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

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

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

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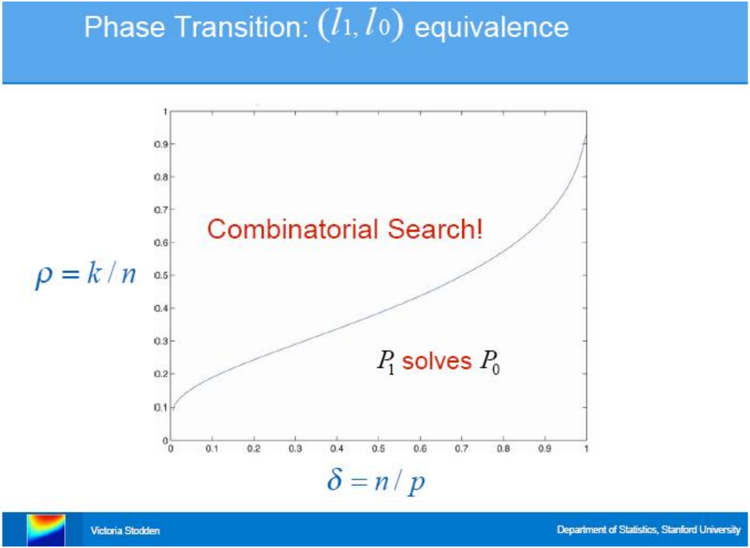
Basis Pursuit can recover β if k is small enough.

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*.


Phase Transition: (l_1, l_0) equivalence
Combinatorial Search!
P_1 solves P_0
$\rho = k/n$
$\delta = n/p$
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
Victoria Stodden
Department of Statistics, Stanford University

Noisy case - multiple regression

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

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

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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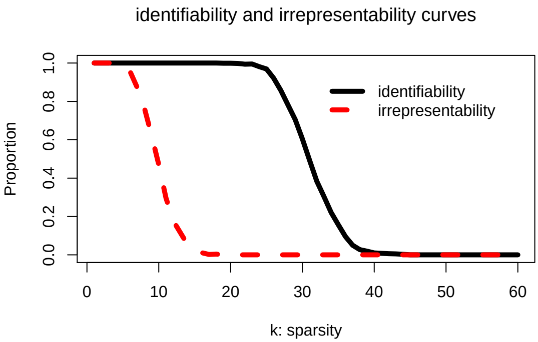
When

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

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]

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

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

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Reduces bias and improves model selection properties

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

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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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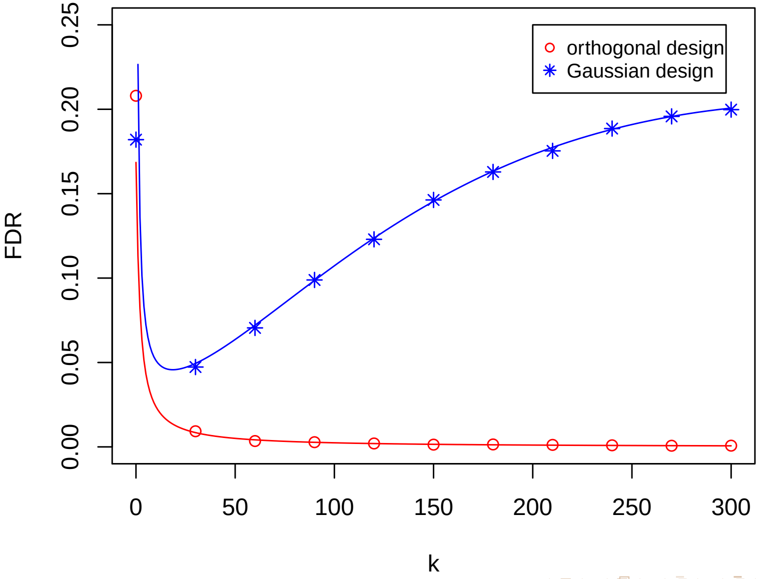
Bogdan, van den Berg, Su and Candés, 2013

