Variable selection with error control: Another look at Stability Selection

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What is Stability Selection?

Stability Selection (Meinshausen and Bühlmann, 2010) **is a very general technique designed to improve the performance of a variable selection algorithm.**

It is based on aggregating the results of applying a selection procedure to subsamples of the data.

A particularly attractive feature of Stability Selection is the error control provided by an upper bound on the expected number of falsely selected variables.

A general model for variable selection

Let $Z_1, \ldots, Z_n$ **be i.i.d. random vectors. We think of the indices** S **of some components of** Z_i **as being 'signal variables', and others** N **as being 'noise variables'.**

E.g. $Z_i = (X_i, Y_i)$, **with covariate** $X_i \in \mathbb{R}^p$, **response** $Y_i \in \mathbb{R}$ **and log-likelihood of the form**

$$\sum_{i=1}^{n} L(Y_i, X_i^T \beta),$$

with $\beta \in \mathbb{R}^p$. **Then** $S = \{k : \beta_k \neq 0\}$ **and** $N = \{k : \beta_k = 0\}$.

Thus $S \subseteq \{1, \ldots, p\}$ **and** $N = \{1, \ldots, p\} \setminus S$. **A *variable selection procedure* is a statistic** $\hat{S}_n := \hat{S}_n(Z_1, \ldots, Z_n)$ **taking values in the set of all subsets of** $\{1, \ldots, p\}$.

How does Stability Selection work?

For a subset $A = \{i_1, \ldots, i_{|A|}\} \subseteq \{1, \ldots, n\}$, **write**

$$\hat{S}(A) := \hat{S}_{|A|}(Z_{i_1}, \ldots, Z_{i_{|A|}}).$$

Meinshausen and Bühlmann defined

$$\hat{\Pi}(k) = \binom{n}{\lfloor n/2 \rfloor}^{-1} \sum_{\substack{A \subseteq \{1,\ldots,n\} \\ |A| = \lfloor n/2 \rfloor}} \mathbb{1}_{\{k \in \hat{S}(A)\}}.$$

Stability Selection fixes $\tau \in [0,1]$ **and selects** $\hat{S}^{\mathrm{SS}}_{n,\tau} = \{k : \hat{\Pi}(k) \geq \tau\}$.

Why subsets of size $\lfloor n/2 \rfloor$?

Both taking subsamples of size m and bootstrap (with-replacement) sampling are examples of exchangeably weighted bootstrap schemes (Mason and Newton, 1992; Præstgaard and Wellner, 1993).

The sum of the weights is n in both cases, and the variance of each component of the bootstrap weights is $\mathrm{Var}\,\mathrm{Bin}(n, 1/n) = 1 - 1/n \to 1$.

For subsampling, the variance of each component is $n/m - 1$, which converges to 1 iff $m/n \to 1/2$.

Error control

Meinshausen and Bühlmann (2010)

Assume that $\{\mathbb{1}_{\{k \in \hat{S}_{\lfloor n/2 \rfloor}\}} : k \in N\}$ is exchangeable, and that $\hat{S}_{\lfloor n/2 \rfloor}$ is not worse than random guessing:

$$\frac{\mathbb{E}(|\hat{S}_{\lfloor n/2 \rfloor} \cap S|)}{\mathbb{E}(|\hat{S}_{\lfloor n/2 \rfloor} \cap N|)} \geq \frac{|S|}{|N|}.$$

Then, for $\tau \in (\frac{1}{2}, 1]$,

$$\mathbb{E}(|\hat{S}^{\mathrm{SS}}_{n,\tau} \cap N|) \leq \frac{1}{2\tau - 1} \frac{(\mathbb{E}|\hat{S}_{\lfloor n/2 \rfloor}|)^2}{p}.$$

Error control discussion

In principle, this theorem helps the practitioner choose the tuning parameter τ. However:

- The theorem requires two conditions, and the exchangeability assumption is very strong
- There are too many subsets to evaluate $\hat{S}^{\mathrm{SS}}_{n,\tau}$ when $n \geq 20$
- The bound tends to be rather weak.

Complementary Pairs Stability Selection

Shah and S. (2013)

Let $\{(A_{2j-1}, A_{2j}) : j = 1, \ldots, B\}$ be randomly chosen independent pairs of subsets of $\{1, \ldots, n\}$ of size $\lfloor n/2 \rfloor$ such that $A_{2j-1} \cap A_{2j} = \emptyset$.

Define

$$\hat{\Pi}_B(k) := \frac{1}{2B} \sum_{j=1}^{2B} \mathbb{1}_{\{k \in \hat{S}(A_j)\}},$$

and select $\hat{S}^{\mathrm{CPSS}}_{n,\tau} = \{k : \hat{\Pi}_B(k) \geq \tau\}$.

