Data splitting for variable selection

Statistical Learning
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References

- Dezeure, Buhlmann, Meier, Meinshausen (2015). High dimensional inference: Confidence intervals, *p*-values and r-software `hdi`. Statistical Science, 533–558

High-dimensional inference

- Consider the gaussian linear model

$$y \sim N_n(1_n\beta_0 + X\beta, \sigma^2 I_n)$$

  with $n \times p$ design matrix X and $p \times 1$ vector of coefficients β
- When $p \geq n$, classical approaches for estimation and inference of β cannot be directly applied
- How to perform inference on β (e.g. confidence intervals and p-values for individual regression parameters β_j, $j = 1, \dots, p$) in a high-dimensional setting?

Support set

- The *support set* is

$$S = \{j \in \{1, \ldots, p\} : \beta_j \neq 0\}$$

  with cardinality $s = |S|$, and its complement is the *null set*, i.e.

$$N = \{j \in \{1, \ldots, p\} : \beta_j = 0\}$$

- Let $\hat{S} \subseteq \{1, \ldots, p\}$ be an estimator of S. Then

$$|\hat{S} \cap N|$$

  is the number of the wrong selections (type I errors) and

$$|S \setminus \hat{S}|$$

  is the number of wrong deselections (type II errors)

Error rates

- Define the *False Discovery Proportion* (FDP) by

$$\mathrm{FDP}(\hat{S}) = \frac{|\hat{S} \cap N|}{|\hat{S}|}$$

  with $\mathrm{FDP}(\emptyset) = 0$
- *FamilyWise Error Rate* (FWER)

$$\mathrm{P}(\mathrm{FDP}(\hat{S}) > 0) = \mathrm{P}(\hat{S} \cap N \neq \emptyset)$$

- *False Discovery Rate* (FDR)

$$\mathbb{E}(\mathrm{FDP}(\hat{S}))$$

Error control

- We would like to *control* the chosen error rate at level α, i.e.

$$P(\hat{S} \cap N \neq \emptyset) \leq \alpha \quad \text{or} \quad \mathbb{E}(\text{FDP}(\hat{S})) \leq \alpha$$

  while maximizing some notion of power e.g. the average power

$$\text{AvgPower} = \frac{\sum_{j \in S} P(\hat{S} \in j)}{|S|}$$

- We are dealing with the trade-off between type I and type II errors, and since FWER is more stringent than FDR, i.e.

$$\mathbb{E}(\text{FDP}(\hat{S})) \leq P(\hat{S} \cap N \neq \emptyset)$$

  methods that control FWER are less powerful

Simulate data as described in Section 3.1 of Hastie et al. (2020)

Given n (number of observations), p (problem dimensions), s (sparsity level), beta-type (pattern of sparsity), ρ (predictor autocorrelation level), and ν (signal-to-noise ratio (SNR) level)

1. we define coefficients $\beta \in \mathbb{R}^p$ according to s and the beta-type; e.g. beta-type 2: β has its first s components equal to 1, and the rest equal to 0
2. we draw the rows of the predictor matrix $X \in \mathbb{R}^{n \times p}$ i.i.d. from $N_p(0, \Sigma)$, where $\Sigma \in \mathbb{R}^{p \times p}$ has entry (i, j) equal to $\rho^{|i-j|}$ (Toeplitz matrix)
3. we draw the response vector $y \in \mathbb{R}^n$ from $N_n(X\beta, \sigma^2 I_n)$ with σ^2 defined to meet the desired SNR level, i.e. $\sigma^2 = \beta^t \Sigma \beta / \nu$

Lasso active set

Lasso with λ chosen by e.g. the 1-se rule

$$\hat{S} = \{j \in \{1, \ldots, p\} : \hat{\beta}_j \neq 0\}$$

Simulated data with $n = 200$, $p = 1000$, $s = 10$, $\rho = 0$, $\nu = 2.5$:

Size $\lvert\hat{S}\rvert$	# Type I $\lvert\hat{S} \cap N\rvert$	# Type II $\lvert S \setminus \hat{S}\rvert$	FDP $\lvert\hat{S} \cap N\rvert / \lvert\hat{S}\rvert$	Sensitivity $\lvert\hat{S} \cap S\rvert / \lvert S\rvert$
23	13	0	56.5%	100%

100 replications

	1	2	3	4	5	6	7
Size	23	20	13	25	23	21	11
# Type I	13	10	3	15	13	11	4
# Type II	0	0	0	0	0	0	3
FDP	0.57	0.50	0.23	0.60	0.57	0.52	0.36
Sensitivity	1	1	1	1	1	1	0.7

