Regularization methods in multiple regression

March 21, 2024

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$X_{n \times p}$ - matrix of regressors

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$$-X'Y + (X'X + \gamma I)b = 0 \quad \Leftrightarrow \quad b = (X'X + \gamma I)^{-1} X'Y$$

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$$Tr[M] = \sum_{i=1}^{n} \lambda_i(M), \quad \text{where} \quad \lambda_1(M), \ldots, \lambda_n(M) \quad \text{are eigenvalues of} \quad M$$

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$$\hat{P}E = RSS + 2\sigma^2 \sum_{i=1}^{n} \frac{\lambda_i(X'X)}{\lambda_i(X'X) + \gamma}$$

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$$E||\hat{\beta} - \beta||^2 = \frac{\gamma^2}{(1+\gamma)^2}||\beta||^2 + \frac{p\sigma^2}{(1+\gamma)^2}$$

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$$\gamma < \frac{2p\sigma^2}{||\beta||^2 - p\sigma^2}$$

Basis Pursuit

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BP can recover β if it is *identifiable* with respect to L_1 norm, i.e.

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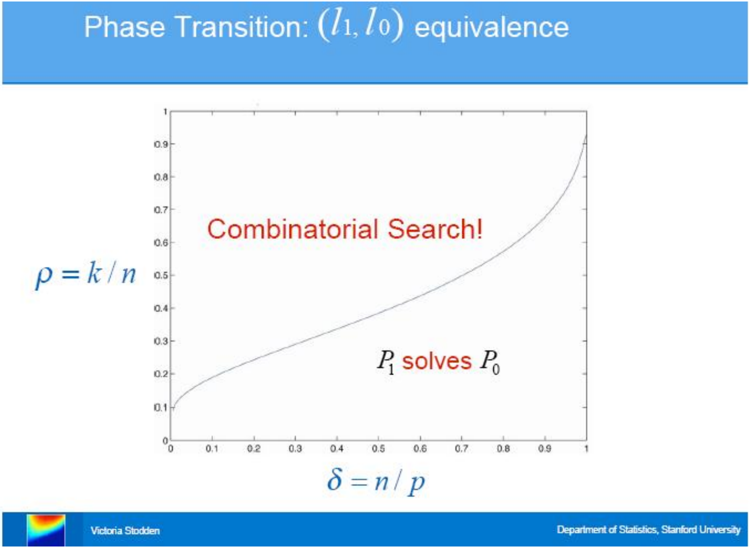
Basis Pursuit can recover β if k is small enough.

Transition curve (Donoho and Tanner, 2005)

Let's assume than $p \to \infty$, $n/p \to \delta$ and $k/n \to \epsilon$.

If X_{ij} are iid $N(0, \tau^2)$ then the probability that BP recovers β converges to 1 if $\epsilon < \rho(\delta)$ and to 0 if $\epsilon > \rho(\delta)$, where $\rho(\delta)$ is the *transition curve*.

Transition curve (2)



Noisy case - multiple regression

$$Y_{n\times 1} = X_{n\times p}\beta_{p\times 1} + z_{n\times 1}, \quad z \sim N(0, \sigma I)$$

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Convex program: Minimize $||b||_1$ subject to $||Y - Xb||_2^2 \leq \epsilon$

Or alternatively: $\min_{b\in R^p} \frac{1}{2}||y - Xb||_2^2 + \lambda||b||_1$

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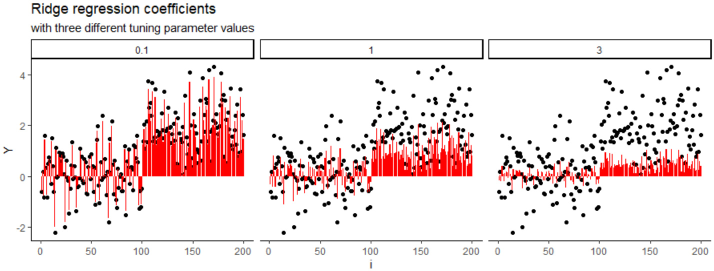
BPDN (Chen and Donoho, 1994) or LASSO (Tibshirani, 1996)

Solution to orthogonal design, ridge

- The Solution for ridge is given by

$$\hat{\beta}_i^{ridge} = \frac{y_i}{1+\lambda} = \frac{\hat{\beta}_i^{LS}}{1+\lambda}.$$

  - Leads to a shrinkage by a factor $\frac{1}{1+\lambda}$ of the coefficients.

