Package: VCBART (via r-universe)

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Title Fit Varying Coefficient Models with Bayesian Additive Regression Trees

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Description Fits linear varying coefficient (VC) models, which assert a linear relationship between an outcome and several covariates but allow that relationship (i.e., the coefficients or slopes in the linear regression) to change as functions of additional variables known as effect modifiers, by approximating the coefficient functions with Bayesian Additive Regression Trees. Implements a Metropolis-within-Gibbs sampler to simulate draws from the posterior over coefficient function evaluations. VC models with independent observations or repeated observations can be fit. For more details see Deshpande et al. (2026) <doi:10.1214/24-BA1470>.

License GPL (>= 3)

LinkingTo Rcpp, RcppArmadillo

Imports Rcpp, MASS

URL https://github.com/skdeshpande91/VCBART

NeedsCompilation yes

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`predict_betas` *Compute posterior predictive evaluates of covariate effect functions.*

Description

Given an object returned by `VCBART_ind` or `VCBART_cs` and matrices of continuous and categorical modifiers, returns MCMC samples of the coefficient functions evaluated the provided points.

Usage

```
predict_betas(fit,
              Z_cont = matrix(0, nrow = 1, ncol = 1),
              Z_cat =  matrix(0, nrow = 1, ncol = 1),
              verbose = TRUE)
```

Arguments

`fit`	A list returned by `VCBART_ind` or `VCBART_cs`
`Z_cont`	Matrix of continuous modifiers at which you wish to evaluate the covariate effect functions. Default is a 1x1 matrix, which signals that no continuous modifiers are required for these evaluations.
`Z_cat`	Integer matrix of categorical modifiers at which you wish to evaluate the covariate effect functions. Default is a 1x1 matrix, which signals that no continuous modifiers are required for these evaluations.
`verbose`	Boolean indicating whether the code should print its progress (`TRUE`). Default is `TRUE`.

Value

An array of size nd x N x (p+1) where nd is the total number of MCMC draws, N is the total number of points at which you are evaluating the covariate effect functions (i.e. `nrow(Z_cont)` or `nrow(Z_cat)`), and p is the number of covariates. Note that the intercept function is included as the first slice in the third dimension.

summarize_beta *Compute posterior mean and 95% credible interval for evaluations of each coefficient function.*

Description

Given an array of posterior samples of coefficient function evaluations, returns the posterior mean and 95% credible interval for each evaluation.

Usage

```
summarize_beta(beta_samples)
```

Arguments

beta_samples	An array, returned by VCBART_ind, VCBART_cs, or predict_betas of posterior samples of coefficient function evaluations

Value

An array of size N x 3 x p where N is the number of inputs at which the coefficient functions are evaluated (i.e. N = dim(beta_samples)[2]) and p is the total number of coefficient functions including the intercept (i.e. p = dim(beta_samples)[3]). The j-th slice is an N x 3 matrix where the columns correspond to the posterior mean, 2.5% quantile, and 97.5% quantile of each evaluation of the (j-1)-th coefficient function. Note the effect of predictor X_j (i.e., $\beta_j(Z)$ is the (j+1)-st coefficient function.

VCBART_cs *Fit a VCBART model with compound symmetry error structure*

Description

Fit a varying coefficient model to panel data. Assumes a compound symmetry error structure in which the residual errors for a given subject are equally correlated. This is equivalent to assuming that there is a normally distributed random effect per subject.

Usage

```
VCBART_cs(Y_train,subj_id_train, ni_train,X_train,
          Z_cont_train = matrix(0, nrow = 1, ncol = 1),
          Z_cat_train = matrix(0L, nrow = 1, ncol = 1),
          X_test = matrix(0, nrow = 1, ncol = 1),
          Z_cont_test = matrix(0, nrow = 1, ncol = 1),
          Z_cat_test = matrix(0, nrow = 1, ncol = 1),
          unif_cuts = rep(TRUE, times = ncol(Z_cont_train)),
          cutpoints_list = NULL,
```

```
cat_levels_list = NULL,
edge_mat_list = NULL,
graph_split = rep(FALSE, times = ncol(Z_cat_train)),
sparse = TRUE,
rho = 0.9,
M = 50,
mu0 = NULL, tau = NULL, nu = NULL, lambda = NULL,
nd = 1000, burn = 1000, thin = 1,
save_samples = TRUE, save_trees = TRUE,
verbose = TRUE, print_every = floor( (nd*thin + burn)/10))
```

