# Package 'ipd'

January 7, 2025

Title Inference on Predicted Data

```
Version 0.1.4
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Description
     Performs valid statistical inference on predicted data (IPD) using recent methods, where for a sub-
     set of the data, the outcomes have been predicted by an algorithm. Provides a wrapper func-
     tion with specified defaults for the type of model and method to be used for estimation and infer-
     ence. Further provides methods for tidying and summarizing re-
     sults. Salerno et al., (2024) <doi:10.48550/arXiv.2410.09665>.
License MIT + file LICENSE
URL https://github.com/ipd-tools/ipd, https://ipd-tools.github.io/ipd/
BugReports https://github.com/ipd-tools/ipd/issues
Depends R (>= 3.5.0)
Imports caret, gam, generics, ranger, splines, stats, MASS,
     randomForest
Suggests knitr, patchwork, rmarkdown, spelling, testthat (>= 3.0.0),
     tidyverse
VignetteBuilder knitr
Config/testthat/edition 3
Encoding UTF-8
RoxygenNote 7.3.2
Language en-US
NeedsCompilation no
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# Repository CRAN

**Date/Publication** 2025-01-07 16:10:02 UTC

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Calculation of the matrix A based on single dataset

# Description

Α

A function for the calculation of the matrix A based on single dataset

# Usage

```
A(X, Y, quant = NA, theta, method)
```

# Arguments

| Χ      | Array or data.frame containing covariates   |
|--------|---|
| Υ      | Array or data.frame of outcomes   |
| quant  | quantile for quantile estimation  |
| theta  | parameter theta   |
| method | indicates the method to be used for M-estimation. Options include "mean", "quantile", "ols", "logistic", and "poisson". |

# Value

matrix A based on single dataset

4 augment.ipd

augment.ipd

Augment Data from an IPD Fit

## **Description**

Augments the data used for an IPD method/model fit with additional information about each observation.

# Usage

```
## S3 method for class 'ipd'
augment(x, data = x$data_u, ...)
```

# **Arguments**

x An object of class ipd.data The data. frame used to fit the model. Default is x\$data.... Additional arguments to be passed to the augment function.

#### Value

A data.frame containing the original data along with fitted values and residuals.

```
#-- Generate Example Data
set.seed(2023)
dat <- simdat(n = c(300, 300, 300), effect = 1, sigma_Y = 1)
head(dat)
formula <- Y - f ~ X1
#-- Fit IPD
fit <- ipd(formula, method = "postpi_analytic", model = "ols",
    data = dat, label = "set_label")
#-- Augment Data
augmented_df <- augment(fit)
head(augmented_df)</pre>
```

calc\_lhat\_glm 5

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Estimate PPI++ Power Tuning Parameter

#### **Description**

Calculates the optimal value of lhat for the prediction-powered confidence interval for GLMs.

# Usage

```
calc_lhat_glm(
  grads,
  grads_hat,
  grads_hat_unlabeled,
  inv_hessian,
  coord = NULL,
  clip = FALSE
)
```

# Arguments

grads (matrix): n x p matrix gradient of the loss function with respect to the parameter

evaluated at the labeled data.

grads\_hat (matrix): n x p matrix gradient of the loss function with respect to the model

parameter evaluated using predictions on the labeled data.

grads\_hat\_unlabeled

(matrix): N x p matrix gradient of the loss function with respect to the parameter

evaluated using predictions on the unlabeled data.

inv\_hessian (matrix): p x p matrix inverse of the Hessian of the loss function with respect to

the parameter.

coord (int, optional): Coordinate for which to optimize 1hat. If None, it optimizes the

total variance over all coordinates. Must be in (1, ..., d) where d is the shape of

the estimand.

clip (boolean, optional): Whether to clip the value of lhat to be non-negative. De-

faults to False.

#### Value

```
(float): Optimal value of 1hat in [0,1].
```

```
dat <- simdat(model = "ols")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])</pre>
```

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```
Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

est <- ppi_plusplus_ols_est(X_l, Y_l, f_l, X_u, f_u)

stats <- ols_get_stats(est, X_l, Y_l, f_l, X_u, f_u)

calc_lhat_glm(stats$grads, stats$grads_hat, stats$grads_hat_unlabeled,

stats$inv_hessian, coord = NULL, clip = FALSE)</pre>
```

compute\_cdf

Empirical CDF of the Data

#### Description

Computes the empirical CDF of the data.

## Usage

```
compute_cdf(Y, grid, w = NULL)
```

#### **Arguments**

```
Y (matrix): n x 1 matrix of observed data.
grid (matrix): Grid of values to compute the CDF at.
w (vector, optional): n-vector of sample weights.
```

#### Value

(list): Empirical CDF and its standard deviation at the specified grid points.

```
Y <- c(1, 2, 3, 4, 5)
grid <- seq(0, 6, by = 0.5)
compute_cdf(Y, grid)</pre>
```

compute\_cdf\_diff 7

compute\_cdf\_diff

Empirical CDF Difference

# Description

Computes the difference between the empirical CDFs of the data and the predictions.

#### Usage

```
compute_cdf_diff(Y, f, grid, w = NULL)
```

#### **Arguments**

```
Y (matrix): n x 1 matrix of observed data.

f (matrix): n x 1 matrix of predictions.

grid (matrix): Grid of values to compute the CDF at.

w (vector, optional): n-vector of sample weights.
```

#### Value

(list): Difference between the empirical CDFs of the data and the predictions and its standard deviation at the specified grid points.

# **Examples**

```
Y <- c(1, 2, 3, 4, 5)

f <- c(1.1, 2.2, 3.3, 4.4, 5.5)

grid <- seq(0, 6, by = 0.5)

compute_cdf_diff(Y, f, grid)
```

est\_ini

Initial estimation

# Description

```
est_ini function for initial estimation
```

# Usage

```
est_ini(X, Y, quant = NA, method)
```

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#### **Arguments**

X Array or data.frame containing covariates

Y Array or data.frame of outcomes quant quantile for quantile estimation

method indicates the method to be used for M-estimation. Options include "mean",

"quantile", "ols", "logistic", and "poisson".

#### Value

initial estimation

glance.ipd

Glance at an IPD Fit

# **Description**

Glances at the IPD method/model fit, returning a one-row summary.

#### Usage

```
## S3 method for class 'ipd'
glance(x, ...)
```

#### **Arguments**

x An object of class ipd.

... Additional arguments to be passed to the glance function.

#### Value

A one-row data frame summarizing the IPD method/model fit.

```
#-- Generate Example Data
set.seed(2023)
dat <- simdat(n = c(300, 300, 300), effect = 1, sigma_Y = 1)
head(dat)
formula <- Y - f ~ X1
#-- Fit IPD
fit <- ipd(formula, method = "postpi_analytic", model = "ols",</pre>
```

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```
data = dat, label = "set_label")
#-- Glance Output
glance(fit)
```

ipd

Inference on Predicted Data (ipd)

#### **Description**

The main wrapper function to conduct ipd using various methods and models, and returns a list of fitted model components.

#### Usage

```
ipd(
  formula,
  method,
  model,
  data,
  label = NULL,
  unlabeled_data = NULL,
  seed = NULL,
  intercept = TRUE,
  alpha = 0.05,
  alternative = "two-sided",
  n_t = Inf,
  na_action = "na.fail",
  ...
)
```

#### **Arguments**

formula

An object of class formula: a symbolic description of the model to be fitted. Must be of the form  $Y - f \sim X$ , where Y is the name of the column corresponding to the observed outcome in the labeled data, f is the name of the column corresponding to the predicted outcome in both labeled and unlabeled data, and X corresponds to the features of interest (i.e., X = X1 + ... + Xp). See **1. Formula** in the **Details** below for more information.

method

The IPD method to be used for fitting the model. Must be one of "postpi\_analytic", "postpi\_boot", "ppi", "ppi\_plusplus", or "pspa". See **3. Method** in the **Details** below for more information.

model

The type of downstream inferential model to be fitted, or the parameter being estimated. Must be one of "mean", "quantile", "ols", "logistic", or "poisson". See **4. Model** in the **Details** below for more information.

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data A data. frame containing the variables in the model, either a stacked data frame

with a specific column identifying the labeled versus unlabeled observations (label), or only the labeled data set. Must contain columns for the observed outcomes (Y), the predicted outcomes (f), and the features (X) needed to specify

the formula. See 2. Data in the Details below for more information.

label A string, int, or logical specifying the column in the data that distinguishes

between the labeled and unlabeled observations. See the Details section for more information. If NULL, unlabeled\_data must be specified. See 2. Data

in the **Details** below for more information.

unlabeled\_data (optional) A data.frame of unlabeled data. If NULL, label must be specified.

Specifying both the label and unlabeled\_data arguments will result in an error message. If specified, must contain columns for the predicted outcomes (f), and the features (X) needed to specify the formula. See **2. Data** in the

**Details** below for more information.

seed (optional) An integer seed for random number generation.

intercept Logical. Should an intercept be included in the model? Default is TRUE.

alpha The significance level for confidence intervals. Default is 0.05.

alternative A string specifying the alternative hypothesis. Must be one of "two-sided",

"less", or "greater".

n\_t (integer, optional) Size of the dataset used to train the prediction function (neces-

sary for the "postpi\_analytic" and "postpi\_boot" methods if  $n_t < n_{X_1}$ .

Defaults to Inf.

na\_action (string, optional) How missing covariate data should be handled. Currently

"na.fail" and "na.omit" are accommodated. Defaults to "na.fail".

... Additional arguments to be passed to the fitting function. See the Details sec-

tion for more information. See 5. Auxiliary Arguments and 6. Other Argu-

ments in the **Details** below for more information.

#### **Details**

#### 1. Formula:

The ipd function uses one formula argument that specifies both the calibrating model (e.g., PostPI "relationship model", PPI "rectifier" model) and the inferential model. These separate models will be created internally based on the specific method called.

# 2. Data:

The data can be specified in two ways:

- 1. Single data argument (data) containing a stacked data. frame and a label identifier (label).
- 2. Two data arguments, one for the labeled data (data) and one for the unlabeled data (unlabeled\_data).

For option (1), provide one data argument (data) which contains a stacked data.frame with both the unlabeled and labeled data and a label argument that specifies the column identifying the labeled versus the unlabeled observations in the stacked data.frame (e.g., label = "set\_label" if the column "set\_label" in the stacked data denotes which set an observation belongs to).

NOTE: Labeled data identifiers can be:

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```
String "1", "lab", "label", "labeled", "labelled", "tst", "test", "true"
```