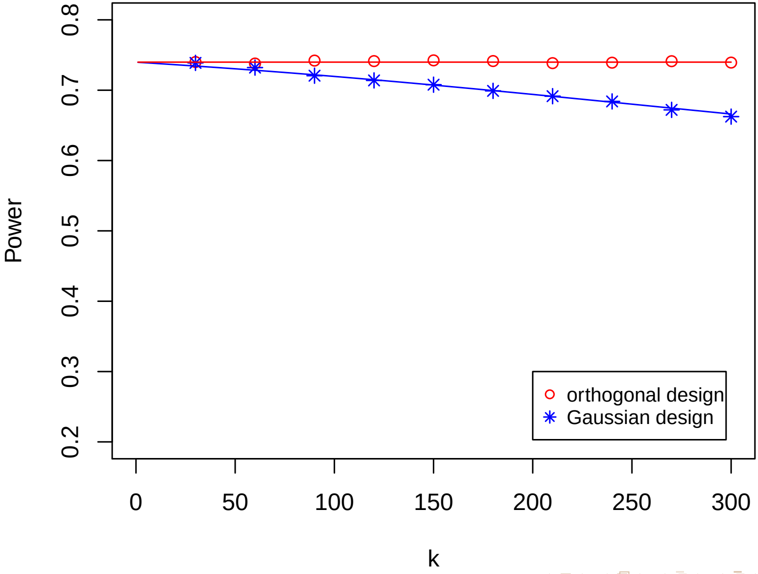
$$\text{FDR} \to \frac{2\mathbb{P}(\Pi = 0)\Phi(-\alpha)}{\mathbb{P}(|\Pi + \tau Z| > \alpha\tau)} \quad ,$$

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

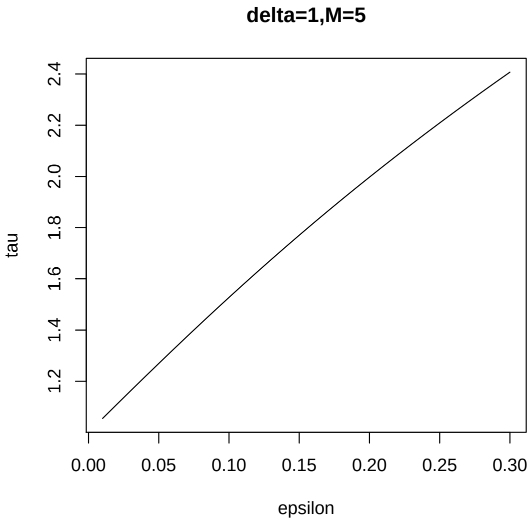
FDR - illustration



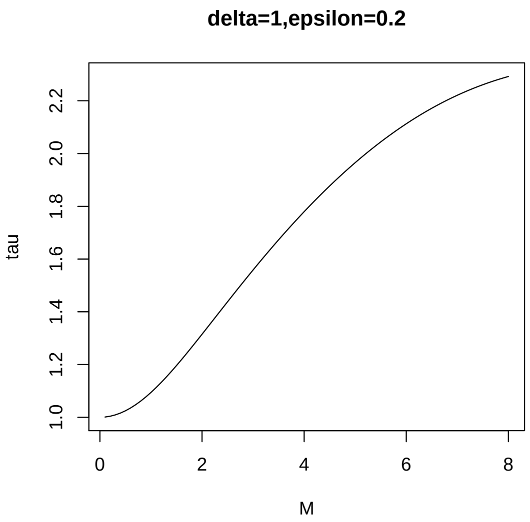
Power - illustration



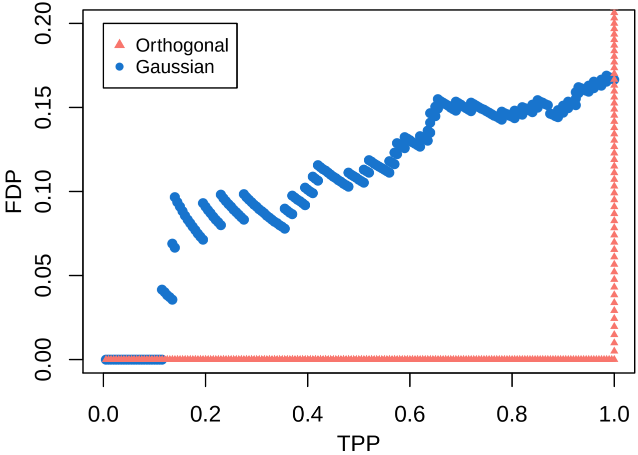
Magnitude of additional noise (1)



