SDRcausal: an R package for causal inference based on sufficient dimension reduction

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Abstract

SDRcausal is a package that implements sufficient dimension reduction methods for causal inference as proposed in Ghosh, Ma, and de Luna (2021). The package implements (augmented) inverse probability weighting and outcome regression (imputation) estimators of an average treatment effect (ATE) parameter. Nuisance models, both treatment assignment probability given the covariates (propensity score) and outcome regression models, are fitted by using semiparametric locally efficient dimension reduction estimators, thereby allowing for large sets of confounding covariates. Techniques including linear extrapolation, numerical differentiation, and truncation have been used to obtain a practicable implementation of the methods. Finding the suitable dimension reduction map (central mean subspace) requires solving an optimization problem, and several optimization algorithms are given as choices to the user. The package also provides estimators of the asymptotic variances of the causal effect estimators implemented. Plotting options are provided. The core of the methods are implemented in C language, and parallelization is allowed for. The user-friendly and freeware R language is used as interface. The package can be downloaded from Github repository: [https://github.com/stat4reg](https://github.com/stat4reg)

- SDRcausal is an R-package to perform causal inference in situations with large amount of potentially confounding covariates.
- Semiparametric sufficient dimension reduction methods are used to deal with high dimensionality.
- Average causal effect of binary treatments can be obtained using different semiparametric estimators.

**Keywords:** average treatment effect; central mean subspace; double robust estimation; semiparametric inference

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**Figure 1: Graphical Abstract**

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**Package installation**

To install and load the package form GitHub, type the following command in an R console:

```r
install.packages("devtools")
library(devtools)
install_github("stat4reg/SDRcausal")
library(SDRcausal)
```

Mac users may also need to run the following command in a terminal window before installing the package:

```
xcode-select --install
```
Assumptions and parameter of interest

Average Treatment Effect

Let \(X_i \in \mathbb{R}^p\) be a set of covariates for the \(i\)th individual in a sample of size \(n\). Assume there is a binary treatment s.t. for each individual \(T_i = 1\) or \(0\) if the \(i\)th individual received treatment or not, respectively. Let \(Y_{i1}\) and \(Y_{i0}\) be potential outcomes, i.e. the outcomes under \(T_i = 1\) and \(T_i = 0\) respectively. Only one potential outcome is observed for each individual. We assume that \(Y_i = Y_{i1}, T + Y_{i0}(1 - T)\) is the observed outcome. This package performs inference on the average causal effect of treatment (or average treatment effect, ATE),

\[D = E(Y_1) - E(Y_0),\]

using sufficient dimension reduction techniques. This parameter is identified under the model given below.

Nuisance Models and Dimension Reduction

Nuisance models are typically considered to identify the causal parameter \(D\). These models are assumed to have signal belonging to three different projections \(\alpha^T x\), \(\beta_0^T x\), and \(\beta_1^T x\), i.e. lower dimensional spaces. First, the propensity score is modeled:

\[pr(T = 1 | X = x, Y_1, Y_0) = pr(T = 1 | X = x) = e^{\eta(x^T x)}/\{1 + e^{\eta(x^T x)}\},\]

where \(\eta(\cdot)\) is a smooth and bounded function. Boundedness also guarantees that the propensity score is strictly in \((0, 1)\). The parameter \(\alpha\) is a one or two dimensional projection matrix, i.e. with dimension \(p \times d\), \(d = 1\) or \(2\).

Furthermore, models for \(Y_1\) and \(Y_0\) given \(X = x\) are specified as

\[Y_1 = m_1(\beta_1^T x) + \varepsilon_1,\]

and

\[Y_0 = m_0(\beta_0^T x) + \varepsilon_0,\]

where \(E(\varepsilon_1 | x) = E(\varepsilon_0 | x) = 0\). Here, \(m_1(\cdot)\) and \(m_0(\cdot)\) are unknown functions, and \(\beta_1\) and \(\beta_0\) are unknown projection matrices with dimension \(p \times d\), \(d = 1, 2\). These three models are estimated separately using the random sample at hand. Then, by combining the models, fitted in various ways, different estimators for the treatment effect \(D = E(Y_1 - Y_0)\) are obtained.

Fitting the Propensity Score and Outcome Models

The algorithms for fitting the outcome and propensity score models through semiparametric dimension reduction are described in detail in Ghosh, Ma, and de Luna (2021). The goal of these algorithms is to find \(\hat{\alpha}, \hat{\eta}(\cdot), \hat{\beta}_1, \hat{\hat{m}}_i(\cdot), t = 0, 1\), that satisfy the following conditions:

\[\sum_{i=1}^{n} t_i \{y_{i1} - \hat{m}_1(\hat{\beta}_1^T x_i)\} \hat{m}_1' (\hat{\beta}_1^T x_i) \otimes \{X_{Li} - \hat{E}(X_{Li} | \hat{\beta}_1^T x_i)\} = 0, \tag{1}\]

\[\sum_{i=1}^{n} t_i \{y_{i0} - \hat{m}_0(\hat{\beta}_0^T x_i)\} \hat{m}_0' (\hat{\beta}_0^T x_i) \otimes \{X_{Li} - \hat{E}(X_{Li} | \hat{\beta}_0^T x_i)\} = 0, \tag{2}\]

\[\sum_{i=1}^{n} \{X_{Li} - \hat{E}(X_{Li} | \hat{\alpha}^T x_i)\} \left[t_i - \frac{e^{\hat{\eta}(\hat{\alpha}^T x_i)}}{1 + e^{\hat{\eta}(\hat{\alpha}^T x_i)}}\right] \hat{\beta}' (\hat{\alpha}^T x_i)^T = 0, \tag{3}\]

where \(X_{Li}\) is the subvector containing the lower \(p - d\) components of \(X_i\), where \(X_i\) is the random vector of covariates corresponding to \(i\)th individual.
The algorithms have two phases. In the first phase, the algorithms start by finding naïve estimates of the functions \( \eta \) and \( m_t \), \( t = 0, 1 \). Initial guesses for \( \alpha \) and \( \beta_t \), \( t = 0, 1 \), matrices of dimension \( p \times d \), \( d = 1, 2 \), are needed for these naïve estimations. Then, the naïve estimates \( \hat{\eta} \) and \( \hat{m}_t \) are in turn used to estimate \( \alpha \) and \( \beta_t \), \( t = 0, 1 \). The second phase consists of a repetition of the first part of phase one by updating the initial estimates of \( \alpha \) and \( \beta_t \), i.e., instead of initial guesses, the estimates of \( \alpha \) and \( \beta_t \), obtained at the end of phase one, are used to make new estimations for \( \eta \) and \( m_t \). Thus, first, \( \hat{E}(X_L|\alpha^T x_t) \) and \( \hat{E}(X_L|\beta_t^T x_t) \) are fitted based on initial guesses of the projection parameters. Here, the Nadaraya-Watson kernel estimator is used:

\[
\hat{E}(X_L|\beta_t^T x) = \sum_{i=1}^n x_L h(\beta_t^T x - \beta_t^T x),
\]

\[
\hat{E}(X_L|\alpha^T x) = \sum_{i=1}^n x_L h(\alpha^T x - \alpha^T x),
\]

where \( h(\alpha^T x - \alpha^T x) \) is such that \( \frac{1}{h} K(\frac{\alpha^T x - \alpha^T x}{h}) \), where different kernel functions and bandwidth \( h \) can be used (see below).

