SLOPE-Adaptive variable selection via convex optimization

Guidelines in ML

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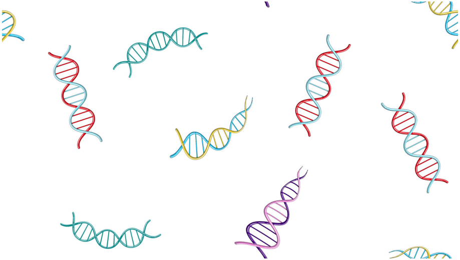
Motivations

Guarentees on variable selection

We aim to select variables based on their importance relative to the target variable, rather than solely for optimal prediction.



A common starting point for exploring relationships between covariates X and a target variable Y is the linear model:

$$\underbrace{Y}_{\text{cholesterol}} = \underbrace{X}_{\text{genes}} \beta + Z$$

where $Z \sim \mathcal{N}(0, \sigma^2 I_n)$ and $X \in \mathscr{M}_{n,p}(\mathbb{R})$ In our example we have p $\gg$ n.

Quick reminder

Common metrics

The challenge is to consider metrics and methods that enable us to achieve our goal of ensuring finite sample guarentees for the selected subsets of variables. Let $\mathscr{R}$ denote the set of rejected variables, and let $V(\mathscr{R}) = |\mathscr{R} \cap \mathscr{H}_0|$ represent the cardinality of the false positives set.

Common metrics	Methods
FWER, $\mathbb{P}(\lvert\mathscr{R} \cap \mathscr{H}_0\rvert \geq 1)$	Bonferroni, $\mathscr{R} = \{i; p_i \leq \frac{\alpha}{p}\}$
FDR, $\mathbb{E}\left[\frac{V(\mathscr{R})}{\lvert\mathscr{R}\rvert \vee 1}\right]$	Benjamini-Hochberg, $\mathscr{R} = \{i : p_i \leq \frac{\alpha \widehat{k}^{\mathrm{BH}}}{p}\}$, where $\widehat{k}^{\mathrm{BH}} = \max\left\{k \in [\![0, p]\!]; p_{(k)} \leq \frac{\alpha k}{p}\right\}$

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Methodology

Introduction: Lasso is commonly used for variable selection. In our study, we will explore variations of Lasso.

Lasso:

$$\min_{b\in\mathbb{R}^p} \frac{1}{2}\|Y - Xb\|_2^2 + \lambda\|b\|_1 \tag{1}$$

SLOPE:

$$\min_{b\in\mathbb{R}^p} \frac{1}{2}\|Y - Xb\|_2^2 + \sum_{i=1}^{p} \lambda_i |b|_{[i]}, \tag{2}$$

where $\lambda_1 \geq \ldots \geq \lambda_pand|b|_{[1]} \geq \ldots \geq |b|_{[p]}$.

Choosing λ sequence: How to select the λ sequence for metric control?

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where $\lambda_1 \geq \ldots \geq \lambda_pand|b|_{[1]} \geq \ldots \geq |b|_{[p]}$.

Choosing λ sequence: How to select the λ sequence for metric control?

Intuitions: Orthogonal design matrix

Asumption: $X^T X = I_p$, σ known.
Our problem: Recover relevant covariates from β, where:

$$Y = X\beta + Z, \quad \text{where } Z \sim \mathcal{N}(0, \sigma^2 I_n)$$

We can see it as a multiple testing problem.

$$\widetilde{Y} \stackrel{\text{def}}{=} X^\top Y = X^\top X\beta + X^\top Z = \beta + X^\top Z \sim \mathcal{N}(\beta, \sigma^2 I_p)$$

How to solve it ?

