Package 'iBART'

Title Iterative Bayesian Additive Regression Trees Descriptor
Selection Method

Version 1.0.0

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Description A statistical method based on Bayesian Additive Regression Trees with Global
Standard Error Permutation Test (BART-G.SE) for descriptor selection
and symbolic regression. It finds the symbolic formula of the regression function
y=f(x) as described in Ye, Senftle, and Li (2023) <doi:10.48550/arXiv.2110.10195>.

URL https://github.com/mattsheng/iBART

BugReports https://github.com/mattsheng/iBART/issues

License GPL (>= 3)

Encoding UTF-8

LazyData true

VignetteBuilder knitr

RoxygenNote 7.2.3

Depends R (>= 4.0.0)

Imports bartMachine (>= 1.2.6), glmnet (>= 4.1-1), foreach, stats

Suggests knitr, rmarkdown, ggplot2, ggpubr

SystemRequirements Java (>= 8.0)

NeedsCompilation no

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Repository CRAN

Date/Publication 2023-11-14 17:40:02 UTC

Contents

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catalysis	*Single-Atom Catalysis Data*

Description

Single-Atom Catalysis Data

Usage

```
catalysis
```

Format

A list with 4 objects:

X Primary feature matrix: physical properties of transition metals and oxide supports

y Reponse variable: binding energy of metal/oxide pairs

head Column names of X

unit Unit of columns of X

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generate_unit	*A helper function to generate unit for iBART input*

Description

A helper function to generate unit for iBART input

Usage

```
generate_unit(unit, dimension)
```

Arguments

unit	A vector of unit of the primary features. For example, unit <- c("cm", "s"). Then the unit of $x1$ is centimeter and the unit of $x2$ is second.
dimension	A vector of dimension of the units. For example, unit <- c("cm", "s") and dimension <- c(2, 1) mean that the unit of $x1$ is square centimeter and the unit of $x2$ is second.

Value

A list that contains unit and dimension information.

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iBART *iBART descriptor selection*

Description

Finds a symbolic formula for the regression function $y = f(X)$ using (y, X) as inputs.

Usage

```
iBART(
  X = NULL,
  y = NULL,
  head = NULL,
  unit = NULL,
  BART_var_sel_method = "global_se",
  num_trees = 20,
  num_burn_in = 10000,
  num_iterations_after_burn_in = 5000,
  num_reps_for_avg = 10,
  num_permute_samples = 50,
  type.measure = "deviance",
  nfolds = 10,
  nlambda = 100,
  relax = FALSE,
  gamma = c(0, 0.25, 0.5, 0.75, 1),
  opt = c("binary", "unary", "binary"),
  sin_cos = FALSE,
  apply_pos_opt_on_neg_x = TRUE,
  hold = 0,
  pre_screen = TRUE,
  corr_screen = TRUE,
  out_sample = FALSE,
  train_idx = NULL,
  train_ratio = 1,
  Lzero = TRUE,
```

```
    parallel = FALSE,
    K = ifelse(Lzero, 5, 0),
    aic = FALSE,
    standardize = TRUE,
    writeLog = FALSE,
    verbose = TRUE,
    count = NULL,
    seed = NULL
)
```

Arguments

X	Input matrix of primary features X.
y	Response variable y.
head	Optional: name of primary features.
unit	Optional: units and their respective dimensions of primary features. This is used to perform dimension analysis for generated descriptors to avoid generating unphyiscal descriptors, such as $size + size^2$. See generate_dimension() for details.
BART_var_sel_method	
	Variable selection criterion used in BART. Three options are available: (1) "global_se", (2) "global_max", (3) "local". The default is "global_se". See var_selection_by_permute in R package bartMachine for more detail.
num_trees	BART parameter: number of trees to be grown in the sum-of-trees model. If you want different values for each iteration of BART, input a vector of length equal to number of iterations. Default is num_trees = 20.
num_burn_in	BART parameter: number of MCMC samples to be discarded as "burn-in". If you want different values for each iteration of BART, input a vector of length equal to number of iterations. Default is num_burn_in = 10000.
num_iterations_after_burn_in	
	BART parameter: number of MCMC samples to draw from the posterior distribution of $hatf(x)$. If you want different values for each iteration of BART, input a vector of length equal to number of iterations. Default is num_iterations_after_burn_in = 5000.
num_reps_for_avg	
	BART parameter: number of replicates to over over to for the BART model's variable inclusion proportions. If you want different values for each iteration of BART, input a vector of length equal to number of iterations. Default is num_reps_for_avg = 10.
num_permute_samples	
	BART parameter: number of permutations of the response to be made to generate the "null" permutation distribution. If you want different values for each iteration of BART, input a vector of length equal to number of iterations. Default is num_permute_samples = 50.
type.measure	glmnet parameter: loss to use for cross-validation. The default is type.measure="deviance", which uses squared-error for Gaussian models (a.k.a type.measure="mse" there). type.measure="mae" (mean absolute error) can be used also.

