

# Spike-and-Slab Additive Models And Fast Algorithms For High-Dimensional Data Analysis

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## Dissertation Committee

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## Outline

# Outline

- ▶ Background
  - ▶ Spline Model Development
  - ▶ Bayesian Regularization
  - ▶ Bayesian Variable Selection
- ▶ Dissertation
  - ▶ Bayesian Hierarchical Additive Models
  - ▶ Additive Cox Proportional Hazards Model
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- ▶ Conclusion
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  - ▶ Questions & Answers
  - ▶ Closing Statement & Acknowledgment

## Background

## Spline Model Development

# Spline Model Development

*“It is extremely unlikely that the true (effect) function  $f(X)$  (on the outcome) is actually linear in  $X$ .”*

— *Hastie, Tibshirani, and Friedman (2009) PP. 139*

## Question

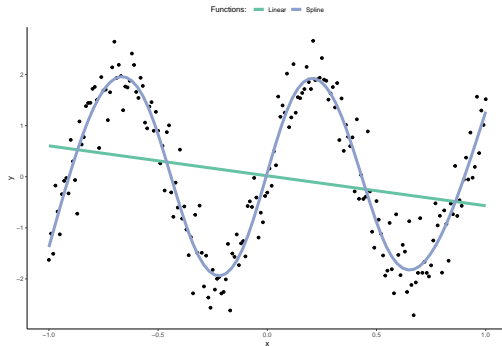
How to model nonlinear effects?

# Spline Functions

A *spline* function is a piece-wise polynomial function

$$B(x) = \sum_{k=1}^K \beta_k b_k(x) \equiv \mathbf{x}^T \boldsymbol{\beta}$$

$b_k(x)$  are the *basis functions*, possibly truncated power basis and b-spline basis.  
(Simon N. Wood 2017)



- For simplicity, we assume all functions have  $K$  basis functions and knots of functions are equidistance.



# Generalized Additive Models with Splines

**Generalized additive model** (Hastie and Tibshirani 1987) is expressed

$$y_i \stackrel{\text{iid}}{\sim} EF(\mu_i, \phi), \quad i = 1, \dots, n$$
$$g(\mu_i) = \beta_0 + B(x_i) = \beta_0 + \mathbf{x}_i^T \boldsymbol{\beta}, \quad \mathbb{E}[B(X)] = 0$$

where  $B(x_i)$  is the spline function,  $g(\cdot)$  is a link function,  $\phi$  is the dispersion parameter

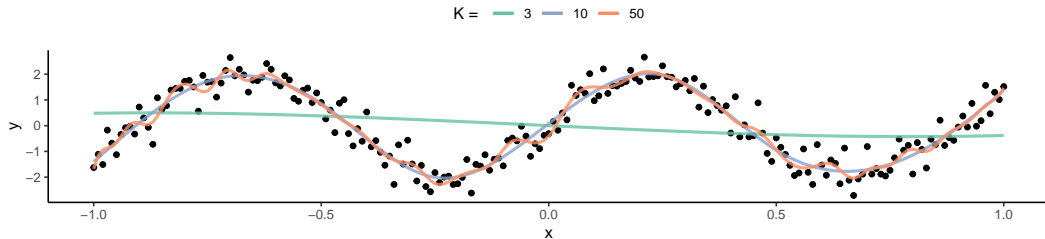
- Model fitting follows the generalized linear models, e.g. ordinary least square for Gaussian outcome

$$\hat{\boldsymbol{\beta}} = \arg \min \sum_{i=1}^n \left[ y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta} \right]^2$$

# Problem: Function Smoothness

## Question

How to mathematically define and estimate the smoothness of spline functions?



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Bayesian Regularization

## Bayesian Regularization

# Smoothing Spline Model

- ▶ Smoothing penalty  $\lambda \int B''(X)^2 dx = \lambda \boldsymbol{\beta}^T \mathbf{S} \boldsymbol{\beta}$ 
  - ▶ The smoothing penalty matrix  $\mathbf{S}$  is known given  $\mathbf{X}$
  - ▶  $\mathbf{S}$  is symmetric and positive semi-definite
- ▶ Penalized Least Square for Gaussian Outcome

$$\hat{\boldsymbol{\beta}} = \arg \min \sum_{i=1}^n \sum_{i=1}^n \left[ y_i - \beta_0 - \mathbf{x}_i^T \boldsymbol{\beta} \right]^2 + \lambda \boldsymbol{\beta}^T \mathbf{S} \boldsymbol{\beta}$$