Arguments

Y_train	Vector of continous responses for training data
ni_train	Vector containing the number of observations per subject in the training data.
subj_id_train	Vector of length length(Y_train) that records which subject contributed each observation. Subjects should be numbered sequentially from 1 to length(ni_train).
X_train	Matrix of covariates for training observations. Do not include intercept as the first column.
Z_cont_train	Matrix of continuous modifiers for training data. Note, modifiers must be rescaled to lie in the interval [-1,1]. Default is a 1x1 matrix, which signals that there are no continuous modifiers in the training data.
Z_cat_train	Integer matrix of categorical modifiers for training data. Note categorical levels should be 0-indexed. That is, if a categorical modifier has 10 levels, the values should run from 0 to 9. Default is a 1x1 matrix, which signals that there are no categorical modifiers in the training data.
X_test	Matrix of covariate for testing observations. Default is a 1x1 matrix, which signals that testing data is not provided.
Z_cont_test	Matrix of continuous modifiers for testing data. Default is a 1x1 matrix, which signals that testing data is not provided.
Z_cat_test	Integer matrix of categorical modifiers for testing data. Default is a 1x1 matrix, which signals that testing data is not provided.
unif_cuts	Vector of logical values indicating whether cutpoints for each continuous modifier should be drawn from a continuous uniform distribution (TRUE) or a discrete set (FALSE) specified in cutpoints_list. Default is TRUE for each variable in Z_cont_train
cutpoints_list	List of length ncol(Z_cont_train) containing a vector of cutpoints for each continuous modifier. By default, this is set to NULL so that cutpoints are drawn uniformly from a continuous distribution.
cat_levels_list	List of length ncol(Z_cat_train) containing a vector of levels for each categorical modifier. If the j-th categorical modifier contains L levels, cat_levels_list[[j]] should be the vector 0:(L-1). Default is NULL, which corresponds to the case that no categorical modifiers are available.

edge_mat_list	List of adjacency matrices if any of the categorical modifiers are network-structured. Default is NULL, which corresponds to the case that there are no network-structured categorical modifiers.
graph_split	Vector of logicals indicating whether each categorical modifier is network-structured. Default is rep(FALSE, times = ncol(Z_cat_train)).
sparse	Logical, indicating whether or not to perform variable selection in each tree ensemble based on a sparse Dirichlet prior rather than uniform prior; see Linero 2018. Default is TRUE
rho	Initial auto-correlation parameter for compound symmetry error structure. Must be between 0 and 1. Default is 0.9.
M	Number of trees in each ensemble. Default is 50.
mu0	Prior mean for jumps/leaf parameters. Default is 0 for each beta function. If supplied, must be a vector of length 1 + ncol(X_train).
tau	Prior standard deviation for jumps/leaf parameters. Default is 1/sqrt(M) for each beta function. If supplied, must be a vector of length 1 + ncol(X_train).
nu	Degrees of freedom for scaled-inverse chi-square prior on sigma^2. Default is 3.
lambda	Scale hyperparameter for scaled-inverse chi-square prior on sigma^2. Default places 90% prior probability that sigma is less than sd(Y_train).
nd	Number of posterior draws to return. Default is 1000.
burn	Number of MCMC iterations to be treated as "warmup" or "burn-in". Default is 1000.
thin	Number of post-warmup MCMC iteration by which to thin. Default is 1.
save_samples	Logical, indicating whether to return all posterior samples. Default is TRUE. If FALSE, only posterior mean is returned.
save_trees	Logical, indicating whether or not to save a text-based representation of the tree samples. This representation can be passed to predict_flexBART to make predictions at a later time. Default is FALSE.
verbose	Logical, inciating whether to print progress to R console. Default is TRUE.
print_every	As the MCMC runs, a message is printed every print_every iterations. Default is floor((nd*thin + burn)/10) so that only 10 messages are printed.