Logical TRUE

**Factor** Non-reference category (i.e., binary 1)

Unlabeled data identifiers can be:

```
String "u", "unlab", "unlabeled", "unlabelled", "val", "validation", "false"
```

Logical FALSE

**Factor** Non-reference category (i.e., binary 0)

For option (2), provide separate data arguments for the labeled data set (data) and the unlabeled data set (unlabeled\_data). If the second argument is provided, the function ignores the label identifier and assumes the data provided are not stacked.

NOTE: Not all columns in data or unlabeled\_data may be used unless explicitly referenced in the formula argument or in the label argument (if the data are passed as one stacked data frame).

#### 3. Method:

Use the method argument to specify the fitting method:

#### 4. Model:

Use the model argument to specify the type of downstream inferential model or parameter to be estimated:

The ipd wrapper function will concatenate the method and model arguments to identify the required helper function, following the naming convention "method\_model".

# 5. Auxiliary Arguments:

The wrapper function will take method-specific auxiliary arguments (e.g., q for the quantile estimation models) and pass them to the helper function through the "..." with specified defaults for simplicity.

#### 6. Other Arguments:

All other arguments that relate to all methods (e.g., alpha, ci.type), or other method-specific arguments, will have defaults.

<sup>&</sup>quot;postpi\_analytic" Wang et al. (2020) Post-Prediction Inference (PostPI) Analytic Correction

<sup>&</sup>quot;postpi\_boot" Wang et al. (2020) Post-Prediction Inference (PostPI) Bootstrap Correction

<sup>&</sup>quot;ppi" Angelopoulos et al. (2023) Prediction-Powered Inference (PPI)

<sup>&</sup>quot;ppi\_plusplus" Angelopoulos et al. (2023) PPI++

<sup>&</sup>quot;pspa" Miao et al. (2023) Assumption-Lean and Data-Adaptive Post-Prediction Inference (PSPA)

<sup>&</sup>quot;mean" Mean value of a continuous outcome

<sup>&</sup>quot;quantile" qth quantile of a continuous outcome

<sup>&</sup>quot;ols" Linear regression coefficients for a continuous outcome

<sup>&</sup>quot;logistic" Logistic regression coefficients for a binary outcome

<sup>&</sup>quot;poisson" Poisson regression coefficients for a count outcome

ipd ipd

#### Value

a summary of model output.

A list containing the fitted model components:

coefficients Estimated coefficients of the model

se Standard errors of the estimated coefficients

ci Confidence intervals for the estimated coefficients

**formula** The formula used to fit the ipd model.

data The data frame used for model fitting.

**method** The method used for model fitting.

model The type of model fitted.

intercept Logical. Indicates if an intercept was included in the model.

fit Fitted model object containing estimated coefficients, standard errors, confidence intervals, and additional method-specific output.

... Additional output specific to the method used.

link\_grad 13

```
#-- PPI++ (Angelopoulos et al., 2023)
ipd(formula, method = "ppi_plusplus", model = "ols",
    data = dat, label = "set_label")
#-- PSPA (Miao et al., 2023)
ipd(formula, method = "pspa", model = "ols",
    data = dat, label = "set_label")
```

link\_grad

Gradient of the link function

# **Description**

link\_grad function for gradient of the link function

## Usage

```
link_grad(t, method)
```

# Arguments

t

method

indicates the method to be used for M-estimation. Options include "mean", "quantile", "ols", "logistic", and "poisson".

#### Value

gradient of the link function

link\_Hessian

Hessians of the link function

# Description

link\_Hessian function for Hessians of the link function

# Usage

```
link_Hessian(t, method)
```

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#### **Arguments**

t t

method

indicates the method to be used for M-estimation. Options include "mean", "quantile", "ols", "logistic", and "poisson".

#### Value

Hessians of the link function

log1pexp

Log1p Exponential

# Description

Computes the natural logarithm of 1 plus the exponential of the input, to handle large inputs.

# Usage

log1pexp(x)

# **Arguments**

Х

(vector): A numeric vector of inputs.

## Value

(vector): A numeric vector where each element is the result of log(1 + exp(x)).

```
x <- c(-1, 0, 1, 10, 100)
log1pexp(x)
```

logistic\_get\_stats 15

#### **Description**

Computes the statistics needed for the logstic regression-based prediction-powered inference.

#### Usage

```
logistic_get_stats(
    est,
    X_1,
    Y_1,
    f_1,
    X_u,
    f_u,
    w_1 = NULL,
    w_u = NULL,
    use_u = TRUE
)
```

#### **Arguments**

| est   | (vector): Point estimates of the coefficients.                 |
|-------|--|
| X_1   | (matrix): Covariates for the labeled data set.                 |
| Y_1   | (vector): Labels for the labeled data set.                     |
| f_1   | (vector): Predictions for the labeled data set.                |
| X_u   | (matrix): Covariates for the unlabeled data set.               |
| f_u   | (vector): Predictions for the unlabeled data set.              |
| w_1   | (vector, optional): Sample weights for the labeled data set.   |
| w_u   | (vector, optional): Sample weights for the unlabeled data set. |
| use_u | (bool, optional): Whether to use the unlabeled data set.       |

# Value

(list): A list containing the following:

grads (matrix): n x p matrix gradient of the loss function with respect to the coefficients.

**grads\_hat** (matrix): n x p matrix gradient of the loss function with respect to the coefficients, evaluated using the labeled predictions.

**grads\_hat\_unlabeled** (matrix): N x p matrix gradient of the loss function with respect to the coefficients, evaluated using the unlabeled predictions.

**inv\_hessian** (matrix): p x p matrix inverse Hessian of the loss function with respect to the coefficients.

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#### **Examples**

```
dat <- simdat(model = "logistic")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

est <- ppi_plusplus_logistic_est(X_l, Y_l, f_l, X_u, f_u)

stats <- logistic_get_stats(est, X_l, Y_l, f_l, X_u, f_u)</pre>
```

mean\_psi

Sample expectation of psi

# Description

mean\_psi function for sample expectation of psi

#### Usage

```
mean_psi(X, Y, theta, quant = NA, method)
```

#### **Arguments**

X Array or data.frame containing covariates

Y Array or data.frame of outcomes

theta parameter theta

quantile for quantile estimation

method indicates the method to be used for M-estimation. Options include "mean",

"quantile", "ols", "logistic", and "poisson".

#### Value

sample expectation of psi

mean\_psi\_pop 17

| mean_psi_pop | Sample expectation of PSPA psi |  |
|--------------|--------------------------------|--|
|--------------|--------------------------------|--|

# Description

 ${\tt mean\_psi\_pop\ function\ for\ sample\ expectation\ of\ PSPA\ psi}$ 

# Usage

```
mean_psi_pop(
  X_lab,
  X_unlab,
  Y_lab,
  Yhat_lab,
  Yhat_unlab,
  w,
  theta,
  quant = NA,
  method
)
```

# Arguments

| X_lab      | Array or data.frame containing observed covariates in labeled data.   |
|------------|---|
| X_unlab    | Array or data.frame containing observed or predicted covariates in unlabeled data.                                      |
| Y_lab      | Array or data.frame of observed outcomes in labeled data.   |
| Yhat_lab   | Array or data.frame of predicted outcomes in labeled data.  |
| Yhat_unlab | Array or data.frame of predicted outcomes in unlabeled data.  |
| W          | weights vector PSPA linear regression (d-dimensional, where d equals the number of covariates).                         |
| theta      | parameter theta   |
| quant      | quantile for quantile estimation  |
| method     | indicates the method to be used for M-estimation. Options include "mean", "quantile", "ols", "logistic", and "poisson". |

# Value

sample expectation of PSPA psi

ols\_get\_stats

ols

Ordinary Least Squares

# **Description**

Computes the ordinary least squares coefficients.

