Package 'HIP'

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Description We present HIP (Heterogeneity in Integration and Prediction) for integration of multiple data views while accounting for subgroup heterogeneity to identify common and subgroupspecific variables of interest for a particular outcome. HIP accommodates Gaussian, multi-class, Poisson, and zero-inflated Poisson outcomes. In addition to this package, HIP may be accessed through an R Shiny application found at https://multi-viewlearn.shinyapps.io/HIP_ShinyApp/ . For details, refer to the paper found on arXiv: https://arxiv.org/abs/2111.06962
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covid_data

Example COVID-19 data

Description

Data taken from a multi-omic study of COVID-19 severity. This particular dataset has Sex (male/female) as the subgroup variable and HFD45 (the number of hospital free days out of the 45 days enrolled in the study) as the outcome variable; a zero indicates the patient was either still in the hospital or died. There are two views in the data: genomic and proteomic data. The genomic data consists of RNAseq expression data for 5800 genes in each patient, while the proteomic data consists of mass spectrometry data for 264 proteins in each patient. Each also has an ID variable such as 'COVID_01' which provides a label for each patient across the data views.

Usage

data("covid_data")

Format

The data is divided up into 6 dataframes: 3 for training data and 3 for testing data. The training datasets consist of 100 observations, while the testing datasets consist of 20 observations. X_train_genomic and X_test_genomic are dataframes of 5801 variables: the first column is the ID variable, while the remaining columns are genes. X_train_proteomic and X_test_proteomic are dataframes of 265 variables, the first column being an ID variable and the remaining are proteins. Y_train and Y_test consist of 3 columns: the first is the ID variable, the second column is the subgroup variable variable Sex, and the third column is the outcome variable HFD45.

Source

Source of data: Overmeyer et al. (2021), https://doi.org/10.1016/j.cels.2020.10.003

Preprocessing of data: Lipman et al. (2022), https://doi.org/10.1371/journal.pone.0267047

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Description

Creates a Python virtual environment and installs necessary packages

Usage

```
create_virtualenv()
```

Details

This function creates a Python virtual environment called "HIP_env" and installs necessary packages such as torch, numpy, and matplotlib into the environment. Once created, the environment will be used when the package is loaded.

Examples

```
create_virtualenv()
```

fixed_lambda

Fits a HIP model given lambda values

Description

fixed_lambda fits a model from X, Y data and fixed λ_{ξ} , λ_{G} supplied by the user.

Usage

```
\label{lambda} fixed\_lambda(X, Y, gamma, family, topn, lambda\_xi=1, lambda\_g=1, K=NULL, k\_thresh=0.2, update\_thresh=10^-5, epsilon=10^-4, max\_iter=50, standardize='subgroup', std_type='scale\_center', std_x=TRUE, std_y=TRUE, verbose=FALSE)
```

Χ	matrix list - list of X^d,s matrices containing covariates
Υ	matrix list - list of Y^s matrices containing outcomes
family	string - family of outcome; options are 'gaussian', 'multiclass', 'poisson' or 'zip'
topn	int or list - number of variables to retain; different values may be specified for each view using a list of length D
lambda_xi	double - value of lambda_xi in penalty term
lambda_g	double - value of lambda_g in penalty term
K	int - number of latent components; will use 'select_K_simple' to choose if not provided

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k_thresh double - threshold to use for 'select K simple' if K not provided; default = 0.2double - threshold to use for suboptimization convergence criterion; default = update_thresh 10**-5 epsilon double - threshold to use for overall convergence criterion; default = $10^{**}-4$ int - maximum number of outer loop iterations; default = 50max_iter string - One of "all", "subgroup", or "none"; default = "subgroup" standardize string - One of "scale_center", "center", or "norm"; default = "scale_center" std_type boolean - indicates whether to standardize X; default = TRUE std_x

boolean - indicates whether to standardize Y: default = TRUE std_y

verbose boolean - whether to print additional information during optimization; default =

FALSE

Value

full list - results returned from optimize_torch on full data

include list - list of length D with a 1 indicating the variable was included in subset fit

and 0 indicating not included in subset fit

subset list - results returned from optimize_torch on subset of variables

In addition, fixed_lambda returns -99 for best_index and NA for criterion to indicate they are not applicable to this case. topn is also returned.