Magnitude of additional noise (2)



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



FDP-Power tradeoff

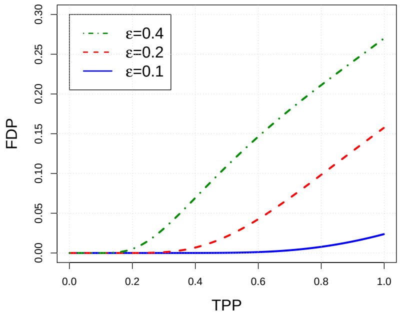
Theorem (Su, Bogdan, Candes, 2017)

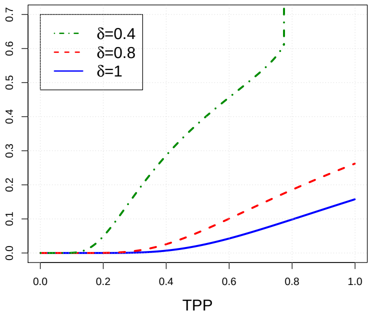
Fix $\delta \in (0, \infty)$ *and* $\epsilon \in (0, 1)$. *Then the event*

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

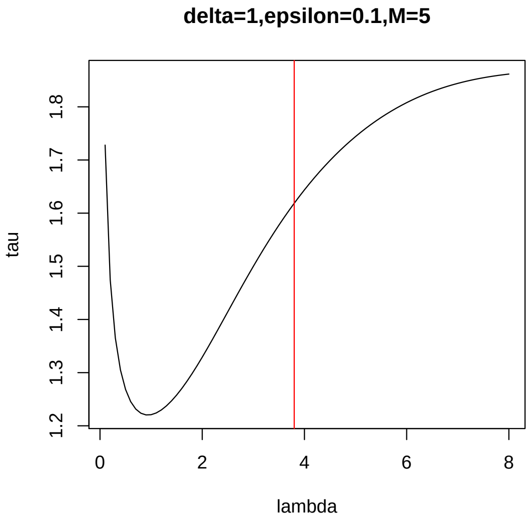
holds with probability tending to one.

FDR-Power trade-off (2)