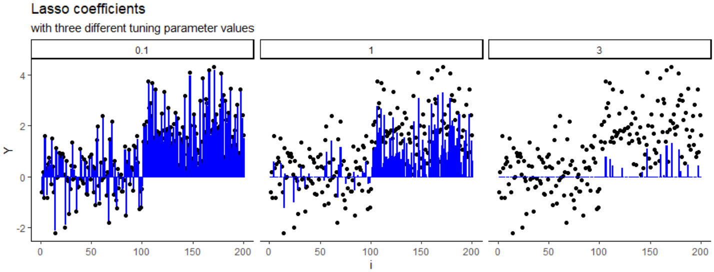


Solution to orthogonal design, lasso

- The Solution for lasso is given by

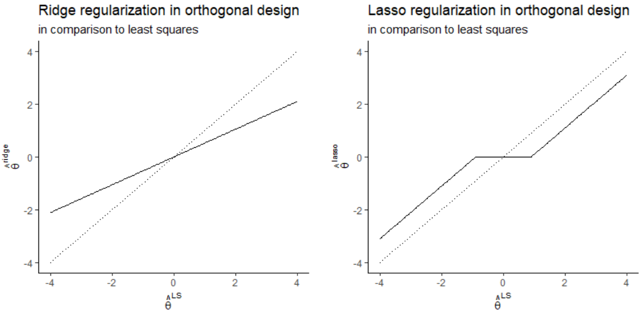
$$\hat{\beta}_i^{lasso} = sign(y_i)\left(|y_i| - \lambda\right)_+ = sign(\hat{\beta}_i^{LS})\left(|\hat{\beta}_i^{LS}| - \lambda\right)_+$$

  - Set small values to exactly zero (sparse solution)
  - Fixed shrinkage of λ for non-zero coefficients.



Solution to orthogonal design, joint

- Common representation: Plot relation between $\hat{\beta}^{LS}$ and $\hat{\beta}^{ridge}$ / $\hat{\beta}^{lasso}$



Selection of the tuning parameter for LASSO

- General rule: the reduction of λ_L results in identification of more elements from the true support (true discoveries) but at the same time it produces more falsely identified variables (false discoveries)
- The choice of λ_L is challenging- e.g. crossvalidation typically leads to many false discoveries
- When $X^T X = I$ Lasso selects X_j iff $|\hat{\beta}_j^{LS}| > \lambda$
- Selection $\lambda = \sigma \Phi^{-1}(1 - \alpha/(2p)) \approx \sigma\sqrt{2 \log p}$ corresponds to Bonferroni correction and controls FWER.

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  - X_i- samples were scanned with a microarray, that measures the expression of 10000s of genes simultaneously.
  - y_i- time for severe breast cancer to metastasize.
  - The goal is to identify patients with poor prognosis in order to administer more aggressive follow-up treatment for them.

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  - $y_i -$ time for severe breast cancer to metastasize.
  - The goal is to identify patients with poor prognosis in order to administer more aggressive follow-up treatment for them.
- Two typical genetic "models"
  - quantitative trait loci (QTL) a single or few important gene.
  - Polygene: many genes with small individual effect.

Which model is lasso which model is ridge?

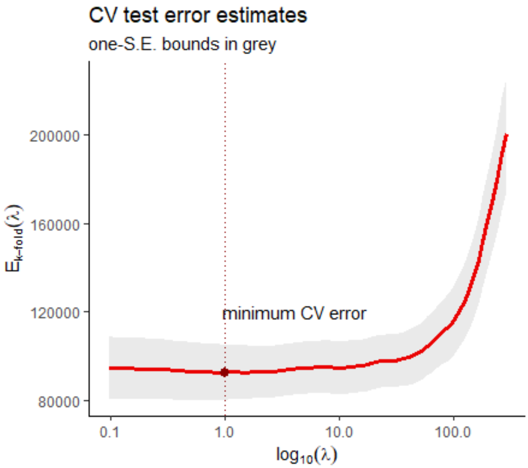
$p >> n$

https://www.mv.helsinki.fi/home/mjxpirin/HDS$_{c}ourse/material/vantveer.txt$
D = read.table("vantveer.txt", header = T)
print(dim(D))
X = as.matrix(D[,2:ncol(D)])
y = D$Months

```
## [1]    98 24189
```

