Sparse Additive Interaction Learning

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1 Introduction

Computational approaches to variable selection have become increasingly important with the advent of high-throughput technologies in genomics and brain imaging studies, where the data has become massive, yet where it is believed that the number of truly important variables is small relative to the total number of variables. Although many approaches have been developed for main effects, there are several applications where interaction models can reflect biological phenomena and improve prediction accuracy. For example, genome wide association studies (GWAS) have been unable to explain a large proportion of heritability (the variance in phenotype attributable to genetic variants) and it has been suggested that this missing heritability may in part be due to gene-environment interactions [1]. Furthermore, diseases are now thought to be the result of changes in entire biological networks whose states are affected by a complex interaction of genetic and environmental factors. In high-dimensional settings ($p >> n$), power to estimate interactions is low, the number of possible interactions could be enormous and their effects may be non-linear. In this paper, we propose a multivariable penalization procedure for detecting non-linear interactions between high dimensional data $\mathbf{X}$ and a single environmental factor E on a response vector Y.

1.1 Sparse additive interaction model

Let $Y = (Y_1, \ldots, Y_n) \in \mathbb{R}^n$ be a continuous or binary outcome variable, $X_E = (E_1, \ldots, E_n) \in \mathbb{R}^n$ a binary or continuous environment vector, and $\boldsymbol{X} = (X_1, \ldots, X_p) \in \mathbb{R}^{n \times p}$ a matrix of predictors. Furthermore let $f_j : \mathbb{R} \to \mathbb{R}$ be a smoothing method for variable X_j by a projection on to a set of basis functions:

$$f_j(X_j) = \sum_{\ell=1}^{m_j} \psi_{j\ell}(X_j)\beta_{j\ell} \tag{1}$$

Here, the $\{\psi_{j\ell}\}_1^{m_j}$ are a family of basis functions in X_j [2]. Let $\boldsymbol{\Psi}_j$ be the $n \times m_j$ matrix of evaluations of the $\psi_{j\ell}$ and $\boldsymbol{\theta}_j = (\beta_{j1}, \ldots, \beta_{jm_j}) \in \mathbb{R}^{m_j}$ for $j = 1, \ldots, p$, i.e., $\boldsymbol{\theta}_j$ is a m_j-dimensional column vector of basis coefficients for the jth main effect. In this article we consider an additive interaction regression model of the form

$$g(\boldsymbol{\mu}) = \beta_0 \cdot \mathbf{1} + \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j + \beta_E X_E + \sum_{j=1}^{p} (X_E \circ \boldsymbol{\Psi}_j)\boldsymbol{\tau}_j \tag{2}$$

where $g(\cdot)$ is a known link function, $\boldsymbol{\mu} = \mathsf{E}\left[Y | \boldsymbol{\Psi}, X_E\right]$, β_0 is the intercept, β_E is the coefficient for the environment variable, $\boldsymbol{\tau}_j = (\tau_{j1}, \ldots, \tau_{jm_j}) \in \mathbb{R}^{m_j}$ are the basis coefficients for the jth interaction term, and $(X_E \circ \boldsymbol{\Psi}_j)$ is the $n \times m_j$ matrix formed by the component-wise multiplication of the column vector X_E by each column of $\boldsymbol{\Psi}_j$. For a continuous response, we use the squared-error loss:

$$\mathcal{L}(\boldsymbol{\Theta}|\mathbf{D}) = \frac{1}{2n}\left\| Y - \beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j - \beta_E X_E - \sum_{j=1}^{p} (X_E \circ \boldsymbol{\Psi}_j)\boldsymbol{\tau}_j \right\|_2^2 \tag{3}$$

and for binary response $Y_i \in \{-1, +1\}$ we use the logistic loss:

$$\mathcal{L}(\boldsymbol{\Theta}|\mathbf{D}) = \frac{1}{n}\sum_i \log\left(1 + \exp\left\{ -Y_i \left(\beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j - \beta_E X_E - \sum_{j=1}^{p} (X_E \circ \boldsymbol{\Psi}_j)\boldsymbol{\tau}_j \right)\right\}\right) \tag{4}$$

where $\boldsymbol{\Theta} := (\beta_0, \beta_E, \boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p, \boldsymbol{\tau}_1, \ldots, \boldsymbol{\tau}_p)$ and $\mathbf{D} := (Y, \boldsymbol{\Psi}, X_E)$ is the working data.

Due to the large number of parameters to estimate with respect to the number of observations, one commonly-used approach is to shrink the regression coefficients by placing a constraint on the values of $(\beta_E, \boldsymbol{\theta}_j, \boldsymbol{\tau}_j)$. Certain constraints have the added benefit of producing a sparse model in the sense that many of the coefficients will be set exactly to 0. This reduced predictor set can lead to a more interpretable model with smaller prediction variance, albeit at the cost of having biased parameter estimates. In light of these goals, we consider the following penalized least squares criterion:

$$\arg\min_{\boldsymbol{\Theta}} \mathcal{L}(\boldsymbol{\Theta}|\mathbf{D}) + \lambda(1-\alpha)\left(w_E \|\beta_E\|_1 + \sum_{j=1}^{p} w_j \|\boldsymbol{\theta}_j\|_2 \right) + \lambda\alpha \sum_{j=1}^{p} w_{jE} \|\boldsymbol{\tau}_j\|_2 \tag{5}$$

where $\|\boldsymbol{\theta}_j\|_2 = \sqrt{\sum_{k=1}^{m_j} \beta_{jk}^2}$, $\|\boldsymbol{\tau}_j\|_2 = \sqrt{\sum_{k=1}^{m_j} \tau_{jk}^2}$, $\|\beta_E\|_1 = |\beta_E|$, $\lambda > 0$ and $\alpha \in (0,1)$ are tuning parameters, w_E, w_j, w_{jE} are adaptive weights for $j = 1, \ldots, p$. These weights serve as a way of allowing parameters to be penalized differently.

An issue with (5) is that since no constraint is placed on the structure of the model, it is possible that an estimated interaction term is nonzero while the corresponding main effects are zero. While there may be certain situations where this is plausible, statisticians have generally argued that interactions should only be included if the corresponding main effects are also in the model [3]. This is known as the strong heredity principle [4]. Indeed, large main effects are more likely to lead to detectable interactions [5]. In the next section we discuss how a simple reparametrization of the model (5) can lead to this desirable property.

