The de-biased Lasso: its Gaussian limiting distribution

$$\underbrace{\sigma^{-1}\sqrt{n}\frac{(X^{(j)})^{T}Z^{(j)}/n}{\|Z^{(j)}\|_{2}/\sqrt{n}}}_{\text{scaling factor}}(\hat{b}_{j} - \beta_{j}^{0}) = W_{j} + \Delta_{j}}_{(W_{1}, \dots, W_{p})^{T}} \sim \mathcal{N}_{p}(0, \Omega), \max_{j=1,\dots,p} |\Delta_{j}| = o_{P}(1)$$

confidence intervals for β_i^0 :

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

 $\hat{\sigma}^2 = \|Y - X\hat{\beta}\|_2^2/n \text{ or } \hat{\sigma}^2 = \|Y - X\hat{\beta}\|_2^2/(n - \|\hat{\beta}\|_0^0)$ 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 $G \subseteq \{1, \ldots, p\}$

$$egin{aligned} &\mathcal{H}_{0,G}:\ eta_j^0\equiv 0\ orall j\in G\ &\mathcal{H}_{A,G}:\exists j\in G ext{ such that }eta_j^0
eq 0 \end{aligned}$$

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

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

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

error due to bias estimation is bounded by:

$$|\ldots| \leq \sqrt{n} \frac{\lambda_j/2}{|(X^{(j)})^T Z^{(j)}/n|} \|\hat{\beta} - \beta^0\|_1 \propto \frac{\lambda_j}{\|Z^{(j)}\|_2^2/n}$$

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

 \rightsquigarrow 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 ≪ n/log(p)

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

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

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

Why the $1/\sqrt{n}$ convergence rate?

de-biased/de-sparsified Lasso is considering

▶ low-dimensional components $\{\beta_i^0; j \in A\}$ with |A| small

$$\sum_{j \in A} c_j \sqrt{n} (\hat{b}_j - \beta_j^0) \Rightarrow \mathcal{N}(0, \sum_{j,j' \in A} c_j c_{j'} V_{j,j'}), V = \lim_n n \operatorname{Cov}(\hat{b})$$

for large |A|: the sum would blow up the variance and the scaling with \sqrt{n} is not correct

• high-dimensional β^0 and ℓ_{∞} -norm:

$$\frac{\sqrt{n}\|\hat{b} - \beta^0\|_{\infty}}{\sim} \underbrace{\max(n, p, p)}_{\text{maximum of } p \text{ dependent Gaussian r.v.'s}}_{\text{maximum of } p \text{ dependent Gaussian r.v.'s}}_{\text{maximum of } p \text{ dependent Gaussian r.v.'s}}$$

 $\rightsquigarrow \sqrt{\log(p)/n}$ convergence rate

Multiple testing adjustment

if we test all hypotheses, for all j = 1, ..., p:

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

we have to adjust/correct for multiple testing different type I error measures: for multiple tests, one can control for:

FamilyWise Error Rate: FWER = P[V > 0], False Discovery Rate: $FDR = \mathbb{E}[V/R]$, V = number of false positives, R = number of rejections null-hyp. rejected although it is true

other measures exist: but these are the two most common ones

 input: raw p-values p_j for jth hypothesis test (e.g. from de-biased Lasso)

output: corrected p-values p_{corr,j}

reject $H_{0,j} \iff p_{\operatorname{corr},j} \leq \alpha$: then,

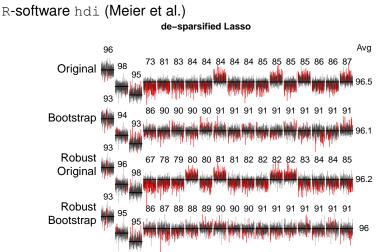
 $\mathsf{FWER} \leq \alpha \text{ or } \mathsf{FDR} \leq \alpha$

depending on the adjustment method

 for controlling FWER: Bonferroni-Holm procedure for controlling FDR: Benjamini-Hochberg procedure (which is only proven to be correct for independent hypotheses)

R-software: p.adjust or also package hdi has some more clever adjustment for dependent p-values from de-biased Lasso

Empirical results



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

Stability Selection (Ch. 10 in Bühlmann and van de Geer (2011))