# Usage

```
ols(X, Y, return_se = FALSE)
```

# **Arguments**

```
    X (matrix): n x p matrix of covariates.
    Y (vector): p-vector of outcome values.
    return_se (bool, optional): Whether to return the standard errors of the coefficients.
```

## Value

```
(list): A list containing the following:
```

```
theta (vector): p-vector of ordinary least squares estimates of the coefficients.
se (vector): If return_se == TRUE, return the p-vector of standard errors of the coefficients.
```

# **Examples**

```
n <- 1000
X <- rnorm(n, 1, 1)
Y <- X + rnorm(n, 0, 1)
ols(X, Y, return_se = TRUE)</pre>
```

 $ols\_get\_stats$ 

OLS Gradient and Hessian

# **Description**

Computes the statistics needed for the OLS-based prediction-powered inference.

ols\_get\_stats 19

#### Usage

```
ols_get_stats(
    est,
    X_1,
    Y_1,
    f_1,
    X_u,
    f_u,
    w_1 = NULL,
    w_u = NULL,
    use_u = TRUE
)
```

## **Arguments**

| est   | (vector): Point estimates of the coefficients.                 |
|-------|--|
| X_1   | (matrix): Covariates for the labeled data set.                 |
| Y_1   | (vector): Labels for the labeled data set.                     |
| f_1   | (vector): Predictions for the labeled data set.                |
| X_u   | (matrix): Covariates for the unlabeled data set.               |
| f_u   | (vector): Predictions for the unlabeled data set.              |
| w_1   | (vector, optional): Sample weights for the labeled data set.   |
| w_u   | (vector, optional): Sample weights for the unlabeled data set. |
| use_u | (boolean, optional): Whether to use the unlabeled data set.    |

# Value

(list): A list containing the following:

grads (matrix): n x p matrix gradient of the loss function with respect to the coefficients.

**grads\_hat** (matrix): n x p matrix gradient of the loss function with respect to the coefficients, evaluated using the labeled predictions.

**grads\_hat\_unlabeled** (matrix): N x p matrix gradient of the loss function with respect to the coefficients, evaluated using the unlabeled predictions.

**inv\_hessian** (matrix): p x p matrix inverse Hessian of the loss function with respect to the coefficients.

```
dat <- simdat(model = "ols")
form <- Y - f ~ X1

X_1 <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_1 <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)
```

optim\_est

```
f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

est <- ppi_plusplus_ols_est(X_l, Y_l, f_l, X_u, f_u)

stats <- ols_get_stats(est, X_l, Y_l, f_l, X_u, f_u, use_u = TRUE)</pre>
```

optim\_est

One-step update for obtaining estimator

## **Description**

optim\_est function for One-step update for obtaining estimator

## Usage

```
optim_est(
   X_lab,
   X_unlab,
   Y_lab,
   Yhat_lab,
   Yhat_unlab,
   w,
   theta,
   quant = NA,
   method
)
```

# Arguments

| X_lab      | Array or data.frame containing observed covariates in labeled data.   |
|------------|---|
| X_unlab    | Array or data.frame containing observed or predicted covariates in unlabeled data.                                      |
| Y_lab      | Array or data.frame of observed outcomes in labeled data.   |
| Yhat_lab   | Array or data.frame of predicted outcomes in labeled data.  |
| Yhat_unlab | Array or data.frame of predicted outcomes in unlabeled data.  |
| W          | weights vector PSPA linear regression (d-dimensional, where d equals the number of covariates).                         |
| theta      | parameter theta   |
| quant      | quantile for quantile estimation  |
| method     | indicates the method to be used for M-estimation. Options include "mean", "quantile", "ols", "logistic", and "poisson". |

optim\_weights 21

## Value

estimator

optim\_weights

One-step update for obtaining the weight vector

## **Description**

optim\_weights function for One-step update for obtaining estimator

# Usage

```
optim_weights(
  X_lab,
  X_unlab,
  Y_lab,
  Yhat_lab,
  Yhat_unlab,
  w,
  theta,
  quant = NA,
  method
)
```

# Arguments

X\_lab Array or data.frame containing observed covariates in labeled data.

X\_unlab Array or data.frame containing observed or predicted covariates in unlabeled

data

Y\_lab Array or data.frame of observed outcomes in labeled data.

Yhat\_lab Array or data.frame of predicted outcomes in labeled data.

Yhat\_unlab Array or data.frame of predicted outcomes in unlabeled data.

w weights vector PSPA linear regression (d-dimensional, where d equals the num-

ber of covariates).

theta parameter theta

quantile for quantile estimation

method indicates the method to be used for M-estimation. Options include "mean",

"quantile", "ols", "logistic", and "poisson".

# Value

weights

22 postpi\_analytic\_ols

#### **Description**

Helper function for PostPI OLS estimation (analytic correction)

## Usage

```
postpi_analytic_ols(X_1, Y_1, f_1, X_u, f_u, scale_se = TRUE, n_t = Inf)
```

# **Arguments**

| X_1      | (matrix): n x p matrix of covariates in the labeled data.   |
|----------|---|
| Y_1      | (vector): n-vector of labeled outcomes.   |
| f_1      | (vector): n-vector of predictions in the labeled data.  |
| X_u      | (matrix): N x p matrix of covariates in the unlabeled data.   |
| f_u      | (vector): N-vector of predictions in the unlabeled data.  |
| scale_se | (boolean): Logical argument to scale relationship model error variance. Defaults to TRUE; FALSE option is retained for posterity. |
| n_t      | (integer, optional) Size of the dataset used to train the prediction function (necessary if $n_t < nrow(X_1)$ . Defaults to Inf.  |

#### **Details**

Methods for correcting inference based on outcomes predicted by machine learning (Wang et al., 2020) https://www.pnas.org/doi/abs/10.1073/pnas.2001238117

# Value

A list of outputs: estimate of the inference model parameters and corresponding standard error estimate.

```
dat <- simdat(model = "ols")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])</pre>
```

postpi\_boot\_logistic 23

```
f_u \leftarrow dat[dat\$set_label == "unlabeled", all.vars(form)[2]] > matrix(ncol = 1)
postpi_analytic_ols(X_l, Y_l, f_l, X_u, f_u)
```

```
postpi_boot_logistic PostPI Logistic Regression (Bootstrap Correction)
```

# Description

Helper function for PostPI logistic regression (bootstrap correction)

## Usage

```
postpi_boot_logistic(
    X_1,
    Y_1,
    f_1,
    X_u,
    f_u,
    nboot = 100,
    se_type = "par",
    seed = NULL
)
```

# Arguments

| X_1     | (matrix): n x p matrix of covariates in the labeled data.   |
|---------|---|
| Y_1     | (vector): n-vector of labeled outcomes.   |
| f_1     | (vector): n-vector of predictions in the labeled data.  |
| X_u     | (matrix): N x p matrix of covariates in the unlabeled data.   |
| f_u     | (vector): N-vector of predictions in the unlabeled data.  |
| nboot   | (integer): Number of bootstrap samples. Defaults to 100.  |
| se_type | (string): Which method to calculate the standard errors. Options include "par" (parametric) or "npar" (nonparametric). Defaults to "par". |
| seed    | (optional) An integer seed for random number generation.  |
|         |   |

#### **Details**

Methods for correcting inference based on outcomes predicted by machine learning (Wang et al., 2020) https://www.pnas.org/doi/abs/10.1073/pnas.2001238117

#### Value

A list of outputs: estimate of inference model parameters and corresponding standard error based on both parametric and non-parametric bootstrap methods.

postpi\_boot\_ols

## **Examples**

```
dat <- simdat(model = "logistic")

form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

postpi_boot_logistic(X_l, Y_l, f_l, X_u, f_u, nboot = 200)
```

postpi\_boot\_ols

PostPI OLS (Bootstrap Correction)

## **Description**

Helper function for PostPI OLS estimation (bootstrap correction)

#### Usage

```
postpi_boot_ols(
   X_l,
   Y_l,
   f_l,
   X_u,
   f_u,
   nboot = 100,
   se_type = "par",
   rel_func = "lm",
   scale_se = TRUE,
   n_t = Inf,
   seed = NULL
)
```

# Arguments

```
X_1 (matrix): n x p matrix of covariates in the labeled data.
```

Y\_l (vector): n-vector of labeled outcomes.

f\_1 (vector): n-vector of predictions in the labeled data.

X\_u (matrix): N x p matrix of covariates in the unlabeled data.

