

Package ‘btml’

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Type Package

Title Bayesian Treed Machine Learning for Personalized Prediction and Precision Diagnostics

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Description Generalization of the Bayesian classification and regression tree (CART) model that partitions subjects into terminal nodes and tailors machine learning model to each terminal node.

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Depends R (>= 4.5.0), glmnet, randomForest, e1071, pROC, stats, graphics

NeedsCompilation no

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btml	<i>Bayesian Treed Machine Learning</i>
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Description

The treed model generalizes the Bayesian classification and regression tree (BCART) model by partitioning subjects into terminal nodes and tailoring machine learning model to each terminal node.

Usage

```
btml(y,x,z,ynew,xnew,znew,MList,sparse,nwarm,niter,minsample,base,power)
```

Arguments

y	Response vector. If a factor coded as 0 or 1, classification is assumed. Otherwise, regression is assumed.
x	Data.frame or matrix of predictors that is used to estimate a tree structure.
z	Data.frame or matrix of predictors that is used in terminal node specific ML models. See the description below about the difference between x and z.
ynew	Response vector for the test set corresponding to y (default ynew=NULL).
xnew	Data.frame or matrix for the test set corresponding to x (default xnew=NULL).
znew	Data.frame or matrix for the test set corresponding to z (default znew=NULL).
MList	Candidate ML models that can be assigned to each terminal node (default MList=c("lasso","rf","svm")). Any other ML models can be included. See the details below.
sparse	Whether to perform variable and machine learning model selections based on a sparse Dirichlet prior rather than simply uniform (default sparse=TRUE).
nwarm	Number of warm-up (default nwarm=1000).
niter	Number of iteration (default niter=1000).
minsample	The number of minimum sample size per each node, i.e., $\text{length}(y) > \text{min_sample}$ if y is continuous and $\min(\text{length}(y==1), \text{length}(y==0)) > \text{min_sample}$ (default min_sample=20).
base	Base parameter for tree prior (default base=0.95).
power	Power parameter for tree prior (default power=0.8).

Details

This treed model uses stochastic search to find the optimal decision-tree based rule that partitions subjects into distinct terminal nodes and assigns the most effective ML model to each terminal node. For high-dimensional variables, increase nwarm=10000 and niter=10000, or more; and increase minsample.

Ideally, there are two sets of predictors, x and z, e.g., demographic variables and biomarkers, where x is used to split trees, and z is assigned to each terminal node. However, if this is not possible, it allows us to use the same x and z in the btml function, e.g., `btml(y=y, x=x, z=x, ...)`.

Regarding the node numbers, an internal node s has left and right child nodes $2*s$ and $2*s+1$, respectively, where node 1 is a root node; nodes 2 and 3 are left and right child nodes of node 1; nodes 4 and 5 are left and right nodes of node 2; and so on.

Currently, `lasso()`, `randomForest()`, and `svm(...,kernel="radial")` functions from R packages `cv.glmnet`, `randomForest`, and `e1071` are supported, but any ML models can be flexibly added to terminal nodes, e.g., see the example #3 below.

Value

An object of class `btml`, which is a list with the following components:

<code>terminal</code>	Node numbers in terminal nodes.
<code>internal</code>	Node numbers in internal nodes.
<code>splitVariable</code>	Variable (i.e., $x[,u]$ if <code>splitVariable[k]=u</code>) used to split the internal node k .
<code>cutoff</code>	<code>cutoff[k]</code> is the cutoff value to split the internal node k .
<code>selML</code>	ML model assigned to the terminal node t .
<code>fitML</code>	<code>fitML[[t]]</code> is the fitted ML model at the terminal node $t \in \text{terminal}$.
<code>y.hat</code>	Estimated y (or estimated probability) on the training set if y is continuous (or binary).
<code>node.hat</code>	Estimated node on the training set.
<code>mse</code>	Training MSE.
<code>bs</code>	Training Brier Score.
<code>roc</code>	Training ROC curve.
<code>auc</code>	Training AUC.
<code>y.hat.new</code>	Estimated y (or estimated probability) on the test set if y is continuous (or binary).
<code>node.hat.new</code>	Estimated node on the test set.
<code>mse.new</code>	Test MSE.
<code>bs.new</code>	Test Brier Score.
<code>roc.new</code>	Test ROC curve.
<code>auc.new</code>	Test AUC.

