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The R Package BHAM: Fast and Scalable Bayeisan Hierarchical Additive Model for High-dimensional Data

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Abstract

\pkg{BHAM} is a freely avaible R pakcage that implments Bayesian hierarchical additive models for high-dimensional clinical and genomic data. The package includes functions that generlized additive model, and Cox additive model with the spike-and-slab LASSO prior. These functions implements scalable and stable algorithms to estimate parameters. \pkg{BHAM} also provides utility functions to construct additive models in high dimensional settings, select optimal models, summarize bi-level variable selection results, and visualize nonlinear effects. The package can facilitate flexible modeling of large-scale molecular data, i.e. detecting succeptable variables and inforing disease diagnostic and prognostic. In this article, we describe the models, algorithms and related features implemented in \pkg{BHAM}. The package is freely avaiable via the public GitHub repository `https://github.com/boyiguo1/BHAM`.

Keywords: additive model, spike-and-slab LASSO, scalable.

1. Introduction

High-dimensional statistics has been an indispensable area of research for its high impact in molecular and clinical data analysis. In recent years, there are continuous efforts to make high-dimensional models more flexible and interpretable, aiming to capture more complex signals. One particular family of such flexible and interpretable models is the additive models where predictors are included in the model as an additive function. These high-dimensional additive models serve for two purposes: variable selection and outcome prediction. In high-dimensional statistics, it is common to assume there is only a small subset of predictors that have effects on the outcome, also known as the signal sparsity assumption. (Bühlmann and van de Geer 2011) The high-dimensional additive models select not only the predictors who

have linear associations with the outcome, but also those who inform the outcome prediction with nonlinearity. As a result, they provide more flexible effect modeling and improve prediction accuracy compared to high-dimensional linear models.

There are many proposals on high-dimensional additive models. The main idea of these proposals focus on the application of grouped sparse penalties, for example, group LASSO penalty (Ravikumar, Lafferty, Liu, and Wasserman 2009; Huang, Horowitz, and Wei 2010) and group SCAD penalty (Wang, Chen, and Li 2007; Xue 2009), on the coefficients of additive functions. There methods are developed primarily for variable selection and may provide inaccurate estimation of the underlying functions due to the excess shrinkage of the sparsity penalty (Scheipl, Kneib, and Fahrmeir 2013). Thus, the prediction performance will be affected. In addition, these methods take an "all-in-all-out" approach for variable selection, and fails to answer if the underlying signals are linear or nonlinear. To address these shortcomings, Guo and his colleagues proposed the two-part spike-and-slab LASSO prior for generalized additive models (Guo, Jaeger, Rahman, Long, and Yi 2022) and additive Cox proportional hazards models (Guo and Yi 2022). Instead of using the computationally prohibitive Markov chain Monte Carlo approximations, optimization-based EM-Coordinate Descent algorithms are developed for model fitting. Monte Carlo studies and real data analysis demonstrate improved prediction and computation performances compare to the state-of-the-art additive models.

In this article, we introduce an R package `BHAM` that implements the spike-and-slab LASSO additive models and computationally efficient algorithms. Notably, `BHAM` provides functions for setting up and fitting various spike-and-slab LASSO additive models, including generalized additive models for various continuous and discrete outcomes and Cox proportional hazards models for censored survival outcomes. The specification of additive functions follows a popular syntax implemented in `mgcv`. We provide a parser function that translates high-dimensional predictors names and their corresponding additive functions to model formulas, rendering convenience to model large datasets with hundreds and thousands of predictors. Other ancillary functions include cross-validation, model summary, and effect visualization. Our objective with `BHAM` is to offer a friendly user experience that emphasizes statistical validity, computational scalability and utility flexibility for high-dimension additive models.

1.1. Literature Review

We enlist current available packages that have similar functionality, i.e. modeling to the best of our knowledge. To note, we don't list packages that are unable of handling high-dimensional data, for example the well known R package `mgcv`, and high-dimensional packages that requires extra steps to construct the design matrix of functional form of predictors (Such implementation can be found with grouped sparse models, for example `SGL`.)