FWER = 99%, FDR = 54.2%, AvgPower = 99.6%

Naïve two-step procedure

1. Perform the lasso in order to obtain the active set

$$\hat{M} = \{j \in \{1, \ldots, p\} : \hat{\beta}_j \neq 0\}$$

2. Use least squares to fit the submodel containing just the variables in $\hat{M}$, i.e. linear regression of the $n \times 1$ response y on the reduced $n \times |\hat{M}|$ submatrix $X_{\hat{M}}$. Obtain

$$\hat{S} = \{j \in \hat{M} : p_j \leq \alpha\}$$

   where p_j is the p-value for testing the null hypothesis $H_j : \beta_j = 0$ in the linear model including only the selected variables

Simulation with $n = 200$, $p = 1000$, $s = 10$, $\rho = 0$, $\nu = 2.5$, $\alpha = 5\%$:

Size $\lvert\hat{S}\rvert$	# Type I $\lvert\hat{S} \cap N\rvert$	# Type II $\lvert S \setminus \hat{S}\rvert$	FDP $\lvert\hat{S} \cap N\rvert / \lvert\hat{S}\rvert$	Sensitivity $\lvert\hat{S} \cap S\rvert / \lvert S\rvert$
15	5	0	33.3%	100%

100 replications

	1	2	3	4	5	6	7
Size	15	18	12	17	18	17	11
# Type I	5	8	2	7	8	7	4
# Type II	0	0	0	0	0	0	3
FDP	0.33	0.44	0.17	0.41	0.44	0.41	0.36
Sensitivity	1	1	1	1	1	1	0.7

FWER = 99%, FDR = 42.1%, AvgPower = 99.6%

j	p_j	Selected
1	0.00	*
2	0.00	*
3	0.00	*
4	0.00	*
5	0.00	*
6	0.00	*
7	0.00	*
8	0.00	*
9	0.00	*
10	0.00	*
37	0.29	
53	0.06	
273	0.00	*
417	0.04	*
427	0.12	
525	0.04	*
577	0.24	
590	0.06	
636	0.16	
673	0.01	*
698	0.31	
721	0.12	
829	0.01	*

- The main problem with the naïve two-step procedure is that it peeks at the data twice: once to select the variables to include in $\hat{M}$, and then again to test hypotheses associated with those variables
- Here $\hat{M}$ is a random variable (it is a function of the data), but inference for linear model assumes it fixed (given a priori)
- A secondary problem is the multiplicity of the tests performed
- A simple idea is to use data-splitting to break up the dependence of variable selection and hypothesis testing (Cox, 1975)

Data-split

The *single-split* approach (Wasserman and Roeder, 2009) splits the data into two parts I and L of equal sizes $n_I = n_L = n/2$:

1. Use variable selection on the L portion (X^L, y^L) to obtain

$$\hat{M}^L \subseteq \{1, \ldots, p\}$$

2. Use the I portion (X^I, y^I) for constructing p-values

$$p_j = \begin{cases} p_j^I & \text{if } j \in \hat{M}^L \\ 1 & \text{if } j \notin \hat{M}^L \end{cases}$$

where p_j^I is the p-value testing $H_j : \beta_j = 0$ in the linear model including only the selected variables, i.e. based on the linear regression of the reduced $n_I \times 1$ response y^I on the reduced $n_I \times |\hat{M}^L|$ matrix $X^I_{\hat{M}^L}$

3. Adjust the p-values for their multiplicity $|\hat{M}^L|$, by e.g. Bonferroni

$$\tilde{p}_j = \min(|\hat{M}^L| \cdot p_j, 1), \quad j = 1, \dots, p$$

4. Selected variables

$$\tilde{S} = \{j \in \hat{M}^L : \tilde{p}_j \leq \alpha\}$$

j	p_j^L	p_j^I	$\tilde{p}_j^I$	Selected
1	0.00	0.08	1.00	
2	0.00	0.00	0.00	*
3	0.00	0.00	0.00	*
4	0.03	0.01	0.09	
6	0.00	0.00	0.00	*
8	0.00	0.00	0.01	*
9	0.16	0.00	0.00	*
10	0.00	0.00	0.00	*
37	0.03	0.38	1.00	
390	0.15	0.79	1.00	
398	0.01	0.21	1.00	
720	0.24	0.04	0.60	
721	0.02	0.82	1.00	
742	0.04	0.21	1.00	
824	0.02	0.24	1.00	
829	0.01	0.38	1.00	
943	0.15	0.66	1.00	

Theorem

Assume that

1. *the linear model* $y \sim N_n(1\beta_0 + X\beta, \sigma^2 I)$ *holds*
2. *the variable selection procedure satisfies the screening property for the first half of the sample, i.e.*

$$P(\hat{M}^L \supseteq S) \geq 1 - \delta$$

   for some $\delta \in (0, 1)$.

3. *The reduced design matrix for the second half of the sample satisfies* $\text{rank}(X^I_{\hat{M}^L}) = |\hat{M}^L|$.