Examples

```
# Generating data
dat_gen <- generate_data()</pre>
# Getting model from fixed_lambda
res <- fixed_lambda(dat_gen$X, dat_gen$Y, c(1,1), 'gaussian', 50)</pre>
```

format_data

Format data for use with HIP

Description

User-supplied data must be formatted properly to work with HIP functions such as select_lambda or HIP_test_eval. Use this function to format the data, which will return a list containing training/testing data converted to PyTorch tensors and useful information such as the number of data views and subgroups. Note, either X or Y data must contain the subgroup variable, and each dataframe must have an ID variable. Y data should contain an outcome variable, which may belong to a Gaussian, multiclass, Poisson, or ZIP family. You may exclude the Y data if you simply want to format X data for use in prediction functions such as HIP_pred. See the example below for a demonstration of the function using a COVID-19 dataset included in the HIP package.

```
format_data(X_train, Y_train=NULL, id_var=NULL,
subgroup_var=NULL, outcome_var=NULL, X_test=NULL, Y_test=NULL,
family="", data_source="")
```

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Arguments

X_train list of dataframes - list of D dataframes containing X training data (where D is the number of data views). NOTE: X_train should also contain the subgroup_var if it is not contained in the Y_train data.
 Y_train list of dataframes - list of D dataframes containing Y training data
 id_var string - name of ID variable in data

string - name of ID variable in data
subgroup_var string - name of subgroup variable in data
outcome_var string - name of outcome variable in data

X_test list of dataframes - list of D dataframes containing X test data, if available
Y_test list of datamframes - list of D dataframes containing Y test data, if available
family string - family of outcome data; one of either "gaussian", "multiclass", "pois-

son", or "zip"

Details

As HIP uses functions integrated in Python, it is necessary to convert dataframes to PyTorch tensors prior to use. This function also gathers training and testing data together for use in functions such as HIP_test_eval. See individual function documentation for examples. Also note that data from the generate_data function is already formatted, so they do not need to be fed into this function.

Value

Returns a list with the following:

```
Χ
             matrix list - Contains training data X^d,s matrices; access as data$X[[d]][[s]]
Υ
             matrix list - Contains training data Y^s matrices; access as data$Y[[d]][[s]]
             matrix list - Contains test data X^d,s matrices; access as data$X_test[[d]][[s]]
X_test
Y_test
             matrix list - Contains test data Y^s matrices; access as data$Y_test[[d]][[s]]
D
            int - Number of data views
S
            int - Number of unique subgroups
sub vec
            int vec - Vector with labels for subgroups
var_list
            string list - D lists containing names of variables in X data
```

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Description

generate_data returns a nested list containing data matrices and values used to generate the data.

Usage

```
generate_data(seed=1, n=c(250,260), p=c(300,350), K=2, D=2, S=2, nonzero=50, offset=25, sigma_x=1, sigma_y=1, family='gaussian', test_data=FALSE, q=1, m = 2, theta_init=NULL, B=NULL, Z=NULL, y_mean=0, y_sd=1, z_mean=25, z_sd=3, beta=0, tau=NULL, t_dist=FALSE, t_df=20)
```

seed	int or string - set a seed for replicability
n	int vector - number of subjects desired in each subgroup; should be length S
р	int vector - number of covariates desired in each data set; should be length D
K	int - number of latent components to use in generating the data
D	int - number of data sets to generate
S	int - number of subgroups
nonzero	int - number of important variables for each subgroup; same for all subgroups
offset	int - how many variables to offset the important variables between subgroups; same for all subgroups
sigma_x	double - factor by which the errors added to X are scaled by
sigma_y	double - factor by which the errors added to Y are scaled by; not applicable when family = 'poisson' or 'zip'
family	string - determines what type of outcome is generated:
	 'gaussian' - q should also be specified or q will default to 1 'multiclass' - m should also be specified or m will default to 2 'poisson' 'zip'
test_data	bool - TRUE to generate test data, FALSE otherwise
q	int - number of continuous outcomes; can be >= 1; default = 1
m	int - number of classes in multiclass outcome; can be ≥ 2 ; default = 2
theta_init	double matrix - matrix to use for theta; if None, then a theta matrix will be generated from a $\mathrm{U}(0,1)$ distribution
В	matrix list - B^d,s matrices used to generate the data; will randomly generate if not provided
Z	matrix list - Z^s matrices used to generate the data; if not provided, will generate as $N(mu = z_mean, sigma = z_sd)$
y_mean	double - Value for mean of Y; default = 0
y_sd	double - Value for sd of Y; default = 1