Scheipl *et al.* (2013) Summarized the software development of additive models in high-dimensional data analysis before 2013.

Generalized Additive Model

- `COSSO`
- `spikeSlabGAM`

- `sparseGAM`

Additive Cox Proportional Hazard Model

- `COSSO`
- `tfCox`

[TODO: Add a sentence in the literature review paragraph describe the additive functions are costimizable, and provide greater flexibility compared to previous models.]

In this article, we focus on the packages that can directly construct additive models for high-dimensional data analysis, instead of requiring additional step of constructing design matrix of functional form of the variables before fitting a sparse model.

There are other methods to model survival outcome and provides proporitonal hazards interpretation, for example Marra, Farcomeni, and Radice (2021) provides a link-based survival additive model for mixed censoring in package `GJRM`.

2. Models and algorithms

In this section, we describe the Bayeisan hiearchical additive model that `BHAM` implements. The basic idea is to impose the two-part spike-and-slab LASSO prior Guo *et al.* (2022) on each additive function in the model. The choices of model includes generalized additive model and Cox proportional hazard model. The proposed two-part spike-and-slab LASSO prior consists of a spike-and-slab LASSO prior for the linear space coefficient β_j of a additive function $B_j(X_j)$ of the jth variables, and a modified group spike-and-slab LASSO prior for the nonlinear space coefficients $\beta^*_{jk}, k = 1, ..., K_j$ of the jth additive function.

$$\begin{aligned} \beta_j|\gamma_j, s_0, s_1 &\sim (1-\gamma_j)DE(0, s_0) + \gamma_j DE(0, s_1) \\ \beta^*_{jk}|\gamma^*_j, s_0, s_1 &\overset{\text{iid}}{\sim} (1-\gamma^*_j)DE(0, s_0) + \gamma^*_j DE(0, s_1), k = 1, \ldots, K_j. \end{aligned} \tag{1}$$

To note, the model matrix of the additive function undergoes a reparameterization process that absorbs the smoothing penalty via eigendecomposition. Meanwhile, the reparameterization also isolate the linear and nonlinear spaces of the additive function, allowing different shrinkages on the two spaces and motivates signal selection via the linear space and function smoothing of the nonlinear space. The spike-and-slab prior use the binary indicator γ to indicate if the the corresponding variable is included in the model. Nevertheless, this selection finalized based on soft-thresholding. the spike-and-slab LASSO prior makes this selection process easier by shrinking the coefficient to exactly 0. In the two-part SSL prior, each additive function have two indicators γ_j and γ^*_j, controlling the linear and nonlinear component selection. Effect hierarchy was implemented via the conditional priors of to ensure the the linear component is more likely to be selected than the nonlinear components.

$$\gamma_j|\theta_j \sim Bin(1, \theta_j) \qquad \gamma^*_j|\gamma_j, \theta_j \sim Bin(1, \gamma_j\theta_j). \tag{2}$$

The inclusion probability parameter θ_j have a beta prior to allow adaptive shrinkage.

To fit the model in a efficient and scalable fashion, we implement the EM-coordinate descent algorithm. The EM-coordinant descent algorithm estimates maximum a posteriori of the coefficients by optimizing the log joint posterior density function. The algorithm re-writes the spike-and-slab LASSO prior as a double exponential distribution with conditional scale parameter, and leverages the relationship between double exponential prior and l_1 penalty. Hence, the log joint posterior density function can be expressed as the summation of a l_1 penalized likelihood function and log beta posterior density. Nevertheless, the nuances parameters $\boldsymbol{\gamma}$ are unknown and requires the EM algorithm to address. In each iterations of the EM procedure, we update the expectation of the log joint posterior density function with respect to the nusance parameters, calculate the penalties based on the estimation from previous iteration, and optimize the penalized likelihood and the posterior density with coordinate descent algorithm and closed-form calculation for the coefficients. The process iterates until convergence. Cross-validation is used to choose the optimal model. We defer Guo *et al.* (2022); Guo and Yi (2022)to for full description of GAM algorithm and Cox additive model algorithm.