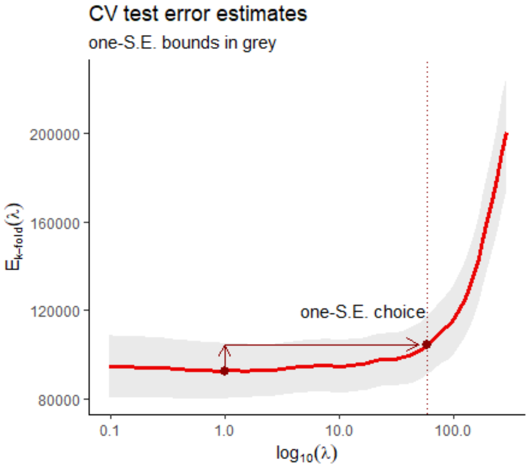
Choosing the regularization parameter

- Cross-validation for choosing λ.
- Often the cross validated error is often flat
- Prediction favours more parameters



Choosing the regularization parameter II

- A solution is instead choose a more regularized solution that have similar error.
- "similar" = within one S.E.

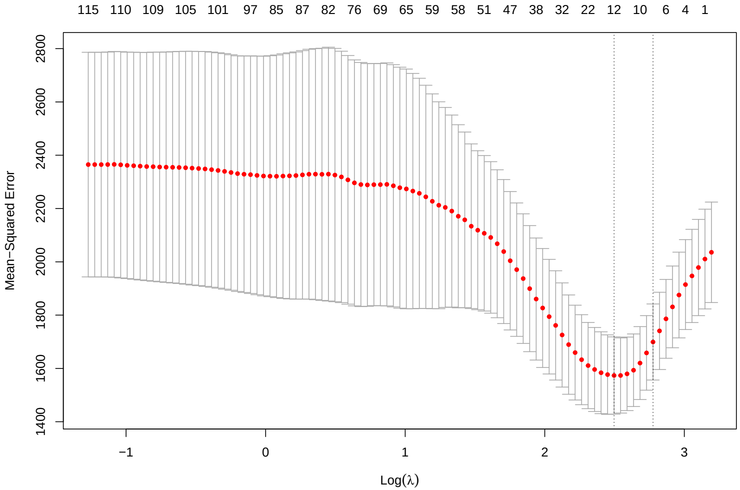


Choosing the regularization parameter (R)

- Go to package in R **glmnet** for both lasso and ridge.
- Need to find λ, use k-fold cross-validation.

[] library(glmnet) cvfit <- cv.glmnet(X, y, alpha=1, nfolds = 10, intercept = T, standardize = T)
plot(cvfit)

fit λ II (lasso)



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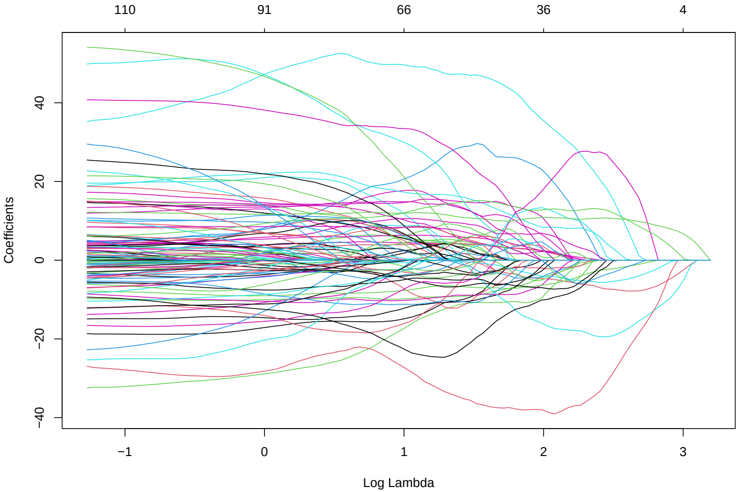
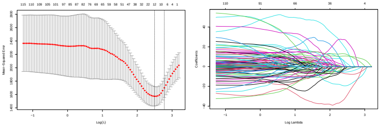


Under the hood

- For each cross validation sample on solves an entire path $\lambda \in \{100, 10, 1, 0.1..., \}$
- Recall that $p = 24189$, thus for each $\lambda \in \{100, 10, 1, 0.1..., \}$ and each cross-validation set we need to estimate 24189 parameters to optimum.