The functions \( \eta \) and \( m_t \), \( t = 0, 1 \), are then fitted using local linear estimation. For the function \( m_t \):

\[
\hat{m}_t(\beta_t^T x) = A_{11} + A_{13}^T (A_{14} - A_{13} A_{13})^{-1} A_{13} A_{11},
\]

where

\[
A_{11} = \frac{\sum_{i=1}^n z_i h(\beta_t^T x_i - \beta_t^T x)}{\sum_{i=2}^n z_i h(\beta_t^T x_i - \beta_t^T x)},
\]

\[
A_{13} = \frac{\sum_{i=1}^n z_i h(\beta_t^T x_i - \beta_t^T x)}{\sum_{i=2}^n z_i h(\beta_t^T x_i - \beta_t^T x)},
\]

\[
A_{14} = \frac{\sum_{i=1}^n z_i h(\beta_t^T x_i - \beta_t^T x)}{\sum_{i=2}^n z_i h(\beta_t^T x_i - \beta_t^T x)}.
\]

The following equations are solved for \( \eta \) and \( \eta' \) (derivative of \( \eta \)) for \( z = \alpha^T x_1, \ldots, \alpha^T x_n \):

\[
\sum_{i=1}^n \left[ t_i - \frac{e^{\eta(\alpha^T x_i) + \eta'(\alpha^T x_i)^T (\alpha^T x_i - z)}}{1 + e^{\eta(\alpha^T x_i) + \eta'(\alpha^T x_i)^T (\alpha^T x_i - z)}} \right] h(\alpha^T x_i - z) = 0,
\]

\[
\sum_{i=1}^n \left[ t_i - \frac{\eta(\alpha^T x_i) + \eta'(\alpha^T x_i)^T (\alpha^T x_i - z)}}{1 + \eta(\alpha^T x_i) + \eta'(\alpha^T x_i)^T (\alpha^T x_i - z)}} \right] (\alpha^T x_i - z) h(\alpha^T x_i - z) = 0.
\]

The default kernel function in the package is “Epanechnikov” (“parabolic”). Users can choose kernels and bandwidths. The package support three kernels: “Epanechnikov”, “Quartic” (“biweight”), and “Gaussian”. The asymptotic properties of the estimators are derived in Ghosh, Ma, and de Luna (2021) based on conditions on the bandwidths; loosely a range of proper bandwidths. In this framework the set of proper bandwidths for \( h(\beta_t^T x_i - \beta_t^T x) \) is \( h_c = c \text{sd}(\beta_t^T x)n^{\frac{2}{4}} \), where \( c \) is an arbitrary scale and \( \text{sd}(\beta_t^T x) \) is the estimated standard deviation of \( \beta_t^T x \). (The same statement is valid for \( \alpha^T x \) ). The package uses these appropriate bandwidths based on a scale \( c \) that is specified by the user.

**Estimation of ATE**

**A Data Generating Process**

The data generating process (Study 1 in Ghosh, Ma, and de Luna (2021)) that we present in this section is used to illustrate the package functions in the next sections. The seed that we used for the data generation process is 48371. We set sample size to \( n = 1000 \) and covariate dimension \( p = 6 \). Then, we generate the covariate vectors \( X_i = (X_{i1}, \ldots, X_{i6})^T \) as:
\begin{itemize}
  \item $X_1 \sim N(1, 1)$ and $X_2 \sim N(0, 1)$,
  \item $X_4 = 0.015X_1 + u_1$, where $u_1$ is uniformly distributed in (-0.5, 0.5),
  \item $X_3 \sim \text{Bernoulli}(0.5 + 0.05X_2)$ and $X_5 \sim \text{Bernoulli}(0.4 + 0.2X_4)$,
  \item $X_6 = 0.04X_2 + 0.15X_3 + 0.05X_4 + u_2$, where $u_2 \sim N(0, 1)$.
\end{itemize}

In addition, we set $\beta_1 = (1, -1, 1, -2, -1.5, 0.5)^T$, $\beta_0 = (1, 1, 0, 0, 0, 0)^T$ and $\alpha = (-0.27, 0.2, -0.15, 0.05, 0.15, -0.1)^T$.

We generate the response variables based on
\[Y_1 = 0.7(\beta_1^T X)^2 + \sin(\beta_1^T X) + \varepsilon_1\] and \[Y_0 = \beta_0^T X + \varepsilon_0.\]
Here $\varepsilon_1$ and $\varepsilon_0$ are normally distributed with mean zero and variances 0.5 and 0.2 respectively. Further, we let $\eta(\alpha^T x) = \alpha^T x$. Thus, the treatment indicator $T$ is generated from the logistic model $\text{pr}(T = 1 | X) = \exp(\alpha^T x)/(1 + \exp(\alpha^T x))$.

The generated dataset is stored in the package, and it is accessible by using the following commands:
\begin{verbatim}
beta0 = SDRcausal::beta0_guess
beta1 = SDRcausal::beta1_guess
alpha = SDRcausal::alpha_guess
covariates = SDRcausal::covariates
y = SDRcausal::outcomes
treated = SDRcausal::treated
\end{verbatim}

\section*{Imputation through outcome regression (IMP)}
\section*{Description}
The first estimator is based on the outcome regression models, often called an imputation approach (Ghosh, Ma, and de Luna (2021), Section 3.1). Let
\[\hat{E}_{\text{IMP}}(Y_1) = n^{-1} \sum_{i=1}^{n} \{t_i y_i + (1 - t_i)\hat{m}_1(\hat{\beta}_1^T x_i)\},\]
and
\[\hat{E}_{\text{IMP}}(Y_0) = n^{-1} \sum_{i=1}^{n} \{(1 - t_i)y_i + t_i\hat{m}_0(\hat{\beta}_0^T x_i)\} .\]

Then the imputation estimator of $D$ is:
\[\hat{D}_{\text{IMP}} = \hat{E}_{\text{IMP}}(Y_1) - \hat{E}_{\text{IMP}}(Y_0).\]

Furthermore, there is an alternative imputation estimator that uses the predicted values everywhere, even when the observed response values are available, i.e.:
\[\hat{E}_{\text{IMP}2}(Y_1) = n^{-1} \sum_{i=1}^{n} \hat{m}_1(\hat{\beta}_1^T x_i),\]
and
\[\hat{E}_{\text{IMP}2}(Y_0) = n^{-1} \sum_{i=1}^{n} \hat{m}_0(\hat{\beta}_0^T x_i),\]
and the IMP2 estimator of $D$ is:
\[\hat{D}_{\text{IMP}2} = \hat{E}_{\text{IMP}2}(Y_1) - \hat{E}_{\text{IMP}2}(Y_0).\]

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Example and Code

The imputation estimators are implemented in the function `imp.ate` in the package. Initial guesses for $\beta_1$ and $\beta_0$ are needed to call the function. Based on how good the initial guesses are, users can choose different optimizers. If the initial guess is close enough to the true values, choosing a local optimizer is more efficient. Otherwise, if the initial guess is entirely random, then using a global optimizer is probably a safer option. Two different functions are available for optimization: `optim` and `cobyla`. The function `optim` includes both global and local optimizers. However, all the `optim` methods need the derivability condition. If derivative-free optimization methods are required, the `cobyla` method in the `nloptr` package is recommended. By default `optim` is used, with the method Nelder-Mead. To use another method, such as the global optimization method SANN, just add `method = "SANN"` to the `imp.ate` inputs. Other methods that can be used in `optim` are: BFGS, CG, L-BFGS-B, and Brent.