1. Bonferroni
2. BH

Bonferroni

$$\mathscr{R}_{\mathrm{Bonf}} = \left\{ i; \quad \check{p}_i = 2\left(1 - \Phi\left(\frac{|\widetilde{Y}_i|}{\sigma}\right)\right) < \frac{\alpha}{p} \right\}$$

$$\text{or equivalently } \left\{ i; \Phi^{-1}\left(1 - \frac{\alpha}{2p}\right) < \frac{|\widetilde{Y}_i|}{\sigma} \right\},$$

where α is the confidence level, and Φ is the cumulative distribution function of a standard Gaussian, with $\widetilde{Y} = X^\top Y$.
This reminds us of the Lasso thresholding with

$$\lambda_{\mathrm{Bonf}} = \sigma\Phi^{-1}\left(1 - \frac{\alpha}{2p}\right)$$

$$\widehat{k}^{\mathrm{BH}} = \max\left\{k \in [\![0,p]\!]; \check{p}_{(k)} \leq \frac{\alpha k}{p}\right\}$$
$$= \max\left\{k \in [\![0,p]\!]; \frac{|\widetilde{Y}_{[k]}|}{\sigma} \geq \Phi^{-1}\left(1 - \frac{k\alpha}{2p}\right)\right\}$$

We can apply the same reasoning as before with the Lasso-Bonf with λ_{BH} written as follows:

$$\lambda_{\mathrm{BH}}(i) = \left(\sigma\Phi^{-1}\left(1 - \frac{i\alpha}{2p}\right)\right), \quad 1 \leq i \leq p$$

Theoretical guarantees of SLOPE

Theorem 1 (SLOPE's FDR control)

Under the linear assumption, orthogonal X, $Z \sim \mathcal{N}(0, \sigma^2 I_n)$ with σ known, then SLOPE verifies $\mathrm{FDR} \leq \alpha p_0/p$.

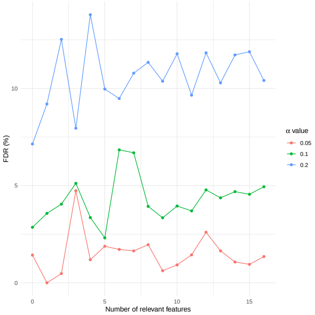

Figure 1: $n = 800, p = 800, \sigma^2 = 1, \alpha \in \{0.05, 0.1, 0.2\}$ and $|\mathcal{H}_1| \in [\![0;16]\!]$.

Relation with other methods

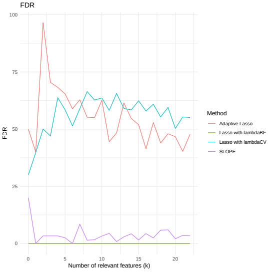

Figure 2: FDR

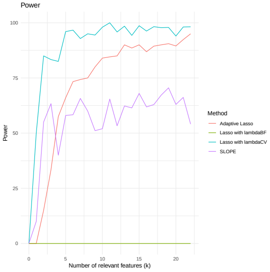

Figure 3: Power

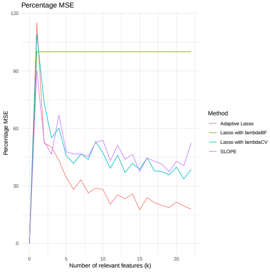

Figure 4: MSE

Figure 5: Different metrics to compare SLOPE, $\mathrm{Lasso} - \lambda_{\mathrm{Bonf}}$, $\mathrm{Lasso} - \lambda_{\mathrm{CV}}$ and $\mathrm{Adaptive} - \mathrm{Lasso}$ (with $\alpha = 0.1, n = p = 500, \sigma^2 = 1$).

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Intuitions to generalize SLOPE

⚠Shrinkage due to penalization.
Define $\eta_\lambda(t) = \mathrm{sign}(t)(|t| - \lambda)_+$ and assume that $X_j^\top X_j = 1$ and $\beta \geq 0$

1. Lasso optimality condition:

$$\widehat{\beta} = \eta_\lambda(\widehat{\beta} - X^\top(X\widehat{\beta} - Y)) = \eta_\lambda(\widehat{\beta} - X^\top X(\widehat{\beta} - \beta) + X^\top z).$$

2. Define $v_i := \langle X_i, \sum_{i \neq j} X_j(\beta_j - \widehat{\beta}_j)\rangle$ so that $\widehat{\beta}_i = \eta_\lambda(\beta_i + X_i^\top z + v_i)$.
💡Estimate v_i to iteratively adapt the penalization sequence.