3. Features

In this section, we demonstrate how to fit Bayesian hierarchical additive model with two-part spike-and-slab LASSO prior, and introduce the model tuning, diagnostic and other utility functions for visualize additive functions, bi-level selection.

In this section, we describe to the users the workflow for of fitting a high-dimensional additive model with the two-part spike-and-slab LASSO prior in `BHAM`. Specifically, we introduce how to 1) prepare the high-dimensional design matrix for fitting the proposed model, 2) fit generalized additive model, 3) Model tuning and performance assessment, and 4) visualize the bi-level variable selection.

3.1. Installation

To install the latest development version of `BHAM` package from **GitHub**, type the following command in R console:

```
R> if (!require(devtools)) install.packages("devtools")
R> if(!require(BHAM)) devtools::install_github("boyiguo1/BHAM", build_vignettes = FALSE)
```

You can also set `build_vignettes=TRUE` but this will slow down the installation drastically (the vignettes can always be accessed online anytime at boyiguo1.github.io/BHAM/articles).

3.2. Preliminaries

We use a simulated data set to demonstrate our package. The data generating mechanism is motivated by Bai (citation) and programmed in the function `sim_Bai`: we assume there are $p = 10$ predictors where the first four predictors have effects on the outcome (see functions below), and the rest of predictors don't, i.e $B_j(x_j) = 0, j = 5, \ldots, p$. [TODO: Insert functions here on what the equations are]. With the data generating mechanism, we simulate two datasets with the binary outcome from Bernoulli trials with logit link function. To note,

the function `sim_Bai` can also simulate Gaussian and Poisson outcomes using the same data generating mechanism. The sample sizes of these two datasets are 500 and 1000 for training and testing respectively. The following code section creates the training and testing datasets.

```
R> library(BHAM)
R> set.seed(1) ## simulate some data...
R> n_train <- 500
R> n_test <- 1000
R> p <- 10
R> # Train Data
R> train_dat <- sim_Bai(n_train, p)
R> dat <- train_dat$dat %>% data.frame
R>
R> # Test Data
R> test_tmp <- sim_Bai(n_test, p)
R> test_dat <- test_tmp$dat %>% data.frame
```

The first ten observation of the data set look like below

```
           x1         x2         x3          x4         x5          x6
1   1.5579537 -1.1346302  0.5205997  0.73911492 -1.8054836 -0.88614959
2  -0.7292970  0.7645571  0.3775619  0.38660873 -0.6780407 -1.92225490
3  -1.5039509  0.5707101 -0.6236588  1.29639717 -0.4733581  1.61970074
4  -0.5667870 -1.3516939 -0.5726105 -0.80355836  1.0274171  0.51926990
5  -2.1044536 -2.0298855  0.3125012 -1.60262567 -0.5973876 -0.05584993
6   0.5307319  0.5904787 -0.7074278  0.93325097  1.1598494  0.69641761
7   1.6176841 -1.4130700  0.5212035  1.80608925 -1.3332269  0.05351568
8   1.1845319  1.6103416  0.4481880 -0.05650363 -0.9257557 -1.31028350
9   1.8763334  1.8404425 -0.5053226  1.88591132 -1.0744951 -2.12306606
10 -0.4557759  1.3682979 -0.2066122  1.57838343 -1.4511165 -0.20807859
           x7          x8          x9         x10 y
1   0.8500435  1.13496509  0.07730312 -0.6264538 0
2  -0.9253130  1.11193185 -0.29686864  0.1836433 1
3   0.8935812 -0.87077763 -1.18324224 -0.8356286 0
4  -0.9410097  0.21073159  0.01129269  1.5952808 0
5   0.5389521  0.06939565  0.99160104  0.3295078 0
6  -0.1819744 -1.66264885  1.59396745 -0.8204684 0
7   0.8917676  0.81083998 -1.37271127  0.4874291 0
8   1.3292082 -1.91234580 -0.24961093  0.7383247 1
9  -0.1034661 -1.24675343  1.15942453  0.5757814 0
10  0.6150646  0.99815445 -1.11422235 -0.3053884 0
```