The default kernel function that is used to do the kernel regressions is Epanechnikov, and it can be changed to Quartic or Gaussian by adding `kernel = "QUARTIC"` or `kernel = "GAUSSIAN"`.

If `explicit_bandwidth` is set as FALSE, bandwidths are computed by the formula $c \text{sd}(\beta^T x)n^{1/5}$, where $c$ is determined by choosing values for `bwc_dim_red1`, `bwc_impute1`, `bwc_dim_red0`, and `bwc_impute0`. The values `bwc_dim_red1` and `bwc_dim_red0` are used for all kernel regressions in the first phase (finding a projection) of estimation of $m_1(\beta_1^T x)$ and $m_0(\beta_0^T x)$, respectively. The values `bwc_impute1` and `bwc_impute0` are used in the second phase (estimating $m_1(\cdot)$ and $m_0(\cdot)$, respectively). If `explicit_bandwidth = TRUE` has been chosen, then the function considers `bwc_dim_red1`, `bwc_impute1`, `bwc_dim_red0`, and `bwc_impute0` as the bandwidth values.

```r
imp <- imp.ate(x = covariates,
                y = y,
                treated = treated,
                beta_guess1 = beta1,
                beta_guess0 = beta0,
                n_threads = 2)
```

The list of all arguments is:

- **x**
  Covariate matrix

- **y**
  Response vector

- **treated**
  A binary vector indicating treatment status

- **beta_guess1**
  Initial guess for $\beta_1$

- **beta_guess0**
  Initial guess for $\beta_0$

- **solver**
  Specifies which solver is to be used. Current options are "optim" and "cobyla" (from `nloptr` package). The default value is "optim".

- **kernel**
  Specifies which kernel function is to be used, current options are: "EPAN"(default), "QUARTIC", and "GAUSSIAN".

- **explicit_bandwidth**
  Specifies if `bandwidth_scale` will be used as the bandwidth or if it will be calculated as `bandwidth_scale \times \text{sd}(\beta^T x) \times n^{1/5}`. The default value is FALSE.

- **recalc_bandwidth**
  Specifies whether the bandwidth should be recalculated after the first stage (the estimations of
dimension reduction step). If `explicit_bandwidth = TRUE`, `recalc_bandwidth` is not used, but if `explicit_bandwidth = FALSE`, then if `recalc_bandwidth = TRUE`, bandwidths are recalculated at the beginning of the second step based on `bwc_impute0` and `bwc_impute1`. If `recalc_bandwidth = FALSE`(default), the first step bandwidths are used.

- **bwc_dim_red1**
  Scaling of calculated bandwidth, or if `explicit_bandwidth = TRUE` used as the bandwidth. It is used in the dimension reduction step for $\hat{m}_1(\beta^T_1 x)$. The default value is 1.

- **bwc_impute1**
  Scaling of calculated bandwidth, or if `explicit_bandwidth = TRUE` used as the bandwidth. It is used in the imputation step for $\hat{m}_1(\beta^T_1 x)$. The default value is 1.25.

- **bwc_dim_red0**
  Scaling of calculated bandwidth, or if `explicit_bandwidth = TRUE` used as the bandwidth. It is used in the dimension reduction step for $\hat{m}_0(\beta^T_0 x)$. The default value is 1.

- **bwc_impute0**
  Scaling of calculated bandwidth, or if `explicit_bandwidth = TRUE` used as the bandwidth. It is used in the imputation step for $\hat{m}_0(\beta^T_0 x)$. The default value is 1.25.

- **gauss_cutoff**
  The cutoff value for Gaussian kernel. The default value is $1e^{-3}$.

- **penalty**
  Penalty for the optimizer if local linear regression fails. Added to the function value in solver as $\text{penalty}(n - n_{\text{before\_pen}})$, where $n$ is the number of times local linear regression fails. The default value is 10.

- **n_before_pen**
  The number of acceptable local linear regression failures during the estimation of $\beta_0$ and $\beta_1$ phase. The default value is 5.

- **to_extrapolate**
  Specifies whether to extrapolate or not. Since in $\hat{m}_0(\beta^T_0 x)$ and $\hat{m}_1(\beta^T_1 x)$ estimates in terms of $\beta^T_0 x$ and $\beta^T_1 x$, local linear regression at the boundaries of $\beta^T_0 X$, and $\beta^T_1 X$, can be very volatile, it is recommended to use extrapolation on those points instead of local linear regression. The default value is TRUE.

- **extrapolation_basis**
  The number of data points to base extrapolation on. Extrapolation at border points can be done based on a different number of neighborhood points. `extrapolation_basis` is how many neighborhood points are used. The default value is 5.

- **to_truncate**
  Specifies whether to truncate $\hat{m}_0(\beta^T_0 x)$ and $\hat{m}_1(\beta^T_1 x)$ or not. After estimating $\hat{m}_0(\beta^T_0 x)$ and $\hat{m}_1(\beta^T_1 x)$, if they are outside the range of observed outputs, they are replaced with the minimum and maximum observed outputs. The default value is TRUE.

- **n_threads**
  Sets the number of threads for parallel computing. Set to 1 serial. If `n_threads` exceeds the maximum number of threads, sets `n_threads` to `max_threads - 1`. To use `max_threads`, set to `n_threads` to `max_threads` of system. The default value is 1.

- **verbose**
  Specifies if the program should print output while running. The default value is TRUE.

• ... Additional parameters passed to optim or cobyla.

Output values include IMP and IMP2 estimators of ATE:
Furthermore, the imputed values computed for each individual, \( \hat{m}_1(\hat{\beta}_T^T x_i) \) and \( \hat{m}_0(\hat{\beta}_0^T x_i) \), are stored in `imp$m1` and `imp$m0`, and derivatives in `imp$m1$dm` and `imp$m0$dm`. Finally, \( \hat{\beta}_0 \) and \( \hat{\beta}_1 \) are also available as output:

```
imp$beta1_hat
#>   [,1]
#> [1,] 1.00000000
#> [2,] -0.98679430
#> [3,]  0.98289033
#> [4,] -2.05234549
#> [5,] -1.39629388
#> [6,]  0.52481479

imp$beta0_hat
#>   [,1]
#> [1,] 1.00000000
#> [2,] 1.02942153
#> [3,] -0.05913347
#> [4,] -0.11466994
#> [5,]  0.03370901
#> [6,]  0.04537406
```

### Visualization

The visualization function provided for the IMP estimator is `plot.imp`. It needs `ggplot2` to run. The function yields three graphs. The first graph displays all observed responses and estimated (imputed) potential outcomes against the index. The second graph shows observed outcomes and estimated potential outcomes against the estimated dimension reduction subspace \( \hat{\beta}_1^T x \). The third graph is the same as the second one, but against the estimated dimension reduction subspace \( \hat{\beta}_0^T x \).