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Intuitions to generalize SLOPE

3. KKT conditions on the Lasso give $X_{\mathscr{S}}^{\top}(Y - X\widehat{\beta}_{\mathscr{S}}) = \lambda 1_{\mathscr{S}}$, or equivalently, $\widehat{\beta}_{\mathscr{S}} = (X_{\mathscr{S}}^{\top}X_{\mathscr{S}})^{-1}(X_{\mathscr{S}}^{\top}Y - \lambda 1_{\mathscr{S}})$
4. Adapting it to SLOPE: $\widehat{\beta}_{\mathscr{S}} = (X_{\mathscr{S}}^{\top}X_{\mathscr{S}})^{-1}(X_{\mathscr{S}}^{\top}Y - \lambda_{\mathscr{S}})$
5. $\mathbb{E}[\beta_{\mathscr{S}} - \widehat{\beta}_{\mathscr{S}}] \approx (X_{\mathscr{S}}^{\top}X_{\mathscr{S}})^{-1}\lambda_{\mathscr{S}}$, i.e. $\mathbb{E}[X_i^{\top}X_{\mathscr{S}}(\beta_{\mathscr{S}} - \widehat{\beta}_{\mathscr{S}})] \approx X_i^{\top}X_{\mathscr{S}}(X_{\mathscr{S}}^{\top}X_{\mathscr{S}})^{-1}\lambda_{\mathscr{S}}$

Finally, if $X \sim \mathscr{N}(0, 1/n)$, we obtain that $\mathbb{E}[(X_i^{\top}X_{\mathscr{S}}(X_{\mathscr{S}}^{\top}X_{\mathscr{S}})^{-1}\lambda_{\mathscr{S}})^2] = \lambda_{\mathscr{S}}^{\top}\mathbb{E}[(X_{\mathscr{S}}^{\top}X_{\mathscr{S}})^{-1}]\lambda_{\mathscr{S}}/n = w(|\mathscr{S}|)\|\lambda_{\mathscr{S}}\|_2^2$ where $w(k) = 1/(n-k-1)$.

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SLOPE with $\lambda_{G^\star}$

1. $\lambda_G(1) = \lambda_{BH}(1)$
2. $\lambda_G(2) = \lambda_{BH}(2)\sqrt{1 + w(1)\lambda_G(1)^2}$
3. $\lambda_G(i) = \lambda_{BH}(i)\sqrt{1 + w(i-1)\sum_{j<i}\lambda_G(j)^2}$

⚠ λ must be decreasing to guarantee convexity of the problem, then if there exist $i_0 \in \{0, \dots, p-1\}$ such that $\lambda_G(i_0) < \lambda_G(i_0+1)$, fix the rest the sequence to $\lambda_G(i_0)$, which gives $\lambda_{G^\star}$.

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Is SLOPE better than BH?

Assume $y \sim \mathcal{N}(\mu, \Sigma)$ with Σ *almost* diagonal, $\Sigma_{i,j} \geq 0$ and known.

Goal:

What are the relevant covariates?(i.e. $\{i \in \{1, \dots p\}; \mu_i \neq 0\}$

- **BH:** Order $|y|_{[1]} \geq \dots \geq |y|_{[p]}$ and then SU with $\tau(i) = (\sigma\Phi^{-1}(1 - i\alpha/2p))_i$.
- **SLOPE:** $\underbrace{\tilde{y}}_{\text{Label}} = \Sigma^{-1/2} y = \underbrace{\Sigma^{-1/2}}_{\text{Design}} \mu + \varepsilon$, with $\varepsilon \sim \mathcal{N}(0, I_p)$ with $\lambda_{\mathrm{G}*}$.

