>	A fitted classification model used to estimate efficiency probabilities. Supported types are: <ul style="list-style-type: none"> <li>• "train": an object fitted with <b>caret</b>.</li> <li>• "glm": a binomial logistic regression model.</li> </ul>
<code>calibration_model</code>	Optional probability-calibration model applied to the raw predicted probabilities from <code>final_model</code> (e.g., Platt scaling or isotonic regression). If provided, calibrated probabilities are used for ranking and threshold-based decisions. Set to <code>NULL</code> to use uncalibrated predictions.
<code>efficiency_thresholds</code>	Numeric vector defining one or more efficiency probability thresholds to determine the attainable frontier or peer set.
<code>targets</code>	A named list containing, for each efficiency threshold, the corresponding attainable targets and estimated $\beta$ values (e.g., obtained from counterfactual analysis). Each element should be a list with a component named "beta".
<code>rank_basis</code>	Character string specifying the ranking criterion. Options are: <ul style="list-style-type: none"> <li>• "predicted": order units by predicted efficiency probability.</li> <li>• "attainable": order by attainable probability, then by <math>\beta</math>, and finally by predicted probability (see Details).</li> </ul>

**Details**

The attainable-based ranking combines predictive efficiency with the modeled potential for improvement ( $\beta$ ) and the probability of reaching a target frontier level. This approach yields a more nuanced and interpretable prioritization of DMUs, reflecting both their current and achievable performance under the estimated model.

When `rank_basis = "attainable"`, ties in attainable probability are broken first by the magnitude of  $\beta$  (ascending), and then by the predicted probability (descending).

**Value**

- If rank\_basis = "predicted": a data.frame sorted by predicted efficiency probability.
- If rank\_basis = "attainable": a named list of data.frames, one per efficiency threshold, each sorted according to the hierarchical ranking scheme described above.

**Examples**

```

data("firms", package = "PEAXAI")

data <- subset(
  firms,
  autonomous_community == "Comunidad Valenciana"
)

x <- 1:4
y <- 5
RTS <- "vrs"
imbalance_rate <- NULL

trControl <- list(
  method = "cv",
  number = 3
)

# glm method
methods <- list(
  "glm" = list(
    weights = "dinamic"
  )
)

metric_priority <- c("Balanced_Accuracy", "ROC_AUC")

models <- PEAXAI_fitting(
  data = data, x = x, y = y, RTS = RTS,
  imbalance_rate = imbalance_rate,
  methods = methods,
  trControl = trControl,
  metric_priority = metric_priority,
  verbose = FALSE,
  seed = 1
)

final_model <- models[["best_model_fit"]][["glm"]]

relative_importance <- PEAXAI_global_importance(
  data = data, x = x, y = y,
  final_model = final_model,
  background = "real", target = "real",
  importance_method = list(name = "PI", n.repetitions = 5)
)

```

```

efficiency_thresholds <- seq(0.75, 0.95, 0.1)

directional_vector <- list(relative_importance = relative_importance,
scope = "global", baseline = "mean")

targets <- PEAXAI_targets(data = data, x = x, y = y, final_model = final_model,
efficiency_thresholds = efficiency_thresholds, directional_vector = directional_vector,
n_expand = 0.5, n_grid = 50, max_y = 2, min_x = 1)

ranking <- PEAXAI_ranking(data = data, x = x, y = y,
final_model = final_model, rank_basis = "predicted")

```

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PEAXAI\_targets

*Projection-Based Efficiency Targets*


---

### Description

Computes efficiency projections for each observation based on a trained classifier from **caret** that provides class probabilities via `predict(type = "prob")`. For each probability threshold, the function finds the direction and magnitude of change in input–output space required for a unit to reach a specified efficiency level, following a directional distance approach.