3.3. Set up Design Matrix of additive functions

Given the raw data, we would like to translate the additive functions to the their matrix form. The challenge here is to allow a customizable and convenient way to specify the high-dimensional model. Our solution here is to use a data frame to accomodate each predictor in

the raw data set, and allows each predictor have their spline function specified. There are three columns for this formulat specification data frame, including `Var` `Func`, `Args`. The `Var` column hosts the variable name; the `Func` column hosts the spline function following the commonly used generalized additive model `mgcv`; the `Args` column hosts the detail specification of the spline function. The data frame can be constructed manually for low-dimensional settings and also be manipulated easily when the number of spline components grows to tens or hundreds. See the examples below.

```
R> # Low-dimensional setting
R> mgcv_df <- dplyr::tribble(
+   ~Var, ~Func, ~Args,
+   "X1",  "s",     "bs='cr', k=5",
+   "X2",  "s",     NA,
+   "X3",  "s",    "",
+ )
R>
R> # High-dimensional setting
R> mgcv_df <- data.frame(
+   Var = setdiff(names(dat), "y"),
+   Func = "s",
+   Args ="bs='cr', k=7"
+ )
```

After having the model specification data frame, the next task is to construct the overall design matrix. We provide a function `construct_smooth_data` to construct the design matrix for each predictor according to their spline specification iteratively, and binding all design matrices together with a systematic naming convention. The linear component of the spline function is named with the suffix `.null` and the nonlinear components are named with the suffix `.pen`. In `construct_smooth_data`, we take three steps of matrix manipulation via the `smoothCon` from the package `mgcv`: 1) linear constraints, 2) eigendecomposition of the smoothing matrix S to isolate linear and nonlinear spaces, 3) scaling of the design matrix such that the coefficients are on the same scale. As we use `mgcv::smoothCon` to decode the spline specification, we carry over the ability to work with user-defined spline functions as long as it follows `mgcv` standard.

The `construct_smooth_data` function have two arguments, the model specification data frame and the raw data, and return the finalized design matrix `data` and the smooth specification functions `Smooth` which will later be used to construct the design matrix of the new datasets for the prediction purpose.

```
R> train_sm_dat <- BHAM::construct_smooth_data(mgcv_df, dat)
R> train_smooth <- train_sm_dat$Smooth
R> train_smooth_data <- train_sm_dat$data
```

3.4. Fitting the Bayesian Hierarchical model

With the additive function design matrix constructed, we are ready to fit the Bayesian hierarchical model with the two-part spike-and-slab LASSO prior for smooth function. The

model fitting algorithm, implementing the EM-coordinate descent algorithm, is wrapped in the function `bamlasso`. The necessary arguments are `x` for the design matrix, `y` for the outcome, `family` for the family distribution of the outcome, and `group` for the additive functions. We provide a utility function `make_group` to automate the grouping, taking the column names from the design matrix. It generates a list of vectors containing the bases of each additive function. Another important argument is `ss`, which is a vector of length 2 for the spike and slab components of the spike-and-slab LASSO scale parameters, i.e. the mixture double exponential distribution. The argument `ss` defaults to a spike double exponential density with scale parameter 0.04, and a slab double exponential density with scale parameter 0.5, which is a general starting prior based on empirical evidence.

```
R> bham_mdl <- bamlasso(x = train_smooth_data, y = dat$y,
+                       family = "binomial",
+                       group = make_group(names(train_smooth_data)))
```