The first plot (Figure 2) can be used, e.g., to check whether the range and dispersion of the imputed values is similar to the distribution of observed values for the treated and untreated groups. The second and third plots (Figures 3 and 4) can be used, e.g., to inspect visually if imputed values seem reasonable. The fitted values represent the functions \( m_1 \) and \( m_0 \), respectively. The smoothness of the estimated functions is related to the kernel bandwidths. In other words, these graphs can also be used to help choosing appropriate bandwidths. If the estimated function is too flexible and sensitive to minor errors in observed values, then this is a sign that the selected bandwidths were too small.

```
plot(imp , covariates = covariates, y=y, treated = treated)
#> [1] "salam"
#> $pl_imp
```

The bandwidths computed are dependent on the standard deviation of the projected covariates. The higher these variances, the larger the bandwidths. Nevertheless, the distribution of data points in the projection
Figure 2: The imputed and observed outcome values for each individual, for the treated (red) and for the controls (blue).
Figure 3: The fitted (estimation of $m_1$) and observed outcome values for the treated (red) and the predicted values for the controls (blue) versus the estimated central mean subspace (CMS) for the treated.
Figure 4: The fitted (estimation of $m_0$) and observed values for the controls (blue) and the predicted values for the treated (red) versus the estimated central mean subspace for the controls.
subspace can be non-uniform. In such settings, the bandwidth may be too small for the low-density intervals, and the support of the kernel function may not include neighboring data. If the kernel method fails because of a low density of data points in some regions, the package uses extrapolation and interpolation to impute missing values. For a point inside the data region, a linear interpolation is performed using two nearest points. For a point outside, extrapolation is used using a user-specified number of nearest points. The package uses the average slope between each pair of neighboring points to obtain a slope for the linear extrapolation. The results of these choices for interpolation and extrapolation may be checked visually using the above plots.

Inverse Probability Weighting (IPW)

Description

The IPW estimator of ATE weighs observed outcomes by the inverse of the estimated propensity score. For details, see Section 3.2 in Ghosh, Ma, and de Luna (2021). The expected potential outcomes are estimated as

\[ \hat{E}(Y_1) = n^{-1} \sum_{i=1}^{n} t_i y_i / \hat{p}_i, \]

and

\[ \hat{E}(Y_0) = n^{-1} \sum_{i=1}^{n} (1 - t_i) y_i / (1 - \hat{p}_i), \]

where \( \hat{p}_i = e^{\hat{\eta}(\hat{\alpha}^T x)}/(1 + e^{\hat{\eta}(\hat{\alpha}^T x)}) \), thereby yielding a corresponding estimator of ATE:

\[ \hat{D}_{IPW} = \hat{E}(Y_1) - \hat{E}(Y_0). \]

Example and Code

The function `ipw.ate` implements such an IPW estimator. Just as the function `imp.ate` needed an initial guess for \( \beta_1 \) and \( \beta_0 \), the function `ipw.ate` needs an initial guess for \( \alpha \). Given how accurate the initial \( \alpha \) guess is, one can choose the relevant optimizer. Selecting the optimizer function is done by using the `solver` = `optim` or `solver` = `cobyla` options. The option `method` can be used to select different methods for the `optim` function.

In estimating the propensity score, the local linear regression estimator may not be between 0 and 1. In such cases, we use linear interpolation to obtain an estimate between 0 and 1. However, a large number of such interpolations will reduce the accuracy of the propensity score estimation. Therefore, controlling the number of interpolations seems necessary. For this purpose, we consider this number as an additive penalty in the optimization problem.

The user can add such a penalty to the optimization. The optimization solver considers the sum of the loss function and the penalty term as the new loss function. There are two variables `penalty` and `n_before_pen` that should be assigned. The additive penalty term is `penalty` to the power of the number of predicted propensity scores falling outside of the interval \([0,1]\), minus `n_before_pen`.

\[ l_{New} = l + \text{penalty}^{(n - \text{n\_before\_pen})}, \]

where \( n \) is the number of estimated propensity scores bigger than 1 or less than 0.

As for `imp.ate`, there is an option `n_threads` allowing parallelization, that one can use to decrease runtime for big datasets. The maximum acceptable number can be found by calling the function `parallel::detectCores()`. Only one thread is possible when using Mac OS because OpenMP is not available on this operative system.
ipw <- ipw.ate(x = covariates,  
                y = y,  
                treated = treated,  
                alpha_initial = alpha)

The complete list of arguments is:

- **x**
  Covariate matrix.

- **y**
  Response vector.

- **treated**
  A binary vector indicating treatment status.

- **alpha_initial**
  Initial guess for \( \alpha \).

- **solver**
  Specifies which solver is to be used. Current options are optm and cobyla (from nloptr package). The default value is "optm".

- **kernel**
  Specifies which kernel function to be used, current options are: "EPAN", "QUARTIC", and "GAUSSIAN". The default is "EPAN".

- **explicit_bandwidth**
  Specifies if bandwidth_scale will be used as the bandwidth or if it will be calculated as bandwidth_scale \( \times \text{sd}(\alpha^T x) \times n^{1/5} \). The default value is FALSE.

- **recalc_bandwidth**
  Specifies whether the bandwidth should be recalculated after the estimation of \( \alpha \). If explicit_bandwidth = TRUE, recalc_bandwidth is not used, but if explicit_bandwidth = FALSE, and recalc_bandwidth = TRUE, bandwidth is recalculated at the beginning of the second step based on bwc_prop_score. If recalc_bandwidth = FALSE, the first step bandwidth is used. The default value is TRUE.

- **bwc_dim_red**
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used in the dimension reduction step for \( \alpha^T x \). The default value is 1.

- **bwc_prop_score**
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used for the estimation of the propensity score. The default value is 10.

- **gauss_cutoff**
  The cutoff value for Gaussian kernel. The default value is 1e-3.

- **penalty**
  Penalty for the optimizer if a probability is outside (0, 1) during the estimation of \( \alpha \) phase. Added to the function value in solver as penalty \(^{(n - n_{before\_pen})} \), where n is the number of probabilities outside (0, 1). The default value is 10.

- **n_before_pen**
  The number of probabilities outside the range (0, 1) to accept during the estimation of \( \alpha \) phase. The default value is 1.

- **n_threads**
  The number of threads for parallel computing. Set it to 1 for serial. If n_threads exceeds the maximum
number of threads, \texttt{n_threads} is set to \texttt{max_threads - 1}. To use \texttt{max_threads}, set \texttt{n_threads} to \texttt{max_threads} of the system. The default value is 1.

