SpS penalty of group Lasso type

for easier computation: instead of

$$\text{SpS penalty} = \lambda_1 \sum_j \|f_j\|_n + \lambda_2 \sum_j I(fj)$$

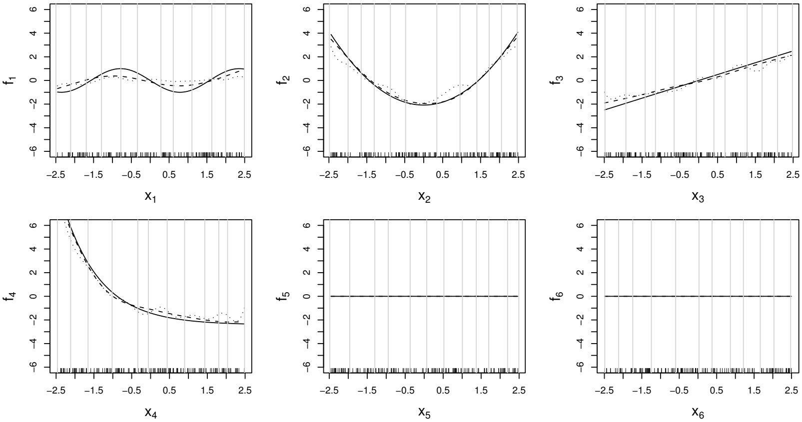
one can also use as an alternative:

$$\text{SpS Group Lasso penalty} = \lambda_1 \sum_j \sqrt{\|f_j\|_n^2 + \lambda_2^2 I^2(f_j)}$$

in parameterized form, the latter becomes:

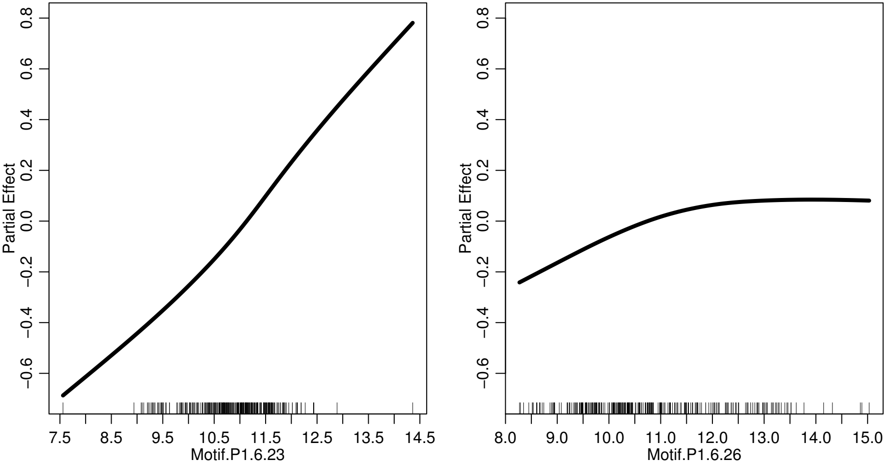
$$\lambda_1 \sum_{j=1}^{p} \sqrt{\|H_j\beta_j\|_2^2/n + \lambda_2^2 \beta_j^T W_j \beta_j} = \lambda_1 \sum_{j=1}^{p} \sqrt{\beta_j^T (H_j^T H_j/n + \lambda_2^2 W_j)\beta_j}$$

$\leadsto$ for every λ_2: a generalized Group Lasso penalty simulated example: $n = 150, p = 200$ and 4 active variables



dotted line: $\lambda_2 = 0$

$\rightsquigarrow \lambda_2$ seems not so important: just consider a few candidate values (solid and dashed line) motif regression: $n = 287, \ p = 195$



$\leadsto$ a linear model would be "fine as well"

Theoretical properties of high-dimensional additive models

- prediction and function estimation:
  compatibility-type assumption for the functions f_j^0
- screening property:
  beta-min analogue assumption for non-zero functions f_j^0

see Chapters 5.6 and 8.4 in Bühlmann and van de Geer (2011)

Conclusions

if the problem is sparse and smooth:
only a few $X^{(j)}$'s influence Y (only a few non-zero f_j^0) and the non-zero f_j^0 are smooth
$\leadsto$ one can often afford to model and fit additive functions in high dimensions

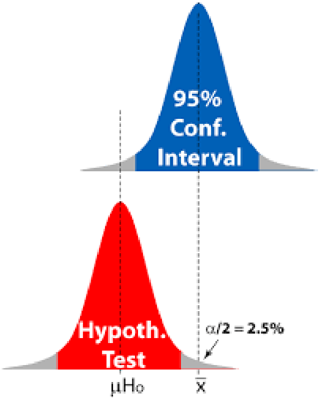
reason:

- dimensionality is of order $\mathrm{dim} = O(pn)$
  $\log(\mathrm{dim})/n = O((\log(p) + \log(n))/n)$ which is still small
- sparsity and smoothness then lead to: if each f_j^0 is twice continuously differentiable

$$\|\hat{f} - f^0\|_2^2/n = O_P(\underbrace{\text{sparsity}}_{\text{no. of non-zero } f_j^0} \sqrt{\log(p)}n^{-4/5})$$

(cf. Ch. 8.4 in Bühlmann & van de Geer (2011))

Uncertainty quantification:
p-values and confidence intervals (slides, denoted as Ch. 10)



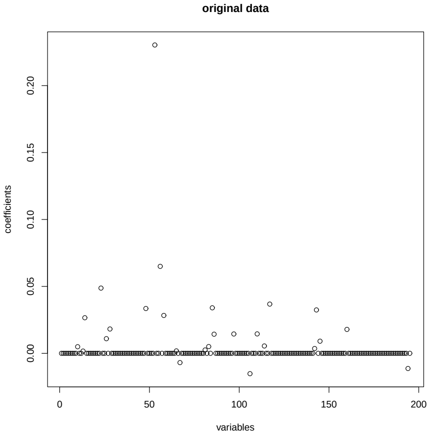
frequentist
uncertainty quantification

(in contrast to Bayesian inference)

classical concepts but in very high-dimensional settings

Toy example: Motif regression ($p = 195, n = 143$)

Lasso estimated coefficients $\hat{\beta}(\hat{\lambda}_{\mathrm{CV}})$



p-values/quantifying uncertainty would be very useful!

$$Y = X\beta^0 + \varepsilon \quad (p \gg n)$$

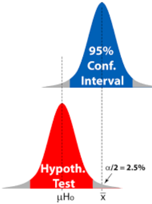
classical goal: statistical hypothesis testing

$$H_{0,j} : \beta_j^0 = 0 \text{ versus } H_{A,j} : \beta_j^0 \neq 0$$

or $$H_{0,G} : \beta_j^0 = 0 \; \forall \, j \in \underbrace{G}_{\subseteq\{1,\ldots,p\}} \quad \text{versus } H_{A,G} : \exists j \in G \text{ with } \beta_j^0 \neq 0$$

background: if we could handle the asymptotic distribution of the Lasso $\hat{\beta}(\lambda)$ under the null-hypothesis

$\leadsto$ could construct p-values



this is very difficult!
asymptotic distribution of $\hat{\beta}$ has some point mass at zero,...
Knight and Fu (2000) for $p < \infty$ and $n \to \infty$

because of “non-regularity” of sparse estimators
“point mass at zero” phenomenon $\rightsquigarrow$ “super-efficiency”


(Hodges, 1951)

$\rightsquigarrow$ standard bootstrapping and subsampling should not be used

$\rightsquigarrow$ de-sparsify/de-bias the Lasso instead

The de-sparsified or de-biased Lasso

Recap: if $p < n$ and $\mathrm{rank}(X) = p$, then:

$$\hat{\beta}_{\mathrm{OLS},j} = Y^T Z^{(j)}/(X^{(j)})^T Z^{(j)} \;\; (\underbrace{=}_{Z^{(j)}=X^{(j)}-\hat{X}^{(j)}} Y^T Z^{(j)}/\|Z^{(j)}\|_2^2)$$

$$Z^{(j)} = X^{(j)} - X^{(-j)}\hat{\gamma}^{(j)}$$

$$= \text{OLS residuals from } X^{(j)} \text{ vs. } X^{(-j)} = \{X^{(k)};\; k \neq j\}$$

$$\hat{\gamma}^{(j)} = \mathrm{argmin}_{\gamma}\|X^{(j)} - X^{(-j)}\gamma\|_2^2$$

that is: partial regression of Y onto residuals Z_j

idea for high-dimensional setting:
use the Lasso for the residuals $Z^{(j)}$

The de-sparsified Lasso

consider

$$\begin{aligned} Z^{(j)} &= X^{(j)} - X^{(-j)}\hat{\gamma}^{(j)} \\ &\quad = \text{Lasso residuals from } X^{(j)} \text{ vs. } X^{(-j)} = \{X^{(k)};\ k \neq j\} \\ \hat{\gamma}^{(j)} &= \text{argmin}_{\gamma}\|X^{(j)} - X^{(-j)}\gamma\|_2^2 + \lambda_j\|\gamma\|_1 \end{aligned}$$

build projection of Y onto $Z^{(j)}$:

$$\frac{Y^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} \underbrace{=}_{Y = X\beta^0 + \varepsilon} \beta_j^0 + \underbrace{\sum_{k \neq j} \frac{(X^{(k)})^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} \beta_k^0}_{\text{bias}} + \frac{\varepsilon^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}}$$

estimate bias and subtract it:

$$\widehat{\text{bias}} = \sum_{k \neq j} \frac{(X^{(k)})^T X^{(j)}}{(X^{(j)})^T Z^{(j)}} \underbrace{\hat{\beta}_k}_{\text{standard Lasso}}$$