Tuning via Cross-validation

With the specified `ss` argument, the function `bamlasso` fit the asked model. Nevertheless, it is not necessary the optimal model. To select the optimal model, we employ a tuning step via cross validation, which is implemented in the function `tune.bgam`. The main arguments are the previously fitted model where the model data, additive function specifications are stored, a sequence of spike density scale parameter s_0, and number of folds. The following example shows to use five-fold cross validation to examine a vector of s_0 options, from 0.005 to 0.1 with 0.01 increment. Currently, we don't consider to examine values of the slab density scale parameter s_1 for computational economy, as the previously literature shows s_1 has modest impact on the model performance. The tuning function also allows nested cross-validation by allowing running multiple cross-validation via `ncv` and user-specified folds via `foldid`.

```
R> s0_seq <- seq(0.005, 0.1, 0.01)
R> cv_res <- tune.bgam(bham_mdl, nfolds = 5, s0= s0_seq, verbose = FALSE)

Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.01 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.006 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.006 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.006 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.006 minutes
```

```
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.005 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.005 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.005 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.006 minutes
Fitting ncv*nfolds = 5 models:
1 2 3 4 5
 Cross-validation time: 0.005 minutes
```

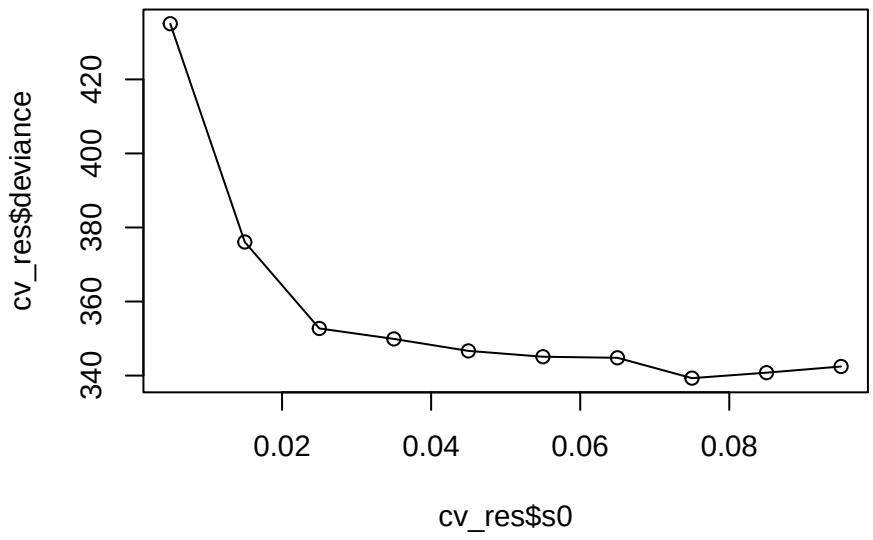
The cross-validation tuning function returns different performance metrics, including deviance, mean squared error, mean absolute error, area under the curve, misclassifcation for binary outcome, and concordance statistics for survival outcome. The following shows the cross-validated performance metrics for the first five values of the s_0 sequence using out-of-bag samples.

```
R> head(cv_res, 5)
```

```
     s0 deviance   auc   mse   mae misclassification
1 0.005  435.044 0.809 0.141 0.281             0.212
2 0.015  376.082 0.865 0.120 0.253             0.166
3 0.025  352.728 0.883 0.111 0.238             0.148
4 0.035  349.896 0.882 0.110 0.226             0.154
5 0.045  346.670 0.884 0.109 0.223             0.158
```

Here we want to caution the reader, if the performance metric varies monotonically with the candidate s_0 values, it would be better to examine a broader range of candidate s_0 values, as the sequence contains a local optimal performance where the global optimal performance is not reached yet. Using some visual aid to examine the s_0 and performance metric relationship would be more helpful.

```
R> plot(cv_res$s0, cv_res$deviance)
R> lines(cv_res$s0, cv_res$deviance)
```



With the cross-validation results, we can choose from all the candidate values of s_0 and select the one with the best performance using the preferred metrics. For example, we can use the s_0 value that gives the minimum cross-validated deviance, and re-fit the model. Hence, this would be the optimal model.

```
R> s0_min <- cv_res$s0[which.min(cv_res$deviance)]
R> bham_final <- bamlasso(x = train_smooth_data, y = dat$y,
+                         family = "binomial",
+                         group = make_group(names(train_smooth_data)),
+                         ss = c(s0_min, 0.5))
```

To note, it is a convention to use some predictive metrics to select the best performed model among all the candidate values, for both predictive purpose and variable selection purpose. However, previous literature shows that when using predictive metrics to select model for variable selection purpose, the variable selection performance may not be optimal.