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z_mean	double - Value for mean of Y; default = 0
z_sd	double - Value for sd of Y; default = 1
beta	double - Value of intercept term; default = 0
t_dist	boolean - if family = "gaussian", setting $t_dist = TRUE$ will generate data with errors drawn from a t-distribution with some specified degrees of freedom
t_df	int - degrees of freedom for t-distribution if t_dist = TRUE; default = 20

Details

generate_data can be used to generate simulated multi-view data across different subgroups. The input parameters specify relevant information such as the number of data views, the number of subgroups, subjects desired for each subgroup, and more. The output of generate_data gives the $X^{d,s}$ data matrices and Y^s outcome matrices, as well as values used to generate the data such as the Z^s and $B^{d,s}$ matrices. See the HIP paper for details.

Value

generate_data returns a nested list object with the following elements:

```
Χ
             matrix list - Contains X^d,s matrices; access as data$X[[d]][[s]]
Υ
             matrix list - Contains Y^s matrices; access as data$Y[[d]][[s]]
X_test
             matrix list - Contains test data X^d,s matrices; access as data$X_test[[d]][[s]]
Y_test
             matrix list - Contains test data Y^s matrices; access as data$Y_test[[d]][[s]]
             int - Number of data sets generated
             int - Number of subgroups
sub_vec
             int vec - Vector with labels for subgroups (from 1 to S)
Ζ
             matrix list - Contains all Z's matrices used to generate the data; access as data[[Z]][[d]][[s]]
В
             matrix list - Contains all B^d,s matrices used to generate the data; access as data[[B]][[d]][[s]]
             matrix - Contains the theta matrix used in generating the data; access as data$theta
theta
beta
             double - Value for intercept
             double - If family = 'zip', proportion of observations in zero state with default = 0.25; None ow
tau
             double - Value for mean of Y
y_mean
             double - Value for sd of Y
y_sd
             double - Value for mean of Z
z_mean
             double - Value for sd of Z
z sd
             int or string - Value of seed used to generate the data
seed
var_list
             vec list - Contains D vectors with labels for variables in each dataset (1 to p^d)
```

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get_best_r

Helper function to get best result from select lambda

Description

'get_best_R' is used within the select_lambda function to get the best result based on model performance. Not generally called by the user.

Usage

```
get_best_r(res_list, criterion="", family)
```

Arguments

res_list list - search_results list from the select_lambda output criterion string - criterion for model selection: one of 'CV', 'BIC', 'AIC', 'eBIC_0',

'eBIC_5', or 'eBIC_1'

family string - family of outcome data ('gaussian', 'multiclass', etc.)

Details

get_best_R takes in the list of results from the select_lambda tuning function, and returns the index of the best result. It also takes in the criterion used in training such as AIC or BIC, in addition to the family the outcome data belongs to.

Value

get_best_R returns the index of the best results from the select_lambda output

```
# Generate data
dat_gen <- generate_data()

# Get results from select_lambda
res <- select_lambda(dat_gen$X, dat_gen$Y, c(1,1), "gaussian", 50, K=2, num_steps=c(4,4))
best_index <- get_best_r(res$out$search_results, "eBIC_0", "gaussian")</pre>
```

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HIP_pred	Make predictions from HIP model	

Description

Outputs predicted Y values given X data and results from select_lambda or fixed_lambda.

Usage

```
HIP_pred(X_dat, res, fix_or_search, standardize="no")
```

Arguments

Value

The function returns a list of S tensors containing predictions for observations in each subgroup.