Worst case error control bounds

Let $p_{k,n} = \mathbb{P}(k \in \hat{S}_n)$**. For** $\theta \in [0,1]$**, let** $L_\theta = \{k : p_{k,\lfloor n/2 \rfloor} \leq \theta\}$ **and** $H_\theta = \{k : p_{k,\lfloor n/2 \rfloor} > \theta\}$**.**

If $\tau \in (\frac{1}{2}, 1]$**, then**

$$\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau} \cap L_\theta| \leq \frac{\theta}{2\tau - 1}\mathbb{E}|\hat{S}_{\lfloor n/2 \rfloor} \cap L_\theta|.$$

Moreover, if $\tau \in [0, \frac{1}{2})$**, then**

$$\mathbb{E}|\hat{N}^{\mathrm{CPSS}}_{n,\tau} \cap H_\theta| \leq \frac{1-\theta}{1 - 2\tau}\mathbb{E}|\hat{N}_{\lfloor n/2 \rfloor} \cap H_\theta|.$$

Illustration and discussion

Suppose $p = 1000$**, and** $q := \mathbb{E}|\hat{S}_{\lfloor n/2 \rfloor}| = 50$**. Then on average, CPSS with** $\tau = 0.6$ **selects no more than a quarter of the variables that have below average selection probability under** $\hat{S}_{\lfloor n/2 \rfloor}$**.**

- **The theorem requires no exchangeability or random guessing conditions**
- **It holds even when** $B = 1$
- **If exchangeability and random guessing conditions do hold, then we recover**

$$\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau} \cap N| \leq \frac{1}{2\tau - 1}\Big(\frac{q}{p}\Big)\mathbb{E}|\hat{S}_{\lfloor n/2 \rfloor} \cap L_{q/p}| \leq \frac{1}{2\tau - 1}\Big(\frac{q^2}{p}\Big).$$

Proof

Let

$$\tilde{\Pi}_B(k) := \frac{1}{B}\sum_{j=1}^{B} \mathbb{1}_{\{k \in \hat{S}(A_{2j-1})\}}\mathbb{1}_{\{k \in \hat{S}(A_{2j})\}},$$

and note that $\mathbb{E}\{\tilde{\Pi}_B(k)\} = p^2_{k,\lfloor n/2 \rfloor}$**. Now**

$$0 \leq \frac{1}{B}\sum_{j=1}^{B}\big\{1 - \mathbb{1}_{\{k \in \hat{S}(A_{2j-1})\}}\big\}\big\{1 - \mathbb{1}_{\{k \in \hat{S}(A_{2j})\}}\big\} = 1 - 2\hat{\Pi}_B(k) + \tilde{\Pi}_B(k).$$

Thus

$$\mathbb{P}\{\hat{\Pi}_B(k) \geq \tau\} \leq \mathbb{P}\big\{\tfrac{1}{2}(1 + \tilde{\Pi}_B(k)) \geq \tau\big\} = \mathbb{P}\{\tilde{\Pi}_B(k) \geq 2\tau - 1\} \leq \frac{1}{2\tau - 1}p^2_{k,\lfloor n/2 \rfloor}.$$

Proof 2

Note that

$$\mathbb{E}|\hat{S}_{\lfloor n/2 \rfloor} \cap L_\theta| = \mathbb{E}\bigg(\sum_{k: p_{k,\lfloor n/2 \rfloor} \leq \theta} \mathbb{1}_{\{k \in \hat{S}_{\lfloor n/2 \rfloor}\}}\bigg) = \sum_{k: p_{k,\lfloor n/2 \rfloor} \leq \theta} p_{k,\lfloor n/2 \rfloor}.$$

It follows that

$$\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau} \cap L_\theta| = \mathbb{E}\bigg(\sum_{k: p_{k,\lfloor n/2 \rfloor} \leq \theta} \mathbb{1}_{\{k \in \hat{S}^{\mathrm{CPSS}}_{n,\tau}\}}\bigg) = \sum_{k: p_{k,\lfloor n/2 \rfloor} \leq \theta} \mathbb{P}(k \in \hat{S}^{\mathrm{CPSS}}_{n,\tau})$$
$$\leq \frac{1}{2\tau - 1}\sum_{k: p_{k,\lfloor n/2 \rfloor} \leq \theta} p^2_{k,\lfloor n/2 \rfloor} \leq \frac{\theta}{2\tau - 1}\mathbb{E}|\hat{S}_{\lfloor n/2 \rfloor} \cap L_\theta|.$$