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| f_u      | (vector): N-vector of predictions in the unlabeled data.  |
|----------|---|
| nboot    | (integer): Number of bootstrap samples. Defaults to 100.  |
| se_type  | (string): Which method to calculate the standard errors. Options include "par" (parametric) or "npar" (nonparametric). Defaults to "par".                                 |
| rel_func | (string): Method for fitting the relationship model. Options include "lm" (linear model), "rf" (random forest), and "gam" (generalized additive model). Defaults to "lm". |
| scale_se | (boolean): Logical argument to scale relationship model error variance. Defaults to TRUE; FALSE option is retained for posterity.   |
| n_t      | (integer, optional) Size of the dataset used to train the prediction function (necessary if $n_t < n_{to}(X_1)$ . Defaults to Inf.  |
| seed     | (optional) An integer seed for random number generation.  |

#### **Details**

Methods for correcting inference based on outcomes predicted by machine learning (Wang et al., 2020) https://www.pnas.org/doi/abs/10.1073/pnas.2001238117

#### Value

A list of outputs: estimate of inference model parameters and corresponding standard error based on both parametric and non-parametric bootstrap methods.

```
dat <- simdat(model = "ols")
form <- Y - f ~ X1

X_1 <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_1 <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_1 <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

postpi_boot_ols(X_1, Y_1, f_1, X_u, f_u, nboot = 200)
```

ppi\_logistic

| ppi_logistic PI | PI Logistic Regression |
|-----------------|------------------------|
|-----------------|------------------------|

## **Description**

Helper function for PPI logistic regression

## Usage

```
ppi_logistic(X_1, Y_1, f_1, X_u, f_u, opts = NULL)
```

# **Arguments**

| X_1  | (matrix): n x p matrix of covariates in the labeled data.                   |
|------|---|
| Y_1  | (vector): n-vector of labeled outcomes.                                     |
| f_l  | (vector): n-vector of predictions in the labeled data.                      |
| X_u  | (matrix): N x p matrix of covariates in the unlabeled data.                 |
| f_u  | (vector): N-vector of predictions in the unlabeled data.                    |
| opts | (list, optional): Options to pass to the optimizer. See ?optim for details. |

#### **Details**

Prediction Powered Inference (Angelopoulos et al., 2023) https://www.science.org/doi/10.1126/science.adi6000

#### Value

```
est (vector): vector of PPI logistic regression coefficient estimates.

se (vector): vector of standard errors of the coefficients.

rectifier_est (vector): vector of the rectifier logistic regression coefficient estimates.

var_u (matrix): covariance matrix for the gradients in the unlabeled data.

var_l (matrix): covariance matrix for the gradients in the labeled data.

grads (matrix): matrix of gradients for the labeled data.

grads_hat_unlabeled (matrix): matrix of predicted gradients for the unlabeled data.

grads_hat (matrix): matrix of predicted gradients for the labeled data.

inv_hessian (matrix): inverse Hessian matrix.
```

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#### **Examples**

```
dat <- simdat(model = "logistic")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_logistic(X_l, Y_l, f_l, X_u, f_u)
```

ppi\_mean

PPI Mean Estimation

## **Description**

Helper function for PPI mean estimation

# Usage

```
ppi_mean(Y_1, f_1, f_u, alpha = 0.05, alternative = "two-sided")
```

## Arguments

| Y_1         | (vector): n-vector of labeled outcomes.  |
|-------------|--|
| f_1         | (vector): n-vector of predictions in the labeled data.   |
| f_u         | (vector): N-vector of predictions in the unlabeled data.                                       |
| alpha       | (scalar): type I error rate for hypothesis testing - values in $(0, 1)$ ; defaults to $0.05$ . |
| alternative | (string): Alternative hypothesis. Must be one of "two-sided", "less", or "greater".            |

#### **Details**

Prediction Powered Inference (Angelopoulos et al., 2023) https://www.science.org/doi/10. 1126/science.adi6000

#### Value

tuple: Lower and upper bounds of the prediction-powered confidence interval for the mean.

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## **Examples**

```
dat <- simdat(model = "mean")
form <- Y - f ~ 1
Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)
f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)
f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)
ppi_mean(Y_l, f_l, f_u)
```

ppi\_ols

PPI OLS

# Description

Helper function for prediction-powered inference for OLS estimation

# Usage

```
ppi_ols(X_1, Y_1, f_1, X_u, f_u, w_1 = NULL, w_u = NULL)
```

## **Arguments**

| X_1 | (matrix): n x p matrix of covariates in the labeled data.                                     |
|-----|---|
| Y_1 | (vector): n-vector of labeled outcomes.   |
| f_1 | (vector): n-vector of predictions in the labeled data.  |
| X_u | (matrix): N x p matrix of covariates in the unlabeled data.                                   |
| f_u | (vector): N-vector of predictions in the unlabeled data.                                      |
| w_1 | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.   |
| w_u | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones. |

#### **Details**

Prediction Powered Inference (Angelopoulos et al., 2023) https://www.science.org/doi/10.1126/science.adi6000

ppi\_plusplus\_logistic 29

## Value

```
(list): A list containing the following:
est (vector): vector of PPI OLS regression coefficient estimates.
se (vector): vector of standard errors of the coefficients.
rectifier_est (vector): vector of the rectifier OLS regression coefficient estimates.
```

#### **Examples**

```
dat <- simdat()
form <- Y - f ~ X1

X_1 <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_1 <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_1 <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_ols(X_1, Y_1, f_1, X_u, f_u)
```

```
ppi_plusplus_logistic PPI++ Logistic Regression
```

#### **Description**

Helper function for PPI++ logistic regression

#### Usage

```
ppi_plusplus_logistic(
   X_l,
   Y_l,
   f_l,
   X_u,
   f_u,
   lhat = NULL,
   coord = NULL,
   opts = NULL,
   w_l = NULL,
   w_u = NULL
)
```

| Arg | um | ents |
|-----|----|------|
|     |    |      |

| X_1   | (matrix): n x p matrix of covariates in the labeled data.  |
|-------|--|
| Y_1   | (vector): n-vector of labeled outcomes.  |
| f_1   | (vector): n-vector of predictions in the labeled data.   |
| X_u   | (matrix): N x p matrix of covariates in the unlabeled data.  |
| f_u   | (vector): N-vector of predictions in the unlabeled data.   |
| lhat  | (float, optional): Power-tuning parameter (see <a href="https://arxiv.org/abs/2311">https://arxiv.org/abs/2311</a> . 01453). The default value, NULL, will estimate the optimal value from the data. Setting lhat = 1 recovers PPI with no power tuning, and setting lhat = 0 recovers the classical point estimate. |
| coord | (int, optional): Coordinate for which to optimize 1hat = 1. If NULL, it optimizes the total variance over all coordinates. Must be in $(1,, d)$ where d is the dimension of the estimand.  |
| opts  | (list, optional): Options to pass to the optimizer. See ?optim for details.  |
| w_1   | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.  |
| w_u   | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.  |

#### **Details**

PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453

#### Value

```
est (vector): vector of PPI++ logistic regression coefficient estimates.
se (vector): vector of standard errors of the coefficients.
lambda (float): estimated power-tuning parameter.
rectifier_est (vector): vector of the rectifier logistic regression coefficient estimates.
var_u (matrix): covariance matrix for the gradients in the unlabeled data.
var_l (matrix): covariance matrix for the gradients in the labeled data.
grads (matrix): matrix of gradients for the labeled data.
grads_hat_unlabeled (matrix): matrix of predicted gradients for the unlabeled data.
grads_hat (matrix): matrix of predicted gradients for the labeled data.
inv_hessian (matrix): inverse Hessian matrix.
```

#### **Examples**

```
dat <- simdat(model = "logistic")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_plusplus_logistic(X_l, Y_l, f_l, X_u, f_u)
```

#### **Description**

Helper function for PPI++ logistic regression (point estimate)

## Usage

```
ppi_plusplus_logistic_est(
   X_l,
   Y_l,
   f_l,
   X_u,
   f_u,
   lhat = NULL,
   coord = NULL,
   opts = NULL,
   w_l = NULL,
   w_u = NULL
)
```

# Arguments

```
    X_1 (matrix): n x p matrix of covariates in the labeled data.
    Y_1 (vector): n-vector of labeled outcomes.
    f_1 (vector): n-vector of predictions in the labeled data.
    X_u (matrix): N x p matrix of covariates in the unlabeled data.
```

| f_u   | (vector): N-vector of predictions in the unlabeled data.  |
|-------|---|
| lhat  | (float, optional): Power-tuning parameter (see <a href="https://arxiv.org/abs/2311.01453">https://arxiv.org/abs/2311.01453</a> ). The default value, NULL, will estimate the optimal value from the data. Setting lhat = 1 recovers PPI with no power tuning, and setting lhat = 0 recovers the classical point estimate. |
| coord | (int, optional): Coordinate for which to optimize $1$ hat = 1. If NULL, it optimizes the total variance over all coordinates. Must be in $(1,, d)$ where d is the dimension of the estimand.  |
| opts  | (list, optional): Options to pass to the optimizer. See ?optim for details.   |
| w_1   | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.   |
| w_u   | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.   |

## **Details**

PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453

#### Value

(vector): vector of prediction-powered point estimates of the logistic regression coefficients.

```
dat <- simdat(model = "logistic")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_plusplus_logistic_est(X_l, Y_l, f_l, X_u, f_u)
```

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ppi\_plusplus\_mean

PPI++ Mean Estimation

# Description

Helper function for PPI++ mean estimation

# Usage

```
ppi_plusplus_mean(
    Y_l,
    f_l,
    f_u,
    alpha = 0.05,
    alternative = "two-sided",
    lhat = NULL,
    coord = NULL,
    w_l = NULL,
    w_u = NULL
)
```

# Arguments

| Y_1         | (vector): n-vector of labeled outcomes.  |
|-------------|--|
| f_1         | (vector): n-vector of predictions in the labeled data.   |
| f_u         | (vector): N-vector of predictions in the unlabeled data.   |
| alpha       | (scalar): type I error rate for hypothesis testing - values in $(0, 1)$ ; defaults to $0.05$ .   |
| alternative | (string): Alternative hypothesis. Must be one of "two-sided", "less", or "greater".  |
| lhat        | (float, optional): Power-tuning parameter (see <a href="https://arxiv.org/abs/2311">https://arxiv.org/abs/2311</a> . 01453). The default value, NULL, will estimate the optimal value from the data. Setting lhat = 1 recovers PPI with no power tuning, and setting lhat = 0 recovers the classical point estimate. |
| coord       | (int, optional): Coordinate for which to optimize $1hat = 1$ . If NULL, it optimizes the total variance over all coordinates. Must be in $(1,, d)$ where d is the dimension of the estimand.   |
| w_1         | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.  |
| w_u         | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.  |

# **Details**

PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453

#### Value

tuple: Lower and upper bounds of the prediction-powered confidence interval for the mean.