1.2 Strong and weak heredity

The strong heredity principle states that the interaction term can only have a non-zero estimate if its corresponding main effects are estimated to be non-zero. The weak heredity principle allows for a non-zero interaction estimate as long as one of the corresponding main effects are estimated to be non-zero [4]. In the context of penalized regression methods, these principles can be formulated as structured sparsity [6] problems. Several authors have proposed to modify the type of penalty in order to achieve the heredity principle [7, 8, 9, 10]. We take an alternative approach. Following Choi et al. [11], we introduce a parameter $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_p) \in \mathbb{R}^p$ and reparametrize the coefficients for the interaction terms $\boldsymbol{\tau}_j$ in (2) as a function of γ_j and the main effect parameters $\boldsymbol{\theta}_j$ and β_E. This reparametrization for both strong and weak heredity is summarized in Table 1.

Table 1: Reparametrization for strong and weak heredity principle for `sail` model

Type	Feature	Reparametrization
Strong heredity	$\hat{\boldsymbol{\tau}}_j \neq 0 \Rightarrow \hat{\boldsymbol{\theta}}_j \neq 0$ and $\hat{\beta}_E \neq 0$	$\alpha_j = \gamma_j \beta_E \boldsymbol{\theta}_j$
Weak heredity	$\hat{\tau}_j \neq 0 \Rightarrow \hat{\boldsymbol{\theta}}_j \neq 0$ or $\hat{\beta}_E \neq 0$	$\alpha_j = \gamma_j (\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j)$

To perform variable selection in this new parametrization, we penalize $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_p)$ instead of penalizing $\boldsymbol{\tau}$ as in (5), leading to the following penalized least squares criterion:

$$\arg\min_{\beta_0, \boldsymbol{\beta}, \boldsymbol{\gamma}} \frac{1}{2} \|Y - g(\boldsymbol{\mu})\|^2 + \lambda_\beta \sum_{j=1}^{p} w_j |\beta_j| + \lambda_\gamma \sum_{j=1}^{p} w_{jE} |\gamma_{jE}| \tag{6}$$

where $g(\boldsymbol{\mu})$ is from (**??**), λ_β and λ_γ are tuning parameters and $\mathbf{w} = (w_1, \ldots, w_q, w_{1E}, \ldots, w_{qE})$ are prespecified adaptive weights. The λ_β tuning parameter controls the amount of shrinkage applied to the main effects, while λ_γ controls the interaction estimates and allows for the possibility of excluding the interaction term from the model even if the corresponding main effects are non-zero.

1.3 Toy example

We begin with a toy example to better illustrate our method. We sample $p = 20$ covariates independently from a $N(0, 1)$ truncated to the interval [0,1] and sample size $N = 100$. We generated data from the model

$$Y = f_1(X_1) + f_2(X_2) + 1.75E + 1.5E \cdot f_2(X_2) + \varepsilon \tag{7}$$

where $f_1(x) = -3x$, $f_2(x) = 2(2x - 1)^3$ and the error term ε is generated from a normal distribution with variance chosen such that the signal-to-noise ratio (SNR) is 2. We run the `sail` method with cubic b-splines and 10-fold CV to choose the optimal value of λ. Default values were used for all other arguments. We plot the solution path for both main effects and interactions in Figure **??** and the estimated functions $\hat{f}_1$ and $\hat{f}_2$ in Figure **??**.

1.4 Existing Literature

2 Regularization Path

The `sail` model has the form

$$\hat{Y} = \beta_0 \cdot \mathbf{1} + \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j + \beta_E X_E + \sum_{j=1}^{p} \gamma_j \beta_E (X_E \circ \boldsymbol{\Psi}_j) \boldsymbol{\theta}_j \tag{8}$$

Type	Model	Software
Linear	`CAP` (Zhao et al. 2009, *Ann. Stat*)	✗
	`SHIM` (Choi et al. 2009, *JASA*)	✗
	`hiernet` (Bien et al. 2013, *Ann. Stat*)	`hierNet(x, y)`
	`GRESH` (She and Jiang 2014, *JASA*)	✗
	`FAMILY` (Haris et al. 2014, *JCGS*)	`FAMILY(x, z, y)`
	`glinternet` (Lim and Hastie 2015, *JCGS*)	`glinternet(x, y)`
	`RAMP` (Hao et al. 2016, *JASA*)	`RAMP(x, y)`
Non-linear	`VANISH` (Radchenko and James 2010, *JASA*)	✗
	`sail` (Bhatnagar et al. 2017+)	`sail(x, e, y)`

The objective function is given by

$$Q(\mathbf{\Theta}) = \frac{1}{2n}\left\|Y - \hat{Y}\right\|_2^2 + \lambda(1-\alpha)\left(w_E|\beta_E| + \sum_{j=1}^{p} w_j \|\boldsymbol{\theta}_j\|_2\right) + \lambda\alpha\sum_{j=1}^{p} w_{jE}|\gamma_j| \tag{9}$$

Denote the n-dimensional residual column vector $R = Y - \hat{Y}$. The subgradient equations are given by

$$\frac{\partial Q}{\partial \beta_0} = \frac{1}{n}\left(Y - \beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \mathbf{\Psi}_j\boldsymbol{\theta}_j - \beta_E X_E - \sum_{j=1}^{p}\gamma_j\beta_E(X_E \circ \mathbf{\Psi}_j)\boldsymbol{\theta}_j\right)^{\top}\mathbf{1} = 0 \tag{10}$$

$$\frac{\partial Q}{\partial \beta_E} = -\frac{1}{n}\left(X_E + \sum_{j=1}^{p}\gamma_j(X_E \circ \mathbf{\Psi}_j)\boldsymbol{\theta}_j\right)^{\top} R + \lambda(1-\alpha)w_E s_1 = 0 \tag{11}$$

$$\frac{\partial Q}{\partial \boldsymbol{\theta}_j} = -\frac{1}{n}\left(\mathbf{\Psi}_j + \gamma_j\beta_E(X_E \circ \mathbf{\Psi}_j)\right)^{\top} R + \lambda(1-\alpha)w_j s_2 = \mathbf{0} \tag{12}$$

$$\frac{\partial Q}{\partial \gamma_j} = -\frac{1}{n}\left(\beta_E(X_E \circ \mathbf{\Psi}_j)\boldsymbol{\theta}_j\right)^{\top} R + \lambda\alpha w_{jE} s_3 = 0 \tag{13}$$

where s_1 is in the subgradient of the ℓ_1 norm:

$$s_1 \in \begin{cases} \text{sign}\left(\beta_E\right) & \text{if } \beta_E \neq 0 \\ [-1, 1] & \text{if } \beta_E = 0, \end{cases}$$

s_2 is in the subgradient of the ℓ_2 norm:

$$s_2 \in \begin{cases} \dfrac{\boldsymbol{\theta}_j}{\|\boldsymbol{\theta}_j\|_2} & \text{if } \boldsymbol{\theta}_j \neq \mathbf{0} \\ u \in \mathbb{R}^{m_j} : \|u\|_2 \leq 1 & \text{if } \boldsymbol{\theta}_j = \mathbf{0}, \end{cases}$$

and s_3 is in the subgradient of the ℓ_1 norm:

$$s_3 \in \begin{cases} \text{sign}\left(\gamma_j\right) & \text{if } \gamma_j \neq 0 \\ [-1, 1] & \text{if } \gamma_j = 0. \end{cases}$$