Bounds with no assumptions whatsoever

If $Z_1, \ldots, Z_n$ **are not identically distributed, the same bound holds, provided in** L_θ **we redefine**

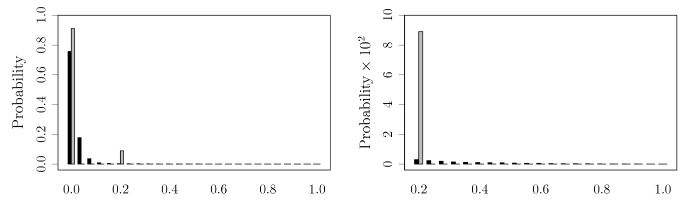
$$p_{k,\lfloor n/2 \rfloor} = \binom{n}{\lfloor n/2 \rfloor}^{-1} \sum_{|A|=n/2} \mathbb{P}\{k \in \hat{S}_{\lfloor n/2 \rfloor}(A)\}.$$

Similarly, if $Z_1, \ldots, Z_n$ **are not independent, the same bound holds, with** $p^2_{k,\lfloor n/2 \rfloor}$ **as the average of**

$$\mathbb{P}\{k \in \hat{S}_{\lfloor n/2 \rfloor}(A_1) \cap \hat{S}_{\lfloor n/2 \rfloor}(A_2)\}$$

over all complementary pairs A_1, A_2**.**

Can we improve on Markov's inequality?



Improved bound under unimodality

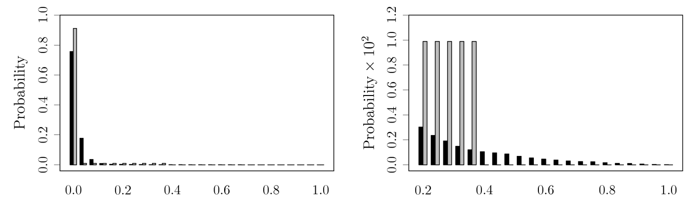
Suppose that the distribution of $\tilde{\Pi}_B(k)$ **is unimodal for each** $k \in L_\theta$**. If** $\tau \in \{\frac{1}{2} + \frac{1}{B}, \frac{1}{2} + \frac{3}{2B}, \frac{1}{2} + \frac{2}{B}, \ldots, 1\}$**, then**

$$\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau} \cap L_\theta| \leq C(\tau, B)\, \theta\, \mathbb{E}|\hat{S}_{\lfloor n/2 \rfloor} \cap L_\theta|,$$

where, when $\theta \leq 1/\sqrt{3}$**,**

$$C(\tau,B) = \begin{cases} \dfrac{1}{2(2\tau - 1 - 1/2B)} & \textbf{if } \tau \in (\min(\frac{1}{2} + \theta^2, \frac{1}{2} + \frac{1}{2B} + \frac{3}{4}\theta^2), \frac{3}{4}] \\ \dfrac{4(1 - \tau + 1/2B)}{1 + 1/B} & \textbf{if } \tau \in (\frac{3}{4}, 1]. \end{cases}$$

Extremal distribution under unimodality



The r-concavity constraint

r-concavity provides a continuum of constraints that interpolate between unimodality and log-concavity.

A non-negative function f on an interval $I \subset \mathbb{R}$ is r-***concave*** with $r < 0$ if for every $x, y \in I$ and $\lambda \in (0, 1)$,

$$f(\lambda x + (1-\lambda)y) \geq \{\lambda f(x)^r + (1-\lambda) f(y)^r\}^{1/r};$$

equivalently iff f^r is convex. A pmf f on $\{0, 1/B, \ldots, 1\}$ is r-concave if the linear interpolant to $\{(i, f(i/B)) : i = 0, 1, \ldots, B\}$ is r-concave. The constraint becomes weaker as r increases to 0.

Further improvements under r-concavity

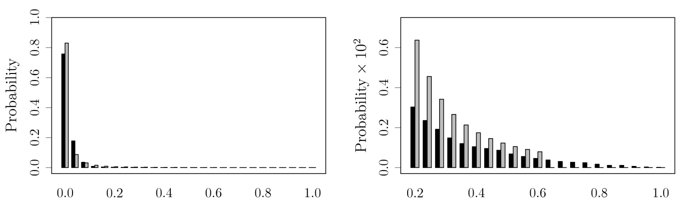
Suppose $\tilde{\Pi}_B(k)$ is r-concave for all $k \in L_\theta$. Then for $\tau \in (\frac{1}{2}, 1]$,

$$\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau} \cap L_\theta| \leq D(\theta^2, 2\tau - 1, B, r)|L_\theta|,$$

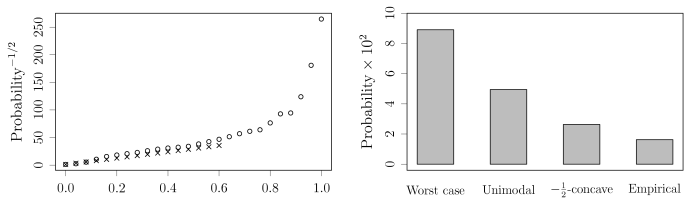
where D can be evaluated numerically.