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Stability selection

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[Read before The Royal Statistical Society at a meeting organized by the Research Section on Wednesday, February 3rd, 2010, Professor D. M. Titterington in the Chair]

has been developed before one knew about the de-biased/de-sparsified Lasso

even with new tools such as the de-biased/de-sparsified Lasso estimation of discrete structures ("relevant" variables in a generalized linear model; edges in a graphical model) is notoriously difficult

e.g. choice of tuning parameters ...?

i.i.d. data Z_1, \ldots, Z_n

main example: $Z_i = (X_i, Y_i)$ from regression or classification

\hat{S}_{λ} is a "feature selection" method/algorithm among $\{1, \dots, p\}$ features

can we assign "relevance" to the selected features in \hat{S}_{λ} ?

prime example: \hat{S}_{λ} from Lasso in linear model with *p* covariates

a "natural" approach: resampling! here: use subsampling:

- ▶ l^* random sub-sample of size $\lfloor n/2 \rfloor$ of $\{1, \ldots, n\}$
- compute $\hat{S}_{\lambda}(I^*)$
- repeat *B* times to obtain $\hat{S}_{\lambda}(I^{*1}), \ldots, \hat{S}_{\lambda}(I^{*B})$
- consider the "overlap" among $\hat{S}_{\lambda}(I^{*1}), \dots, \hat{S}_{\lambda}(I^{*B})$ regarding the latter, for example:

$$\hat{\Pi}_{\mathcal{K}}(\lambda) = \mathbb{P}^*[\mathcal{K} \subseteq \hat{S}_{\lambda}(I^*)] \approx B^{-1} \sum_{b=1}^{B} I(\mathcal{K} \subseteq \hat{S}_{\lambda}(I^{*b}))$$

e.g. $\hat{\Pi}_j(\lambda) \ (j \in \{1, \dots, p\})$

the probability \mathbb{P}^* is with respect to subsampling: a sum over $\binom{n}{m}$ terms, $m = \lfloor n/2 \rfloor$, i.e., all possible subsampling combinations

ightarrow it is approximated by *B* (pprox 500) times random subsampling

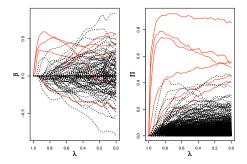
The stability regularization path

Riboflavin data: n = 115, p = 4088

Y: log-production rat of riboflavin by bacillus subtilis

X: gene expressions of bacillus subtilis

all X-variables permuted except 6 "a-priori relevant" genes



left: Lasso regularization path (red: the 6 non-permuted "relevant" genes) right: Stability path with $\hat{\Pi}_j$ on y-axis (red: the 6 non-permuted "relevant" variables stick out much more clearly from the noise covariates)

What is a good truncation value (for $\hat{\Pi}$)?

aim: choose π_{thr} such that

$$\hat{S}_{ ext{stable}} = \{j; \max_{\lambda \in \Lambda} \hat{\Pi}_j(\lambda) \geq \pi_{ ext{thr}} \}$$

has not too many false positives Λ can be a singleton or a range of values

as a measure for type I error control (against false positives):

$$V =$$
 number of false positives $= |\hat{S}_{\text{stable}} \cap S_0^c|$

where S_0 is the set of the true relevant features, e.g.:

- active variables in regression
- true edges in a graphical model

"the miracle":

a simple formula connecting π_{thr} with $\mathbb{E}[V]$

consider a setting with *p* possible features \hat{S}_{λ} is a feature selection algorithm $\hat{S}_{\Lambda} = \bigcup_{\lambda \in \Lambda} \hat{S}_{\lambda}$ $q_{\Lambda} = \mathbb{E}[\hat{S}_{\Lambda}(\underbrace{I}_{\text{random subsample}})]$

Theorem 10.1 Assume:

- exchangeability condition: $\{l(j \in \hat{S}_{\lambda}), j \in S_0^c\}$ is exchangeable for all $\lambda \in \Lambda$
- \hat{S} is not worse than random guessing

$$\frac{\mathbb{E}|\mathcal{S}_0 \cap \hat{\mathcal{S}}_{\Lambda}|)}{\mathbb{E}(|\mathcal{S}_0^c \cap \hat{\mathcal{S}}_{\Lambda}|)} \ \geq \ \frac{|\mathcal{S}_0|}{|\mathcal{S}_0^c|}.$$