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The Hessian Screening Rule

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The Strong Screening Rule for SLOPE

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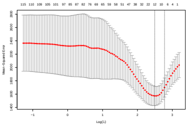
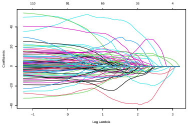
Abstract



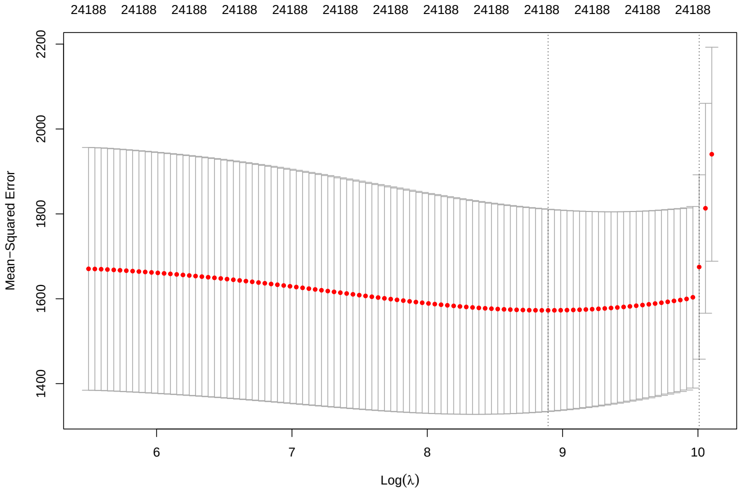


ridge

- Then ridge ($\alpha = 0$), fitting λ the same way

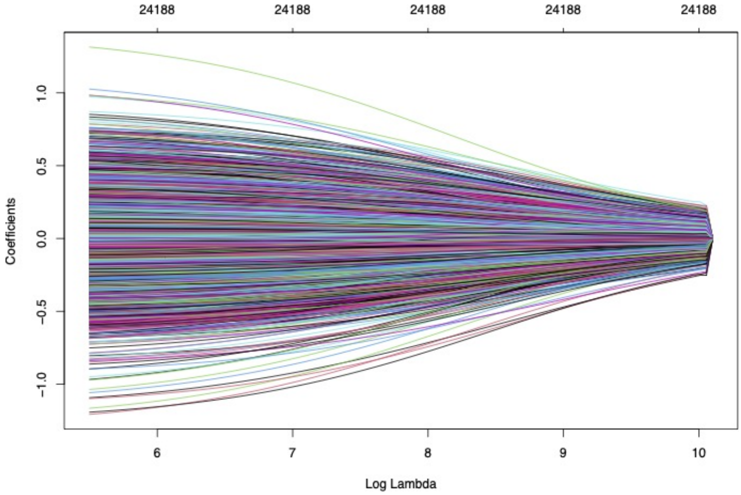
[] cvfit <- cv.glmnet(X, y, alpha=0, nfolds = 10, intercept = T, standardize = T) plot(cvfit)

ridge II



24188 24188 24188 24188 24188 24188 24188 24188 24188 24188 24188 24188 24188
Mean−Squared Error
2200
2000
1800
1600
1400
6
7
8
9
10
Log(λ)

ridge III



24188
24188
24188
24188
24188
Coefficients
1.0
0.5
0.0
−0.5
−1.0
6
7
8
9
10
Log Lambda

LASSO Irrepresentability condition

The sign vector of β is defined as
$S(\beta) = (S(\beta_1), \ldots, S(\beta_p)) \in \{-1, 0, 1\}^p$,
where for $x \in \mathbb{R}$, $S(x) = 1_{x>0} - 1_{x<0}$

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Let $I := \{i \in \{1, \dots, p\} \mid \beta_i \neq 0\}$, and let $X_I, X_{\bar{I}}$ be matrices whose columns are respectively $(X_i)_{i \in I}$ and $(X_i)_{i \notin I}$.