- ▶ The smoothing parameter  $\lambda$  is a tuning parameter, selected via cross-validation

## Problem: Multiple Predictor Model

When a model contains multiple spline functions for variables  $X_1, \dots, X_p$ , the penalized least square estimator is

$$\hat{\beta} = \arg \min \sum_{i=1}^n \left[ y_i - \beta_0 - \sum_{j=1}^p \mathbf{x}_{ij}^T \beta_j \right]^2 + \sum_{j=1}^p \lambda_j \beta_j^T \mathbf{S}_j \beta_j$$

### Question

How to choose  $\lambda_i$  for  $i = 1, \dots, p$ ?

- ▶ Global smoothing:  $\lambda_1 = \dots = \lambda_p$
- ▶ Adaptive smoothing: unique  $\lambda_i$  for  $i = 1, \dots, p$

# Bayesian Regularization

- ▶ Bayesian regularization is the Bayesian analogy of penalized models by using regularizing priors

$$\text{Bayesian ridge: } \beta \sim N(0, \tau^2) \rightarrow \lambda = \sigma^2 / \tau^2$$

- ▶ Adaptive shrinkage with hierarchical priors

$$\tau_j^2 \stackrel{\text{iid}}{\sim} IG(a, b)$$

- ▶ Adaptive smoothing
  - ▶ Random walk prior on b-spline bases with IG hyperprior (Lang and Brezger 2004)
  - ▶ Log-normal spline model for coefficient variance (Baladandayuthapani, Mallick, and Carroll 2005)

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Bayesian Variable Selection

## Bayesian Variable Selection

## Problem: Functional Selection

In the context of variable selection and high-dimensional statistics, we always assume some variables are not effective or predictive of the outcome.

### Question

How to statistically detect

- ▶ if a variable is predictive to the outcome,  $B_j(X_j) = 0$
- ▶ if a variable has a nonlinear relationship with the outcome,  $B_j(X_j) = \beta_j X_j$

*Bi-level selection* is the procedure that simultaneously addresses the two questions above



# Spike-and-Slab Priors

Spike-and-slab priors are a family of mixture distributions that deploys a characterizing structure

$$\beta|\gamma \sim (1 - \gamma)f_{spike}(\beta) + \gamma f_{slab}(\beta)$$

- ▶ Latent indicator  $\gamma$  follows a Bernoulli distribution with probability  $\theta$
- ▶ Spike density  $f_{spike}(x)$  concentrates around 0 for small effects
- ▶ Slab density  $f_{slab}(x)$  is a flat density for large effects
- ▶ Natural procedure to select variables via posterior distribution of  $\gamma$
- ▶ Markov chain Monte Carlo is not compelling for high-dimensional data analysis

# Spike-and-Slab LASSO Priors

- ▶ Double exponential distributions as the spike and slab distributions

$$\beta|\gamma \sim (1 - \gamma)DE(0, s_0) + \gamma DE(0, s_1), 0 < s_0 < s_1$$

- ▶ Computation advantages via Expectation-Maximization (EM) algorithms
  - ▶ Seamless variable selection as coefficients shrinkage to 0
- ▶ Group spike-and-slab LASSO prior
  - ▶ Structure among predictors, e.g. gene pathways, bases of a spline function
  - ▶ Structured prior  $\gamma_k|\theta_j \stackrel{\text{iid}}{\sim} \text{Binomial}(1, \theta_j), k \in j$

## Problem: High-dimensional Spline Model

### Question

How to jointly model signal sparsity and function smoothness, while capable of bi-level selection?

- ▶ Excess shrinkage due to negligence of smooth penalty
  - ▶ Group lasso penalty (Ravikumar et al. 2009; Huang, Horowitz, and Wei 2010), group SCAD penalty (Wang, Chen, and Li 2007; Xue 2009)
- ▶ All-in-all-out selection
  - ▶ Failed to select function as whole, e.g. group spike-and-slab LASSO prior
  - ▶ Can not detect if a function is linear, e.g. spike-and-slab grouped LASSO prior (Bai et al. 2020; Bai 2021)

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## Dissertation

# Objectives

- ▶ To develop statistical models that improve curve interpolation and outcome prediction
  - ▶ Local adaption of sparse penalty and smooth penalty
  - ▶ Bi-level selection for linear and nonlinear effect
- ▶ To develop a fast and scalable algorithm
- ▶ To implement a user-friendly statistical software

