Regularization methods in multiple regression

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

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

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

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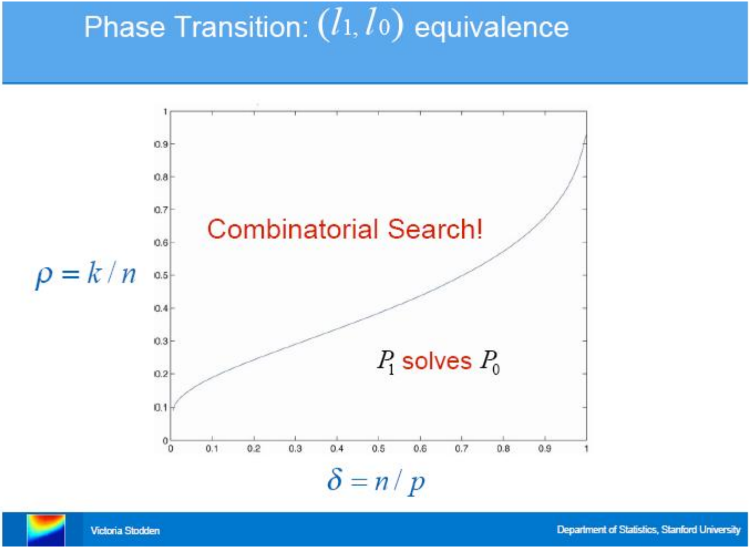
Basis Pursuit can recover β if k is small enough.

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

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

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

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$$\partial_f(b) = \{v \in \mathbb{R}^p : f(z) - f(b) \geq v'(z - b) \ \forall z \in \mathbb{R}^p\}.$$

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The convex function $f(x)$ attains a minimum at x_0 if and only if $0 \in \partial_f(x_0)$.

LASSO for the orthogonal design $X'X = I$

$$\beta^{LS} = Y'X, \;\; ||Y - Xb||^2 + \lambda||b||_1 = Y'Y + \sum_{i=1}^{p} f_i(b_i)$$

$$f_i(x) = x^2 - 2\beta_i^{LS} x + \lambda|x|$$

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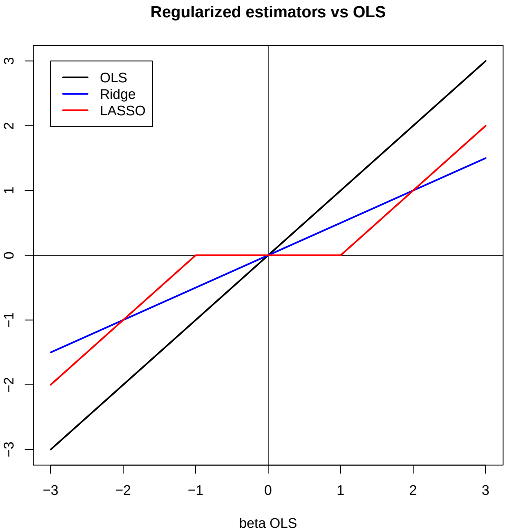
$$\lambda\partial_{|x|}(x_0) = \begin{cases} \lambda & \text{for} \quad x_0 > 0 \\ -\lambda & \text{for} \quad x_0 < 0 \\ < -\lambda, \lambda > & \text{for} \quad x_0 = 0 \end{cases}$$

LASSO for the orthogonal design

$$\hat{\beta}_i^L = \begin{cases} \beta^{LS} - \lambda/2 & \text{when} \quad \beta_i^{LS} > \lambda/2 \\ -\beta_i^{LS} + \lambda/2 & \text{when} \quad \beta_i^{LS} < -\lambda/2 \\ 0 & \text{when} \quad |\beta_i^{LS}| < \lambda/2 \end{cases}$$

Regularized estimators vs OLS



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.