$\leadsto$ de-sparsified Lasso estimator

$$\hat{b}_j = \frac{Y^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} - \sum_{k \neq j} \frac{(X^{(k)})^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} \hat{\beta}_k \quad (j = 1, \ldots, p)$$

not sparse! Never equal to zero for all $j = 1, \ldots, p$

can also be represented as (Exercise!)

$$\hat{b}_j = \underbrace{\hat{\beta}_j}_{\text{standard Lasso}} + \frac{(Y - X\hat{\beta})^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}}$$

name: “de-biased Lasso”

using that

$$\frac{Y^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} = \beta_j^0 + \sum_{k \neq j} \frac{(X^{(k)})^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} \beta_k^0 + \frac{\varepsilon^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}}$$

we obtain

$$\sqrt{n}(\hat{b}_j - \beta_j^0) = \underbrace{\sqrt{n} \sum_{k \neq j} \frac{(X^{(k)})^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} (\beta_k^0 - \hat{\beta}_k)}_{\sqrt{n} \cdot \text{ (bias term of de-biased Lasso)}} + \underbrace{\sqrt{n} \frac{\varepsilon^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}}}_{\text{fluctuation term}}$$

so far, this holds for any $Z^{(j)}$

assume fixed design X, e.g. condition on X
Gaussian error $\varepsilon \sim \mathcal{N}_n(0, \sigma^2 I)$

fluctuation term:

$$\sqrt{n}\frac{\varepsilon^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}} = \frac{n^{-1/2}\varepsilon^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}/n} \sim \mathcal{N}(0, \frac{\sigma^2 \|Z^{(j)}\|_2^2/n}{|(X^{(j)})^T Z^{(j)}/n|^2})$$

bias term of de-biased Lasso: we exploit two things

- $\|\hat{\beta} - \beta^0\|_1 = O_P(s_0\sqrt{\log(p)/n})$
- KKT condition for Lasso (on $X^{(j)}$ versus $X^{(-j)}$): $|(X^{(k)})^T Z^{(j)}/n| \le \lambda_j/2 \; \forall k \ne j$

therefore:

$$
\begin{aligned}
& \sqrt{n}\sum_{k\ne j}\frac{(X^{(k)})^T Z^{(j)}}{(X^{(j)})^T Z^{(j)}}(\beta_k^0 - \hat{\beta}_k) \\
= \;& \sqrt{n}\sum_{k\ne j}\frac{(X^{(k)})^T Z^{(j)}/n}{(X^{(j)})^T Z^{(j)}/n}(\beta_k^0 - \hat{\beta}_k) \\
\le \;& \sqrt{n}\max_{k\ne j}\left|\frac{(X^{(k)})^T Z^{(j)}/n}{(X^{(j)})^T Z^{(j)}/n}\right|\|\hat{\beta} - \beta^0\|_1 \\
\le \;& \sqrt{n}\frac{\lambda_j/2}{(X^{(j)})^T Z^{(j)}/n}O_P(s_0\sqrt{\log(p)/n}) \\
= \;& O_P(s_0\log(p)/\sqrt{n}) = o_P(1) \text{ if } s_0 \ll \frac{\sqrt{n}}{\log(p)}
\end{aligned}
$$

if $\lambda_j \asymp \sqrt{\log(p)/n}$ and $(X^{(j)})^T Z^{(j)}/n \asymp O(1)$

summarizing $\rightsquigarrow$
Theorem 10.1 in the notes
assume:

- $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$
- $\lambda_j = C_j \sqrt{\log(p)/n}$ and $\|Z^{(j)}\|_2^2/n \geq L > 0$
- $s_0 = o(\sqrt{n}/\log(p))$ (a bit sparser than "usual")
- $\|\hat{\beta} - \beta^0\|_1 = O_P(s_0 \sqrt{\log(p)/n})$
  (i.e., compatibility constant ϕ_o^2 bounded away from zero)

Then:

$$\sigma^{-1}\sqrt{n}\frac{(X^{(j)})^T Z^{(j)}/n}{\|Z^{(j)}\|_2/\sqrt{n}}(\hat{b}_j - \beta_j^0) \Longrightarrow \mathcal{N}(0,1) \quad (j = 1, \ldots, p)$$

more precisely:

$$\sigma^{-1}\sqrt{n}\frac{(X^{(j)})^T Z^{(j)}/n}{\|Z^{(j)}\|_2/\sqrt{n}}(\hat{b}_j - \beta_j^0) = W_j + \Delta_j$$

$$(W_1, \ldots, W_p)^T \sim \mathcal{N}_p(0, \sigma^2\Omega), \ \max_{j=1,\ldots,p} |\Delta_j| = o_P(1)$$

confidence intervals for β_j^0:

$$\hat{b}_j \pm \hat{\sigma} n^{-1/2} \frac{\|Z^{(j)}\|_2/\sqrt{n}}{|(X^{(j)})^T Z^{(j)}/n} \Phi^{-1}(1 - \alpha/2)$$