Details

Given p covariates $X_1, \ldots, X_p$ and r effect modifiers $Z_1, \ldots, Z_r$, the varying coefficient model asserts that

$E[Y|X = x, Z =] = \beta_0(z) + \beta_1(z) * x_1 + ...\beta_p(z) * X_p.$

That is, for any r-vector Z, the relationships between X and Y is linear. However, the specific relationship is allowed to vary with respect tp Z. VCBART approximates the covariate effect functions $\beta_0(Z), \ldots, \beta_p(Z)$ using ensembles of regression trees. This function assumes that the within-subject errors are equi-correlated (i.e. a compound symmetry error structure).

Value

A list containing

`y_mean` Mean of the training observations (needed by `predict_VCBART`)

`y_sd` Standard deviation of the training observations (needed by `predict_VCBART`)

`x_mean` Vector of means of columns of `X_train`, including the intercept (needed by `predict_VCBART`).

`x_sd` Vector of standard deviations of `X_trian`, including the intercept (needed by `predict_VCBART`).

`yhat.train.mean`
Vector containing posterior mean of evaluations of regression function E[y|x,z] on training data.

`betahat.train.mean`
Matrix with `length(Y_train)` rows and `ncol(X_train)+1` columns containing the posterior mean of evaluations of each coefficient function evaluated on the training data. Each row corresponds to a training set observation and each column corresponds to a coefficient function. Note the first column is for the intercept function.

`yhat.train` Matrix with `nd` rows and `length(Y_train)` columns. Each row corresponds to a posterior sample of the regression function E[y|x,z] and each column corresponds to a training set observation. Only returned if `save_samples == TRUE`.

`betahat.train` Array of dimension with `nd` x `length(Y_train)` x `ncol(X_train)+1` containing posterior samples of evaluations of the coefficient functions. The first dimension corresponds to posterior samples/MCMC iterations, the second dimension corresponds to individual training set observations, and the third dimension corresponds to coefficient functions. Only returned if `save_samples == TRUE`.

`yhat.test.mean` Vector containing posterior mean of evaluations of regression function E[y|x,z] on testing data.

`betahat.test.mean`
Matrix with `nrow(X_test)` rows and `ncol(X_testn)+1` columns containing the posterior mean of evaluations of each coefficient function evaluated on the training data. Each row corresponds to a training set observation and each column corresponds to a coefficient function. Note the first column is for the intercept function.

`yhat.test` Matrix with `nd` rows and `nrow(X_test)` columns. Each row corresponds to a posterior sample of the regression function E[y|x,z] and each column corresponds to a testing set observation. Only returned if `save_samples == TRUE`.

`betahat.test` Array of size `nd` x `nrow(X_test)` x `ncol(X_test)+1` containing posterior samples of evaluations of the coefficient functions. The first dimension corresponds to posterior samples/MCMC iterations, the second dimension corresponds to individual training set observations, and the third dimension corresponds to coefficient functions. Only returned if `save_samples == TRUE`.

`sigma` Vector containing ALL samples of the residual standard deviation, including warmup.

rho	Vector containing ALL samples of the auto-correlation parameter rho, including warmup.
varcounts	Array of size nd x R x ncol(X)+1 that counts the number of times a variable was used in a decision rule in each posterior sample of each ensemble. Here R is the total number of potential modifiers (i.e. R = ncol(Z_cont_train) + ncol(Z_cat_train)).
theta	If sparse=TRUE, an array of size nd x R ncol(X)+1 containing samples of the variable splitting probabilities.
trees	A list (of length nd) of lists (of length ncol(X_train)+1) of character vectors (of length M) containing textual representations of the regression trees. The string for the s-th sample of the m-th tree in the j-th ensemble is contaiend in trees[[s]][[j]][m]. These strings are parsed by predict_VCBART to reconstruct the C++ representations of the sampled trees.

VCBART_ind *Fit a VCBART model with independent error structure*

Description

Fit a varying coefficient model to panel data. Assumes residual errors are independent within and between subjects. See Deshpande et al. (2024) for details about the model and MCMC sampler.