- \texttt{verbose}
  Specifies if the program should print output while running. The default value is \texttt{TRUE}.
- ...
  Additional parameters passed to \texttt{optim} or \texttt{cobyla}.

The IPW estimate of the average treatment effect is the main output of the function:

```
ipw$ate
#> [1] 2.174172
```

Other outputs are the fitted propensity scores and their first derivatives.

```
P = ipw$pr
dP = ipw$d_pr
```

If the function is run by setting \texttt{explicit_bandwidth = TRUE}, then the bandwidths are computed based on the coefficients \texttt{bwc_dim_red} and \texttt{bwc_prop_score}. The bandwidths used are given as output:

```
ipw$bw_dr
#> [1] 0.08774137

ipw$bw_pr
#> [1] 0.8641581
```

as well as the estimated value of \(\alpha\):

```
ipw$alpha_hat
#> [,1]
#> [1,] -0.27000000
#> [2,] 0.19668843
#> [3,] -0.14153543
#> [4,] 0.03486261
#> [5,] 0.15451347
#> [6,] -0.08843496
```

Visualization

The \texttt{plot.ipw} function visualizes the fitted propensity scores versus the estimated central mean subspace \(\hat{\alpha}^T x\), together with the treatment status of each individual; see Figure 5.

```
plot(ipw, treated = treated, covariates = covariates)
```

Augmented Inverse Probability Weighting (AIPW)

Description

The AIPW estimator combines fits from outcome and propensity score models, and is thereby doubly robust, i.e. consistent and asymptotically normal when either the outcome models or the propensity score model is correctly specified; see Ghosh, Ma, and de Luna (2021). The estimator is obtained as follows:

\[
\hat{E}(Y_1) = n^{-1} \sum_{i=1}^{n} \{t_i y_i / \hat{p}_i + (1 - t_i / \hat{p}_i) \hat{m}_1(\hat{\beta}_1^T x_i)\},
\]

\[
\hat{E}(Y_0) = n^{-1} \sum_{i=1}^{n} \{(1 - t_i) y_i / (1 - \hat{p}_i) + [1 - (1 - t_i) / (1 - \hat{p}_i)] \hat{m}_0(\hat{\beta}_0^T x_i)\},
\]
Figure 5: The estimated propensity score (red) and the treatment status (blue) versus the estimated central mean subspace.
\( \hat{D}_{\text{AIPW}} = \hat{E}(Y_1) - \hat{E}(Y_0). \)

**Example and Code**

The function `aipw.ate` that implements AIPW, asks for `imp.ate` and `ipw.ate` objects as inputs as well as observed values for outcome and treatment status.

```r
ate_aipw <- aipw.ate( y=y, treated = treated, imp = imp, ipw = ipw)
```

Thus, inputs are:
- `y` Observed response
- `treated` A binary vector indicating treatment
- `imp` The imp function output object from `imp.ate`
- `ipw` The ipw function output object from `ipw.ate`

Furthermore, the function returns the AIPW estimation of the average treatment effect:

```r
ate_aipw
#> [1] 2.025275
```

**Improved Augmented Inverse Probability Weighting (AIPW2)**

**Description**

An improved version of the AIPW estimator is also implemented; see details in Section 3.3 of Ghosh, Ma, and de Luna (2021):

\[
\hat{E}(Y_1) = n^{-1} \sum_{i=1}^{n} \{t_i y_i / \hat{p}_i + \hat{\gamma}_1 (1 - t_i / \hat{p}_i) \hat{m}_1 (\hat{\beta}_1^T x_i) \},
\]

\[
\hat{E}(Y_0) = n^{-1} \sum_{i=1}^{n} \{(1 - t_i) y_i / (1 - \hat{p}_i) + \hat{\gamma}_0 [1 - (1 - t_i) / (1 - \hat{p}_i)] \hat{m}_0 (\hat{\beta}_0^T x_i) \},
\]

and

\[
\hat{D}_{\text{IAIPW}} = \hat{E}(Y_1) - \hat{E}(Y_0),
\]

where \( \hat{\gamma}_0 \), and \( \hat{\gamma}_1 \) are:

\[
\hat{\gamma}_1 = \text{cov}\{\hat{m}_1 (\hat{\beta}_1^T x_i) t_i / \hat{p}_i, (1 - t_i / \hat{p}_i) \hat{m}_1 (\hat{\beta}_1^T x_i) \}^{-1} \times \text{cov}\{t_i y_i / \hat{p}_i, (1 - t_i / \hat{p}_i) \hat{m}_1 (\hat{\beta}_1^T x_i) \},
\]

\[
\hat{\gamma}_0 = \text{cov}\{(1 - t_i) / (1 - \hat{p}_i) \hat{m}_0 (\hat{\beta}_0^T x_i), (t_i - \hat{p}_i) / (1 - \hat{p}_i) \hat{m}_0 (\hat{\beta}_0^T x_i) \}^{-1} \times \text{cov}\{(1 - t_i) y_i / (1 - \hat{p}_i), (t_i - \hat{p}_i) / (1 - \hat{p}_i) \hat{m}_0 (\hat{\beta}_0^T x_i) \}.
\]

**Example and Code**

The AIPW2 function has as same inputs as the AIPW function.

```r
ate_aipw
#> [1] 2.025275
```
ate_iaipw <- aipw.ate(y=y, treated = treated, imp = imp, ipw=ipw)

- `y`
  Observed response
- `treated`
  A binary vector indicating treatment
- `imp`
  The imp function output object from `imp.ate`
- `ipw`
  The ipw function output object from `ipw.ate`

As output, the ATE estimation is given:

```
ate_iaipw
#> [1] 2.025727
```

**Variance of the ATE estimators**

In this section, we describe functions designed to calculate the asymptotic variances of the estimators discussed above. These asymptotic variances are obtained under regularity conditions, including:

- **C1** The univariate $m$th order kernel function $K(\cdot)$ is symmetric, Lipschitz continuous on its support $[-1, 1]$, which satisfies

  \[
  \int K(u)du = 1, \quad \int u^i K(u)du = 0, 1 \leq i \leq m - 1, 0 \neq \int u^m K(u)du < \infty.
  \]

- **C2** The bandwidths satisfy $nh^{2m} \to 0$, $nh^{2d} \to \infty$.

Theorems with asymptotic properties are given in Ghosh, Ma, and de Luna (2021), Section 3.4. For the estimators described above, we have \( \sqrt{n}(\hat{D}_{est} - D) \xrightarrow{d} N(0, var_{est}) \), where \( var_{est} \), the asymptotic variance for each estimator, are implemented in the functions described below.