Author(s)

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References

Yaliang Zhang and Yunro Chung, Bayesian treed machine learning model (in preperation)

Examples

```
set.seed(123)
###
#1. continuous y
###
n=200*2 #n=200 & 200 for training & test sets

x=matrix(rnorm(n*10),n,10) #10 predictors
z=matrix(rnorm(n*10),n,10) #10 biomarkers

xcut=median(x[,1])
subgr=1*(x[,1]<xcut)+2*(x[,1]>=xcut) #2 subgroups
```

```

lp=rep(NA,n)
for(i in 1:n)
  lp[i]=1+3*z[i,subgr[i]]
y=lp+rnorm(n,0,1)

idx.nex=sample(1:n,n*1/2,replace=FALSE)
ynew=y[idx.nex]
xnew=x[idx.nex,]
znew=z[idx.nex,]

y=y[-idx.nex]
x=x[-idx.nex,]
z=z[-idx.nex,]

fit1=btml(y,x,z,ynew=ynew,xnew=xnew,znew=znew)
fit1$mse.new
plot(fit1$y.hat.new~ynew,ylab="Predicted y",xlab="ynew")

###
#2. binary y
###
x=matrix(rnorm(n*10),n,10) #10 predictors
z=matrix(rnorm(n*10),n,10) #10 biomarkers

xcut=median(x[,1])
subgr=1*(x[,1]<xcut)+2*(x[,1]>=xcut) #2 subgroups

lp=rep(NA,n)
for(i in 1:n)
  lp[i]=1+3*z[i,subgr[i]]
prob=1/(1+exp(-lp))
y=rbinom(n,1,prob)
y=as.factor(y)

idx.nex=sample(1:n,n*1/2,replace=FALSE)
ynew=y[idx.nex]
xnew=x[idx.nex,]
znew=z[idx.nex,]

y=y[-idx.nex]
x=x[-idx.nex,]
z=z[-idx.nex,]

fit2=btml(y,x,z,ynew=ynew,xnew=xnew,znew=znew)
fit2$auc.new
plot(fit2$roc.new)

###
#3. add new ML models
# 1) write two functions:
#   c_xx & c_xx_predict if y is continuous or
#   b_xx & b_xx.predict if y is binary

```

```
# 2) MLlist includes xx, not c.xx nor b.xx.
# 3) run btml using the updated MLlist.
# The below is an example of adding ridge regression.
###
#3.1. ridge regression for continuous y.
c_ridge=function(y,x){
  x=data.matrix(x)
  fit=NULL
  suppressWarnings(try(fit<-glmnet::cv.glmnet(x,y,alpha=0),silent=TRUE))
  return(fit)
}
c_ridge_predict=function(fit,xnew){
  y.hat=rep(NA,nrow(xnew))
  if(!is.null(fit)){
    xnew=data.matrix(xnew)
    y.hat=as.numeric(predict(fit,newx=xnew,s="lambda.min",type="response"))
  }
  return(y.hat)
}

#3.2. ridge regression for binary y.
b_ridge=function(y,x){
  x=data.matrix(x)
  fit=NULL
  suppressWarnings(try(fit<-glmnet::cv.glmnet(x,y,alpha=1,family="binomial"),silent=TRUE))
  return(fit)
}
b_ridge_predict=function(fit,xnew){
  y.hat=rep(NA,nrow(xnew))
  if(!is.null(fit)){
    xnew=data.matrix(xnew)
    y.hat=as.numeric(predict(fit,newx=xnew,s="lambda.min",type="response"))
  }
  return(y.hat)
}

#3.3. update MLlist
MLlist=c("lasso","ridge")
fit3=btml(y,x,z,ynew=ynew,xnew=xnew,znew=znew,MLlist=MLlist)
fit3$auc.new
plot(fit3$roc.new)
```

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