Our simulations suggest $r = -1/2$ is a safe and sensible choice.

Extremal distribution under r-concavity



$r = -1/2$ is sensible



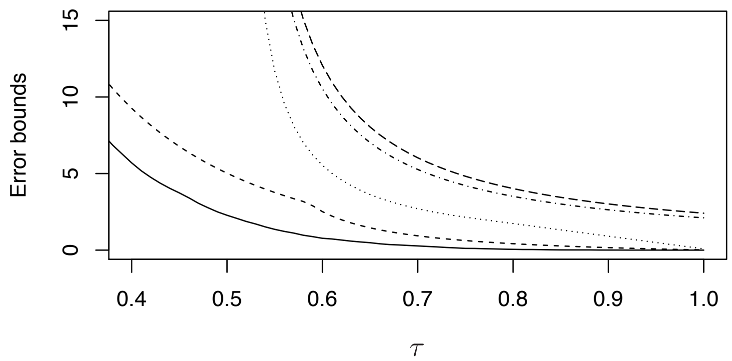
Reducing the threshold τ

Suppose $\tilde{\Pi}_B(k)$ is $-1/2$-concave for all $k \in L_\theta$, and that $\hat{\Pi}_B(k)$ is $-1/4$-concave for all $k \in L_\theta$. Then

$$\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau} \cap L_\theta| \leq \min\{D(\theta^2, 2\tau - 1, B, -1/2), D(\theta, \tau, 2B, -1/4)\}|L_\theta|,$$

for all $\tau \in (\theta, 1]$. (We take $D(\cdot, t, \cdot, \cdot) = 1$ for $t \leq 0$.)

Improved bounds



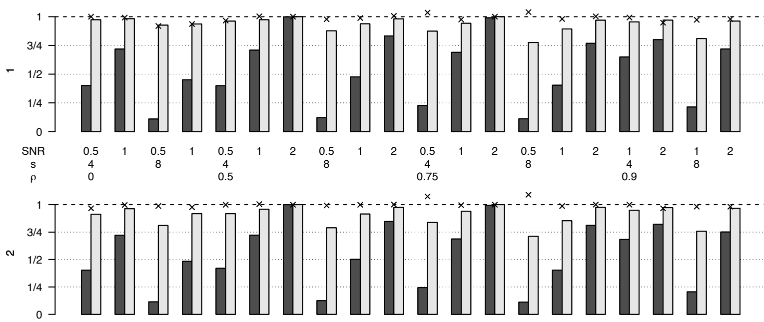
Simulation study

Linear model $Y_i = X_i^T \beta + \epsilon_i$ with $X_i \sim N_p(0, \Sigma)$. Take Σ Toeplitz with $\Sigma_{ij} = \rho^{||i-j|-p/2|-p/2}$. Let β have sparsity s, with $s/2$ equally spaced within $[-1, -0.5]$ and $s/2$ equally spaced in $[0.5, 1]$. Fix $n = 200$, $p = 1000$.

Use Lasso and seek $\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau} \cap L_{q/p}| \leq l$. Fix $q = \sqrt{0.8lp}$ and for worst-case bound choose $\tau = 0.9$. Choose $\tilde{\tau}$ from r-concave bound, oracle τ^*, and oracle λ^* for Lasso $\hat{S}_n^{\lambda^*}$. Compare

$$\frac{\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,0.9} \cap S|}{\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau^*} \cap S|}, \frac{\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tilde{\tau}} \cap S|}{\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau^*} \cap S|} \quad \textbf{and} \quad \frac{\mathbb{E}|\hat{S}_n^{\lambda^*} \cap S|}{\mathbb{E}|\hat{S}^{\mathrm{CPSS}}_{n,\tau^*} \cap S|}.$$

Simulation results



Summary

- CPSS can be used in conjunction with any variable selection procedure.
- We can bound the average number of low selection probability variables chosen by CPSS under no conditions on the model or original selection procedure
- Under mild conditions, e.g. r-concavity, the bounds can be strengthened, yielding tight error control.
- This allows the practitioner to choose the threshold τ in an effective way.

References

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