3.5. Varible Selection and Curve Intropolation

In the proposed R package, we also provide some utility functions to provide more insights for the additive function inferences.

Variable Selecrtion

We provide a function to summarize the variable selection of the produced model, namely `bamlasso_var_selection`. The input of the function is a fitted BHAM model, and the output of the function is a list of two components, `parametric` and `non-parametric`. The `parametrc` component is a vector contains the selected variables that were fitted in the model in its

parameteric form, i.e. not specified via additive functions. The `non-parametric` component contains a dataframe with 3 columns, `Variable`, `Linear`, `Nonlinear`. While `Variable` column includes the variable names of selected aadditive functions, `Linear` and `Nonlinear` columns are logical vectors indicating if the linear and nonlinear components of the additive function are included in the model respectively.

```
R> bamlasso_vs_part <- bamlasso_var_selection(bham_final)
```

Here, we shows the variable selection result from previously tuned model. Since, the model didn't include any variables in their parametric form. Hence, the `parametric` is an empty vector. Meanwhile, the `nonparametric` data frame contains the bi-level selection result.

```
R> bamlasso_vs_part
```

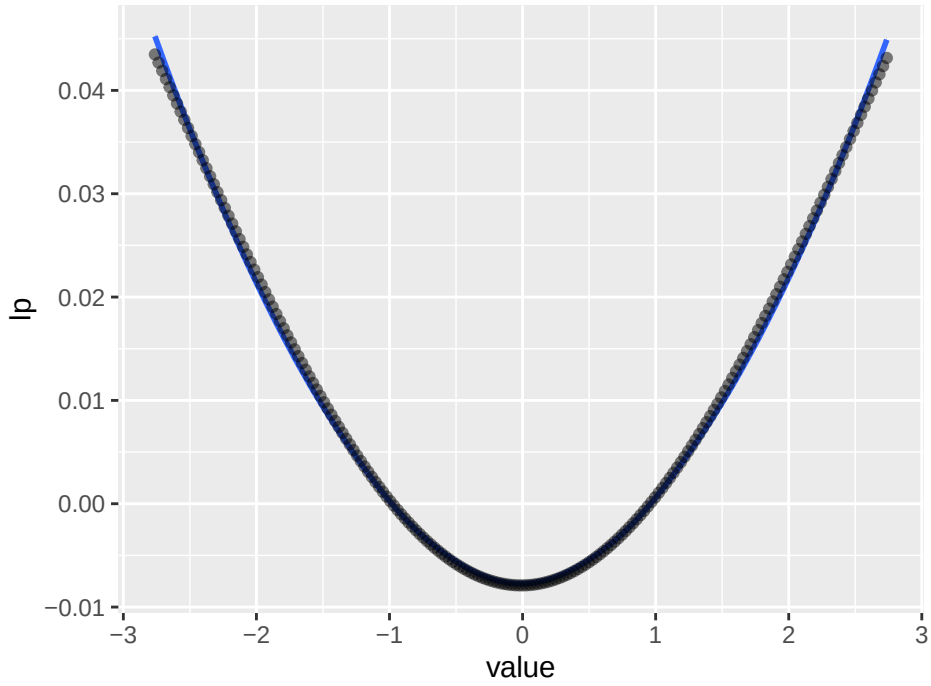
```
$Parametric
character(0)

$`Non-parametric`
  Variable Linear Nonlinear
1       x1  FALSE      TRUE
2       x2  FALSE      TRUE
3       x3   TRUE     FALSE
4       x4  FALSE      TRUE
5       x5  FALSE      TRUE
6       x7  FALSE      TRUE
7       x9  FALSE      TRUE
8      x10  FALSE      TRUE
```