Define the partial residuals, without the jth predictor for $j = 1, \ldots, p$, as

$$R_{(-j)} = Y - \beta_0 \cdot \mathbf{1} - \sum_{\ell \neq j} \boldsymbol{\Psi}_\ell \boldsymbol{\theta}_\ell - \beta_E X_E - \sum_{\ell \neq j} \gamma_\ell \beta_E (X_E \circ \boldsymbol{\Psi}_\ell) \boldsymbol{\theta}_\ell$$

the partial residual without X_E as

$$R_{(-E)} = Y - \beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j$$

and the partial residual without the jth interaction for $j = 1, \ldots, p$

$$R_{(-jE)} = Y - \beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j - \beta_E X_E - \sum_{\ell \neq j} \gamma_\ell \beta_E (X_E \circ \boldsymbol{\Psi}_\ell) \boldsymbol{\theta}_\ell$$

From the subgradient Equation (11), we see that $\beta_E = 0$ is a solution if

$$\frac{1}{w_E}\left|\frac{1}{n}\left(X_E + \sum_{j=1}^{p}\gamma_j (X_E \circ \boldsymbol{\Psi}_j)\boldsymbol{\theta}_j\right)^\top R_{(-E)}\right| \leq \lambda(1-\alpha) \tag{14}$$

From the subgradient Equation (12), we see that $\boldsymbol{\theta}_j = \mathbf{0}$ is a solution if

$$\frac{1}{w_j}\left\|\frac{1}{n}\left(\boldsymbol{\Psi}_j + \gamma_j \beta_E (X_E \circ \boldsymbol{\Psi}_j)\right)^\top R_{(-j)}\right\|_2 \leq \lambda(1-\alpha) \tag{15}$$

From the subgradient Equation (13), we see that $\gamma_j = 0$ is a solution if

$$\frac{1}{w_{jE}}\left|\frac{1}{n}\left(\beta_E (X_E \circ \boldsymbol{\Psi}_j)\boldsymbol{\theta}_j\right)^\top R_{(-jE)}\right| \leq \lambda\alpha \tag{16}$$

2.1 Lambda Max

Due to the strong heredity property, the parameter vector $(\beta_E, \boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p, \gamma_1, \ldots, \gamma_p)$ will be equal to $\mathbf{0}$ if $(\beta_E, \boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p) = \mathbf{0}$. Therefore, the smallest value of λ for which the entire parameter vector (excluding the intercept) is $\mathbf{0}$ is:

$$\lambda_{max} = \frac{1}{n(1-\alpha)} \max\left\{\frac{1}{w_E}\left(X_E + \sum_{j=1}^{p}\gamma_j (X_E \circ \boldsymbol{\Psi}_j)\boldsymbol{\theta}_j\right)^\top R_{(-E)}, \right.$$
$$\left. \max_j \frac{1}{w_j}\left\|\left(\boldsymbol{\Psi}_j + \gamma_j \beta_E (X_E \circ \boldsymbol{\Psi}_j)\right)^\top R_{(-j)}\right\|_2 \right\} \tag{17}$$

which reduces to

$$\lambda_{max} = \frac{1}{n(1-\alpha)} \max\left\{\frac{1}{w_E}\left(X_E\right)^\top R_{(-E)}, \max_j \frac{1}{w_j}\left\|\left(\boldsymbol{\Psi}_j\right)^\top R_{(-j)}\right\|_2\right\}$$

2.2 Optimization of Parameters

From the subgradient equations we see that

$$\hat{\beta}_0 = \left(Y - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \hat{\boldsymbol{\theta}}_j - \hat{\beta}_E X_E - \sum_{j=1}^{p} \hat{\gamma}_j \hat{\beta}_E (X_E \circ \boldsymbol{\Psi}_j) \hat{\boldsymbol{\theta}}_j \right)^\top \mathbf{1} \tag{18}$$

$$\hat{\beta}_E = S\left(\frac{1}{n \cdot w_E} \left(X_E + \sum_{j=1}^{p} \hat{\gamma}_j (X_E \circ \boldsymbol{\Psi}_j) \hat{\boldsymbol{\theta}}_j \right)^\top R_{(-E)}, \lambda(1-\alpha) \right) \tag{19}$$

$$\lambda(1-\alpha) w_j \frac{\boldsymbol{\theta}_j}{\|\boldsymbol{\theta}_j\|_2} = \frac{1}{n} \left(\boldsymbol{\Psi}_j + \gamma_j \beta_E (X_E \circ \boldsymbol{\Psi}_j) \right)^\top R_{(-j)} \tag{20}$$

$$\hat{\gamma}_j = S\left(\frac{1}{n \cdot w_{jE}} \left(\beta_E (X_E \circ \boldsymbol{\Psi}_j) \boldsymbol{\theta}_j \right)^\top R_{(-jE)}, \lambda\alpha \right) \tag{21}$$

where $S(x,t) = \text{sign}(x)(|x| - t)$ is the soft-thresholding operator

3 Algorithm

For each function f_j, we use a cubic B-spline parameterization with 5 degrees of freedom implemented in the `bs` function in `R` [12].

3.1 Details on update for $\boldsymbol{\theta}$

Here we discuss a computational speedup in the updates for the $\boldsymbol{\theta}$ parameter. The partial residual (R_s) used for updating $\boldsymbol{\theta}_s$ ($s \in 1, \ldots, p$) at the kth iteration is given by

$$R_s = Y - \widetilde{Y}_{(-s)}^{(k)} \tag{22}$$

Algorithm 1 Coordinate descent for least-squares `sail` with strong heredity

function `sail`$(Y, \boldsymbol{X}, X_E, \texttt{df}, \texttt{degree}, \epsilon)$ ▷ Algorithm for solving (9)

  $\Psi_j \leftarrow$ `splines::bs`$(X_j,$ `df`, `degree`$)$ for $j = 1, \ldots, p$

  $\widetilde{\Psi}_j \leftarrow X_E \circ \Psi_j$ for $j = 1, \ldots, p$

  Initialize: $\beta_0^{(0)} \leftarrow \bar{Y}$, $\beta_E^{(0)} = \boldsymbol{\theta}_j^{(0)} \leftarrow 0$ for $j = 1, \ldots, p$.