## Projects

- ▶ **Guo, B.**, Jaeger, B. C., Rahman, A. F., Long, D. L., Yi, N. (2022). Spike-and-Slab least absolute shrinkage and selection operator generalized additive models and scalable algorithms for high-dimensional data analysis. *Statistics in Medicine*. doi: <https://doi.org/10.1002/sim.9483>
- ▶ **Guo, B.**, Jaeger, B. C., Rahman, A. F., Long, D. L., Yi, N. (2022). A scalable and flexible Cox proportional hazard model for high-dimensional survival prediction and functional selection *arXiv*. doi: <https://doi.org/10.48550/arXiv.2205.11600>
- ▶ **Guo, B.**, Yi, N. (2022). BHAM: An R Package to Fit Bayesian Hierarchical Additive Models for High-dimensional Data Analysis *Work in Progress*

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Bayesian Hierarchical Additive Models

## Bayesian Hierarchical Additive Models

# Generalized Additive Model

Given the data  $\{y_i, x_{i1}, \dots, x_{ip}\}_{i=1}^n$  where  $p \gg n$

$$y_i \stackrel{\text{i.i.d.}}{\sim} EF(\mu_i, \phi),$$

$$g(\mu_i) = \beta_0 + \sum_{j=1}^p B_j(x_{ij}), \quad i = 1, \dots, n.$$



# Spline Function Reparameterization

- ▶ Smoothing penalty from smoothing spline regression (Simon N. Wood 2017)

$$\lambda_j \int B_j''(x) dx = \lambda_j \beta_j^T \mathbf{S}_j \beta_j,$$

where  $S_j$  is a known smoothing penalty matrix.

- ▶ Isolate the linear and nonlinear components via eigendecomposing  $S_j$

$$\mathbf{X}\beta = \mathbf{X}^0\beta + \mathbf{X}^*\beta^*$$

- ▶ Benefits
  - ▶ Motivate bi-level selection
  - ▶ Implicit modeling of function smoothness
  - ▶ Reduce computation load with conditionally independent prior of basis coefficients

## Two-part Spike-and-slab LASSO (SSL) Prior

- ▶ SSL prior for the linear coefficient and group SSL priors for nonlinear coefficients

$$\beta_j | \gamma_j, s_0, s_1 \sim DE(0, (1 - \gamma_j)s_0 + \gamma_j s_1)$$

$$\beta_{jk}^* | \gamma_j^*, s_0, s_1 \stackrel{\text{iid}}{\sim} DE(0, (1 - \gamma_j^*)s_0 + \gamma_j^* s_1), k = 1, \dots, K_j$$

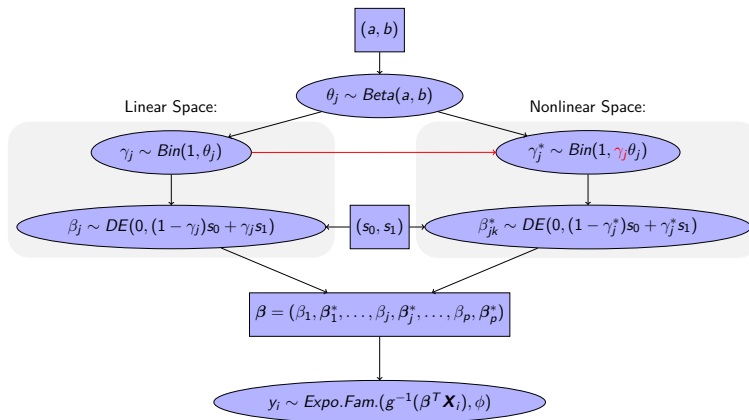
- ▶ Effect hierarchy enforced latent inclusion indicators  $\gamma_j$  and  $\gamma_j^*$  for bi-level selection

$$\gamma_j | \theta_j \sim \text{Bin}(\gamma_j | 1, \theta_j), \quad \gamma_j^* | \gamma_j, \theta_j \sim \text{Bin}(1, \gamma_j \theta_j),$$

- ▶ Local adaptivity of signal sparsity and function smoothness

$$\theta_j \sim \text{Beta}(a, b)$$

# Visual Representation



# EM-Coordinate Descent Algorithm for Scalable Model Fitting

We are interested in estimating  $\Theta = \{\beta, \theta, \phi\}$  using optimization based algorithm for scalability purpose