nfolds	glmnet parameter: number of folds - default is 10. Smallest value allowable is nfolds=3.
nlambda	glmnet parameter: the number of `lambda` values - default is 100.
relax	glmnet parameter: If `TRUE`, then CV is done with respect to the mixing parameter gamma as well as `lambda`. Default is `relax=FALSE`.
gamma	glmnet parameter: the values of the parameter for mixing the relaxed fit with the regularized fit, between 0 and 1; default is gamma = c(0, 0.25, 0.5, 0.75, 1)
opt	A vector of operation order. For example, opt = c("unary", "binary", "unary") will apply unary operators, then binary operators, then unary operators. Available operator sets are "unary", "binary", and "all", where "all" is the union of "unary" and "binary".
sin_cos	Logical flag for using $sin(\pi * x)$ and $cos(\pi * x)$ to generate descriptors. This is useful if you think there is periodic relationship between predictors and response. Default is sin_cos = FALSE.
apply_pos_opt_on_neg_x	
	Logical flag for applying non-negative-valued operators, such as $\sqrt{x}$ and $log(x)$, when some values of x is negative. If apply_pos_opt_on_neg_x == TRUE, apply absolute value operator first then non-negative-valued operator, i.e. generate $\sqrt{|x|}$ and $log(|x|)$ instead. Default is apply_pos_opt_on_neg_x = TRUE.
hold	Number of iterations to hold. This allows iBART to run consecutive operator transformations before screening. Note hold = 0 is equivalent to no skipping of variable selection in each iBART iterations. It should be less than `iter`.
pre_screen	Logical flag for pre-screening the primary features X using BART. Only selected primary features will be used to generate descriptors. Note that pre_screen = FALSE is equivalent to hold = 1.
corr_screen	Logical flag for screening out primary features that are independet of the response variable y.
out_sample	Logical flag for out of sample assessment. Default is out_sample = FALSE.
train_idx	Numerical vector storing the row indices for training data. Please set out_sample = TRUE if you supplied train_idx.
train_ratio	Proportion of data used to train model. Value must be between (0,1]. This is only needed when out_sample = TRUE and train_idx == NULL. Default is train_ratio = 1.
Lzero	Logical flag for L-zero variable selection. Default is Lzero = TRUE.
parallel	Logical flag for parallel L-zero variable selection. Default is parallel = FALSE.
K	If Lzero == TRUE, K sets the maximum number of descriptors to be selected.
aic	If Lzero == TRUE, logical flag for selecting best number of descriptors using AIC. Possible number of descriptors are $1 \le k \le K$.
standardize	Logical flag for data standardization prior to model fitting in BART and LASSO. Default is standardize = TRUE.
writeLog	Logical flag for writing log file to working directory. The log file will contain information such as the descriptors selected by iBART, RMSE of the linear model build on the selected descriptors, etc. Default is writeLog = FALSE.

verbose	Logical flag for printing progress to console. Default is verbose = TRUE.
count	Internal parameter. Default is count = NULL.
seed	Optional: sets the seed in both R and Java. Default is seed = NULL which does not set the seed in R nor Java.

Value

A list of iBART output.

iBART_model	The LASSO output of the last iteration of iBART. The predictors with non-zero coefficient are called the iBART selected descriptors.
X_selected	The numerical values of the iBART selected descriptors.
descriptor_names	
	The names of the iBART selected descriptors.
coefficients	Coefficients of the iBART model. The first element is an intercept.
X_train	The training matrix used in the last iteration.
X_test	The testing matrix used in the last iteration.
iBART_gen_size	The number of descriptors generated by iBART in each iteration.
iBART_sel_size	The number of descriptors selected by iBART in each iteration.
iBART_in_sample_RMSE	
	In sample RMSE of the LASSO model.
iBART_out_sample_RMSE	
	Out of sample RMSE of the LASSO model if out_sample == TRUE.
Lzero_models	The l_0-penalized regression models fitted on the iBART selected descriptors for $1 \leq k \leq K$.
Lzero_names	The name of the best kD descriptors selected by the l_0-penalized regression model for $1 \leq k \leq K$.
Lzero_in_sample_RMSE	
	In sample RMSE of the l_0-penalized regression model for $1 \leq k \leq K$.
Lzero_out_sample_RMSE	
	Out of sample RMSE of the l_0-penalized regression model for $1 \leq k \leq K$ if out_sample == TRUE.
Lzero_AIC_model	
	The best l_0-penalized regression model selected by AIC.
Lzero_AIC_names	
	The best kD descriptors where $1 \leq k \leq K$ is chosen via AIC.
Lzero_AIC_in_sample_RMSE	
	In sample RMSE of the best l_0-penalized regression models chosen by AIC.
Lzero_AIC_out_sample_RMSE	
	Out of sample RMSE of the best l_0-penalized regression models chosen by AIC if out_sample == TRUE.
runtime	Runtime in second.

Author(s)

Shengbin Ye

References

Ye, S., Senftle, T.P., and Li, M. (2023) *Operator-induced structural variable selection for identifying materials genes*, <https://arxiv.org/abs/2110.10195>.

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iBART_real_data	*iBART Real Data Result*

Description

iBART result in the real data vignette

Usage

```
iBART_real_data
```

Format

A list of iBART outputs

iBART_model A cv.glmnet object storing the iBART selected model ...

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iBART_sim	*iBART Simulation Result*

Description

iBART result in the simulation vignette

Usage

```
iBART_sim
```

Format

A list of iBART outputs

iBART_model A cv.glmnet object storing the iBART selected model ...

k_var_model *Best subset selection for linear regression*

Description

Best subset selection for linear regression

Usage

```
k_var_model(
  X_train,
  y_train,
  X_test = NULL,
  y_test = NULL,
  k = 1,
  parallel = FALSE
)
```

Arguments

X_train	The design matrix used during training.
y_train	The response variable used during training.
X_test	The design matrix used during testing. Default is X_test = NULL and full data will be used to train the best subset linear regression model.
y_test	The response variable used during testing. Default is y_test = NULL and full data will be used to train the best subset linear regression model.
k	The maximum number of predictors allowed in the model. For example, k = 5 will produce the best model 5 predictors.
parallel	Logical flag for parallelization. Default is parallel = FALSE.

Value

A list of outputs.

models	An lm object storing the best k-predictor linear model.
names	The variable name of the best k predictors.
rmse_in	In-sample RMSE of the model.
rmse_out	Out-of-sample RMSE of the model.

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