  Set iteration counter $k \leftarrow 0$

  $R^* \leftarrow Y - \beta_0^{(k)} - \beta_E^{(k)} X_E - \sum_j (\boldsymbol{\Psi}_j + \gamma_j^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_j) \boldsymbol{\theta}_j^{(k)}$

  repeat

    • To update $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_p)$

      $\widetilde{X}_j \leftarrow \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_j \boldsymbol{\theta}_j^{(k)}$ for $j = 1, \ldots, p$

      $R \leftarrow R^* + \sum_{j=1}^p \gamma_j^{(k)} \widetilde{X}_j$

$$\boldsymbol{\gamma}^{(k)(new)} \leftarrow \arg\min_{\boldsymbol{\gamma}} \frac{1}{2n} \left\| R - \sum_j \gamma_j \widetilde{X}_j \right\|_2^2 + \lambda\alpha \sum_j w_{jE} |\gamma_j|$$

      $\Delta = \sum_j (\gamma_j^{(k)} - \gamma_j^{(k)(new)}) \widetilde{X}_j$

      $R^* \leftarrow R^* + \Delta$

    • To update $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p)$

      $\widetilde{X}_j \leftarrow \boldsymbol{\Psi}_j + \gamma_j^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_j$ for $j = 1, \ldots, p$

      for $j = 1, \ldots, p$ **do**

        $R \leftarrow R^* + \widetilde{X}_j \boldsymbol{\theta}_j^{(k)}$

$$\boldsymbol{\theta}_j^{(k)(new)} \leftarrow \arg\min_{\boldsymbol{\theta}_j} \frac{1}{2n} \left\| R - \widetilde{X}_j \boldsymbol{\theta}_j \right\|_2^2 + \lambda(1-\alpha) w_j \|\theta_j\|_2$$

        $\Delta = \widetilde{X}_j (\boldsymbol{\theta}_j^{(k)} - \boldsymbol{\theta}_j^{(k)(new)})$

        $R^* \leftarrow R^* + \Delta$

    • To update β_E

      $\widetilde{X}_E \leftarrow X_E + \sum_j \gamma_j^{(k)} \widetilde{\boldsymbol{\Psi}}_j \boldsymbol{\theta}_j^{(k)}$

      $R \leftarrow R^* + \beta_E^{(k)} \widetilde{X}_E$

$$\beta_E^{(k)(new)} \leftarrow S\left(\frac{1}{n \cdot w_E} \widetilde{X}_E^\top R, \lambda(1-\alpha) \right)$$

▷ $S(x,t) = \mathrm{sign}(x)(|x| - t)_+$

      $\Delta = (\beta_E^{(k)} - \beta_E^{(k)(new)}) \widetilde{X}_E$

      $R^* \leftarrow R^* + \Delta$

    • To update β_0

      $R \leftarrow R^* + \beta_0^{(k)}$

$$\beta_0^{(k)(new)} \leftarrow \frac{1}{n} R^* \cdot \mathbf{1}$$

      $\Delta = \beta_0^{(k)} - \beta_0^{(k)(new)}$

      $R^* \leftarrow R^* + \Delta$

    $k \leftarrow k + 1$

  until convergence criterion is satisfied: $\left\| \boldsymbol{\Theta}^{(k)} - \boldsymbol{\Theta}^{(k-1)} \right\|_2^2 < \epsilon$

where $\widetilde{Y}_{(-s)}^{(k)}$ is the fitted value at the kth iteration excluding the contribution from $\boldsymbol{\Psi}_s$:

$$\widetilde{Y}_{(-s)}^{(k)} = \beta_0^{(k)} - \beta_E^{(k)} X_E - \sum_{\ell \neq s} \boldsymbol{\Psi}_\ell \boldsymbol{\theta}_\ell^{(k)} - \sum_{\ell \neq s} \gamma_\ell^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_\ell \boldsymbol{\theta}_\ell^{(k)} \tag{23}$$

Using (23), (22) can be re-written as

$$\begin{aligned} R_s &= Y - \beta_0^{(k)} - \beta_E^{(k)} X_E - \sum_{j=1}^{p} (\boldsymbol{\Psi}_j + \gamma_j^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_j) \boldsymbol{\theta}_j^{(k)} + (\boldsymbol{\Psi}_s + \gamma_s^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_s) \boldsymbol{\theta}_s^{(k)} \\ &= R^* + (\boldsymbol{\Psi}_s + \gamma_s^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_s) \boldsymbol{\theta}_s^{(k)} \end{aligned} \tag{24}$$

where

$$R^* = Y - \beta_0^{(k)} - \beta_E^{(k)} X_E - \sum_{j=1}^{p} (\boldsymbol{\Psi}_j + \gamma_j^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_j) \boldsymbol{\theta}_j^{(k)} \tag{25}$$

Denote $\boldsymbol{\theta}_s^{(k)(\text{new})}$ the solution for predictor s at the kth iteration, given by:

$$\boldsymbol{\theta}_s^{(k)(new)} = \arg\min_{\boldsymbol{\theta}_j} \frac{1}{2n} \left\| R_s - (\boldsymbol{\Psi}_s + \gamma_s^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_s) \boldsymbol{\theta}_j \right\|_2^2 + \lambda(1-\alpha) w_s \|\theta_j\|_2 \tag{26}$$

Now we want to update the parameters for the next predictor $\boldsymbol{\theta}_{s+1}$ $(s+1 \in 1, \ldots, p)$ at the kth iteration. The partial residual used to update $\boldsymbol{\theta}_{s+1}$ is given by

$$R_{s+1} = R^* + (\boldsymbol{\Psi}_{s+1} + \gamma_{s+1}^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_{s+1}) \boldsymbol{\theta}_{s+1}^{(k)} + (\boldsymbol{\Psi}_s + \gamma_s^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_s)(\boldsymbol{\theta}_s^{(k)} - \boldsymbol{\theta}_s^{(k)(new)}) \tag{27}$$

where R^* is given by (25), $\boldsymbol{\theta}_s^{(k)}$ is the parameter value prior to the update, and $\boldsymbol{\theta}_s^{(k)(new)}$ is the updated value given by (26). Taking the difference between (24) and (27) gives

$$\begin{aligned} \Delta &= R_t - R_s \\ &= (\boldsymbol{\Psi}_t + \gamma_t^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_t) \boldsymbol{\theta}_t^{(k)} + (\boldsymbol{\Psi}_s + \gamma_s^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_s)(\boldsymbol{\theta}_s^{(k)} - \boldsymbol{\theta}_s^{(k)(new)}) - (\boldsymbol{\Psi}_s + \gamma_s^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_s) \boldsymbol{\theta}_s^{(k)} \\ &= (\boldsymbol{\Psi}_t + \gamma_t^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_t) \boldsymbol{\theta}_t^{(k)} - (\boldsymbol{\Psi}_s + \gamma_s^{(k)} \beta_E^{(k)} \widetilde{\boldsymbol{\Psi}}_s) \boldsymbol{\theta}_s^{(k)(new)} \end{aligned} \tag{28}$$

Therefore $R_t = R_s + \Delta$, and the partial residual for updating the next predictor can be computed by updating the previous partial residual by Δ, given by (28). This formulation can lead to computational speedups especially when $\Delta = 0$, meaning the partial residual does not need to be re-calculated.