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 $x \in \mathbb{R}$, $S(x) = \mathbf{1}_{x>0} - \mathbf{1}_{x<0}$

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

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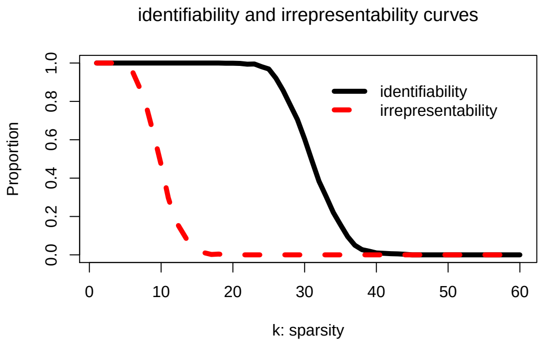
When

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

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

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



Identifiability condition

Definition (Identifiability)

Let X be a $n \times p$ matrix. The vector $\beta \in R^p$ is said to be identifiable with respect to the l^1 norm if the following implication holds

$$X\gamma = X\beta \text{ and } \gamma \neq \beta \Rightarrow \|\gamma\|_1 > \|\beta\|_1. \tag{1}$$

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.

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]

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

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

AMP theory for LASSO, (Bayati and Montanari, 2012)

$$X_{ij} \sim \mathcal{N}(0, 1/n), \quad z_i \sim \mathcal{N}(0, \sigma^2)$$

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$$\tau^2 = \sigma^2 + \frac{1}{\delta}\mathbb{E}\Big(\eta_{\alpha\tau}(\Pi + \tau Z) - \Pi\Big)^2,$$

$$\lambda = \Big(1 - \frac{1}{\delta}\mathbb{P}(|\Pi + \tau Z| > \alpha\tau)\Big)\alpha\tau.$$

AMP theory for LASSO, (Bayati and Montanari, 2012)

Theorem

For any pseudo-Lipschitz function φ*, the lasso solution* $\hat{\beta}$ *with fixed* λ *obeys*

$$\frac{1}{p}\sum_{i=1}^{p}\varphi(\hat{\beta}_i,\beta_i) \longrightarrow \mathbb{E}\varphi(\eta_{\alpha\tau}(\Pi+\tau Z),\Pi)$$

AMP formulas for FDR and Power

$\widehat{\mathcal{S}}$ - set of variables selected by LASSO

$$\mathsf{FDP} \equiv \frac{|\widehat{\mathcal{S}} \cap \mathcal{H}_0|}{|\widehat{\mathcal{S}}|}$$

$$FDR = E(FDP)$$

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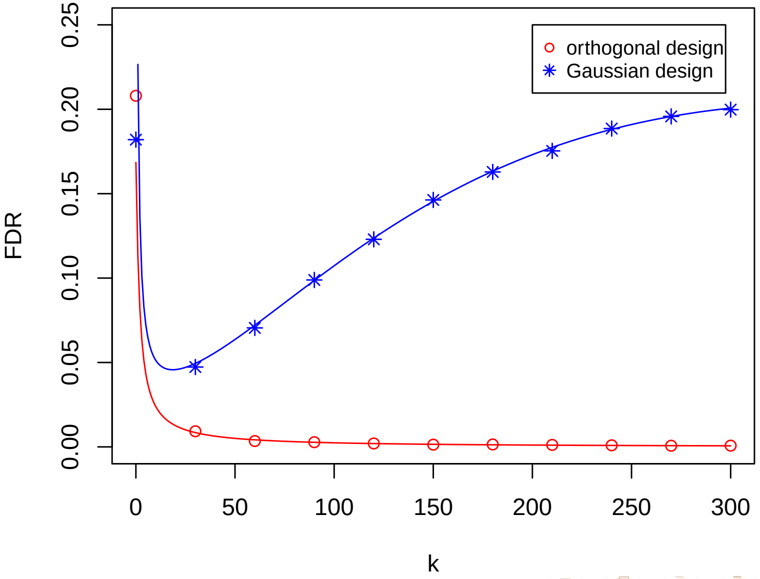
Bogdan, van den Berg, Su and Candés, 2013