- ▶ Basic Ideas

- ▶ Treat  $\gamma$ s as the “missing data” in the EM procedure
- ▶ Quantify the expectation of log posterior density function of  $\Theta$  with respect to  $\gamma$  conditioning on  $\Theta^{(t-1)}$
- ▶ Maximize two parts of the objective function independently

- ▶ Previous applications in high-dimensional data analysis

- ▶ EMVS (Ročková and George 2014), Spike-and-slab lasso (Ročková and George 2018)
- ▶ BhGLM (Yi et al. 2019)

## Decomposition of Objective Function

We aim to maximize the log posterior density of  $\Theta$  by averaging over all possible values of  $\gamma$

$$\log f(\Theta, \gamma | \mathbf{y}, \mathbf{X}) = Q_1(\beta, \phi) + Q_2(\gamma, \theta),$$

- $L_1$ -penalized likelihood function of  $\beta, \phi$

$$Q_1 \equiv Q_1(\beta, \phi) = \log f(\mathbf{y} | \beta, \phi) + \sum_{j=1}^p \left[ \log f(\beta_j | \gamma_j) + \sum_{k=1}^{K_j} \log f(\beta_{jk}^* | \gamma_{jk}^*) \right]$$

- Posterior density of  $\theta$  given data points  $\gamma$ s

$$Q_2 \equiv Q_2(\gamma, \theta) = \sum_{j=1}^p \left[ (\gamma_j + \gamma_j^*) \log \theta_j + (2 - \gamma_j - \gamma_j^*) \log(1 - \theta_j) \right] + \sum_{j=1}^p \log f(\theta_j).$$

- $Q_1$  and  $Q_2$  are independent conditioning on  $\gamma$ s

# Summary of EM-Coordinate Descent Algorithm

- ▶ E-step
  - ▶ Formulate  $E_{\gamma|\Theta^{(t)}} [Q(\Theta, \gamma)] = E(Q_1) + E(Q_2)$ 
    - ▶  $E(Q_1)$  is a penalized likelihood function of  $\beta, \phi$
    - ▶  $E(Q_2)$  is a posterior density of  $\theta$  given  $E(\gamma)$
    - ▶  $E(Q_1)$  and  $E(Q_2)$  are conditionally independent
  - ▶ Calculate  $E(\gamma_j)$ ,  $E(\gamma_j^*)$  and the penalties parameters by Bayes' theorem
- ▶ M-step:
  - ▶ Use Coordinate Descent to fit the penalized model in  $E(Q_1)$  to update  $\beta, \phi$
  - ▶ Closed form calculation via  $E(Q_2)$  to update  $\theta$

# Tuning Parameter Selection

- ▶  $s_0$  and  $s_1$  are tuning parameters
- ▶ Empirically,  $s_1$  has extremely small effect on changing the estimates
- ▶ Focus on tuning  $s_0$
- ▶ Consider a sequence of  $L$  ordered values  $\{s_0^l\} : 0 < s_0^1 < s_0^2 < \dots < s_0^L < s_1$
- ▶ Cross-validation to choose optimal value for  $s_0$

## Simulation Study

- ▶ Follow the data generating process introduced in Bai et al. (2020).
- ▶  $n_{train} = 500$ ,  $n_{test} = 1000$
- ▶  $p = 4, 10, 50, 200$

$$\mu = 5 \sin(2\pi x_1) - 4 \cos(2\pi x_2 - 0.5) + 6(x_3 - 0.5) - 5(x_4^2 - 0.3),$$

- ▶  $f_j(x_j) = 0$  for  $j = 5, \dots, p$ .
- ▶ 2 types of outcome: Gaussian ( $\phi = 1$ ), Binomial
- ▶ Splines are constructed using 10 knots
- ▶ 50 Iterations



# Comparison & Metrics

- ▶ Methods of comparison
  - ▶ Proposed model BHAM
  - ▶ Linear LASSO model as the benchmark
  - ▶ mgcv (S. N. Wood 2004)
  - ▶ COSSO (Zhang and Lin 2006) and adaptive COSSO (Storlie et al. 2011)
  - ▶ Sparse Bayesian GAM (Bai 2021)
  - ▶ spikeSlabGAM (Scheipl, Fahrmeir, and Kneib 2012)
- ▶ Metrics
  - ▶ Prediction:  $R^2$  for continuous outcomes, out-of-sample AUC for binary outcomes
  - ▶ Variable Selection: positive predictive value (precision), true positive rate (recall), and Matthews correlation coefficient (MCC)