Then, for $\pi_{\text{thr}} \in (1/2, 1)$:

$$\mathbb{E}[V] \quad \leq \quad rac{1}{2\pi_{ ext{thr}}-1} \; rac{q_{\Lambda}^2}{
ho}$$

suppose we know q_{Λ} (see later) strategy: specify $\mathbb{E}[V] = v_0$ (e.g. = 5) \sim for $\pi_{\text{thr}} := \frac{1}{2} + \frac{q_{\Lambda}^2}{2\rho v_0}$: $\mathbb{E}[V] \le v_0$ example: regression model with p = 1000 variables

 \hat{S}_{λ} = the top 10 variables from Lasso (e.g. the different λ from Lasso by CV and choose the top 10 variables with the largest absolute values of the corresponding estimated coefficients; if less than 10 variables are selected, take the selected variables) the value λ corresponds to the "top 10"; Λ is a singleton

we then know that $q_{\Lambda} = \mathbb{E}[|\hat{S}_{\lambda}(I)|] \leq 10$

For $\mathbb{E}[V] = v_0 := 5$ we then obtain

$$\pi_{\rm thr} = \frac{1}{2} + \frac{q_{\Lambda}^2}{2\rho v_0} = 0.5 + \frac{10^2}{2*1000*5} = 0.51$$

there is room to play around recommendation: take $|\hat{S}_{\lambda}|$ rather large and stability selection will reduce again to reasonable size

when taking the "top 30", the threshold becomes

$$\pi_{\rm thr} = \frac{1}{2} + \frac{q_{\Lambda}^2}{2\rho v_0} = 0.5 + \frac{30^2}{2*1000*5} = 0.59$$

adding noise... can always add (e.g. independent $\mathcal{N}(0, 1)$) noise covariates enlarged dimension p_{enlarged}

error control becomes better (for the same threshold)

$$\mathbb{E}[V] \leq \frac{1}{2\pi_{\rm thr}-1} \frac{q_{\Lambda}^2}{p_{\rm enlarged}}$$

this sometimes helps indeed in practice – at the cost of loss in power

The assumptions for mathematical guarantees

not worse than random guessing

$$rac{\mathbb{E}|S_0 \cap \hat{S}_{\Lambda}|)}{\mathbb{E}(|S_0^c \cap \hat{S}_{\Lambda}|)} \ \geq \ rac{|S_0|}{|S_0^c|}$$

perhaps hard to check but very reasonable...

for Lasso in linear models it holds assuming the variable screening property asymptotically: if beta-min and compatibility condition hold

exchangeability condition: $\{l(j \in \hat{S}_{\lambda}), j \in S_0^c\}$ is exchangeable for all $\lambda \in \Lambda$

a restrictive assumption but the theorem is very general, for any algorithm \hat{S}

a very special case where exchangeability condition holds: random equi-correlation design linear model

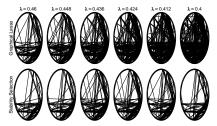
$$Y = X\beta^0 + \varepsilon$$
, $\operatorname{Cov}(X)_{i,j} \equiv \rho \ (i \neq j)$, $\operatorname{Var}(X_j) \equiv 1 \forall j$

distributions of $(Y, X^{(S_0)}, \{X^{(j)}; j \in S_0^c\})$ and of $(Y, X^{(S_0)}, \{X^{(\pi(j))}; j \in S_0^c\})$ are the same for any permutation $\pi : S_0^c \to S_0^c$

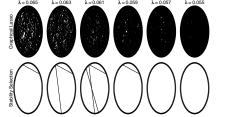
- distribution of X^(S₀), {X^{(π(j))}; j ∈ S₀^c} is the same for all π (because of equi-correlation)
- ► distribution of Y|X^(S₀), {X^{(π(j))}; j ∈ S^c₀} is the same for all π (because it depends only on X^(S₀))
- therefore: distribution of Y, X^(S₀), {X^{(π(j))}; j ∈ S₀^c} is the same for all π and hence exchangeability condition holds for any (measurable) function Ŝ_λ

An illustration for graphical modeling

p = 160 gene expressions, n = 115GLasso estimator, selecting among the $\binom{p}{2} = 12'720$ features stability selection with $\mathbb{E}[V] \le v_0 = 30$



with permutation (empty graph is correct)



Stability Selection is extremely easy to use and super-generic

the sufficient assumptions (far from necessary) for mathematical guarantees are restrictive but the method seems to work very well in practice