

Recap

Group Lasso: $\text{pen}(\beta) = \lambda \sum_{j=1}^q m_j \|\beta_{\mathcal{G}_j}\|_2$

The generalized Group Lasso penalty:

$$\text{pen}(\beta) = \lambda \sum_{j=1}^q m_j \sqrt{\beta_{\mathcal{G}_j}^T A_j \beta_{\mathcal{G}_j}}, \quad A_j \text{ positive definite}$$

important example: **groupwise prediction penalty**

$$\text{pen}(\beta) = \lambda \sum_{j=1}^q m_j \|\mathbf{X}_{\mathcal{G}_j} \beta_{\mathcal{G}_j}\|_2 = \lambda \sum_{j=1}^q m_j \sqrt{\beta_{\mathcal{G}_j}^T \mathbf{X}_{\mathcal{G}_j}^T \mathbf{X}_{\mathcal{G}_j} \beta_{\mathcal{G}_j}}$$

$\mathbf{X}_{\mathcal{G}_j}^T \mathbf{X}_{\mathcal{G}_j}$ typically positive definite for $|\mathcal{G}_j| < n$

- ▶ penalty is **invariant** under arbitrary reparameterizations (bijective mappings) within every group \mathcal{G}_j : important!
- ▶ when using an orthogonal parameterization such that $\mathbf{X}_{\mathcal{G}_j}^T \mathbf{X}_{\mathcal{G}_j} = I$: it is the standard Group Lasso

High-dimensional additive models

$$Y_i = \mu + \sum_{j=1}^p f_j^0(X_i^{(j)}) + \varepsilon_i \quad (i = 1, \dots, n; p \gg n)$$

$$f_j^0 : \mathbb{R} \rightarrow \mathbb{R} \text{ smooth, } \mathbb{E}[f_j^0(X_i^{(j)})] \equiv 0 \quad \forall j$$

aim: estimator such that either $\hat{f}_j(\cdot) \equiv 0$ or $\hat{f}_j(\cdot)$ is not the zero function

\leadsto Group Lasso type problem

for $p < n$: regularize w.r.t. smoothness

for $p \gg n$: need to additionally regularize w.r.t. sparsity

Basis expansion and Group Lasso

- ▶ basis functions
 $h_{j,k}(\cdot)$, $k = 1, \dots, K$ for every component $j = 1, \dots, p$
- ▶ $n \times K$ matrices

$$H_j : (H_j)_{ik} = h_{j,k}(X_i^{(j)})$$

- ▶ approximation

$$f_j^0(X_i^{(j)}) \approx \sum_{k=1}^K \beta_{j,k} h_{j,k}(X_i^{(j)})$$

$$(f_j^0(X_1^{(j)}), \dots, f_j^0(X_n^{(j)}))^T \approx H_j \beta_j, \quad \beta_j = (\beta_{j,1}, \dots, \beta_{j,K})^T$$

Group Lasso with groupwise prediction penalty (and assume $\mu = 0$):

$$\hat{\beta}_1, \dots, \hat{\beta}_p = \operatorname{argmin}_{\beta_1, \dots, \beta_p} \|Y - \sum_{j=1}^p \underbrace{H_j \beta_j}_{=: f_j}\|_2^2 + \lambda \sum_{j=1}^p \underbrace{\|H_j \beta_j\|_2 / \sqrt{n}}_{=:\|f_j\|_n}$$

Sparsity Smoothness (SpS) penalty

$$\hat{f}_1, \dots, \hat{f}_p = \operatorname{argmin}_{f_1, \dots, f_p \in \mathcal{F}} \left(\|Y - \sum_{j=1}^p f_j\|_n^2 + \lambda_1 \sum_{j=1}^p \|f_j\|_n + \lambda_2 \sum_{j=1}^p I(f_j) \right)$$

$$\|f_j\|_n^2 = n^{-1} \sum_{i=1}^n |f_j(X_i^{(j)})|^2, \quad I(f_j)^2 = \int f_j''(x)^2 dx$$

where \mathcal{F} = Sobolev space of functions that are continuously differentiable with square integrable second derivatives

$$\hat{f}_1, \dots, \hat{f}_p = \operatorname{argmin}_{f_1, \dots, f_p \in \mathcal{F}} \left(\|Y - \sum_{j=1}^p f_j\|_n^2 + \lambda_1 \sum_{j=1}^p \|f_j\|_n + \lambda_2 \sum_{j=1}^p I(f_j) \right)$$

is a parametric problem of dimension $d \approx 3pn$, parametrized by natural cubic splines with basis functions encoded in a matrix

$$H_{n \times d} = (H_1, \dots, H_p)^T$$

and integrated squared second derivatives encoded in a matrix

$$(W_j)_{k,l} = \int h''_{j,k}(x) h''_{j,l}(x) dx$$

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$$\hat{\beta} = \operatorname{argmin}_{\beta} \left(\|Y - H\beta\|_2^2/n + \lambda_1 \sum_{j=1}^p \sqrt{\beta_j^T H_j^T H_j \beta_j/n} + \lambda_2 \sum_{j=1}^p \sqrt{\beta_j^T W_j \beta_j} \right)$$