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Irrepresentable condition:

$$\|X_{\bar{I}}' X_I (X_I' X_I)^{-1} S(\beta_I)\|_\infty \leq 1$$

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Irrepresentable condition:

$$\|X_{\bar{I}}' X_I (X_I' X_I)^{-1} S(\beta_I)\|_\infty \leq 1$$

When

$$\|X_{\bar{I}}' X_I (X_I' X_I)^{-1} S(\beta_I)\|_\infty > 1$$

then probability of the support recovery by LASSO is smaller than 0.5 (Wainwright, 2009).

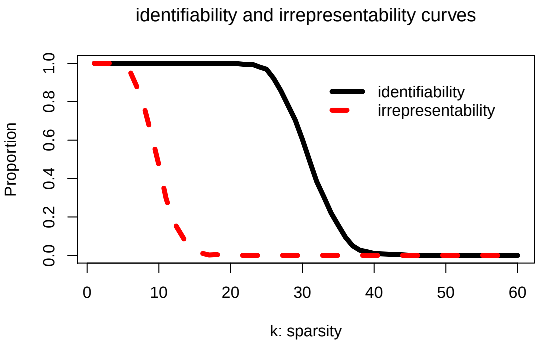
Separation of true and false predictors

Theorem (Tardivel, Bogdan, 2019)

For any $\lambda > 0$ LASSO can separate well the causal and null features if and only if vector β is identifiable with respect to l_1 norm and $min_{i \in I}|\beta_i|$ is sufficiently large.

Irrepresentability and identifiability curves

n=100, p=300, elements of X were generated as iid N(0,1)



Modifications of LASSO

Corollary

Appropriately thresholded LASSO can properly identify the sign of sufficiently large β if and only if β is identifiable with respect to l_1 norm.

Conjecture

Adaptive (reweighted) LASSO can properly identify the sign of sufficiently large β if and only if β is identifiable with respect to l_1 norm.

Adaptive LASSO

Adaptive LASSO [Zou, *JASA* 2006], [Candès, Wakin and Boyd, *J. Fourier Anal. Appl.* 2008]

$$\beta_{aL} = argmin_b \left\{ \frac{1}{2} \|y - Xb\|_2^2 + \lambda \sum_{i=1}^{p} w_i |b|_i \right\}, \tag{1}$$

where $w_i = \frac{1}{\hat{\beta}_i}$, and $\hat{\beta}_i$ is some consistent estimator of β_i.

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where $w_i = \frac{1}{\hat{\beta}_i}$, and $\hat{\beta}_i$ is some consistent estimator of β_i.
Reduces bias and improves model selection properties

Numerical experiments

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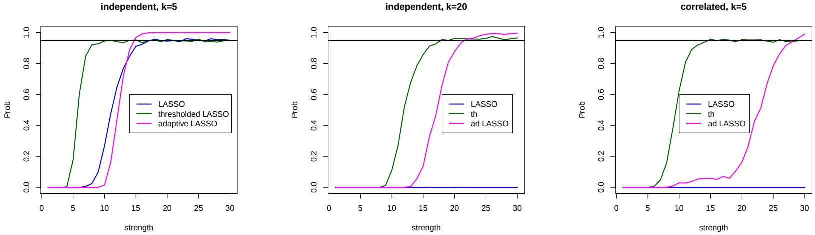
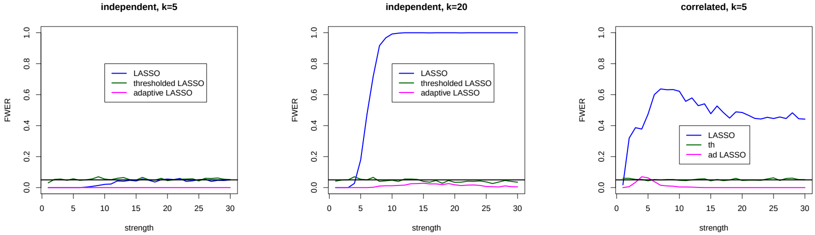
5. Threshold selected by using knockoff control variables (Foygel-Barber and Candès, 2015; Candès, Fan, Janson, Lv, 2016)