Then the single-split procedure yields FWER control at α *against inclusion of null predictors up to the additional (small) value* δ, *i.e.*

$$P(\tilde{S} \cap N \neq \emptyset) \leq \alpha + \delta$$

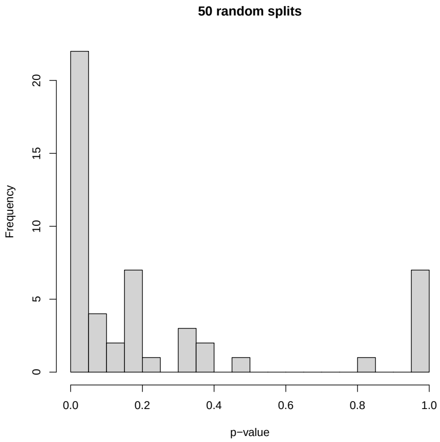
Proof.
Let $E = \{\hat{M}^L \supseteq S\}$ with $\mathrm{P}(E^c) \leq \delta$ by assumption. If E happens, then p_j^I is a valid p-value, i.e. $\mathrm{P}(p_j^I \leq u|E) \leq u$ for $j \in N \cap \hat{M}^L$. We have

$$\begin{aligned}
& \mathrm{P}(\tilde{S} \cap N \neq \emptyset) = \mathrm{P}(\bigcup_{j \in \hat{M}^L \cap N} \{\tilde{p}_j \leq \alpha\}) \\
= \;& \mathrm{P}(\bigcup_{j \in \hat{M}^L \cap N} \{\tilde{p}_j \leq \alpha\}|E)\mathrm{P}(E) + \mathrm{P}(\bigcup_{j \in \hat{M}^L \cap N} \{\tilde{p}_j \leq \alpha\}|E^c)\mathrm{P}(E^c) \\
\leq \;& \Big[\sum_{j \in \hat{M}^L \cap N} \mathrm{P}(p_j^I \leq \frac{\alpha}{|\hat{M}^L|}|E)\Big]\mathrm{P}(E) + \mathrm{P}(\bigcup_{j \in \hat{M}^L \cap N} \mathbb{1}\{\tilde{p}_j \leq \alpha\}|E^c)\mathrm{P}(E^c) \\
\leq \;& |\hat{M}^L \cap N|\frac{\alpha}{|\hat{M}^L|} \cdot 1 + 1 \cdot \delta \\
\leq \;& \alpha + \delta
\end{aligned}$$

□

P-value lottery

A major problem of the single data-splitting method is that different data splits lead to different *p*-values



Multi-split

The *multi-split* approach (Meinshausen et al., 2009)

1. For $b = 1, \ldots, B$
   apply the single-split procedure (L^b, I^b) to obtain

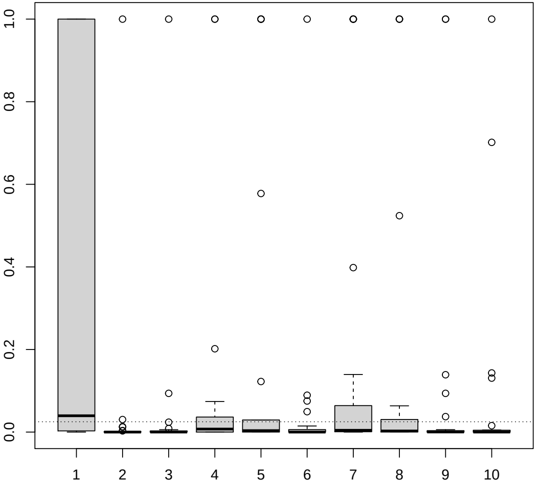
$$\{\tilde{p}_j^b, j = 1, \ldots, p\}$$

2. Aggregate the p-values as

$$\bar{p}_j = 2 \cdot \text{median}(\tilde{p}_j^1, \ldots, \tilde{p}_j^B), \quad j = 1, \ldots, p$$

3. Selected predictors:

$$\bar{S} = \{j \in \{1, \ldots, p\} : \bar{p}_j \leq \alpha\}$$



0.0
0.2
0.4
0.6
0.8
1.0
1
2
3
4
5
6
7
8
9
10

Simultaneous confidence intervals

$$\mathrm{P}(\beta_j \in [\hat{L}_j, \hat{U}_j] \ \forall j \in \{1, \ldots, p\}) \geq 1 - \alpha$$

j	$\hat{L}_j$	$\hat{U}_j$
1	-∞	∞
2	0.69	1.84
3	0.48	1.73
4	0.36	1.49
5	0.47	1.70
6	0.56	1.78
7	0.27	1.57
8	0.40	1.69
9	0.41	1.56
10	0.44	1.56
11	-∞	∞
...		