### Usage

```

PEAXAI_targets(
  data,
  x,
  y,
  final_model,
  calibration_model = NULL,
  efficiency_thresholds,
  directional_vector,
  n_expand,
  n_grid,
  max_y = 2,
  min_x = 1
)

```

### Arguments

<code>data</code>	A <code>data.frame</code> or matrix containing input and output variables.
<code>x</code>	A numeric vector indicating the column indexes of input variables in <code>data</code> .
<code>y</code>	A numeric vector indicating the column indexes of output variables in <code>data</code> .
<code>final_model</code>	A fitted <b>caret</b> model of class "train" that supports <code>predict(type = "prob")</code> and returns a probability column for the efficient class.

calibration_model	Optional probability-calibration model applied to the raw predicted probabilities from <code>final_model</code> (e.g., Platt scaling or isotonic regression). If provided, calibrated probabilities are used for ranking and threshold-based decisions. Set to <code>NULL</code> to use uncalibrated predictions.
efficiency_thresholds	A numeric vector of probability levels in (0,1) that define the efficiency classes (e.g., <code>c(0.75, 0.9, 0.95)</code> ).
directional_vector	A list with the required information to construct the directional vector, including: <ul style="list-style-type: none"> <li>• <code>relative_importance</code>: Numeric vector of variable importances that sum to 1.</li> <li>• <code>scope</code>: "global" (currently supported) or "local".</li> <li>• <code>baseline</code>: "mean", "median", "self" or "ones".</li> </ul>
n_expand	Numeric. Number of expansion steps used to enlarge the initial search range for $\beta$ .
n_grid	Integer. Number of grid points evaluated during each iteration to refine the cutoff value of $\beta$ .
max_y	Numeric. Upper-limit multiplier for output expansion in the search procedure (default = 2).
min_x	Numeric. Lower-limit multiplier for input contraction in the search procedure (default = 1).

### Details

For each observation and for each probability level in `efficiency_thresholds`, the function searches for the smallest directional distance  $\beta$  such that the predicted probability of belonging to the efficient class reaches the target.

### Value

A named list with one element per threshold. Each element contains:

- `data`: A data.frame of projected input–output values at that threshold.
- `beta`: A two-column data.frame with the optimal  $\beta$  and the corresponding predicted probability.

### See Also

[find\\_beta\\_maxmin](#) for initializing search bounds; [train](#) for model training.

### Examples

```
data("firms", package = "PEAXAI")

data <- subset(
  firms,
```

```
    autonomous_community == "Comunidad Valenciana"
  )

  x <- 1:4
  y <- 5
  RTS <- "vrs"
  imbalance_rate <- NULL

  trControl <- list(
    method = "cv",
    number = 3
  )

  # glm method
  methods <- list(
    "glm" = list(
      weights = "dinamic"
    )
  )

  metric_priority <- c("Balanced_Accuracy", "ROC_AUC")

  models <- PEAXAI_fitting(
    data = data, x = x, y = y, RTS = RTS,
    imbalance_rate = imbalance_rate,
    methods = methods,
    trControl = trControl,
    metric_priority = metric_priority,
    verbose = FALSE,
    seed = 1
  )

  final_model <- models[["best_model_fit"]][["glm"]]

  relative_importance <- PEAXAI_global_importance(
    data = data, x = x, y = y,
    final_model = final_model,
    background = "real", target = "real",
    importance_method = list(name = "PI", n.repetitions = 5)
  )

  efficiency_thresholds <- seq(0.75, 0.95, 0.1)

  directional_vector <- list(relative_importance = relative_importance,
    scope = "global", baseline = "mean")

  targets <- PEAXAI_targets(data = data, x = x, y = y, final_model = final_model,
    efficiency_thresholds = efficiency_thresholds, directional_vector = directional_vector,
    n_expand = 0.5, n_grid = 50, max_y = 2, min_x = 1)
```

---

```
preprocessing          Prepare Data and Handle Errors
```

---

**Description**

This function arranges the data in the required format and displays some error messages.