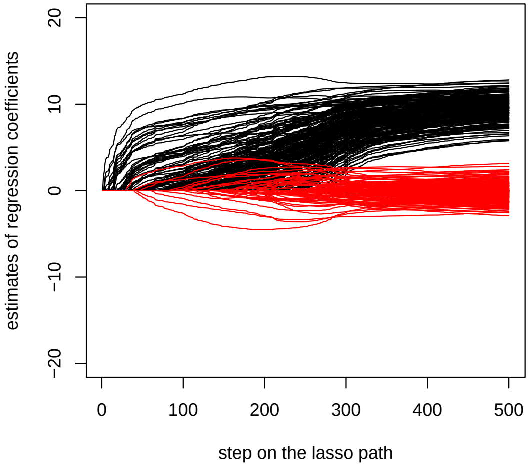
Probability of the sign recovery



Family Wise Error Rate



Thresholded LASSO (1)



Knockoffs and LCD statistics

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When X_{ij} are iid $N(0, 1/n)$ then $\tilde{X}_{ij}$ are also iid $N(0, 1/n)$.

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$$W_j = |\widehat{\beta}_j| - |\widehat{\beta}_{p+j}|$$

Knockoff filter

Define a random threshold as

$$\hat{t}(\lambda) = \min\left\{ t > 0 : \frac{1 + \#\{j : W_j(\lambda) \leq -t\}}{\#\{j : W_j(\lambda) \geq t\}} \leq q \right\}$$

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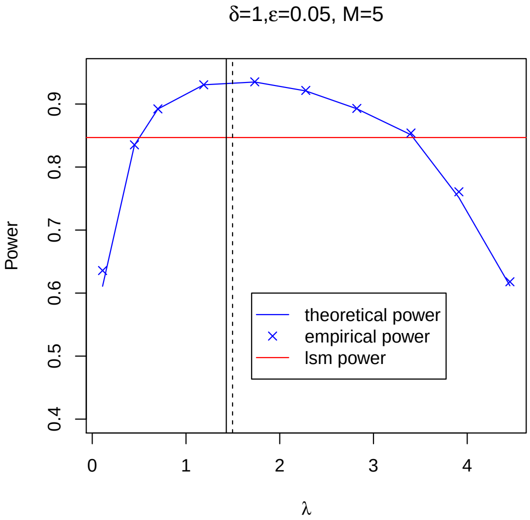
Foygel-Barber and Candès (2015), Candès, Fan, Janson and Lv (2017) - The above knockoff procedure $KN(\lambda, q)$ controls FDR at the level q.

Gain in power over LSM



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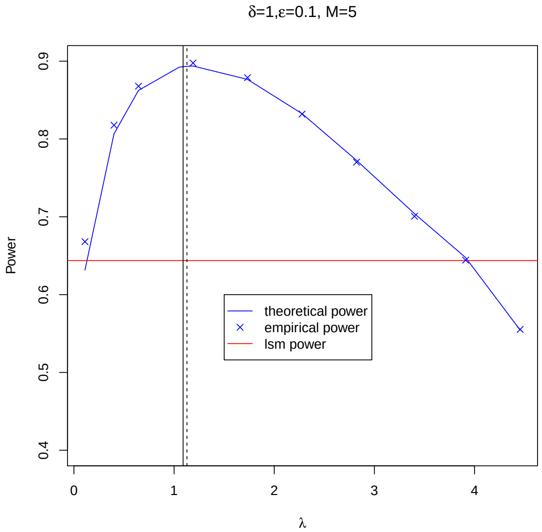

Theoretical results using the mean field asymptotics

Su, Bogdan, Candès, Ann. Stat. 2017 - FDR-Power Tradeoff Diagram for LASSO

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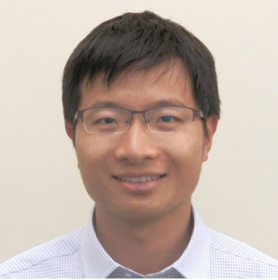
Weinstein, Su, Bogdan, Barber, Candés, Ann. Stat. 2023 - Breaking the tradoff diagram with thresholded LASSO

Sorted L-One Penalized Estimation

M.B., E.van den Berg, C.Sabatti, W.Su, E.J.Candès, AOAS 2015






Sorted L-One Penalized Estimation

$$\hat{\beta} = argmin_{b \in \mathbb{R}^p} \frac{1}{2}\|y - Xb\|_{\ell_2}^2 + \sum_{i=1}^{p} \lambda_i |b|_{(i)}.$$

where $\left|b\right|_{(1)} \geq \ldots \geq \left|b\right|_{(p)}$ are ordered magnitudes of coefficients of b and $\lambda_1 \geq \ldots \geq \lambda_p \geq 0$ is the sequence of tuning parameters.