**IMP**

**Description**

The asymptotic variance of the IMP estimator is

\[
var_{IMP} = E(\{m_1(\beta_1^T x_i) - m_0(\beta_0^T x_i) - E(Y_1) - E(Y_0)\})
+ E[1 + e^{-\eta(\alpha^T X_i)}|\beta_1^T x_i|t_i\{y_{1i} - m_1(\beta_1^T x_i)\}]
- E[1 + e^{\eta(\alpha^T X_i)}|\beta_0^T x_i|(1 - t_i)\{y_{0i} - m_0(\beta_0^T x_i)\}]
- E[(1 - p_i)vec(X_{Li}m_1^T(\beta_1^T X_i)^T)B_1t_i\{y_{1i} - m_1(\beta_1^T x_i)\}]
\times vec|m_1(\beta_1^T x_i) \otimes \{x_{Li} - E(X_{Li}|\beta_1^T x_i)\}|
+ E[p_i vec(X_{Li}m_0^T(\beta_0^T X_i)^T)^TB_0(1 - t_i)\{y_{0i} - m_0(\beta_0^T x_i)\}]
\times vec|m_0^T(\beta_0^T x_i) \otimes \{x_{Li} - E(X_{Li}|\beta_0^T x_i)\}|^2,
\] (6)
and for IMP2

\[ v_{IMP2} = E\{m_1(\beta_1^T x_i) - m_0(\beta_0^T x_i) - E(Y) + E(Y_0)\} \\
+ E[p_1^{-1}|\beta_1^T x_i|t_i\{y_{1i} - m_1(\beta_1^T x_i)\}] \\
- E[(1 - p_0)^{-1}|\beta_0^T x_i|(1 - t_i)\{y_{0i} - m_0(\beta_0^T x_i)\}] \\
- E[vec(X_L|m_1(\beta_1^T X_i)^T)|T B_1 t_i\{y_{1i} - m_1(\beta_1^T x_i)\}] \\
\times vec(m_1^T x_i) \otimes \{x_{Li} - E(X_{Li}|\beta_1^T x_i)\}] \\
+ E[vec(X_L|m_0(\beta_0^T X_i)^T)|T B_0(1 - t_i)\{y_{0i} - m_0(\beta_0^T x_i)\}] \\
\times vec(m_0^T x_i) \otimes \{x_{Li} - E(X_{Li}|\beta_0^T x_i)\}]^2, \]

where \( B_0 \) and \( B_1 \) are

\[
B_0 = \left( E\left( \frac{\partial vec[(1 - T_i)\{Y_{0i} - m_0(\beta_0^T X_i)\} m_0^T X_i \otimes \{X_{Li} - E(X_{Li}|\beta_0^T x_i)\}]}{\partial vec(\beta_0)^T} \right) \right)^{-1},
\]

\[
B_1 = \left( E\left( \frac{\partial vec[T_i\{Y_{1i} - m_1(\beta_1^T X_i)\} m_1^T X_i \otimes \{X_{Li} - E(X_{Li}|\beta_1^T x_i)\}]}{\partial vec(\beta_1)^T} \right) \right)^{-1}.
\]

Here \( vec[M] \) is the concatenation of the lower \((p - d) \times d\) block of a \( p \times d \) matrix \( M \), and \( vec[M] \) is a vector made by concatenation of a matrix \( M \).

**Example and Code**

The functions `imp.var` and `imp2.var` implement the above variance estimators. These functions require `imp.ate` and `ipw.ate` objects as input. The above variances require an estimation of \( E(X_{Li}|\beta_i^T x_i) \). As before, the kernel regression is used, so the variance functions require bandwidths as input. A suggestion is to use the bandwidths used by `imp.ate`. In this case, `explicit_bandwidth` must be set to `TRUE` (default value) in `imp.var` and `imp2.var`.

```r
imp <- imp.ate(x = covariates, 
    y = y, 
    treated = treated, 
    beta_guess1 = beta1, 
    beta_guess0 = beta0)

ipw <- ipw.ate(x = covariates, 
    y = y, 
    treated = treated, 
    alpha_initial = alpha)

vimp <- imp.var(x = covariates, 
    y = y, 
    treated = treated, 
    imp = imp, 
    ipw = ipw)

evimp2 <- imp2.var(x = covariates, 
    y = y, 
    treated = treated, 
    imp = imp, 
    ipw = ipw)
```

• \( x \)
  
  Covariate matrix
• \( y \)
  Response vector

• \( \text{treated} \)
  A binary vector indicating treatment

• \( \text{imp} \)
  The imp function output object from \( \text{imp.ate} \)

• \( \text{ipw} \)
  The ipw function output object from \( \text{ipw.ate} \)

• \( \text{bandwidth_scale1} \)
  Scaling of the calculated bandwidth, or in case of \( \text{explicit_bandwidth = TRUE} \)
  the actual bandwidth for the estimation of \( E(\cdot|\beta_1^T X) \). The default value is \( \text{imp$bw1} \). If this default value is used, one should use the default value \( \text{TRUE} \) for \( \text{explicit_bandwidth} \).

• \( \text{bandwidth_scale0} \)
  Scaling of the calculated bandwidth, or in case of \( \text{explicit_bandwidth = TRUE} \)
  the actual bandwidth for the estimation of \( E(\cdot|\beta_0^T X) \). The default value is \( \text{imp$bw0} \). If this default value is used, one should use the default value \( \text{TRUE} \) for \( \text{explicit_bandwidth} \).

• \( \text{kernel} \)
  Specifies which kernel function is to be used, current options are: "EPAN" (default), "QUARTIC", and "GAUSSIAN".

• \( \text{explicit_bandwidth} \)
  Specifies if bandwidth_scale will be used as the bandwidth or if it will be calculated as \( \text{bandwidth_scale} \times \text{sd}(\beta_1^T x) \times n^{(1/5)} \). The default value is \( \text{TRUE} \).

• \( \text{gauss_cutoff} \)
  The cutoff value for Gaussian kernel. The default value is \( 1e-3 \).

The output is an estimate of the asymptotic variance that can be used to construct confidence intervals based on the asymptotic normal distribution.

\[
vimp
\#
\text{[1]} \ 0.01671471
\]
\[
vimp2
\#
\text{[1]} \ 0.0166378
\]

**IPW**

**Description**

The asymptotic variance for the IPW estimator is:

\[
\begin{align*}
\text{var}_{IPW} &= E\left\{ (t_i y_{1i}/p_i - (1-t_i)y_{0i}/(1-p_i) - E(Y_1) + E(Y_0)) \right\} \\
&\quad + (1-t_i/p_i)E[m_1(\beta_1^T X_i)|\alpha^T x_i] \\
&\quad - (t_i - p_i)/(1 - p_i)E[m_0(\beta_0^T X_i)|\alpha^T x_i] \\
&\quad + (E[(m_1(\beta_1^T X_i)(1-p_i) + m_0(\beta_0^T X_i)p_i)vec\{X_Li\eta'(\alpha^T X_i)^T\}]^T B(t_i - p_i) \\
&\quad \times vec\{x_{Li} - E(X_{Li}|\alpha^T x_i)\eta'(\alpha^T x_i)^T\}^2, \\
\end{align*}
\]

where:

\[
B = \left\{ E\left( \frac{\partial vec\{X_{Li} - E(X_{Li}|\alpha^T X_i)\}(T_i - p_i)\eta'(\alpha^T X_i)^T}{\partial vec(\alpha)^T} \right) \right\}^{-1}.
\]
Example and Code