Usage

```
VCBART_ind(Y_train,subj_id_train, ni_train,X_train,
           Z_cont_train = matrix(0, nrow = 1, ncol = 1),
           Z_cat_train = matrix(0L, nrow = 1, ncol = 1),
           X_test = matrix(0, nrow = 1, ncol = 1),
           Z_cont_test = matrix(0, nrow = 1, ncol = 1),
           Z_cat_test = matrix(0, nrow = 1, ncol = 1),
           unif_cuts = rep(TRUE, times = ncol(Z_cont_train)),
           cutpoints_list = NULL,
           cat_levels_list = NULL,
           edge_mat_list = NULL,
           graph_split = rep(FALSE, times = ncol(Z_cat_train)),
           sparse = TRUE,
           M = 50,
           mu0 = NULL, tau = NULL, nu = NULL, lambda = NULL,
           nd = 1000, burn = 1000, thin = 1,
           save_samples = TRUE, save_trees = TRUE,
           verbose = TRUE, print_every = floor( (nd*thin + burn)/10))
```

Arguments

Y_train	Vector of continous responses for training data
ni_train	Vector containing the number of observations per subject in the training data.

subj_id_train	Vector of length length(Y_train) that records which subject contributed each observation. Subjects should be numbered sequentially from 1 to length(ni_train).
X_train	Matrix of covariates for training observations. Do not include intercept as the first column.
Z_cont_train	Matrix of continuous modifiers for training data. Note, modifiers must be rescaled to lie in the interval [-1,1]. Default is a 1x1 matrix, which signals that there are no continuous modifiers in the training data.
Z_cat_train	Integer matrix of categorical modifiers for training data. Note categorical levels should be 0-indexed. That is, if a categorical modifier has 10 levels, the values should run from 0 to 9. Default is a 1x1 matrix, which signals that there are no categorical modifiers in the training data.
X_test	Matrix of covariate for testing observations. Default is a 1x1 matrix, which signals that testing data is not provided.
Z_cont_test	Matrix of continuous modifiers for testing data. Default is a 1x1 matrix, which signals that testing data is not provided.
Z_cat_test	Integer matrix of categorical modifiers for testing data. Default is a 1x1 matrix, which signals that testing data is not provided.
unif_cuts	Vector of logical values indicating whether cutpoints for each continuous modifier should be drawn from a continuous uniform distribution (TRUE) or a discrete set (FALSE) specified in cutpoints_list. Default is TRUE for each variable in Z_cont_train
cutpoints_list	List of length ncol(Z_cont_train) containing a vector of cutpoints for each continuous modifier. By default, this is set to NULL so that cutpoints are drawn uniformly from a continuous distribution.
cat_levels_list	List of length ncol(Z_cat_train) containing a vector of levels for each categorical modifier. If the j-th categorical modifier contains L levels, cat_levels_list[[j]] should be the vector 0:(L-1). Default is NULL, which corresponds to the case that no categorical modifiers are available.
edge_mat_list	List of adjacency matrices if any of the categorical modifiers are network-structured. Default is NULL, which corresponds to the case that there are no network-structured categorical modifiers.
graph_split	Vector of logicals indicating whether each categorical modifier is network-structured. Default is rep(FALSE, times = ncol(Z_cat_train)).
sparse	Logical, indicating whether or not to perform variable selection in each tree ensemble based on a sparse Dirichlet prior rather than uniform prior; see Linero 2018. Default is TRUE
M	Number of trees in each ensemble. Default is 50.
mu0	Prior mean for jumps/leaf parameters. Default is 0 for each beta function. If supplied, must be a vector of length 1 + ncol(X_train).
tau	Prior standard deviation for jumps/leaf parameters. Default is 1/sqrt(M) for each beta function. If supplied, must be a vector of length 1 + ncol(X_train).
nu	Degrees of freedom for scaled-inverse chi-square prior on sigma^2. Default is 3.