# **Examples**

```
dat <- simdat(model = "mean")
form <- Y - f ~ 1

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_plusplus_mean(Y_l, f_l, f_u)
```

## **Description**

Helper function for PPI++ mean estimation (point estimate)

#### Usage

```
ppi_plusplus_mean_est(
    Y_l,
    f_l,
    f_u,
    lhat = NULL,
    coord = NULL,
    w_l = NULL,
    w_u = NULL
)
```

#### **Arguments**

```
Y_1 (vector): n-vector of labeled outcomes.

f_1 (vector): n-vector of predictions in the labeled data.

f_u (vector): N-vector of predictions in the unlabeled data.

lhat (float, optional): Power-tuning parameter (see https://arxiv.org/abs/2311.
01453). The default value, NULL, will estimate the optimal value from the data.

Setting lhat = 1 recovers PPI with no power tuning, and setting lhat = 0 recovers the classical point estimate.
```

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| coord | (int, optional): Coordinate for which to optimize 1hat = 1. If NULL, it optimizes the total variance over all coordinates. Must be in (1,, d) where d is the dimension of the estimand. |
|-------|---|
| w_1   | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.   |
| w_u   | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.   |

#### **Details**

```
PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453
```

## Value

float or ndarray: Prediction-powered point estimate of the mean.

## **Examples**

```
dat <- simdat(model = "mean")
form <- Y - f ~ 1
Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)
f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)
f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)
ppi_plusplus_mean_est(Y_l, f_l, f_u)
```

```
ppi_plusplus_ols PPI++OLS
```

## **Description**

Helper function for PPI++ OLS estimation

# Usage

```
ppi_plusplus_ols(
    X_1,
    Y_1,
    f_1,
    X_u,
    f_u,
    lhat = NULL,
```

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```
coord = NULL,
w_1 = NULL,
w_u = NULL
)
```

#### **Arguments**

| X_1   | (matrix): n x p matrix of covariates in the labeled data.   |
|-------|---|
| Y_1   | (vector): n-vector of labeled outcomes.   |
| f_1   | (vector): n-vector of predictions in the labeled data.  |
| X_u   | (matrix): N x p matrix of covariates in the unlabeled data.   |
| f_u   | (vector): N-vector of predictions in the unlabeled data.  |
| lhat  | (float, optional): Power-tuning parameter (see <a href="https://arxiv.org/abs/2311">https://arxiv.org/abs/2311</a> .  01453). The default value, NULL, will estimate the optimal value from the data. Setting lhat = 1 recovers PPI with no power tuning, and setting lhat = 0 recovers the classical point estimate. |
| coord | (int, optional): Coordinate for which to optimize $1hat = 1$ . If NULL, it optimizes the total variance over all coordinates. Must be in $(1,, d)$ where d is the dimension of the estimand.  |
| w_1   | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.   |
| w_u   | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.   |

# **Details**

PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453

# Value

```
est (vector): vector of PPI++ OLS regression coefficient estimates.
se (vector): vector of standard errors of the coefficients.
lambda (float): estimated power-tuning parameter.
rectifier_est (vector): vector of the rectifier OLS regression coefficient estimates.
var_u (matrix): covariance matrix for the gradients in the unlabeled data.
var_l (matrix): covariance matrix for the gradients in the labeled data.
grads (matrix): matrix of gradients for the labeled data.
grads_hat_unlabeled (matrix): matrix of predicted gradients for the unlabeled data.
grads_hat (matrix): matrix of predicted gradients for the labeled data.
inv_hessian (matrix): inverse Hessian matrix.
```

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#### **Examples**

```
dat <- simdat(model = "ols")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_plusplus_ols(X_l, Y_l, f_l, X_u, f_u)
```

## **Description**

Helper function for PPI++ OLS estimation (point estimate)

#### Usage

```
ppi_plusplus_ols_est(
    X_1,
    Y_1,
    f_1,
    X_u,
    f_u,
    lhat = NULL,
    coord = NULL,
    w_1 = NULL,
    w_u = NULL
)
```

# **Arguments**

```
X_1 (matrix): n x p matrix of covariates in the labeled data.
Y_1 (vector): n-vector of labeled outcomes.
f_1 (vector): n-vector of predictions in the labeled data.
X_u (matrix): N x p matrix of covariates in the unlabeled data.
f_u (vector): N-vector of predictions in the unlabeled data.
```

| lhat  | (float, optional): Power-tuning parameter (see https://arxiv.org/abs/2311. 01453). The default value, NULL, will estimate the optimal value from the data. Setting lhat = 1 recovers PPI with no power tuning, and setting lhat = 0 recovers the classical point estimate. |
|-------|--|
| coord | (int, optional): Coordinate for which to optimize $lhat = 1$ . If NULL, it optimizes the total variance over all coordinates. Must be in $(1,, d)$ where d is the dimension of the estimand.   |
| w_1   | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.  |
| w_u   | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.  |

## **Details**

PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453

#### Value

(vector): vector of prediction-powered point estimates of the OLS coefficients.

## **Examples**

```
dat <- simdat(model = "ols")
form <- Y - f ~ X1

X_1 <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_1 <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_1 <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_plusplus_ols_est(X_1, Y_1, f_1, X_u, f_u)
```

```
ppi_plusplus_quantile PPI++ Quantile Estimation
```

## Description

Helper function for PPI++ quantile estimation

## Usage

```
ppi_plusplus_quantile(
  Y_l,
  f_l,
  f_u,
  q,
  alpha = 0.05,
  exact_grid = FALSE,
  w_l = NULL,
  w_u = NULL
)
```

## **Arguments**

| Y_1        | (vector): n-vector of labeled outcomes.   |
|------------|---|
| f_1        | (vector): n-vector of predictions in the labeled data.  |
| f_u        | (vector): N-vector of predictions in the unlabeled data.  |
| q          | (float): Quantile to estimate. Must be in the range (0, 1).   |
| alpha      | (scalar): type I error rate for hypothesis testing - values in $(0, 1)$ ; defaults to $0.05$ .  |
| exact_grid | (bool, optional): Whether to compute the exact solution (TRUE) or an approximate solution based on a linearly spaced grid of 5000 values (FALSE). |
| w_1        | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.   |
| w_u        | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.   |

## **Details**

```
PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453
```

## Value

tuple: Lower and upper bounds of the prediction-powered confidence interval for the quantile.

```
dat <- simdat(model = "quantile")
form <- Y - f ~ X1

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)
```

```
ppi_plusplus_quantile(Y_l, f_l, f_u, q = 0.5)
```

# Description

Helper function for PPI++ quantile estimation (point estimate)

# Usage

```
ppi_plusplus_quantile_est(
   Y_l,
   f_l,
   f_u,
   q,
   exact_grid = FALSE,
   w_l = NULL,
   w_u = NULL
)
```

## **Arguments**

| Y_1        | (vector): n-vector of labeled outcomes.   |
|------------|---|
| f_1        | (vector): n-vector of predictions in the labeled data.  |
| f_u        | (vector): N-vector of predictions in the unlabeled data.  |
| q          | (float): Quantile to estimate. Must be in the range (0, 1).   |
| exact_grid | (bool, optional): Whether to compute the exact solution (TRUE) or an approximate solution based on a linearly spaced grid of $5000$ values (FALSE). |
| w_1        | (ndarray, optional): Sample weights for the labeled data set. Defaults to a vector of ones.   |
| w_u        | (ndarray, optional): Sample weights for the unlabeled data set. Defaults to a vector of ones.   |
|            |   |

# **Details**

```
PPI++: Efficient Prediction Powered Inference (Angelopoulos et al., 2023) https://arxiv.org/abs/2311.01453
```

## Value

(float): Prediction-powered point estimate of the quantile.

ppi\_quantile 41

## **Examples**

```
dat <- simdat(model = "quantile")
form <- Y - f ~ 1
Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)
f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)
f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)
ppi_plusplus_quantile_est(Y_l, f_l, f_u, q = 0.5)
```

ppi\_quantile

PPI Quantile Estimation

## **Description**

Helper function for PPI quantile estimation

#### Usage

```
ppi_quantile(Y_1, f_1, f_u, q, alpha = 0.05, exact_grid = FALSE)
```

## **Arguments**

| Y_1        | (vector): n-vector of labeled outcomes.   |
|------------|---|
| f_1        | (vector): n-vector of predictions in the labeled data.  |
| f_u        | (vector): N-vector of predictions in the unlabeled data.  |
| q          | (float): Quantile to estimate. Must be in the range $(0, 1)$ .  |
| alpha      | (scalar): type I error rate for hypothesis testing - values in $(0, 1)$ ; defaults to $0.05$ .  |
| exact_grid | (bool, optional): Whether to compute the exact solution (TRUE) or an approximate solution based on a linearly spaced grid of 5000 values (FALSE). |

#### **Details**

Prediction Powered Inference (Angelopoulos et al., 2023) https://www.science.org/doi/10. 1126/science.adi6000

#### Value

tuple: Lower and upper bounds of the prediction-powered confidence interval for the quantile.

42 print.ipd

#### **Examples**

```
dat <- simdat(model = "quantile")
form <- Y - f ~ X1

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

ppi_quantile(Y_l, f_l, f_u, q = 0.5)
```

print.ipd

Print IPD Fit

## **Description**

Prints a brief summary of the IPD method/model combination.

## Usage

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

#### **Arguments**

x An object of class ipd.

... Additional arguments to be passed to the print function.

#### Value

The input x, invisibly.