Curve Plotting

We also provide a utility function `plot_smooth_term` to plot the estimated functions. The function takes in the fitted model, the variable name, the previously constructed smooth objective to construct the design matrix, minimum and maximum of the range of the predictors. The function outputs a `ggplot` object to show the estimated curve.

```
R> plot_smooth_term(bham_final, "x1", train_smooth,
+                       min = min(dat[, "x1"]),
+                       max = max(dat[, "x1"]))
```

```
`geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



3.6. Prediction

To predict new datasets, we need to go through a two-step procedure as previously building the model. First of all, we need to translate the new dataset to their matrix form using the function `make_predict_dat`. This step is necessary because of the reparameterization of the design matrix. The function `make_predict_dat` is based on the function `PredictMat` from `mgcv`. The function asks for an additional input argument besides the new dataset, i.e. the Smooth object when constructing the design matrix for the training data. The output of the function is the new dataset design matrix with conformable dimension and variable name. We show the first six columns of the first five observations in the following example.

```
R> train_smooth <- train_sm_dat$Smooth
R> test_sm_dat <- make_predict_dat(train_sm_dat$Smooth, dat = test_dat)

     x1.pen1     x1.pen2    x1.pen3     x1.pen4    x1.pen5   x1.null1
1  0.2105822 -0.51339049 -0.7087016  1.48599984 -1.6282845 -0.6187856
2  0.1401345 -0.04244866  0.4101826 -2.49600416 -0.5234851  1.2762868
3 -0.1157559 -0.28695472  0.3280699  0.08111065  9.0232660  3.6778234
4 -0.1551403 -0.57575563  1.1032603 -2.71644734  1.1193043  1.8444025
5  0.1841429 -0.50899800 -0.7593021  1.41065378 -1.6744694 -0.5829544
```

With the new dataset in the conformable design matrix format, we can easily produce the prediction using the function `predict`. Under the hood, we use `predict.glmnet` to produce the prediction, and hence, it is robust. For the GLM, we can produce the linear predictors using `type = "link"` and the fitted probability/mean using `type = "response"`.

```
R> bham_final$offset = 0
R> pred_res <- predict(bham_final, newx = as.matrix(test_sm_dat),
+                      newoffset = 0, type = "link")
```

To note, we suggest to use `BhGLM::measure.bh` to provide a quick prediction performance of the new dataset.

```
R> if(!require("devtools")) install.packages("devtools")
R> if(!require("BhGLM")) devtools::install_github("nyiuab/BhGLM")
R>
R> BhGLM::measure.bh(bham_final, as.matrix(test_sm_dat), test_dat$y)
```

4. Discussion

In this article, we introduce the R package `BHAM` to fit Bayesian Hierarchical additive models with two-part spike-and-slab LASSO prior for high-dimensional data analysis. The R package can be widely used to analyze large-scale molecular and clinical data with the flexibility to model both linear and nonlinear signals, and hence provide improved prediction accuracy. Meanwhile, compared to the more complicated machine learning method, the additive models can provide more interpretable inference of the underlying signals. In addition, the two-part spike-and-slab LASSO prior for smooth function and the EM-CD algorithm provides a natural solution to the bi-level selection problem, without further requirement of thresholding or hypothesis testing. Fitting a high-dimensional Bayesian model is normally computationally intensive. We provide an economic solution by integrate coordinate descent algorithm with the EM procedure. The implementation of the algorithm leverage some commonly used modeling interface form the standard R packages and hence granting robustness.

To help the users to familiarize the utilities of `BHAM`, we provide a analysis pipeline in this manuscript. We demonstrate the construction of the design matrix, model fitting and tuning, signal selection and visualization, and prediction via the analysis of a simulated data set. Due to the space constraint, we can't showcase all the functionality offered by `BHAM` for example fitting a Cox proportional hazard model, time-varying effect model, or fitting the model with the EM-Newton or EM-IWLS algorithms. We recommand the user to visit an interactive website for more details via https://boyiguo1.github.io/BHAM/.

Optimal goal is to provide interface for optimal customizability.

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