lambda	Scale hyperparameter for scaled-inverse chi-square prior on sigma^2. Default places 90% prior probability that sigma is less than sd(Y_train).
nd	Number of posterior draws to return. Default is 1000.
burn	Number of MCMC iterations to be treated as "warmup" or "burn-in". Default is 1000.
thin	Number of post-warmup MCMC iteration by which to thin. Default is 1.
save_samples	Logical, indicating whether to return all posterior samples. Default is TRUE. If FALSE, only posterior mean is returned.
save_trees	Logical, indicating whether or not to save a text-based representation of the tree samples. This representation can be passed to predict_flexBART to make predictions at a later time. Default is FALSE.
verbose	Logical, inciating whether to print progress to R console. Default is TRUE.
print_every	As the MCMC runs, a message is printed every print_every iterations. Default is floor((nd*thin + burn)/10) so that only 10 messages are printed.

Details

Given p covariates $X_1, \ldots, X_p$ and r effect modifiers $Z_1, \ldots, Z_r$, the varying coefficient model asserts that

$E[Y|X = x, Z =] = \beta_0(z) + \beta_1(z) * x_1 + ...\beta_p(z) * X_p.$

That is, for any r-vector Z, the relationships between X and Y is linear. However, the specific relationship is allowed to vary with respect tp Z. VCBART approximates the covariate effect functions $\beta_0(Z), \ldots, \beta_p(Z)$ using ensembles of regression trees. This function assumes that the within-subject errors are independent.

Value

A list containing

y_mean	Mean of the training observations (needed by predict_VCBART)
y_sd	Standard deviation of the training observations (needed by predict_VCBART)
x_mean	Vector of means of columns of X_train, including the intercept (needed by predict_VCBART).
x_sd	Vector of standard deviations of X_trian, including the intercept (needed by predict_VCBART).
yhat.train.mean	Vector containing posterior mean of evaluations of regression function E[y|x,z] on training data.
betahat.train.mean	Matrix with length(Y_train) rows and ncol(X_train)+1 columns containing the posterior mean of evaluations of each coefficient function evaluated on the training data. Each row corresponds to a training set observation and each colunn corresponds to a coefficient function. Note the first column is for the intercept function.

`yhat.train` Matrix with `nd` rows and `length(Y_train)` columns. Each row corresponds to a posterior sample of the regression function E[y|x,z] and each column corresponds to a training set observation. Only returned if `save_samples == TRUE`.

`betahat.train` Array of dimension with `nd` x `length(Y_train)` x `ncol(X_train)+1` containing posterior samples of evaluations of the coefficient functions. The first dimension corresponds to posterior samples/MCMC iterations, the second dimension corresponds to individual training set observations, and the third dimension corresponds to coefficient functions. Only returned if `save_samples == TRUE`.

`yhat.test.mean` Vector containing posterior mean of evaluations of regression function E[y|x,z] on testing data.

`betahat.test.mean`
Matrix with `nrow(X_test)` rows and `ncol(X_testn)+1` columns containing the posterior mean of evaluations of each coefficient function evaluated on the training data. Each row corresponds to a training set observation and each colunn corresponds to a coefficient function. Note the first column is for the intercept function.

`yhat.test` Matrix with `nd` rows and `nrow(X_test)` columns. Each row corresponds to a posterior sample of the regression function E[y|x,z] and each column corresponds to a testing set observation. Only returned if `save_samples == TRUE`.

`betahat.test` Array of size `nd` x `nrow(X_test)` x `ncol(X_test)+1` containing posterior samples of evaluations of the coefficient functions. The first dimension corresponds to posterior samples/MCMC iterations, the second dimension corresponds to individual training set observations, and the third dimension corresponds to coefficient functions. Only returned if `save_samples == TRUE`.

`sigma` Vector containing ALL samples of the residual standard deviation, including warmup.

`varcounts` Array of size `nd` x R x `ncol(X)+1` that counts the number of times a variable was used in a decision rule in each posterior sample of each ensemble. Here R is the total number of potential modifiers (i.e. `R = ncol(Z_cont_train) + ncol(Z_cat_train)`).

`theta` If `sparse=TRUE`, an array of size `nd` x R `ncol(X)+1` containing samples of the variable splitting probabilities.