```
#-- Generate Example Data
set.seed(2023)
dat <- simdat(n = c(300, 300, 300), effect = 1, sigma_Y = 1)
head(dat)
formula <- Y - f ~ X1
#-- Fit IPD</pre>
```

print.summary.ipd 43

```
fit <- ipd(formula, method = "postpi_analytic", model = "ols",
   data = dat, label = "set_label")
#-- Print Output
print(fit)</pre>
```

print.summary.ipd

Print Summary of IPD Fit

## **Description**

Prints a detailed summary of the IPD method/model combination.

## Usage

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

# Arguments

x An object of class summary.ipd.

... Additional arguments to be passed to the print function.

#### Value

The input x, invisibly.

```
#-- Generate Example Data
set.seed(2023)
dat <- simdat(n = c(300, 300, 300), effect = 1, sigma_Y = 1)
head(dat)
formula <- Y - f ~ X1
#-- Fit IPD
fit <- ipd(formula, method = "postpi_analytic", model = "ols",
    data = dat, label = "set_label")
#-- Summarize Output</pre>
```

pspa\_logistic

```
summ_fit <- summary(fit)
print(summ_fit)</pre>
```

psi

Estimating equation

## **Description**

psi function for estimating equation

## Usage

```
psi(X, Y, theta, quant = NA, method)
```

## **Arguments**

X Array or data.frame containing covariates

Y Array or data.frame of outcomes

theta parameter theta

quantile for quantile estimation

method indicates the method to be used for M-estimation. Options include "mean",

"quantile", "ols", "logistic", and "poisson".

#### Value

esimating equation

pspa\_logistic

PSPA Logistic Regression

# Description

Helper function for PSPA logistic regression

# Usage

```
pspa_logistic(X_l, Y_l, f_l, X_u, f_u, weights = NA, alpha = 0.05)
```

pspa\_mean 45

## **Arguments**

| X_1     | (matrix): n x p matrix of covariates in the labeled data.   |
|---------|---|
| Y_1     | (vector): n-vector of binary labeled outcomes.  |
| f_1     | (vector): n-vector of binary predictions in the labeled data.   |
| X_u     | (matrix): N x p matrix of covariates in the unlabeled data.   |
| f_u     | (vector): N-vector of binary predictions in the unlabeled data.   |
| weights | (array): p-dimensional array of weights vector for variance reduction. PSPA will estimate the weights if not specified. |
| alpha   | (scalar): type I error rate for hypothesis testing - values in (0, 1); defaults to 0.05                                 |

#### **Details**

Post-prediction adaptive inference (Miao et al. 2023) https://arxiv.org/abs/2311.14220

#### Value

A list of outputs: estimate of inference model parameters and corresponding standard error.

## **Examples**

```
dat <- simdat(model = "logistic")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

pspa_logistic(X_l, Y_l, f_l, X_u, f_u)
```

pspa\_mean

PSPA Mean Estimation

## **Description**

Helper function for PSPA mean estimation

## Usage

```
pspa_mean(Y_1, f_1, f_u, weights = NA, alpha = 0.05)
```

pspa\_ols

## **Arguments**

| Y_1     | (vector): n-vector of labeled outcomes.   |
|---------|---|
| f_1     | (vector): n-vector of predictions in the labeled data.  |
| f_u     | (vector): N-vector of predictions in the unlabeled data.  |
| weights | (array): 1-dimensional array of weights vector for variance reduction. PSPA will estimate the weights if not specified. |
| alpha   | (scalar): type I error rate for hypothesis testing - values in $(0, 1)$ ; defaults to $0.05$ .                          |

#### **Details**

Post-prediction adaptive inference (Miao et al., 2023) https://arxiv.org/abs/2311.14220

## Value

A list of outputs: estimate of inference model parameters and corresponding standard error.

## **Examples**

```
dat <- simdat(model = "mean")
form <- Y - f ~ 1
Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)
f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)
f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)
pspa_mean(Y_l, f_l, f_u)
```

pspa\_ols

PSPA OLS Estimation

# Description

Helper function for PSPA OLS for linear regression

## Usage

```
pspa_ols(X_1, Y_1, f_1, X_u, f_u, weights = NA, alpha = 0.05)
```

pspa\_poisson 47

## **Arguments**

| X_1     | (matrix): n x p matrix of covariates in the labeled data.   |
|---------|---|
| Y_1     | (vector): n-vector of labeled outcomes.   |
| f_1     | (vector): n-vector of predictions in the labeled data.  |
| X_u     | (matrix): N x p matrix of covariates in the unlabeled data.   |
| f_u     | (vector): N-vector of predictions in the unlabeled data.  |
| weights | (array): p-dimensional array of weights vector for variance reduction. PSPA will estimate the weights if not specified. |
| alpha   | (scalar): type I error rate for hypothesis testing - values in (0, 1); defaults to 0.05.                                |

#### **Details**

Post-prediction adaptive inference (Miao et al. 2023) https://arxiv.org/abs/2311.14220

#### Value

A list of outputs: estimate of inference model parameters and corresponding standard error.

## **Examples**

```
dat <- simdat(model = "ols")
form <- Y - f ~ X1

X_1 <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_1 <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_1 <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

pspa_ols(X_1, Y_1, f_1, X_u, f_u)
```

pspa\_poisson

PSPA Poisson Regression

# Description

Helper function for PSPA Poisson regression

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#### Usage

```
pspa_poisson(X_1, Y_1, f_1, X_u, f_u, weights = NA, alpha = 0.05)
```

## **Arguments**

| X_1     | (matrix): n x p matrix of covariates in the labeled data.   |
|---------|---|
| Y_1     | (vector): n-vector of count labeled outcomes.   |
| f_1     | (vector): n-vector of binary predictions in the labeled data.   |
| X_u     | (matrix): N x p matrix of covariates in the unlabeled data.   |
| f_u     | (vector): N-vector of binary predictions in the unlabeled data.   |
| weights | (array): p-dimensional array of weights vector for variance reduction. PSPA will estimate the weights if not specified. |
| alpha   | (scalar): type I error rate for hypothesis testing - values in (0, 1); defaults to 0.05                                 |

## **Details**

Post-prediction adaptive inference (Miao et al. 2023) https://arxiv.org/abs/2311.14220

## Value

A list of outputs: estimate of inference model parameters and corresponding standard error.

```
dat <- simdat(model = "poisson")
form <- Y - f ~ X1

X_l <- model.matrix(form, data = dat[dat$set_label == "labeled",])

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

X_u <- model.matrix(form, data = dat[dat$set_label == "unlabeled",])

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

pspa_poisson(X_l, Y_l, f_l, X_u, f_u)
```

pspa\_quantile 49

| pspa_quantile PSPA | A Quantile Estimatio |
|--------------------|----------------------|
|--------------------|----------------------|

# Description

Helper function for PSPA quantile estimation

# Usage

```
pspa_quantile(Y_1, f_1, f_u, q, weights = NA, alpha = 0.05)
```

# Arguments

| Y_1     | (vector): n-vector of labeled outcomes.   |
|---------|---|
| f_1     | (vector): n-vector of predictions in the labeled data.  |
| f_u     | (vector): N-vector of predictions in the unlabeled data.  |
| q       | (float): Quantile to estimate. Must be in the range (0, 1).   |
| weights | (array): 1-dimensional array of weights vector for variance reduction. PSPA will estimate the weights if not specified. |
| alpha   | (scalar): type I error rate for hypothesis testing - values in $(0, 1)$ ; defaults to $0.05$ .                          |

#### **Details**

Post-prediction adaptive inference (Miao et al. 2023) https://arxiv.org/abs/2311.14220

## Value

A list of outputs: estimate of inference model parameters and corresponding standard error.