4 Weak Heredity

We can also enforce the weak heredity property:

$$\hat{\alpha}_{jE} \neq 0 \qquad \Rightarrow \qquad \hat{\beta}_j \neq 0 \qquad \text{or} \qquad \hat{\beta}_E \neq 0 \tag{29}$$

That is, an interaction term can only be present if at least one of it's corresponding main effects is nonzero. To do so, we reparametrize the coefficients for the interaction terms in (2) as $\boldsymbol{\alpha}_j = \gamma_j(\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j)$, where $\mathbf{1}_{m_j}$ is a vector of ones with dimension m_j (i.e. the length of $\boldsymbol{\theta}_j$).

4.1 Regularization Path

The `sail` model with weak heredity has the form

$$\hat{Y} = \beta_0 \cdot \mathbf{1} + \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j + \beta_E X_E + \sum_{j=1}^{p} \gamma_j (X_E \circ \boldsymbol{\Psi}_j)(\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j) \tag{30}$$

The objective function is given by

$$Q(\boldsymbol{\Theta}) = \frac{1}{2n} \left\| Y - \hat{Y} \right\|_2^2 + \lambda(1-\alpha)\left(w_E|\beta_E| + \sum_{j=1}^{p} w_j \|\boldsymbol{\theta}_j\|_2 \right) + \lambda\alpha \sum_{j=1}^{p} w_{jE}|\gamma_j| \tag{31}$$

Denote the n-dimensional residual column vector $R = Y - \hat{Y}$. The subgradient equations are given by

$$\frac{\partial Q}{\partial \beta_0} = \frac{1}{n}\left(Y - \beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j - \beta_E X_E - \sum_{j=1}^{p} \gamma_j (X_E \circ \boldsymbol{\Psi}_j)(\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j)\right)^\top \mathbf{1} = 0 \quad (32)$$

$$\frac{\partial Q}{\partial \beta_E} = -\frac{1}{n}\left(X_E + \sum_{j=1}^{p} \gamma_j (X_E \circ \boldsymbol{\Psi}_j)\mathbf{1}_{m_j}\right)^\top R + \lambda(1-\alpha) w_E s_1 = 0 \quad (33)$$

$$\frac{\partial Q}{\partial \boldsymbol{\theta}_j} = -\frac{1}{n}\left(\boldsymbol{\Psi}_j + \gamma_j (X_E \circ \boldsymbol{\Psi}_j)\right)^\top R + \lambda(1-\alpha) w_j s_2 = \mathbf{0} \quad (34)$$

$$\frac{\partial Q}{\partial \gamma_j} = -\frac{1}{n}\left((X_E \circ \boldsymbol{\Psi}_j)(\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j)\right)^\top R + \lambda \alpha w_{jE} s_3 = 0 \quad (35)$$

where s_1 is in the subgradient of the ℓ_1 norm:

$$s_1 \in \begin{cases} \text{sign}\,(\beta_E) & \text{if } \beta_E \neq 0 \\ [-1, 1] & \text{if } \beta_E = 0, \end{cases}$$

s_2 is in the subgradient of the ℓ_2 norm:

$$s_2 \in \begin{cases} \dfrac{\boldsymbol{\theta}_j}{\|\boldsymbol{\theta}_j\|_2} & \text{if } \boldsymbol{\theta}_j \neq \mathbf{0} \\ u \in \mathbb{R}^{m_j} : \|u\|_2 \leq 1 & \text{if } \boldsymbol{\theta}_j = \mathbf{0}, \end{cases}$$

and s_3 is in the subgradient of the ℓ_1 norm:

$$s_3 \in \begin{cases} \text{sign}\,(\gamma_j) & \text{if } \gamma_j \neq 0 \\ [-1, 1] & \text{if } \gamma_j = 0. \end{cases}$$

Define the partial residuals, without the jth predictor for $j = 1, \ldots, p$, as

$$R_{(-j)} = Y - \beta_0 \cdot \mathbf{1} - \sum_{\ell \neq j} \boldsymbol{\Psi}_\ell \boldsymbol{\theta}_\ell - \beta_E X_E - \sum_{\ell \neq j} \gamma_\ell (X_E \circ \boldsymbol{\Psi}_\ell)(\beta_E \cdot \mathbf{1}_{m_\ell} + \boldsymbol{\theta}_\ell)$$

the partial residual without X_E as

$$R_{(-E)} = Y - \beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j - \sum_{j=1}^{p} \gamma_j (X_E \circ \boldsymbol{\Psi}_j) \boldsymbol{\theta}_j$$

and the partial residual without the jth interaction for $j = 1, \ldots, p$

$$R_{(-jE)} = Y - \beta_0 \cdot \mathbf{1} - \sum_{j=1}^{p} \boldsymbol{\Psi}_j \boldsymbol{\theta}_j - \beta_E X_E - \sum_{\ell \neq j} \gamma_\ell (X_E \circ \boldsymbol{\Psi}_\ell)(\beta_E \cdot \mathbf{1}_{m_\ell} + \boldsymbol{\theta}_\ell)$$

From the subgradient Equation (33), we see that $\beta_E = 0$ is a solution if

$$\frac{1}{w_E} \left| \frac{1}{n} \left(X_E + \sum_{j=1}^{p} \gamma_j (X_E \circ \boldsymbol{\Psi}_j) \mathbf{1}_{m_j} \right)^\top R_{(-E)} \right| \leq \lambda(1 - \alpha) \tag{36}$$

From the subgradient Equation (34), we see that $\boldsymbol{\theta}_j = \mathbf{0}$ is a solution if

$$\frac{1}{w_j} \left\| \frac{1}{n} \left(\boldsymbol{\Psi}_j + \gamma_j (X_E \circ \boldsymbol{\Psi}_j) \right)^\top R_{(-j)} \right\|_2 \leq \lambda(1 - \alpha) \tag{37}$$

From the subgradient Equation (35), we see that $\gamma_j = 0$ is a solution if

$$\frac{1}{w_{jE}} \left| \frac{1}{n} \left((X_E \circ \boldsymbol{\Psi}_j)(\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j) \right)^\top R_{(-jE)} \right| \leq \lambda \alpha \tag{38}$$