Examples

HIP_test_eval

Evaluate model on test data

Description

HIP_test_eval is used to get model performance metrics (e.g. MSE or classification accuracy) on test data. It can be used with models generated by select_lambda or fixed_lambda.

```
HIP_test_eval(data, res, fix_or_search, outcome_var=NULL)
```

HIP_train_eval

Arguments

data data object such as from generate_data or py_data containing both X, Y data

and X test, Y test data

res training result such as from select_lambda or fixed_lambda

fix_or_search string - 'fixed' for results from fixed_lambda, 'search' for results from select_lambda

outcome_var string - label of outcome variable, if available

Value

HIP_test_eval returns a list with the following:

each tensor(double) - (for gaussian outcomes) tensor of MSEs for each of the q out-

comes

comp_val tensor(double) - MSE for gaussian outcomes, classification accuracy for multi-

class outcomes, fraction of deviance explained for poisson/ZIP outcomes

pred list<tensor(double) - predicted values from fitted model. For multiclass out-

comes, single integer to represent class, starting with 0. For poisson/ZIP, pre-

dicted means from fitted model

dev_sum list(tensor(double)) - (for poisson/ZIP outcomes), list with more detailed de-

viance information

Also returns a histogram plot for predicted vs. true values in each subgroup.

Examples

HIP_train_eval

Evaluate model on training data

Description

HIP_train_eval is used to get training metrics (e.g. MSE or classification accuracy) from a model built using HIP. It can be used with models generated by select_lambda or fixed_lambda.

```
HIP_train_eval(data, res, fix_or_search)
```

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Arguments

data object such as from generate_data or py_data

res training result such as from select_lambda or fixed_lambda

fix_or_search string - 'fixed' for results from fixed_lambda, 'search' for results from select_lambda

Value

HIP_train_eval returns a list with the following:

each tensor(double) - (for gaussian outcomes) tensor of MSEs for each of the q out-

comes

comp_val tensor(double) - MSE for gaussian outcomes, classification accuracy for multi-

class outcomes, fraction of deviance explained for poisson/ZIP outcomes

pred list<tensor(double) - predicted values from fitted model. For multiclass out-

comes, single integer to represent class, starting with 0. For poisson/ZIP, pre-

dicted means from fitted model

dev_sum list(tensor(double)) - (for poisson/ZIP outcomes), list with more detailed de-

viance information

Also returns a histogram plot for predicted vs. true values in each subgroup.

Examples

optimize_torch

Main optimization function for continuous outcomes

Description

This function is used to fit a HIP model given X and Y training data, a set of lambda values, and gamma values. This largely exists as a helper function, as the user will more often use select_lambda or fixed_lambda to fit HIP models (which then access optimize_torch). However, the function is available if the user needs to access the optimization function directly.

```
\label{lem:continuous} optimze\_torch(X, Y, lambda\_xi, lambda\_g, gamma, family, K=NULL, k\_thresh=0.2, update\_thresh=10^-5, epsilon=10^-4, max\_iter=50, standardize='subgroup', std\_type='scale\_center', std\_x=TRUE, std\_y=TRUE, verbose=FALSE)
```

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Arguments

Y matrix list - list of Y^s matrices containing outcomes

lambda_xi double - value of lambda_xi in penalty term lambda_g double - value of lambda_g in penalty term

gamma list - indicators of whether to penalize each data view; should be length D string - family of outcome; options are 'gaussian', 'multiclass', 'poisson' or

'zip'

K int - number of latent components; will use 'select_K_simple' to choose if not

provided

k_thresh double - threshold to use for 'select_K_simple' if K not provided; default = 0.2 update_thresh double - criteria for convergence in Z, G, Xi, and theta optimization functions;