In calculating this variance, \( E(X_{L_i} | \alpha^T x_i) \) needs to be estimated. Similar to the estimation of \( E(X_{L_i} | \beta^T x_i) \) in the functions \texttt{imp.var} and \texttt{imp2.var}, a kernel regression is used to estimate \( E(X_{L_i} | \alpha^T x_i) \) here. Therefore, \texttt{ipw.var} needs a bandwidth as input too. The function uses the bandwidth that comes from the output of \texttt{ipw.ate} as long as the default values are used for \texttt{explicit_bandwidth} and \texttt{bandwidth_scale}, i.e. \texttt{explicit_bandwidth = TRUE} and \texttt{bandwidth_scale = ipw$bw_dr}. The derivative in \( B \) is difficult to find analytically, and numerical derivation is performed. The argument \texttt{num_deriv_h} determines the accuracy of the numerical derivation.

```r
vipw <- ipw.var(x = covariates, 
y = y, 
treated = treated, 
imp = imp, 
ipw = ipw)
```

- `x`  
  Covariate matrix
- `y`  
  Response vector
- `treated`  
  A binary vector indicating treatment
- `imp`  
  imp output object from \texttt{imp.ate}
- `ipw`  
  ipw output object from \texttt{ipw.ate}
- `bandwidth_scale`  
  Scaling of the calculated bandwidth, or in case of \texttt{explicit_bandwidth = TRUE}, the actual bandwidth for the estimation of \( E(· | \alpha^T X) \). The default value is \texttt{ipw$bw_dr}. If this default value is used, one should use the default value \texttt{TRUE} for \texttt{explicit_bandwidth}.
- `kernel`  
  Specifies which kernel function is to be used, current options are: \"EPAN\"(default), \"QUARTIC\", and \"GAUSSIAN\".
- `explicit_bandwidth`  
  Specifies if bandwidth\_scale will be used as the bandwidth or if it will be calculated as \texttt{bandwidth_scale} \times sd(\( \alpha^T x \)) \times n(1/5). The default value is \texttt{TRUE}.
- `gauss_cutoff`  
  The cutoff value for Gaussian kernel. The default value is \texttt{1e}-3.
- `num_deriv_h`  
  Step size of numerical derivative. The default value is \texttt{1e}-8.
- `verbose`  
  Specifies if the program should print output while running. The default value if \texttt{FALSE}.

The output is an estimate of the asymptotic variance.

```r
vipw
#> [1] 0.03044004
```
AIPW and IAIPW

Description

The asymptotic variances of the AIPW and the IAIPW estimators are equal. One can obtain the variance by calling \texttt{aipw.var} and report it for both estimators.

\[
\text{var}_{\text{AIPW}} = v_{\text{AIPW}} = \text{E}\{\{m_1(\beta_1^T x_i) - m_0(\beta_0^T x_i) - E(Y_1) + E(Y_0)\} + [1 + e^{-\eta(\alpha^T X_i)}]t_i\{y_{1i} - m_1(\beta_1^T x_i)\} - [1 + e^{\eta(\alpha^T X_i)}](1 - t_i)\{y_{0i} - m_0(\beta_0^T x_i)\}
- C_1 B_1 t_i\{y_{1i} - m_1(\beta_1^T x_i)\} vec[m'_1(\beta_1^T x_i) \otimes \{x_{Li} - E(X_{Li}|\beta_1^T x_i)\}]
+ C_0 B_0 (1 - t_i)\{y_{0i} - m_0(\beta_0^T x_i)\} vec[m'_0(\beta_0^T x_i) \otimes \{x_{Li} - E(X_{Li}|\beta_0^T x_i)\}]
+ D_1 B(t_i - p_i) vec[\{x_{Li} - E(X_{Li}|\alpha^T X_i)\} \eta'(\alpha^T X_i)^T]
+ D_0 B(t_i - p_i) vec[\{x_{Li} - E(X_{Li}|\alpha^T X_i)\} \eta'(\alpha^T X_i)^T]\}^2,
\]

where \( C_1, C_0, D_1, \) and \( D_0 \) are defined as:

\[
\begin{align*}
C_1 &= E[\{\partial m_1(\beta_1^T X_i)/\partial \text{vec}(\beta_1)^T\}(1 - T_i/p_i)] \\
C_0 &= E[\{\partial m_0(\beta_0^T X_i)/\partial \text{vec}(\beta_0)^T\}(1 - (1 - T_i)/(1 - p_i))] \\
D_1 &= E[\{Y_{1i} - m_1(\beta_1^T X_i)\} T_i e^{-\eta(\alpha^T X_i)} vec(X_{Li} \eta'(\alpha^T X_i)^T)] \\
D_0 &= E[\{Y_{0i} - m_0(\beta_0^T X_i)\} (1 - T_i) e^{\eta(\alpha^T X_i)} vec(X_{Li} \eta'(\alpha^T X_i)^T)].
\end{align*}
\]

Example and Code

Estimation of the variance of the AIPW estimator requires both estimation of \( E(X_{Li}|\alpha^T x_i) \) and \( E(X_{Li}|\beta_i^T x_i) \). As before, these estimates are performed by kernel regression. Therefore, the function needs input values for the bandwidths. The default is set to take the bandwidths used in the \texttt{imp.ate} and \texttt{ipw.ate} functions.

```r
vaipw = aipw.var(x = covariates,
    y = y,
    treated = treated,
    imp = imp,
    ipw = ipw)
```

- **x**
  Covariate matrix

- **y**
  Response vector

- **treated**
  A binary vector indicating treatment

- **imp**
  imp output object from \texttt{imp.ate}

- **ipw**
  ipw output object from \texttt{ipw.ate}

- **bandwidth_scale1**
  Scaling of the calculated bandwidth, or in case of \texttt{explicit_bandwidth = TRUE}, the actual bandwidth for the estimation of \( E(\cdot|\beta_1^T X) \). The default value is \texttt{imp$bw1}. If this default value is used, one should use the default value \texttt{TRUE} for \texttt{explicit_bandwidth}.
• **bandwidth_scale0**
  Scaling of the calculated bandwidth, or in case of `explicit_bandwidth = TRUE`, the actual bandwidth for the estimation of \( E(\cdot|\beta_0^T X) \). The default value is `imp$bw0`. If this default value is used, one should use the default value **TRUE** for `explicit_bandwidth`.

• **bandwidth_scale_pr**
  Scaling of the calculated bandwidth, or in case of `explicit_bandwidth = TRUE`, the actual bandwidth for the estimation of \( E(\cdot|\alpha^T X) \). The default value is `ipw$bw_dr`. If this default value is used, one should use the default value **TRUE** for `explicit_bandwidth`.

• **kernel**
  Specifies which kernel function is to be used, current options are: "EPAN" (default), "QUARTIC", and "GAUSSIAN".

• **explicit_bandwidth**
  Specifies if `bandwidth_scale` will be used as the bandwidth or if it will be calculated as `bandwidth_scale \times \text{sd}(\beta^T x) \times n^{(1/5)}`. The default value is **TRUE**.

• **gauss_cutoff**
  Cutoff value for Gaussian kernel. The default value is 1e-3.