```
dat <- simdat(model = "quantile")
form <- Y - f ~ 1

Y_l <- dat[dat$set_label == "labeled", all.vars(form)[1]] |> matrix(ncol = 1)

f_l <- dat[dat$set_label == "labeled", all.vars(form)[2]] |> matrix(ncol = 1)

f_u <- dat[dat$set_label == "unlabeled", all.vars(form)[2]] |> matrix(ncol = 1)

pspa_quantile(Y_l, f_l, f_u, q = 0.5)
```

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pspa\_y

PSPA M-Estimation for ML-predicted labels

# Description

pspa\_y function conducts post-prediction M-Estimation.

# Usage

```
pspa_y(
    X_lab = NA,
    X_unlab = NA,
    Y_lab,
    Yhat_lab,
    Yhat_unlab,
    alpha = 0.05,
    weights = NA,
    quant = NA,
    intercept = FALSE,
    method
)
```

# Arguments

| X_lab      | Array or data.frame containing observed covariates in labeled data.   |
|------------|---|
| X_unlab    | Array or data.frame containing observed or predicted covariates in unlabeled data.                                      |
| Y_lab      | Array or data.frame of observed outcomes in labeled data.   |
| Yhat_lab   | Array or data.frame of predicted outcomes in labeled data.  |
| Yhat_unlab | Array or data.frame of predicted outcomes in unlabeled data.  |
| alpha      | Specifies the confidence level as 1 - alpha for confidence intervals.   |
| weights    | weights vector PSPA linear regression (d-dimensional, where d equals the number of covariates).                         |
| quant      | quantile for quantile estimation  |
| intercept  | Boolean indicating if the input covariates' data contains the intercept (TRUE if the input data contains)               |
| method     | indicates the method to be used for M-estimation. Options include "mean", "quantile", "ols", "logistic", and "poisson". |

# Value

A summary table presenting point estimates, standard error, confidence intervals (1 - alpha), P-values, and weights.

rectified\_cdf 51

## **Examples**

```
data <- sim_data_y()
X_lab <- data$X_lab
X_unlab <- data$X_unlab
Y_lab <- data$Y_lab
Yhat_lab <- data$Yhat_lab
Yhat_unlab <- data$Yhat_unlab
pspa_y(X_lab = X_lab, X_unlab = X_unlab,
    Y_lab = Y_lab, Yhat_lab = Yhat_lab, Yhat_unlab = Yhat_unlab,
alpha = 0.05, method = "ols")</pre>
```

 $rectified\_cdf$ 

Rectified CDF

# Description

Computes the rectified CDF of the data.

## Usage

```
rectified\_cdf(Y_l, f_l, f_u, grid, w_l = NULL, w_u = NULL)
```

# Arguments

| Y_1  | (vector): Gold-standard labels.                                  |
|------|--|
| f_1  | (vector): Predictions corresponding to the gold-standard labels. |
| f_u  | (vector): Predictions corresponding to the unlabeled data.       |
| grid | (vector): Grid of values to compute the CDF at.                  |
| w_1  | (vector, optional): Sample weights for the labeled data set.     |
| w_u  | (vector, optional): Sample weights for the unlabeled data set.   |

#### Value

(vector): Rectified CDF of the data at the specified grid points.

52 rectified\_p\_value

## **Examples**

```
Y_1 <- c(1, 2, 3, 4, 5)

f_1 <- c(1.1, 2.2, 3.3, 4.4, 5.5)

f_u <- c(1.2, 2.3, 3.4)

grid <- seq(0, 6, by = 0.5)

rectified_cdf(Y_1, f_1, f_u, grid)
```

rectified\_p\_value

Rectified P-Value

# Description

Computes a rectified p-value.

## Usage

```
rectified_p_value(
  rectifier,
  rectifier_std,
  imputed_mean,
  imputed_std,
  null = 0,
  alternative = "two-sided"
)
```

# Arguments

```
rectifier (float or vector): Rectifier value.

rectifier_std (float or vector): Rectifier standard deviation.

imputed_mean (float or vector): Imputed mean.

imputed_std (float or vector): Imputed standard deviation.

null (float, optional): Value of the null hypothesis to be tested. Defaults to 0.

alternative (str, optional): Alternative hypothesis, either 'two-sided', 'larger' or 'smaller'.
```

#### Value

(float or vector): The rectified p-value.

Sigma\_cal 53

# Examples

```
rectifier <- 0.7
rectifier_std <- 0.5
imputed_mean <- 1.5
imputed_std <- 0.3
rectified_p_value(rectifier, rectifier_std, imputed_mean, imputed_std)</pre>
```

Sigma\_cal

Variance-covariance matrix of the estimation equation

# Description

Sigma\_cal function for variance-covariance matrix of the estimation equation

## Usage

```
Sigma_cal(
  X_lab,
  X_unlab,
  Y_lab,
  Yhat_lab,
  Yhat_unlab,
  w,
  theta,
  quant = NA,
  method
)
```

# Arguments

| X_lab      | Array or data.frame containing observed covariates in labeled data.   |  |
|------------|---|--|
| X_unlab    | Array or data.frame containing observed or predicted covariates in unlabeled data.                                      |  |
| Y_lab      | Array or data.frame of observed outcomes in labeled data.   |  |
| Yhat_lab   | Array or data.frame of predicted outcomes in labeled data.  |  |
| Yhat_unlab | Array or data.frame of predicted outcomes in unlabeled data.  |  |
| W          | weights vector PSPA linear regression (d-dimensional, where d equals the number of covariates).                         |  |
| theta      | parameter theta   |  |
| quant      | quantile for quantile estimation  |  |
| method     | indicates the method to be used for M-estimation. Options include "mean", "quantile", "ols", "logistic", and "poisson". |  |

54 simdat

#### Value

variance-covariance matrix of the estimation equation

simdat

Data generation function for various underlying models

## **Description**

Data generation function for various underlying models

## Usage