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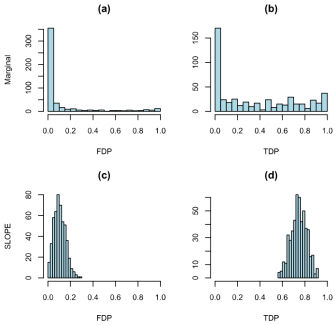

Figure 6: (From [Bogdan et al.(2015a)])The FDP of BH is either 0 or uniformly concentrated on $[0, 1]$, thus the discoveries are not trustworthy. ($\alpha = 0.1$)

Open question:

Can we get guarantees on the FDP instead of on the FDR for SLOPE?

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Conclusions and Perspectives

- ✓ Tractable convex optimization problem.
- ✓ Adaptability of BH.
- ✓ Control of the FDR(under strong assumptions).
- **?** Control of the FDP instead of just FDR?
- **?** SLOPE with $\lambda_{\mathrm{G}^\star}$, is it that general?
- × Reproducibility of the experiments from the article.

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Online Appendix containing proofs of some technical results discussed in the text.

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Thank You, Questions?

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Article figures: FDR not controlled by SLOPE-BH

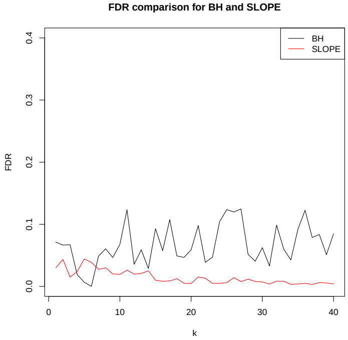

Figure 7: FDR controlled for the experience of BH vs SLOPE. However, SLOPE looks too restrictive...

Article figures: FDR not controlled by SLOPE-BH

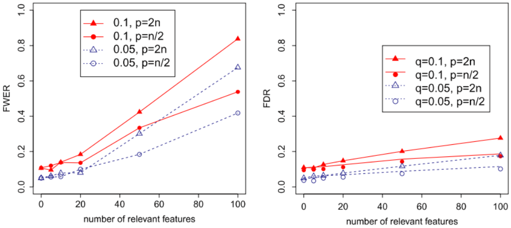

Figure 8: (From [Bogdan et al.(2015a)]) On the left FWER for Lasso-λ_{Bonf} and on the right the FDR for SLOPE with λ_{BH} under Gaussian correlated design.

Article figures: Relation with other methods

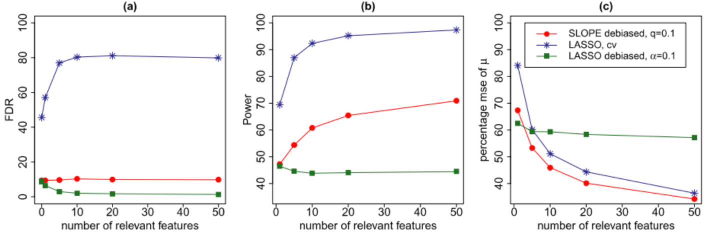

Figure 9: (From [Bogdan et al.(2015a)])SLOPE-$\lambda_{G^\star}$ vs Lasso-λ_{CV} and Lasso-λ_{Bonf} with design entries i.i.d. $\mathcal{N}(0,1/n)$, $n = p = 5000, \sigma^2 = 1$ and non zeros coefficients of the order of $2\sqrt{\log p}$.

Article figures: BH vs SLOPE

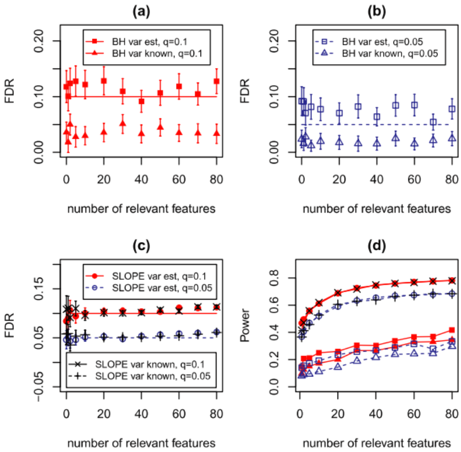

Figure 10: (From [Bogdan et al.(2015a)])Experiences to compare SLOPE-$\lambda_{G^\star}$ with BH procedure, with either known or unknown variance.