4.2 Lambda Max

The smallest value of λ for which the entire parameter vector $(\beta_E, \boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p, \gamma_1, \ldots, \gamma_p)$ is $\mathbf{0}$ is:

$$\lambda_{max} = \frac{1}{n} \max \Bigg\{ \frac{1}{(1-\alpha)w_E} \left(X_E + \sum_{j=1}^{p} \gamma_j (X_E \circ \mathbf{\Psi}_j) \mathbf{1}_{m_j} \right)^\top R_{(-E)},$$
$$\max_j \frac{1}{(1-\alpha)w_j} \left\| \left(\mathbf{\Psi}_j + \gamma_j (X_E \circ \mathbf{\Psi}_j) \right)^\top R_{(-j)} \right\|_2,$$
$$\max_j \frac{1}{\alpha w_{jE}} \left((X_E \circ \mathbf{\Psi}_j)(\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j) \right)^\top R_{(-jE)} \Bigg\} \quad (39)$$

which reduces to

$$\lambda_{max} = \frac{1}{n(1-\alpha)} \max \left\{ \frac{1}{w_E} \left(X_E \right)^\top R_{(-E)}, \max_j \frac{1}{w_j} \left\| \left(\mathbf{\Psi}_j \right)^\top R_{(-j)} \right\|_2 \right\}$$

4.3 Optimization of Parameters

From the subgradient equations we see that

$$\hat{\beta}_0 = \left(Y - \sum_{j=1}^{p} \mathbf{\Psi}_j \hat{\boldsymbol{\theta}}_j - \hat{\beta}_E X_E - \sum_{j=1}^{p} \hat{\gamma}_j (X_E \circ \mathbf{\Psi}_j)(\hat{\beta}_E \cdot \mathbf{1}_{m_j} + \hat{\boldsymbol{\theta}}_j) \right)^\top \mathbf{1} \quad (40)$$

$$\hat{\beta}_E = S\left(\frac{1}{n \cdot w_E} \left(X_E + \sum_{j=1}^{p} \hat{\gamma}_j (X_E \circ \mathbf{\Psi}_j) \mathbf{1}_{m_j} \right)^\top R_{(-E)}, \lambda(1-\alpha) \right) \quad (41)$$

$$\lambda(1-\alpha) w_j \frac{\boldsymbol{\theta}_j}{\|\boldsymbol{\theta}_j\|_2} = \frac{1}{n} \left(\mathbf{\Psi}_j + \gamma_j (X_E \circ \mathbf{\Psi}_j) \right)^\top R_{(-j)} \quad (42)$$

$$\hat{\gamma}_j = S\left(\frac{1}{n \cdot w_{jE}} \left((X_E \circ \mathbf{\Psi}_j)(\beta_E \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j) \right)^\top R_{(-jE)}, \lambda\alpha \right) \quad (43)$$

where $S(x,t) = \text{sign}(x)(|x| - t)$ is the soft-thresholding operator

Algorithm 2 Coordinate descent for least-squares `sail` with weak heredity

function `sail`$(Y, \boldsymbol{X}, X_E, \texttt{df}, \texttt{degree}, \epsilon)$ ▷ Algorithm for solving (31)

  $\Psi_j \leftarrow$ `splines::bs`$(X_j,$ `df`, `degree`$)$ for $j = 1, \ldots, p$

  $\widetilde{\Psi}_j \leftarrow X_E \circ \Psi_j$ for $j = 1, \ldots, p$

  Initialize: $\beta_0^{(0)} \leftarrow \bar{Y}$, $\beta_E^{(0)} = \boldsymbol{\theta}_j^{(0)} \leftarrow 0$ for $j = 1, \ldots, p$.

  Set iteration counter $k \leftarrow 0$

  $R^* \leftarrow Y - \beta_0^{(k)} - \beta_E^{(k)} X_E - \sum_j \boldsymbol{\Psi}_j \boldsymbol{\theta}_j^{(k)} - \sum_j \gamma_j^{(k)} \widetilde{\boldsymbol{\Psi}}_j (\beta_E^{(k)} \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j^{(k)})$

  repeat

  • To update $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_p)$

   $\widetilde{X}_j \leftarrow \widetilde{\boldsymbol{\Psi}}_j (\beta_E^{(k)} \cdot \mathbf{1}_{m_j} + \boldsymbol{\theta}_j^{(k)})$ for $j = 1, \ldots, p$

   $R \leftarrow R^* + \sum_{j=1}^{p} \gamma_j^{(k)} \widetilde{X}_j$

$$\boldsymbol{\gamma}^{(k)(new)} \leftarrow \arg\min_{\boldsymbol{\gamma}} \frac{1}{2n} \left\| R - \sum_j \gamma_j \widetilde{X}_j \right\|_2^2 + \lambda\alpha \sum_j w_{jE} |\gamma_j|$$

   $\Delta = \sum_j (\gamma_j^{(k)} - \gamma_j^{(k)(new)}) \widetilde{X}_j$

   $R^* \leftarrow R^* + \Delta$

  • To update $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p)$

   $\widetilde{X}_j \leftarrow \boldsymbol{\Psi}_j + \gamma_j^{(k)} \widetilde{\boldsymbol{\Psi}}_j$ for $j = 1, \ldots, p$

   for $j = 1, \ldots, p$ **do**

    $R \leftarrow R^* + \widetilde{X}_j \boldsymbol{\theta}_j^{(k)}$

$$\boldsymbol{\theta}_j^{(k)(new)} \leftarrow \arg\min_{\boldsymbol{\theta}_j} \frac{1}{2n} \left\| R - \widetilde{X}_j \boldsymbol{\theta}_j \right\|_2^2 + \lambda(1-\alpha) w_j \|\theta_j\|_2$$

    $\Delta = \widetilde{X}_j (\boldsymbol{\theta}_j^{(k)} - \boldsymbol{\theta}_j^{(k)(new)})$

    $R^* \leftarrow R^* + \Delta$

  • To update β_E

   $\widetilde{X}_E \leftarrow X_E + \sum_j \gamma_j^{(k)} \widetilde{\boldsymbol{\Psi}}_j \mathbf{1}_{m_j}$

   $R \leftarrow R^* + \beta_E^{(k)} \widetilde{X}_E$

$$\beta_E^{(k)(new)} \leftarrow S\left(\frac{1}{n \cdot w_E} \widetilde{X}_E^{\top} R, \lambda(1-\alpha) \right)$$

▷ $S(x,t) = \text{sign}(x)(|x| - t)_+$

   $\Delta = (\beta_E^{(k)} - \beta_E^{(k)(new)}) \widetilde{X}_E$

   $R^* \leftarrow R^* + \Delta$

  • To update β_0

   $R \leftarrow R^* + \beta_0^{(k)}$

$$\beta_0^{(k)(new)} \leftarrow \frac{1}{n} R^* \cdot \mathbf{1}$$

   $\Delta = \beta_0^{(k)} - \beta_0^{(k)(new)}$

   $R^* \leftarrow R^* + \Delta$

  $k \leftarrow k + 1$

  until convergence criterion is satisfied: $\left\| \boldsymbol{\Theta}^{(k)} - \boldsymbol{\Theta}^{(k-1)} \right\|_2^2 < \epsilon$