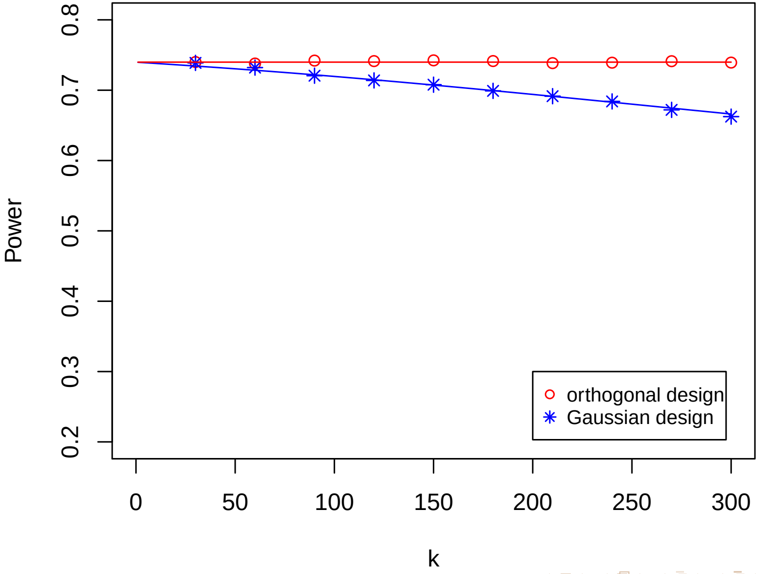
$$\text{FDR} \to \frac{2\mathbb{P}(\Pi = 0)\Phi(-\alpha)}{\mathbb{P}(|\Pi + \tau Z| > \alpha\tau)} \quad ,$$

$$\text{Power} \to \mathbb{P}(|\Pi + \tau Z| > \alpha\tau | \Pi \neq 0).$$

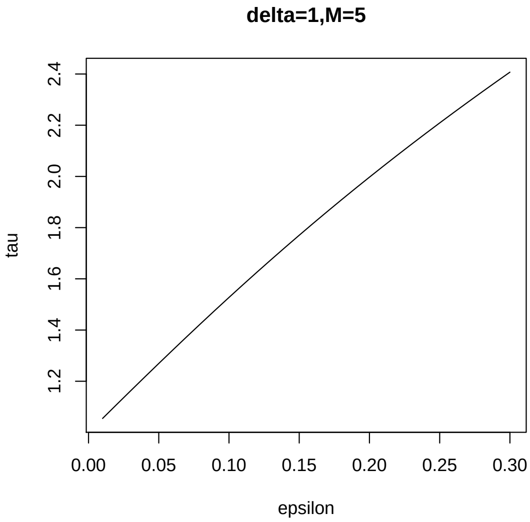
FDR - illustration



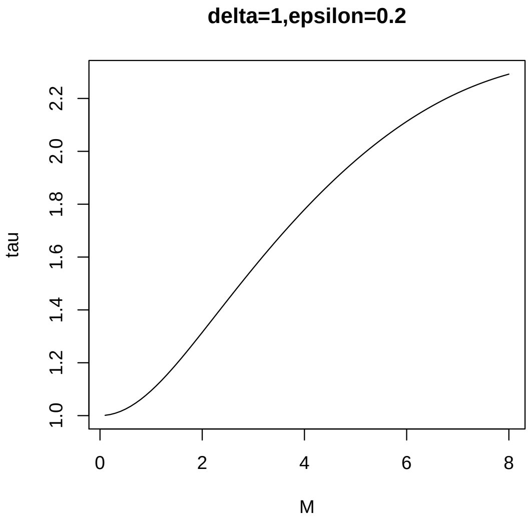
Power - illustration



Magnitude of additional noise (1)

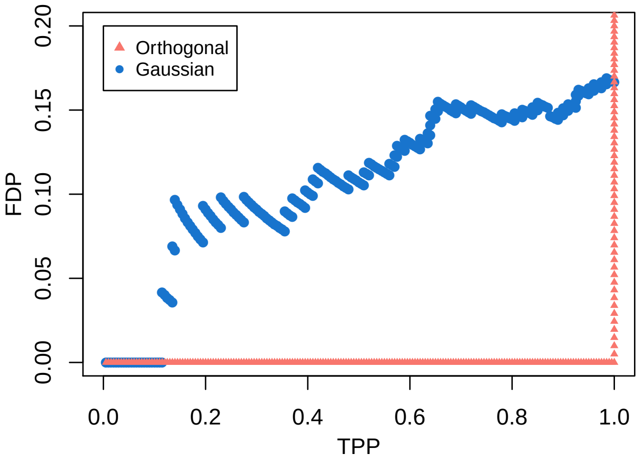


Magnitude of additional noise (2)