`trees` A list (of length `nd`) of lists (of length `ncol(X_train)+1`) of character vectors (of length `M`) containing textual representations of the regression trees. The string for the s-th sample of the m-th tree in the j-th ensemble is contaiend in `trees[[s]][[j]][m]`. These strings are parsed by `predict_VCBART` to reconstruct the C++ representations of the sampled trees.

References

Deshpande, S.K, Bai, R., Balocchi, C., Starling, J., and Weiss, J. (2026). VCBART: Bayesian trees for varying coefficients. *Bayesian Analysis*. 21(1):281–308. doi:10.1214/24BA1470

Examples

```
############
```

```
# True beta functions
beta0_true <- function(Z){
  tmp_Z <- (Z+1)/2
  return( 3 * tmp_Z[,1] +
  (2 - 5 * (tmp_Z[,2] > 0.5)) * sin(pi * tmp_Z[,1]) -
  2 * (tmp_Z[,2] > 0.5))
}
beta1_true <- function(Z){
  tmp_Z <- (Z+1)/2
  return(sin(2*tmp_Z[,1] + 0.5)/(4*tmp_Z[,1] + 1) + (2*tmp_Z[,1] - 0.5)^3)
}
beta2_true <- function(Z){
  tmp_Z <- (Z+1)/2
  return( (3 - 3*cos(6*pi*tmp_Z[,1]) * tmp_Z[,1]^2) * (tmp_Z[,1] > 0.6) -
  (10 * sqrt(tmp_Z[,1])) * (tmp_Z[,1] < 0.25) )
}


################
# Set problem dimensions
###############

set.seed(417)
n_all <- 500
ni_all <- rep(4, times = n_all) # 4 observations per subject
subj_id_all <- rep(1:n_all, each = 4) # give every subject an id number
N_all <- sum(ni_all) # total number of observations

p <- 2 # number of covariates
R_cont <- 20 # number of continuous modifiers
R_cat <- 0 # number of categorical modifiers
R <- R_cont + R_cat
################
# Generate covariates & modifiers
################

X_all <-
  matrix(rnorm(N_all*p, mean = 0, sd = 1), nrow = N_all, ncol = p)
Z_cont_all <-
  matrix(runif(N_all * R_cont, min = -1, max = 1), nrow = N_all, ncol = R_cont)

################
# Define true coefficient functions & noise level
###############
beta0_all <- beta0_true(Z_cont_all)
beta1_all <- beta1_true(Z_cont_all)
beta2_all <- beta2_true(Z_cont_all)
beta_all <- cbind(beta0_all, beta1_all, beta2_all)
sigma <- 0.1

################
# Generate response surface & outcomes
###############
```

```
mu_all <- beta0_all + X_all[,1] * beta1_all + X_all[,2] * beta2_all
Y_all <- mu_all + sigma * rnorm(n = N_all, mean = 0, sd = 1)


## Token run to ensure installation works

fit <-
  VCBART_ind(Y_train = Y_all,
             subj_id_train = subj_id_all,
             ni_train = ni_all,
             X_train = X_all,
             Z_cont_train = Z_cont_all,
             nd = 5, burn = 5,
             verbose = FALSE)


## Longer example
  fit <-
    VCBART_ind(Y_train = Y_all,
               subj_id_train = subj_id_all,
               ni_train = ni_all,
               X_train = X_all,
               Z_cont_train = Z_cont_all,
               verbose = FALSE)

oldpar <- par(no.readonly = TRUE)
par(mar = c(3,3,2,1), mgp = c(1.8, 0.5, 0), mfrow = c(1,2))
plot(beta_all, fit$betahat.train.mean,
     pch = 16, cex = 0.5,
     xlab = "Actual", ylab = "Posterior Mean",
     main = "Coefficients")
abline(a = 0, b = 1, col = 'blue')
plot(mu_all, fit$yhat.train.mean,
     pch = 16, cex = 0.5,
     xlab = "Actual", ylab = "Posterior Mean",
     main = "Regression Function E[Y|X,Z]")
abline(a = 0, b = 1, col = 'blue')

par(oldpar)
```

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