## Prediction Performance

- ▶ Linear LASSO Model performs bad and mgcv performs well
- ▶ BHAM performs better than COSSO, adaptive COSSO and spikeSlabGAM
- ▶ BHAM performs better than SB-GAM in low-dimensional case but slightly worse in the high-dimensional setting
- ▶ BHAM is much faster than SB-GAM in fitting models

# Variable Selection Performance

- ▶ SB-GAM has the best variable selection performance
- ▶ BHAM has conservative selection
- ▶ BHAM and spikeSlabGAM have trade-offs for bi-level selection
  - ▶ spikeSlabGAM tends to select either linear or nonlinear components of the function
  - ▶ BHAM is more likely to select both parts

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Additive Cox Proportional Hazards Model

## Additive Cox Proportional Hazards Model

# Model & Objective Functions

- ▶ Cox proportional hazard model with event time  $t_i$

$$h(t_i) = h_0(t_i) \exp\left(\sum_{j=1}^p B_j(x_{ij})\right), \quad i = 1, \dots, n.$$

- ▶ No intercept term because of the baseline hazard function
- ▶ Model fitting
  - ▶ Replace likelihood function with partial likelihood function

$$\hat{h}_0(t_i|\beta) = d_i / \sum_{i' \in R(t_i)} \exp(X_{i'}\beta).$$

## Two-part Spike-and-slab LASSO (SSL) Prior

- ▶ SSL prior for the linear coefficient and group SSL priors for nonlinear coefficients

$$\beta_j | \gamma_j, s_0, s_1 \sim DE(0, (1 - \gamma_j)s_0 + \gamma_j s_1)$$

$$\beta_{jk}^* | \gamma_j^*, s_0, s_1 \stackrel{\text{iid}}{\sim} DE(0, (1 - \gamma_j^*)s_0 + \gamma_j^* s_1), k = 1, \dots, K_j$$

- ▶ Effect hierarchy enforced latent inclusion indicators  $\gamma_j$  and  $\gamma_j^*$  for bi-level selection

$$\gamma_j | \theta_j \sim \text{Bin}(\gamma_j | 1, \theta_j), \quad \gamma_j^* | \gamma_j, \theta_j \sim \text{Bin}(1, \gamma_j \theta_j),$$

- ▶ Local adaptivity of signal sparsity and function smoothness

$$\theta_j \sim \text{Beta}(a, b)$$

# Summary of EM-Coordinate Descent Algorithm

- ▶ E-step
  - ▶ Formulate  $E_{\gamma|\Theta^{(t)}} [Q(\Theta, \gamma)] = E(Q_1) + E(Q_2)$ 
    - ▶  $E(Q_1)$  is a penalized likelihood function of  $\beta, \phi$
    - ▶  $E(Q_2)$  is a posterior density of  $\theta$  given  $E(\gamma)$
    - ▶  $E(Q_1)$  and  $E(Q_2)$  are conditionally independent
  - ▶ Calculate  $E(\gamma_j)$ ,  $E(\gamma_j^*)$  and the penalties parameters by Bayes' theorem
- ▶ M-step:
  - ▶ Use Coordinate Descent to fit the penalized model in  $E(Q_1)$  to update  $\beta, \phi$
  - ▶ Closed form calculation via  $E(Q_2)$  to update  $\theta$

## Simulation Study

- ▶ Follow the data generating process introduced in Bai et al. (2020).
- ▶  $n_{train} = 500$ ,  $n_{test} = 1000$
- ▶  $p = 4, 10, 50, 100, 200$
- ▶ Survival and censoring time follow Weibull distribution

$$\log \eta = (x_1 + 1)^2/5 + \exp(x_2 + 1)/25 + 3\sin(x_3)/2 + (1.4x_4 + 0.5)/2$$

- ▶ Censoring rate is controlled at  $\{0.15, 0.3, 0.45\}$
- ▶ Splines are constructed using 10 knots
- ▶ 50 Iterations



# Comparison & Metrics

- ▶ Methods of comparison
  - ▶ Proposed model BHAM
  - ▶ Linear LASSO model as the benchmark
  - ▶ mgcv (S. N. Wood 2004)
  - ▶ COSSO (Zhang and Lin 2006) and adaptive COSSO (Storlie et al. 2011)
- ▶ Metrics
  - ▶ Out-of-sample deviance & Concordance