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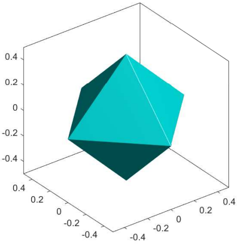
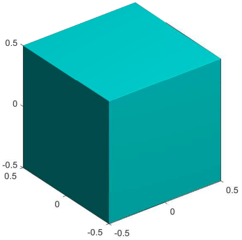
Sorted L-One Norm: $J_\lambda(b) = \sum_{i=1}^{p} \lambda_i \left|b\right|_{(i)}$ reduces to $||b||_1$ if $\lambda_1 = \ldots = \lambda_p$ and to $||b||_\infty$ if $\lambda_1 > \lambda_2 = \ldots = \lambda_p = 0$.

Unit balls for different SLOPE sequences by D.Brzyski

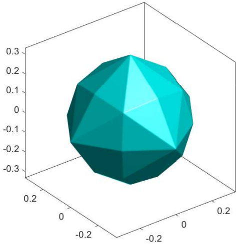
[(2,2,2)]



[(2,0,0)]



[(3,2,1)]



FDR control with SLOPE

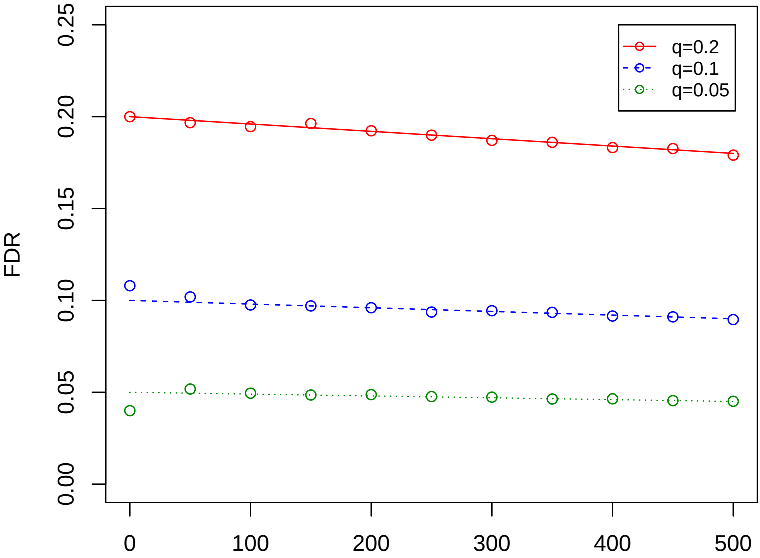
Theorem (B,van den Berg, Sabatti, Su and Candès (2015))

When $X^T X = I$ SLOPE with

$$\lambda_i := \sigma \Phi^{-1}\left(1 - i \cdot \frac{q}{2p}\right)$$

controls FDR at the level $q\frac{p_0}{p}$.

Orthogonal design, $n = p = 5000$



Asymptotic optimality of SLOPE

Let $k = ||\beta||_0$ and consider the setup where $k/p \to 0$ and $\frac{k \log p}{n} \to 0$.

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LASSO rate of the estimation error - $k \log p$

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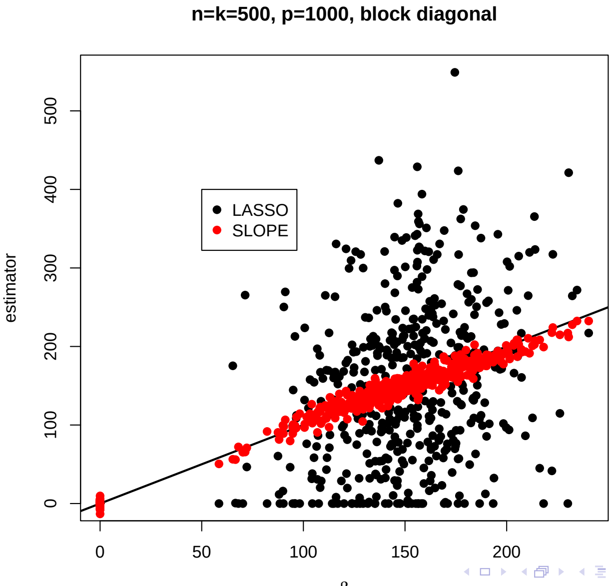
Extension to logistic regression by Abramovich and Grinshtein (2018, IEEE Trans. Inf. Theory)