 $default = 10^{-5}$

epsilon double - criteria for outer loop convergence; default = 10^-4

max_iter int - maximum number of outer loop iterations allowed; default = 50 standardize string - One of "all", "subgroup", or "none"; default = "subgroup"

std_type string - One of "scale_center", "center", or "norm"; default = "scale_center"

std_x boolean - indicates whether to standardize X; default = True std_y boolean - indicates whether to standardize Y; default = True

verbose boolean - indicates whether to print additional info during run; default = False

matrix list - list of X^d,s matrices containing covariates

Value

Returns a list with the possible following elements based on status:

theta tensor - estimate of theta beta tensor - estimate of beta

B list<tensor> - estimates of each B^d,s
G list<tensor> - estimates of each G^d
Xi list<tensor> - estimates of each Xi^d,s
Z list<tensor> - estimates of each Z^s

Lambda tuple - values of lambda_xi and lambda_g used

BIC double - calculated BIC

AIC double - calculated AIC

pred double - prediction loss evaluated at final estimates

train_err nested list - list returned from function to calculate training error

message string - message with the status of the result; "Converged" if converged success-

fully, "MAX ITERS" if algorithm reached max_iter without converging.

paths list - history of losses until convergence
iter int - number of iterations to converge
iter_time double - time to find solution in seconds
conv_criterion double - value of last convergence criterion
std_x boolean - whether X was standardized
std_y boolean - whether Y was standardized

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Examples

```
# Generating data
dat_gen <- generate_data()

# Run the optimization algorithm given the data, lambdas, and gamma
optimization_out <- optimize_torch(dat_gen$Y, dat_gen$X, 0.5, 0.5, c(1,1), 'gaussian', K=3)</pre>
```

select_lambda

Fit HIP models across multiple lambda values

Description

select_lambda searches across lambda values (either grid search or random) and fits HIP models given training data. The best model is chosen based on selection criteria such as cross-validation, BIC, or AIC. Results can then be used for model evaluation, prediction, and plotting.

Usage

Χ	matrix list - list of X^d,s matrices containing covariates
Υ	matrix list - list of Y^s matrices containing outcomes
gamma	list - indicators of whether to penalize each data view; should be length D
family	string - family of outcome; options are 'gaussian', 'multiclass', 'poisson' or 'zip'
topn	int or list - number of variables to retain; different values may be specified for each view using a list of length D
ncore	int - number of cores to use in parallel processing; default is half of available cores
K	int - number of latent components; will use 'select_K_simple' to choose if not provided
k_thresh	• double - threshold to use for 'select_K_simple' if K not provided; default = 0.2
epsilon	double - threshold to use for overall convergence criterion; default = $10**-4$
max_iter	int - maximum number of outer loop iterations; default = 50
search	string - what type of search to perform for lambda parameter; default = "random"
	• "random" - tries a random selection of rand_prop*num_steps lambda values

- in grid
- "grid" tries all lambda values in grid

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xi_range list - minimum and maximum values to consider for lambda_xi; default = c(0.0,

2.0)

g_range list - minimum and maximum values to consider for lambda_g; default = c(0.0,

2.0)

num_steps list - list of two integers; the first is the number of steps for lambda_xi (default

= 8) and the second is the number of steps for lambda_g. Together these define

the number of steps to use in lambda grid

standardize string - One of "all", "subgroup", or "none"; default = "subgroup"

std_type string - One of "scale_center", "center", or "norm"; default = "scale_center"

std_x boolean - indicates whether to standardize X; default = True std_y boolean - indicates whether to standardize Y; default = True

verbose whether to print additional information during optimization; default = False

selection_criterion

string - criterion to use for selecting the best model; one of 'CV', 'BIC', 'AIC',

'eBIC_0', 'eBIC_5', or 'eBIC_1'. eBIC_0 by default.

folds int - number of folds to use if CV is selected as the selection criterion; default =

5

Value

The output is quite large, but most items do not need to be accessed directly by the user and instead are accessed by functions such as HIP_train_eval or HIP_pred. First, select_lambda returns a nested list called out which contains the following:

search_results list - list with results returned from the optimize_torch Python function for each

lambda value tried (see below for detailed output information)

total_time double - time to complete entire search in seconds

xi_range list - minimum and maximum values considered for lambda_xi g_range list - minimum and maximum values considered for lambda_g

num_steps dict - number of steps used in lambda grid

search string - type of search performed for selecting lambda parameters

select_lambda also returns the following:

best_index int - index of the best model chosen by the selection criterion

criterion string - criterion for model selection: one of 'CV', 'BIC', 'AIC', 'eBIC_0',