**Usage**

```
preprocessing(data, x, y)
```

**Arguments**

data	A data.frame or matrix containing the variables in the model.
x	Column indexes of input variables in data.
y	Column indexes of output variables in data.

**Value**

It returns a matrix in the required format and displays some error messages.

---

```
SMOTE_data           Create New SMOTE Units to Balance Data combinations of m + s
```

---

**Description**

This function creates new DMUs to address data imbalances. If the majority class is efficient, it generates new inefficient DMUs by worsening the observed units. Conversely, if the majority class is inefficient, it projects inefficient DMUs to the frontier. Finally, a random selection is performed to keep a proportion of 0.65 for the majority class and 0.35 for the minority class.

**Usage**

```
SMOTE_data(data, x, y, RTS = "vrs", balance_data, seed)
```

**Arguments**

data	A data.frame containing the variables used in the model.
x	Column indexes of the input variables in the data.
y	Column indexes of the output variables in the data.
RTS	Text string or number defining the underlying DEA technology / returns-to-scale assumption (default: "vrs"). Accepted values: 0 / "fdh" Free disposability hull, no convexity assumption. 1 / "vrs" Variable returns to scale, convexity and free disposability.

	2 / "drs" Decreasing returns to scale, convexity, down-scaling and free disposability.
	3 / "crs" Constant returns to scale, convexity and free disposability.
	4 / "irs" Increasing returns to scale (up-scaling, not down-scaling), convexity and free disposability.
	5 / "add" Additivity (scaling up and down, but only with integers), and free disposability.
balance_data	Indicate level of efficient units to achieve and the number of efficient and not efficient units.
seed	Integer. Seed for reproducibility.

**Value**

It returns a data.frame with the newly created set of DMUs incorporated.

---

train\_PEAXAI

*Training a Classification Machine Learning Model*


---

**Description**

This function trains a set of models and selects best hyperparameters for each of them.

**Usage**

```
train_PEAXAI(data, method, parameters, trControl, metric_priority, seed)
```

**Arguments**

data	A data.frame or matrix containing the variables in the model.
method	Parameters for controlling the training process (from the 'caret' package).
parameters	A list of selected machine learning models and their hyperparameters.
trControl	A list of selected machine learning learning.
metric_priority	A string specifying the summary metric for classification to select the optimal model. Default includes "Balanced_Accuracy" due to (normally) unbalanced data.
seed	Integer. Seed for reproducibility.

**Value**

It returns a list with the chosen model.

---

xai_prepare_sets	<i>Prepare Training and Target Datasets from a caret Model</i>
------------------	--

---

### Description

Extracts and formats the training and/or target datasets from a machine learning model trained with `caret::train`, allowing for distinction between using the full training data or only the original subset used for modeling. It standardizes the class column to be named "class\_efficiency" and positions it as the last column.

### Usage

```
xai_prepare_sets(
  data,
  x,
  y,
  final_model,
  background,
  target,
  type,
  threshold,
  levels_order
)
```

### Arguments

<code>data</code>	A <code>data.frame</code> containing the original dataset used to train the model. Only needed when using "real" as background or target.
<code>x</code>	Not currently used. Reserved for future input variable selection.
<code>y</code>	Not currently used. Reserved for future output variable specification.
<code>final_model</code>	A trained model object of class "train" from the <b>caret</b> package.
<code>background</code>	A character string, either "train" or "real", specifying the background dataset used for explainability.
<code>target</code>	A character string, either "train" or "real", specifying the target dataset to be explained.
<code>type</code>	Not currently used. Reserved for future prediction types.
<code>threshold</code>	Not currently used. Reserved for future thresholding logic.
<code>levels_order</code>	A character vector specifying the levels of the response factor, typically <code>c("not_efficient", "efficient")</code> . Not currently used, but can help in reordering or relabeling.

### Value

A list with two elements:

`train_data` A `data.frame` representing the background dataset, with the class column renamed to "class\_efficiency" and positioned last.

`target_data` A `data.frame` representing the target dataset, formatted in the same way.

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