SLOPE vs LASSO



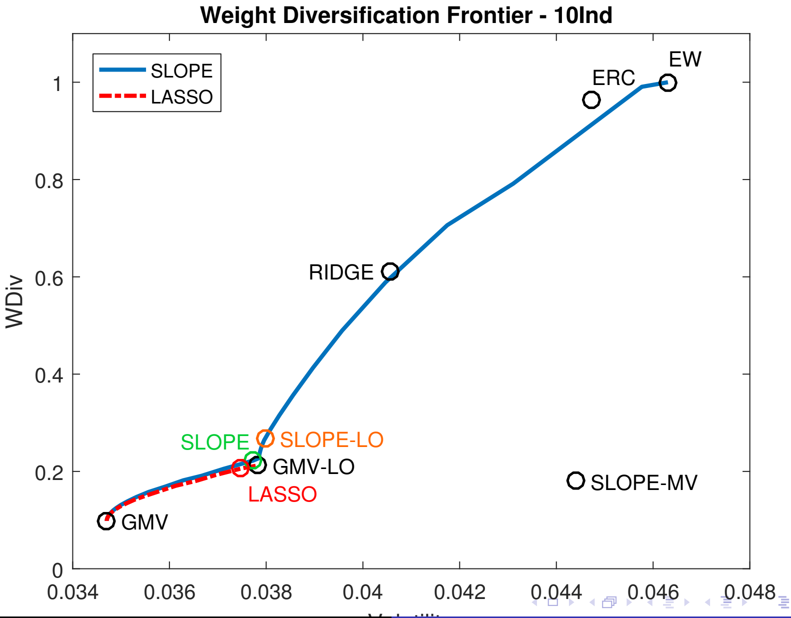
Portfolio Optimization, (P. Kremmer, S. Lee, M. Bogdan, S. Paterlini, JBF 2020)

$R_{t\times k} = (R_1, \dots, R_k)$ - asset returns,
Σ - the covariance matrix of R

$$\min_{w\in\mathbb{R}^k} \frac{\phi}{2} w'\Sigma w + J_\lambda(w) \tag{2}$$

$$\text{s.t.} \sum_{i=1}^{k} w_i = 1 \tag{3}$$

Evolution of Portfolio



Extensions

- Elastic net

$$ {}_{\beta}||y - X\beta||_2^2 + \lambda \left(\alpha|\beta|_1 + (1-\alpha)\, ||\beta||_2^2 \right) $$

where $w_j = \frac{1}{\hat{\beta}^{LS}}$

- Adaptive lasso:

$$ {}_{\beta}||y - X\beta||_2^2 + \lambda \sum_{j=1}^{p} w_j|\beta_j| $$

where $w_j = \frac{1}{|\hat{\beta}^{LS}|^{\gamma}}$ or $w_j = \frac{1}{|\hat{\beta}^{ridge}|^{\gamma}}$

  - Sparser then lasso,
  - less regularization on parameters.

- Group lasso:

$$ {}_{\beta}||y - X\beta||_2^2 + \lambda \sum_{j=1}^{J} ||\beta_j||_2 $$

- The respective versions of SLOPE

The Bayesian connection I:ridge

- Ridge regression solution:

$$\hat{\beta}^{ridge} = argmin_{\beta} \frac{1}{2} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \frac{1}{2} \lambda \sum_{j=1}^{p} \beta_j^2 \quad (3.41)$$

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- And the ridge solution is thus the MAP (maximum a posteriori) estimate of:

$$\pi(\beta | y, \lambda) \propto \mathcal{N}(y; X\beta, I) \mathcal{N} \left(\beta; 0, \frac{1}{\lambda} I \right)$$

The Bayesian connection II:lasso

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