4.4 Algorithm

5 Simulations

The covariates are simulated as follows. First, we generate $w_1, \ldots, w_p, u, v$ independently from a standard normal distribution truncated to the interval [0,1] for $i = 1, \ldots, n$. Then we set $x_j = (w_j + t \cdot u)/(1 + t)$ for $j = 1, \ldots, 4$ and $x_j = (w_j + t \cdot v)/(1 + t)$ for $j = 5, \ldots, p$, where the parameter t controls the amount of correlation among predictors. This leads to a compound symmetry correlation structure where $Corr(x_j, x_k) = t^2/(1 + t^2)$, for $1 \leq j \leq 4, 1 \leq k \leq 4$, and $Corr(x_j, x_k) = t^2/(1 + t^2)$, for $5 \leq j \leq p, 5 \leq k \leq p$, but the covariates of the nonzero and zero components are independent [13, 14]

We evaluate the performance of our method on three of its defining characteristics: 1) the strong heredity property, 2) non-linearity of predictor effects and 3) interactions.

1. **Hierarchy**

   (a) Truth obeys strong hierarchy.

   $$Y = \sum_{j=1}^{4} f_j(X_j) + \beta_E \cdot X_E + X_E \cdot f_3(X_3) + X_E \cdot f_4(X_4) + \varepsilon$$

   (b) Truth obeys weak hierarchy.

   $$Y = f_1(X_1) + f_2(X_2) + \beta_E \cdot X_E + X_E \cdot f_3(X_3) + X_E \cdot f_4(X_4) + \varepsilon$$

   (c) Truth only has interactions.

   $$Y = X_E \cdot f_3(X_3) + X_E \cdot f_4(X_4) + \varepsilon$$

2. **Non-linearity**

   (a) Truth is linear

$$Y = \sum_{j=1}^{4} \beta_j X_j + \beta_E \cdot X_E + X_E \cdot X_3 + X_E \cdot X_4 + \varepsilon$$