False Discoveries along the lasso path

Su, Bogdan and Candes, (2017), $\delta = 1$, $\epsilon = 0.2$



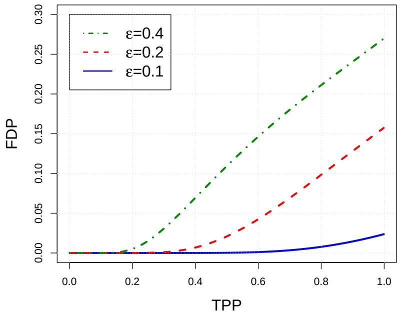
Theorem (Su, Bogdan, Candes, 2017)

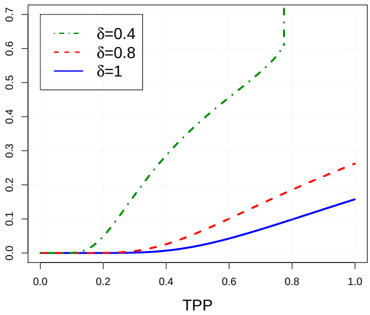
Fix $\delta \in (0, \infty)$ *and* $\epsilon \in (0, 1)$. *Then the event*

$$\bigcap_{\lambda \geq 0.01} \left\{ FDP(\lambda) \geq q^\star \left(TPP(\lambda) \right) - 0.001 \right\} \tag{3}$$

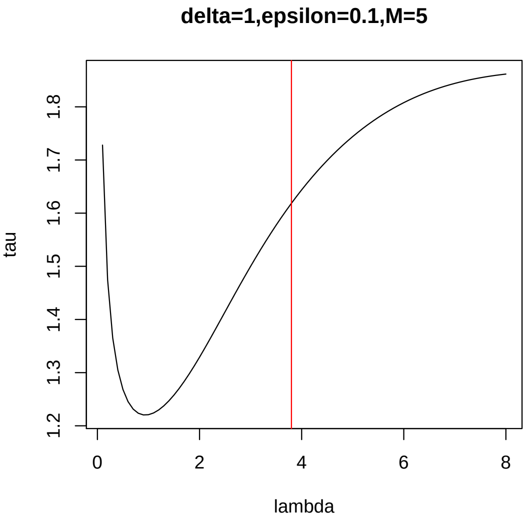
holds with probability tending to one.

FDR-Power trade-off (2)

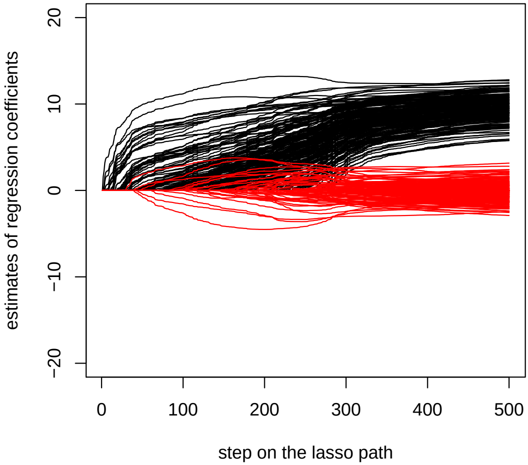




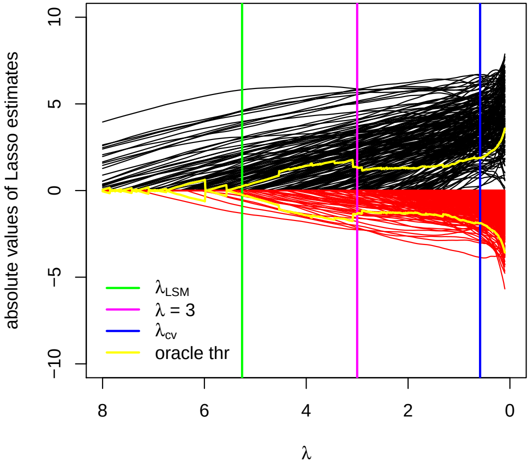
Magnitude of noise



Thresholded LASSO (1)



Thresholded LASSO (2)



Thresholded LASSO (3)