$\hat{\sigma}^2 = \|Y - X\hat{\beta}\|_2^2/n$ or $\hat{\sigma}^2 = \|Y - X\hat{\beta}\|_2^2/(n - \|\hat{\beta}\|_0^0)$

all is very easy!

can also test

$$H_{0,j}:\ \beta_j^0 = 0 \text{ versus } H_{A,j}:\ \beta_j^0 \neq 0$$

can also test group hypothesis: for $G \subseteq \{1, \ldots, p\}$

$$H_{0,G}:\ \beta_j^0 \equiv 0 \forall j \in G$$
$$H_{A,G}: \exists j \in G \text{ such that } \beta_j^0 \neq 0$$

under $H_{0,G}$:

$$\max_{j \in G} \sigma^{-1} \sqrt{n} \frac{|(X^{(j)})^T Z^{(j)}/n|}{\|Z^{(j)}\|_2/\sqrt{n}} |\hat{b}_j| = \max_{j \in G} |W_j + \Delta_j| \asymp \underbrace{\max_{j \in G} |W_j|}_{\text{distr. simulated}}$$

and plug-in $\hat{\sigma}$ for σ

Choice of tuning parameters

as usual: $\hat{\beta} = \hat{\beta}(\hat{\lambda}_{\mathrm{CV}})$; what is the role of λ_j?

$$\text{variance} = \sigma^2 n^{-1} \frac{\|Z^{(j)}\|_2^2/n}{|(X^{(j)})^T Z^{(j)}/n|^2} \asymp \sigma^2/\|Z^{(j)}\|_2^2$$

if $\lambda_j \searrow$ then $\|Z^{(j)}\|_2^2 \searrow$, i.e. large variance

error due to bias estimation is bounded by:

$$|\ldots| \leq \sqrt{n} \frac{\lambda_j/2}{|(X^{(j)})^T Z^{(j)}/n|} \|\hat{\beta} - \beta^0\|_1 \propto \lambda_j$$

assuming λ_j is not too small
if $\lambda_j \searrow$ (but not too small) then bias estimation error $\searrow$

$\leadsto$ inflate the variance a bit to have low error due to bias estimation: control type I error at the price of slightly decreasing power

How good is the de-biased Lasso?

asymptotic efficiency:
for the de-biased Lasso to "work" we require

- sparsity: $s_0 = o(\sqrt{n}/\log(p))$
  this cannot be beaten in a minimax sense
- compatibility condition for X

for optimality in terms of the lowest possible asymptotic variance achieving the "Cramer-Rao" lower bound:

- require in addition that $X^{(j)}$ versus $X^{(-j)}$ is sparse:
  $s_j \ll n/\log(p)$

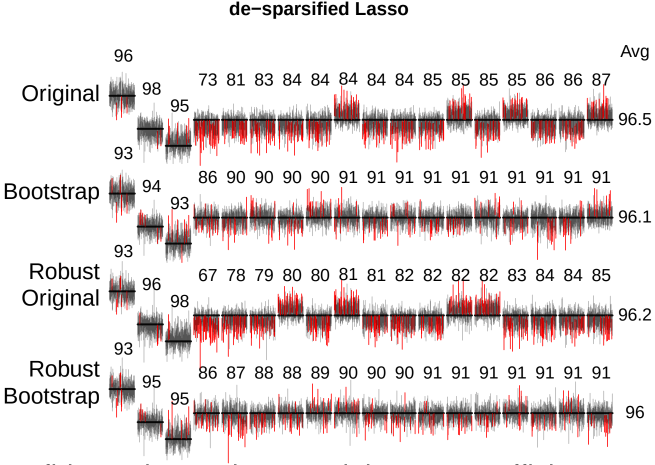
then... skipping details, the de-biased Lasso achieves (see Theorem 10.2):

$$\sqrt{n}(\hat{b}_j - \beta_j^0) \Longrightarrow \mathcal{N}(0, \underbrace{\sigma^2 \Theta_{jj}}_{\text{Cramer-Rao lower bound}})$$

$\Theta = \Sigma_X^{-1} = \mathrm{Cov}(X)^{-1} \rightsquigarrow$ as for OLS in low dimensions!

Empirical results

R-software `hdi` (Meier et al.)



black: confidence interval covered the true coefficient
red: confidence interval failed to cover