3. **Interactions**

   (a) Truth only has main effects

$$Y = \sum_{j=1}^{4} f_j(X_j) + \beta_E \cdot X_E + \varepsilon$$

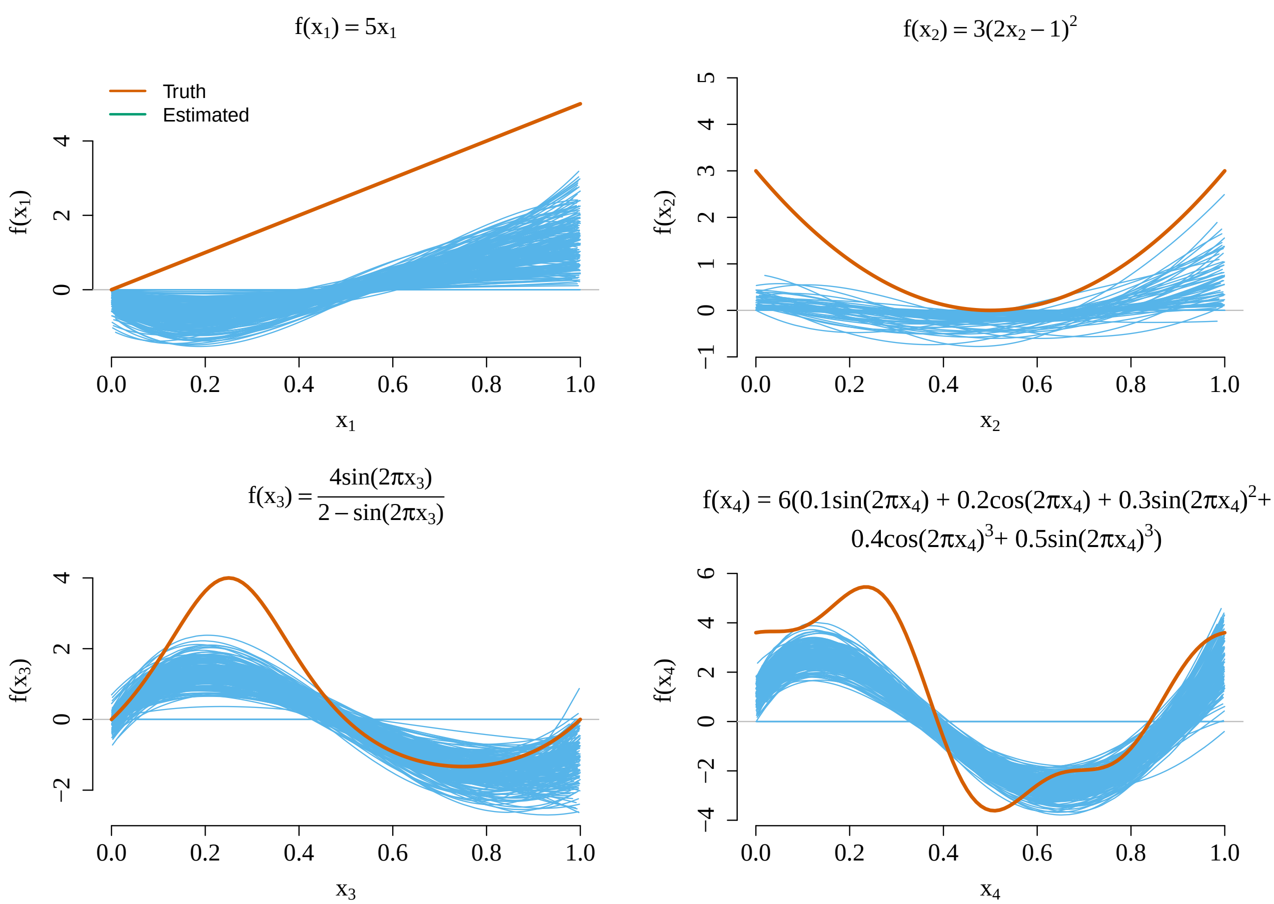

Figure 1: text

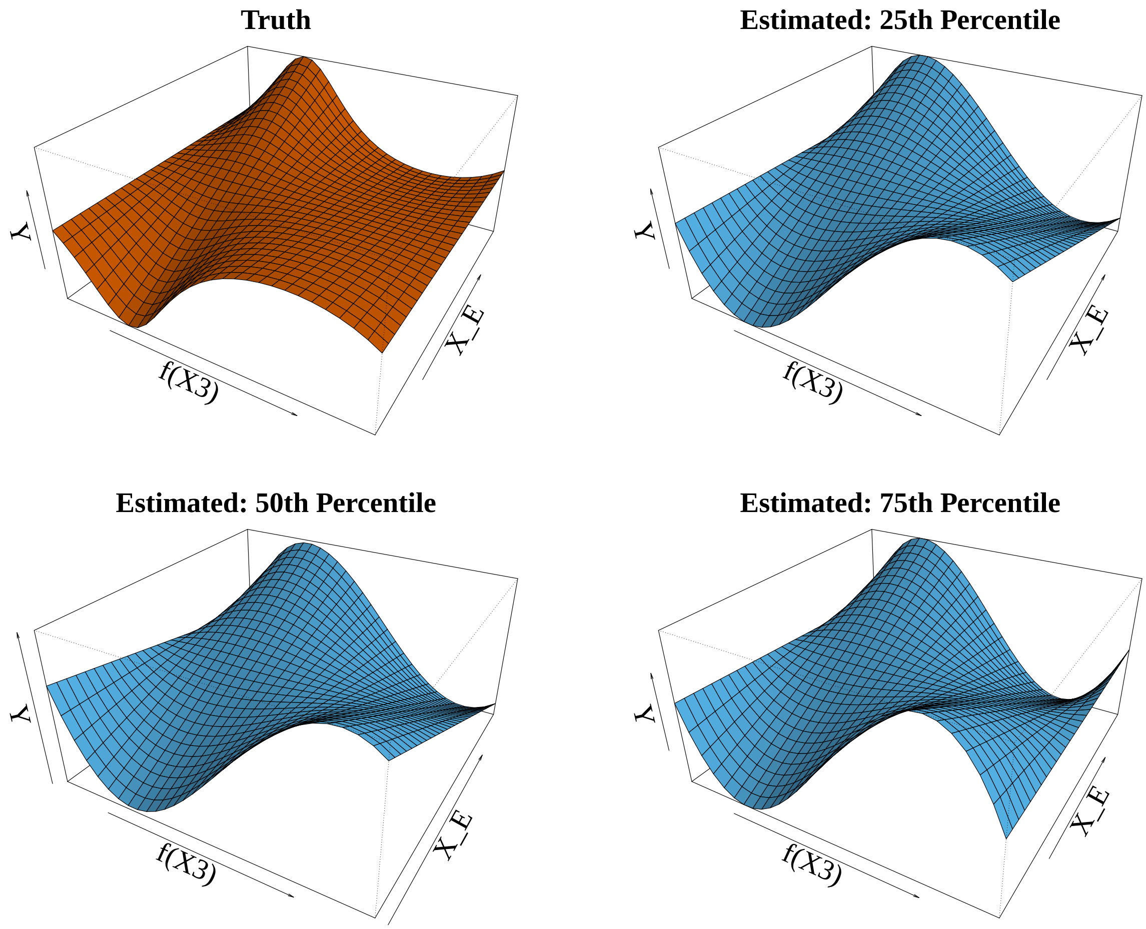

Figure 2: True and estimated interaction effects for $E \cdot f(X_3)$ in simulation scenario 1a).

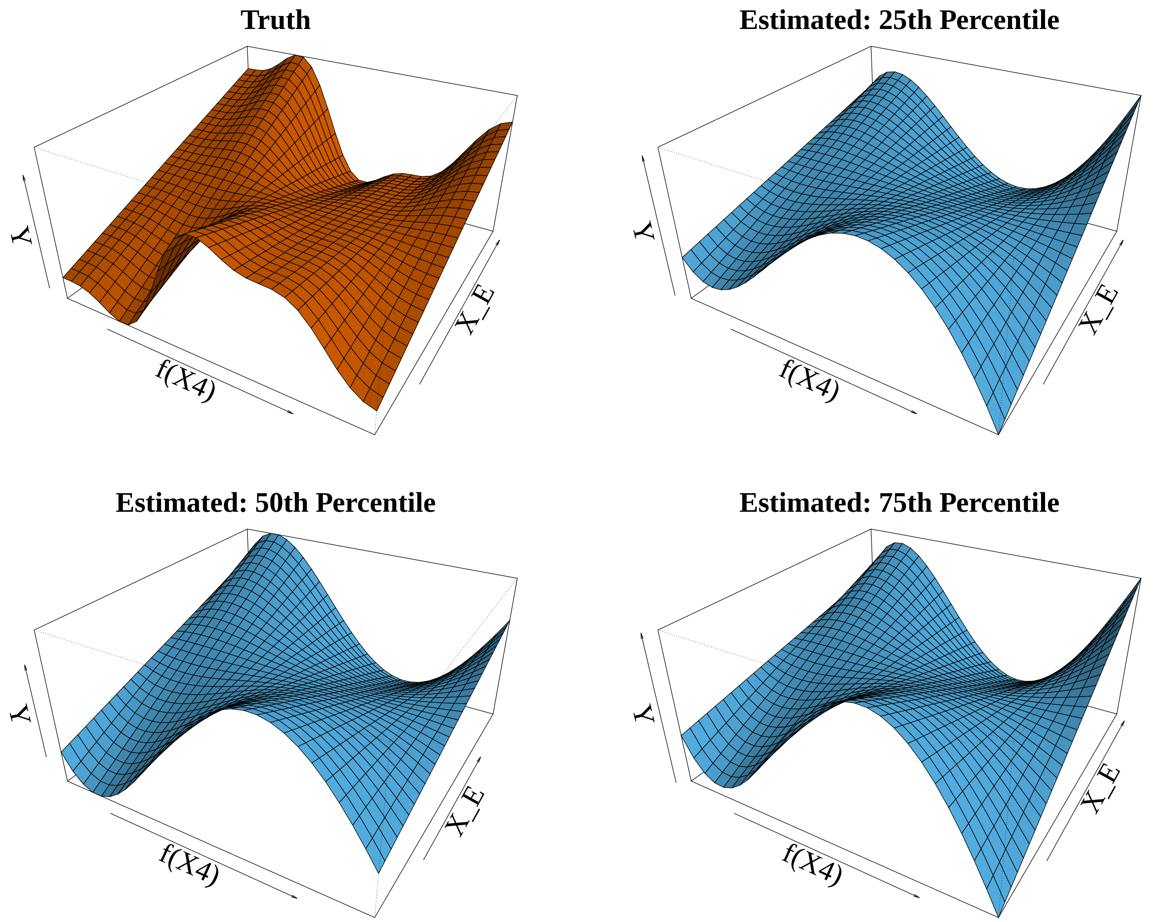

Figure 3: True and estimated interaction effects for $E \cdot f(X_4)$ in simulation scenario 1a).

6 Real Data Application

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