'eBIC_5', or 'eBIC_1'. eBIC_0 by default.

topn int or list - number of variables retained
standardize string - stores option used to standardize data
family string - stores family label for outcome data

search_results is a large list containing results from fit models. First, it contains multiple fit models which have the following items:

full list - results returned from optimize_torch on full data

include list - list of length D with a 1 indicating the variable was included in subset fit

and 0 indicating not included in subset fit

subset list - results returned from optimize_torch on subset of variables

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full and subset are large lists which contain the following:

theta	tensor - estimate of theta
beta	tensor - estimate of beta
В	list <tensor> - estimates of each B^d,s</tensor>
G	list <tensor> - estimates of each G^d</tensor>
Xi	list <tensor> - estimates of each Xi^d,s</tensor>
Z	list <tensor> - estimates of each Z^s</tensor>
Lambda	tuple - values of lambda_xi and lambda_g used
BIC	double - calculated BIC
AIC	double - calculated AIC
pred	double - prediction loss evaluated at final estimates
train_err	nested list - list returned from function to calculate training error
message	string - message with the status of the result; "Converged" if converged successfully, "MAX ITERS" if algorithm reached max_iter without converging.
paths	list - history of losses until convergence
iter	int - number of iterations to converge
iter_time	double - time to find solution in seconds
conv_criterion	double - value of last convergence criterion

Examples

std_x
std_y

```
dat_gen <- generate_data()
res <- select_lambda(dat_gen$X, dat_gen$Y, c(1,1), 'gaussian', 50)</pre>
```

boolean - whether X was standardized

boolean - whether Y was standardized

standardize_dat

Standardizes input data

Description

Helper function used to standardize testing data from training data.

```
standardize_dat(
    standardize,
    std_type,
    X = NULL,
    Y = NULL,
    X_train = NULL,
    Y_train = NULL,
    std_x = TRUE,
    std_y = TRUE,
    verbose = TRUE
)
```

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Arguments

standardize	string - One of "all", "subgroup", or "none"
std_type	string - One of "scale_center", "center", or "norm"
Χ	matrix list - list of X ^d ,s matrices containing covariates
Υ	matrix list - list of Y^s matrices containing outcomes
X_train	matrix list - list of X^d ,s matrices whose mean and sd will be used to standardize X
Y_train	matrix list - list of Y^s matrices whose mean andd sd will be used to standardize Υ
std_x	boolean - indicates whether to standardize X; default = True
std_y	boolean - indicates whether to standardize Y; default = True

Value

Returns a nested list with the following elements:

X matrix list - standardized X^d,s if standardization was requested
Y matrix list - standardized Y^s if standardization was requested

|--|

Description

Outputs plots showing the highest ranking variables contributing to model performance. Plots are shown for each data view and subgroup.

Usage

```
variable_plots(data, res, fix_or_search, top_plotted=15, compact=TRUE,
output_table=FALSE, file_path=NA)
```

data	data object from generate_data or format_data
res	output from select_lambda or fixed_lambda
fix_or_search	string - 'fixed' if results obtained from fixed_lambda, 'search' otherwise
top_plotted	int - number of variables to include in each variable importance plot; 15 by default
compact	boolean - if TRUE (default), only plots top_plotted variables; if set to FALSE, plots as many as possible
output_table	boolean - set to TRUE to write variable importance results to an Excel file; FALSE by default
file_path	string - if output_table is TRUE, you may also specify a file path and file name; make sure to add the .xlsx extension to your file name. By default, it will be written to your current working directory with the name "variable_importance_table.xlsx"

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Value

Returns the variable importance plot as a ggplot object

```
# Generate data
dat_gen <- generate_data()

# Get results from select_lambda
res <- select_lambda(dat_gen$X, dat_gen$Y, c(1,1), 'gaussian', 50)

# Variable importance plots
variable_plots(dat_gen, res, 'search', output_table=TRUE)</pre>
```

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