# Prediction Performance

- ▶ Linear LASSO Model performs bad in general
- ▶ Low dimensional settings:
  - ▶ mgcv performs the best
  - ▶ BHAM performs as good as mgcv
- ▶ High dimensional setting:
  - ▶ BHAM performs better than COSSO models as  $p$  increases and more censoring events



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R Package BHAM

R Package BHAM

# R Package BHAM

- ▶ Model formulation for high-dimensional data
- ▶ Model fitting and tuning
- ▶ Model summary and variable selection
- ▶ Spline function visualization
- ▶ Website via *[boyiguo1.github.io/BHAM](https://boyiguo1.github.io/BHAM)*

## Design Matrix of Spline Functions

- Flexible spline function formulation for high-dimensional data

```
spline_df <- dplyr::tribble(  
  ~Var, ~Func, ~Args,  
  "X1",  "s",  "bs='cr', k=5",  
  "X2",  "s",  NA,  
  "X3",  "s",  "")  
spline_df <- data.frame(  
  Var = setdiff(names(dat), "y"),  
  Func = "s",  
  Args = "bs='cr', k=7")  
train_sm_dat <- BHAM::construct_smooth_data(spline_df, dat)
```

# Model Fitting Functions

- ▶ Model fitting via `bamlasso`
  - ▶ Argument `family` for generalized and survival outcomes
  - ▶ Argument `ss` for spike-and-slab LASSO scale parameters
  - ▶ Argument `group` for group structures among predictors
- ▶ Model tuning via `tune`
  - ▶ Argument `nfolds`, `ncv` for nested cross-validation
  - ▶ Argument `s0` for tuning candidates

# Post Fitting Functions

- ▶ Bi-level selection via `bamlasso_var_selection`
- ▶ Make prediction data for splines `make_predict_dat`
- ▶ Plot spline functions via `plot_smooth_term`



## Future Research

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## Modeling Interactions

# Modeling Interactions

## Varying coefficient models

- ▶ Assume the coefficient of a variable  $X_j$  is a function of a covariate  $Z_j$ 
  - ▶ linear model:  $\beta(Z_j) = \beta$
  - ▶ VC model:  $\beta(Z_j) = B(Z_j)$
- ▶ Replace each spline function  $B(z_{ij})$  with  $B(z_{ij})x_{ij} \equiv (x_{ij}\mathbf{Z}_{ij}^T)\beta_j$
- ▶ Model fitting with EM-Coordinate Descent

### Question

Can  $Z_j$  be continuous? Is it possible to have a more flexible model?

# Smooth Surface Fitting

- ▶ Tensor product of spline functions

$$B_{js}(x_{ij}, x_{is}) = \sum_{\rho=1}^K \sum_{v=1}^K \beta_{jspv} b_{j\rho}(x_{ij}) b_{sv}(x_{is})$$

- ▶ Smooth Surface

$$B_j(x_{ij}) + B_s(x_{is}) + B_{js}(x_{ij}, x_{is}),$$

## Question

Can we have a generalized model that accounts fixed effects, nonlinear curves, smooth surfaces, and random effects?

# Structural Additive Model

High-dimensional structural additive model can be formulated as

$$g(\mathbb{E}(y_i)) = \mathbf{x}_i^T \boldsymbol{\theta} + \mathbf{u}_i^T \boldsymbol{\gamma} + B(z_{i1}) + B(z_{i2}, z_{i3}) + B_{\text{spat}}(s_i)$$

- ▶ Un-regularized predictors  $\mathbf{x}_i$
- ▶ Regularized predictors  $\mathbf{u}_i$
- ▶ Predictors with nonlinear effects  $\mathbf{z}_i$
- ▶ Spatial random effects with coordinates  $s_i$

Spike-and-slab LASSO prior motivates a seamless process of variable/functional selection and a scalable optimization-based model fitting algorithm

# Conclusion

# Conclusion

- ▶ Identify challenges in high-dimensional GAM with spline functions
  - ▶ Balance between signal sparsity and function smoothness
  - ▶ Bi-level selection to automatically detect linear and nonlinear effects
- ▶ Statistical contribution
  - ▶ Two-part spike-and-slab LASSO prior for spline functions
  - ▶ Scalable EM-Coordinate Descent algorithms for generalized and survival outcomes
  - ▶ R package BHAM
- ▶ Future Research
  - ▶ Extension of spike-and-slab LASSO prior in structured additive model

Outline  
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Conclusion  
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References  
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