• **num_deriv_h**
  Step size of numerical derivative. The default value is 1e-6.

• **verbose**
  Specifies if the program should print output while running. The default value is **FALSE**.

The output is an estimate of the asymptotic variance that can be used to construct confidence intervals based on the asymptotic normal distribution.

```r
vaipw
#> [1] 0.01640422
```

### General function

The comprehensive function `inf.ate` executes all the functions listed above, and the output contains all the outputs from these functions. The input variables for the general function includes the combination of the inputs for `ate.imp` and `ate.ipw`. The functions `aipw.ate` and `aipw2.ate`, and the variance functions use their default input values.

```r
inf = inf.ate(x = covariates,
             y = y,
             treated = treated,
             beta_guess1 = beta1,
             beta_guess0 = beta0,
             alpha_initial = alpha)
```

• **x**
  Covariate matrix

• **y**
  Response vector

• **treated**
  A binary vector indicating treatment status

• **beta_guess1**
  Initial guess for \( \beta_1 \)
• beta_guess0
  Initial guess for $\beta_0$

• alpha_initial
  Initial guess for $\alpha$

• imp.solver
  Specifies which solver is to be used for the imputation estimator. Current options are optim and cobyla (from nloptr package). The default value is "optim".

• imp.kernel
  Specifies which kernel function is to be used for the imputation estimator, current options are: "EPAN", "QUARTIC", and "GAUSSIAN". The default value is "EPAN".

• imp.explicit_bandwidth
  Specifies if bandwidth_scale will be used as the bandwidth or if it will be calculated as bandwidth_scale \times \text{sd}(\beta^T x) \times n^{(1/5)}. The default value is FALSE.

• imp.recalc_bandwidth
  Specifies whether the bandwidth should be recalculated after the first stage. If explicit_bandwidth is TRUE, imp.recalc_bandwidth is not used, but if explicit_bandwidth is FALSE, then if recalc_bandwidth is TRUE, bandwidths are recalculated at the beginning of the second step based on bwc_impute0 and bwc_impute1. If recalc_bandwidth is FALSE, the first step bandwidths are used. The default value is FALSE.

• bwc_dim_red1
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used in the dimension reduction step for $\hat{m}_1(\beta^T_1 x)$. The default value is 1.

• bwc_impute1
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used in the imputation step for $\hat{m}_1(\beta^T_1 x)$. The default value is 1.25.

• bwc_dim_red0
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used in the dimension reduction step for $\hat{m}_0(\beta^T_0 x)$. The default value is 1.

• bwc_impute0
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used in the imputation step for $\hat{m}_0(\beta^T_0 x)$. The default value is 1.25.

• imp.gauss_cutoff
  The cutoff value for Gaussian kernel. The default value is 1e-3.

• imp.penalty
  Penalty for the optimizer if local linear regression fails. Added to the function value in solver as penalty*(n - n_before_pen), where n is the number of times local linear regression fails. The default value is 10.

• imp.n_before_pen
  The number of acceptable local linear regression failures during the estimation of $\beta_0$ and $\beta_1$ phase. The default value is 5.

• imp.to_extrapolate
  Specifies whether to extrapolate or not. Since in $\hat{m}_0(\beta^T_0 x)$ and $\hat{m}_1(\beta^T_1 x)$ estimates in terms of $\beta_0$ and $\beta_1$, local linear regression at the boundaries of $\beta_0^T X$, and $\beta_1^T X$, can be very volatile, it is recommended to use extrapolation on those points instead of local linear regression. The default value is TRUE.

• imp.extrapolation_basis
  The number of data points to base extrapolation on. Extrapolation at border points can be done based on a different number of neighborhood points. extrapolation_basis is how many neighborhood points are used. The default value is 5.
• **imp.to_truncate**
  Specifies whether to truncate \( \hat{m}_0(\beta_0^T x) \) and \( \hat{m}_1(\beta_1^T x) \) or not. After estimating \( \hat{m}_0(\beta_0^T x) \) and \( \hat{m}_1(\beta_1^T x) \), if they are outside the range of observed outputs, they are replaced with the minimum and maximum observed outputs. The default value is TRUE.

• **n_threads**
  Sets the number of threads for parallel computing. Set to 1 serial. If n_threads exceeds the maximum number of threads, sets n_threads to max_threads - 1. To use max_threads, set to n_threads to max_threads of system. The default value is 1.

• **imp.solver.options**
  List of parameters passed to optim or cobyla. The default value is NA.

• **ipw.solver**
  Specifies which solver is to be used for the IPW estimator. Current options are optim and cobyla from nloptr package. The default value is 'optim'.

• **ipw.kernel**
  Specifies which kernel function to be used for the IPW estimator, current options are: "EPAN", "QUARTIC", and "GAUSSIAN". The default is "EPAN".

• **ipw.explicit_bandwidth**
  Specifies if bandwidth_scale will be used as the bandwidth or if it will be calculated as \( \text{bandwidth\_scale} \times \text{sd}(\alpha^T x) \times n^{1/5} \). The default value is FALSE.

• **ipw.recalc_bandwidth**
  Specifies whether the bandwidth should be recalculated after the estimation of \( \alpha \) (the estimation of dimension reduction step). If explicit_bandwidth is TRUE, ipw.recalc_bandwidth is not used, but if explicit_bandwidth is FALSE, then if recalc_bandwidth is TRUE, bandwidth is recalculated at the beginning of the second step based on bwc_prop_score. If recalc_bandwidth is FALSE, the first step bandwidth is used. The default value is TRUE.

• **bwc_dim_red**
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used in the dimension reduction step for \( \alpha^T x \). The default value is 1.

• **bwc_prop_score**
  Scaling of calculated bandwidth, or if explicit_bandwidth = TRUE used as the bandwidth. It is used for the estimation of the propensity score. The default value is 10.

• **ipw.gauss_cutoff**
  The cutoff value for Gaussian kernel. The default value is 1e-3.

• **ipw.penalty**
  Penalty for the optimizer if a probability is outside (0, 1) during the estimation of \( \alpha \) phase. Added to the function value in solver as \( \text{penalty}(n - n\_before\_pen) \), where \( n \) is the number of probabilities outside (0, 1). The default value is 10.

• **ipw.n_before_pen**
  The number of probabilities outside the range (0, 1) to accept during the estimation of \( \alpha \) phase. The default value is 1.

• **ipw.solver.options**
  List of parameters passed to optim or cobyla. The default value is NA.

• **verbose**
  Specifies if the program should print output while running. The default value is TRUE.

Output is a list containing:
• **imp**
  The output object of the function `imp.ate`.

• **ipw**
  The output object of the function `ipw.ate`.

• **aipw**
  The AIPW estimation of the average treatment effect.

• **aipw2**
  The improved AIPW estimation of the average treatment effect.

• **imp_var**
  The asymptotic variance of the IMP estimator.

• **imp2_var**
  The asymptotic variance of the IMP2 estimator.

• **ipw_var**
  The asymptotic variance of the IPW estimator.

• **aipw_var**
  The asymptotic variance for the AIPW and AIPW2 estimators.

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**Declaration of interests**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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