```
simdat(
  n = c(300, 300, 300),
  effect = 1,
  sigma_Y = 1,
  model = "ols",
  shift = 0,
  scale = 1
)
```

## **Arguments**

| n       | Integer vector of size 3 indicating the sample sizes in the training, labeled, and unlabeled data sets, respectively     |
|---------|--|
| effect  | Regression coefficient for the first variable of interest for inference. Defaults is 1.                                  |
| sigma_Y | Residual variance for the generated outcome. Defaults is 1.  |
| model   | The type of model to be generated. Must be one of "mean", "quantile", "ols", "logistic", or "poisson". Default is "ols". |
| shift   | Scalar shift of the predictions for continuous outcomes (i.e., "mean", "quantile", and "ols"). Defaults to 0.            |
| scale   | Scaling factor for the predictions for continuous outcomes (i.e., "mean", "quantile", and "ols"). Defaults to 1.         |

## **Details**

The simdat function generates three datasets consisting of independent realizations of Y (for model = "mean" or "quantile"), or  $\{Y, X\}$  (for model = "ols", "logistic", or "poisson"): a *training* dataset of size  $n_t$ , a *labeled* dataset of size  $n_l$ , and an *unlabeled* dataset of size  $n_u$ . These sizes are specified by the argument n.

NOTE: In the *unlabeled* data subset, outcome data are still generated to facilitate a benchmark for comparison with an "oracle" model that uses the true  $Y^{\mathcal{U}}$  values for estimation and inference.

## **Generating Data**

simdat 55

For "mean" and "quantile", we simulate a continuous outcome,  $Y \in \mathbb{R}$ , with mean given by the effect argument and error variance given by the sigma\_y argument.

For "ols", "logistic", or "poisson" models, predictor data,  $X \in \mathbb{R}^4$  are simulated such that the *i*th observation follows a standard multivariate normal distribution with a zero mean vector and identity covariance matrix:

$$X_i = (X_{i1}, X_{i2}, X_{i3}, X_{i4}) \sim \mathcal{N}_4(\mathbf{0}, \mathbf{I}).$$

For "ols", a continuous outcome  $Y \in \mathbb{R}$  is simulated to depend on  $X_1$  through a linear term with the effect size specified by the effect argument, while the other predictors,  $X \setminus X_1$ , have nonlinear effects:

$$Y_i = effect \times Z_{i1} + \frac{1}{2}Z_{i2}^2 + \frac{1}{3}Z_{i3}^3 + \frac{1}{4}Z_{i4}^2 + \varepsilon_y,$$

and  $\varepsilon_y \sim \mathcal{N}(0, sigma_y)$ , where the sigma\_y argument specifies the error variance.

For "logistic", we simulate:

$$\Pr(Y_i = 1 \mid \mathbf{X}) = logit^{-1}(effect \times Z_{i1} + \frac{1}{2}Z_{i2}^2 + \frac{1}{3}Z_{i3}^3 + \frac{1}{4}Z_{i4}^2 + \varepsilon_y)$$

and generate:

$$Y_i \sim Bern[1, \Pr(Y_i = 1 \mid \boldsymbol{X})]$$

where  $\varepsilon_y \sim \mathcal{N}(0, sigma_y)$ .

For "poisson", we simulate:

$$\lambda_Y = exp(effect \times Z_{i1} + \frac{1}{2}Z_{i2}^2 + \frac{1}{3}Z_{i3}^3 + \frac{1}{4}Z_{i4}^2 + \varepsilon_y)$$

and generate:

$$Y_i \sim Poisson(\lambda_Y)$$

#### **Generating Predictions**

To generate predicted outcomes for "mean" and "quantile", we simulate a continuous variable with mean given by the empirical mean of the training data and error variance given by the sigma\_y argument.

For "ols", we fit a generalized additive model (GAM) on the simulated *training* dataset and calculate predictions for the *labeled* and *unlabeled* datasets as deterministic functions of X. Specifically, we fit the following GAM:

$$Y^{\mathcal{T}} = s_0 + s_1(X_1^{\mathcal{T}}) + s_2(X_2^{\mathcal{T}}) + s_3(X_3^{\mathcal{T}}) + s_4(X_4^{\mathcal{T}}) + \varepsilon_p,$$

where  $\mathcal{T}$  denotes the *training* dataset,  $s_0$  is an intercept term, and  $s_1(\cdot)$ ,  $s_2(\cdot)$ ,  $s_3(\cdot)$ , and  $s_4(\cdot)$  are smoothing spline functions for  $X_1$ ,  $X_2$ ,  $X_3$ , and  $X_4$ , respectively, with three target equivalent degrees of freedom. Residual error is modeled as  $\varepsilon_p$ .

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Predictions for labeled and unlabeled datasets are calculated as:

$$f(\mathbf{X}^{\mathcal{L}\cup\mathcal{U}}) = \hat{s}_0 + \hat{s}_1(X_1^{\mathcal{L}\cup\mathcal{U}}) + \hat{s}_2(X_2^{\mathcal{L}\cup\mathcal{U}}) + \hat{s}_3(X_3^{\mathcal{L}\cup\mathcal{U}}) + \hat{s}_4(X_4^{\mathcal{L}\cup\mathcal{U}}),$$

where  $\hat{s}_0, \hat{s}_1, \hat{s}_2, \hat{s}_3$ , and  $\hat{s}_4$  are estimates of  $s_0, s_1, s_2, s_3$ , and  $s_4$ , respectively.

NOTE: For continuous outcomes, we provide optional arguments shift and scale to further apply a location shift and scaling factor, respectively, to the predicted outcomes. These default to shift = 0 and scale = 1, i.e., no location shift or scaling.

For "logistic", we train k-nearest neighbors (k-NN) classifiers on the simulated *training* dataset for values of k ranging from 1 to 10. The optimal k is chosen via cross-validation, minimizing the misclassification error on the validation folds. Predictions for the *labeled* and *unlabeled* datasets are obtained by applying the k-NN classifier with the optimal k to X.

Specifically, for each observation in the labeled and unlabeled datasets:

$$\hat{Y} = \operatorname{argmax}_{c} \sum_{i \in \mathcal{N}_{k}} I(Y_{i} = c),$$

where  $\mathcal{N}_k$  represents the set of k nearest neighbors in the training dataset, c indexes the possible classes (0 or 1), and  $I(\cdot)$  is an indicator function.

For "poisson", we fit a generalized linear model (GLM) with a log link function to the simulated *training* dataset. The model is of the form:

$$\log(\mu^{T}) = \gamma_0 + \gamma_1 X_1^{T} + \gamma_2 X_2^{T} + \gamma_3 X_3^{T} + \gamma_4 X_4^{T},$$

where  $\mu^{\mathcal{T}}$  is the expected count for the response variable in the *training* dataset,  $\gamma_0$  is the intercept, and  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$ , and  $\gamma_4$  are the regression coefficients for the predictors  $X_1$ ,  $X_2$ ,  $X_3$ , and  $X_4$ , respectively.

Predictions for the *labeled* and *unlabeled* datasets are calculated as:

$$\hat{\mu}^{\mathcal{L} \cup \mathcal{U}} = \exp(\hat{\gamma}_0 + \hat{\gamma}_1 X_1^{\mathcal{L} \cup \mathcal{U}} + \hat{\gamma}_2 X_2^{\mathcal{L} \cup \mathcal{U}} + \hat{\gamma}_3 X_3^{\mathcal{L} \cup \mathcal{U}} + \hat{\gamma}_4 X_4^{\mathcal{L} \cup \mathcal{U}}),$$

where  $\hat{\gamma}_0$ ,  $\hat{\gamma}_1$ ,  $\hat{\gamma}_2$ ,  $\hat{\gamma}_3$ , and  $\hat{\gamma}_4$  are the estimated coefficients.

#### Value

A data.frame containing n rows and columns corresponding to the labeled outcome (Y), the predicted outcome (f), a character variable (set\_label) indicating which data set the observation belongs to (training, labeled, or unlabeled), and four independent, normally distributed predictors (X1, X2, X3, and X4), where applicable.

```
#-- Mean
dat_mean <- simdat(c(100, 100, 100), effect = 1, sigma_Y = 1,
    model = "mean")</pre>
```

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```
head(dat_mean)
#-- Linear Regression

dat_ols <- simdat(c(100, 100, 100), effect = 1, sigma_Y = 1,
    model = "ols")

head(dat_ols)</pre>
```

sim\_data\_y

Simulate the data for testing the functions

## **Description**

sim\_data\_y for simulation with ML-predicted Y

# Usage

```
sim_data_y(r = 0.9, binary = FALSE)
```

# Arguments

r imputation correlation

binary simulate binary outcome or not

## Value

simulated data

summary.ipd

Summarize IPD Fit

## **Description**

Produces a summary of the IPD method/model combination.

## Usage

```
## S3 method for class 'ipd'
summary(object, ...)
```

# Arguments

object An object of class ipd.

... Additional arguments to be passed to the summary function.

58 tidy.ipd

#### Value

A list containing:

coefficients Model coefficients and related statistics.performance Performance metrics of the model fit.... Additional summary information.

## **Examples**

```
#-- Generate Example Data
set.seed(2023)
dat <- simdat(n = c(300, 300, 300), effect = 1, sigma_Y = 1)
head(dat)
formula <- Y - f ~ X1
#-- Fit IPD
fit <- ipd(formula, method = "postpi_analytic", model = "ols",
    data = dat, label = "set_label")
#-- Summarize Output
summ_fit <- summary(fit)
summ_fit</pre>
```

tidy.ipd

Tidy an IPD Fit

# Description

Tidies the IPD method/model fit into a data frame.

#### Usage

```
## S3 method for class 'ipd' tidy(x, ...)
```

# Arguments

x An object of class ipd.

... Additional arguments to be passed to the tidy function.

wls 59

#### Value

A tidy data frame of the model's coefficients.

#### **Examples**

```
#-- Generate Example Data
set.seed(2023)
dat <- simdat(n = c(300, 300, 300), effect = 1, sigma_Y = 1)
head(dat)
formula <- Y - f ~ X1
#-- Fit IPD
fit <- ipd(formula, method = "postpi_analytic", model = "ols",
    data = dat, label = "set_label")
#-- Tidy Output
tidy(fit)</pre>
```

wls

Weighted Least Squares

#### **Description**

Computes the weighted least squares estimate of the coefficients.

#### Usage

```
wls(X, Y, w = NULL, return_se = FALSE)
```

## **Arguments**

```
    X (matrix): n x p matrix of covariates.
    Y (vector): p-vector of outcome values.
    w (vector, optional): n-vector of sample weights.
    return_se (bool, optional): Whether to return the standard errors of the coefficients.
```

# Value

```
(list): A list containing the following:
```

```
theta (vector): p-vector of weighted least squares estimates of the coefficients.se (vector): If return_se == TRUE, return the p-vector of standard errors of the coefficients.
```

60 zconfint\_generic

#### **Examples**

```
n <- 1000

X <- rnorm(n, 1, 1)

w <- rep(1, n)

Y <- X + rnorm(n, 0, 1)

wls(X, Y, w = w, return_se = TRUE)</pre>
```

zconfint\_generic

Normal Confidence Intervals

# Description

Calculates normal confidence intervals for a given alternative at a given significance level.

# Usage

```
zconfint_generic(mean, std_mean, alpha, alternative)
```

## **Arguments**

```
mean (float): Estimated normal mean.
std_mean (float): Estimated standard error of the mean.
```

alpha (float): Significance level in [0,1]

alternative (string): Alternative hypothesis, either 'two-sided', 'larger' or 'smaller'.

#### Value

```
(vector): Lower and upper (1 - alpha) * 100% confidence limits.
```

```
n <- 1000
Y <- rnorm(n, 1, 1)
se_Y <- sd(Y) / sqrt(n)
zconfint_generic(Y, se_Y, alpha = 0.05, alternative = "two-sided")</pre>
```

zstat\_generic 61

| zstat_generic | Compute Z-Statistic and P-Value |  |
|---------------|---------------------------------|--|
|---------------|---------------------------------|--|

# Description

Computes the z-statistic and the corresponding p-value for a given test.

# Usage

```
zstat_generic(value1, value2, std_diff, alternative, diff = 0)
```

# Arguments

| value1      | (numeric): The first value or sample mean.   |
|-------------|--|
| value2      | (numeric): The second value or sample mean.  |
| std_diff    | (numeric): The standard error of the difference between the two values.  |
| alternative | (character): The alternative hypothesis. Can be one of "two-sided" (or "2-sided", "2s"), "larger" (or "l"), or "smaller" (or "s"). |
| diff        | (numeric, optional): The hypothesized difference between the two values. Default is 0.   |

## Value

```
(list): A list containing the following:zstat (numeric): The computed z-statistic.pvalue (numeric): The corresponding p-value for the test.
```

```
value1 <- 1.5
value2 <- 1.0
std_diff <- 0.2
alternative <- "two-sided"
result <- zstat_generic(value1, value2, std_diff, alternative)</pre>
```

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