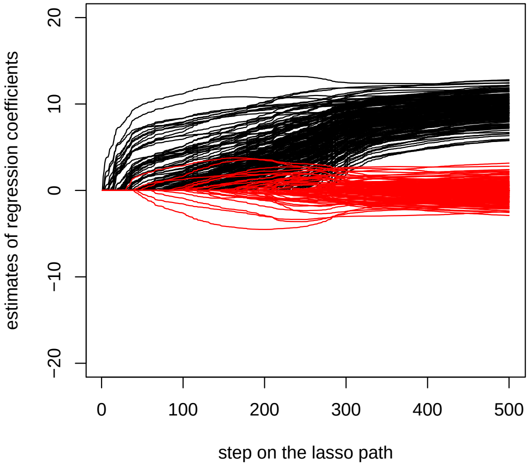




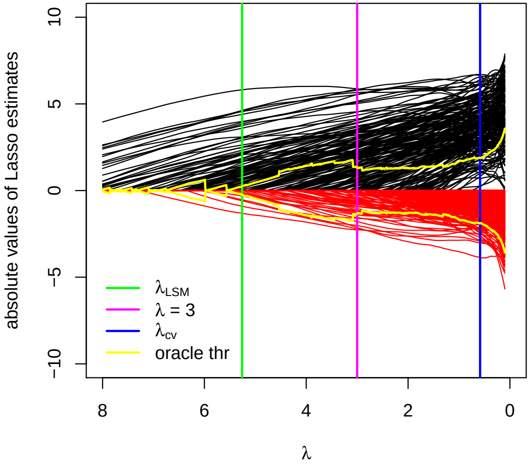
Magnitude of noise



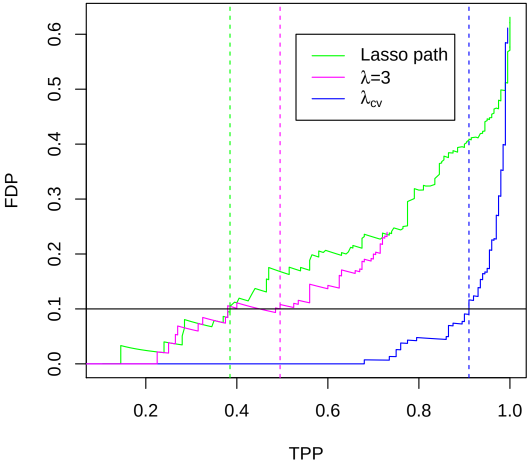
Thresholded LASSO (1)



Thresholded LASSO (2)



Thresholded LASSO (3)



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Consider n i.i.d random vectors $(Y_i, X_{1i}, \ldots, X_{pi})$

Variable X_j is a null variable, if $Y \perp X_j \mid X_{-j}$, where X_{-j} denotes the remaining $p-1$ variables excluding X_j

Construct a set of "fake" covariates $\tilde{X} = (\tilde{X}_1, \tilde{X}_2, \cdots, \tilde{X}_p)$ which satisfy:

1. *Exchangeability:* for any subset $S \subset \{1, \ldots, p\}$,
$$(X, \tilde{X})_{\text{swap}(S)} \stackrel{d}{=} (X, \tilde{X}), \tag{4}$$
where $swap(S)$ is obtained by swapping the entries X_j and $\tilde{X}_j$ for each $j \in S$.
2. *Unimportant variables:* $\tilde{X} \perp Y | X$, which can be guaranteed if $\tilde{X}$ is constructed without looking at Y.

Model Free Knockoffs for Gaussian Designs (1)

If $X \sim \mathcal{N}(0, \Sigma)$, then a joint distribution of $(X, \tilde{X})$ can be:

$$(X, \tilde{X}) \sim \mathcal{N}(0, G), \quad \text{where } G = \begin{bmatrix} \Sigma & \Sigma - \mathsf{diag}(s) \\ \Sigma - \mathsf{diag}(s) & \Sigma \end{bmatrix}, \tag{5}$$

with any choice of the diagonal matrix $\mathsf{diag}(s)$ *s.t.* G is positive semidefinite. Possible choice of s:

$$s_j = 2\lambda_{\min}(\Sigma) \wedge 1, \ \forall j \,, \tag{6}$$

Model Free Knockoffs for Gaussian Designs (2)

Sample $\tilde{X}$ from its conditional distribution:

$$\tilde{X} \mid X \overset{d}{=} \mathcal{N}(\mu_c, \Sigma_c),$$

where

$$\begin{aligned} \mu_c &= X - X\Sigma^{-1}\mathrm{diag}(s) \\ \Sigma_c &= 2\mathrm{diag}(s) - \mathrm{diag}(s)\Sigma^{-1}\mathrm{diag}(s). \end{aligned} \tag{7}$$

Knockoff statistics (1)

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flip-sign property:

$$w_j([X, \tilde{X}]_{swap(S)}, Y) = \begin{cases} w_j([X, \tilde{X}], Y), & j \notin S \\ -w_j([X, \tilde{X}], Y), & j \in S \end{cases}$$

Knockoff statistics (2)

Example:

$$T = (Z, \tilde{Z}) = t([X, \tilde{X}], Y)$$

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Lasso Coefficient Difference (LCD) statistic:

$$W_j = |\hat{\beta}_j(\lambda)| - |\hat{\beta}_{j+p}(\lambda)|$$

Knockoff filter

Define a random threshold as

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

and select

$$\widehat{\mathcal{S}(\lambda)} = \{j : W_j(\lambda) \ge \hat{t}(\lambda)\},$$

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

Breaking through FDR-Power diagram

Weinstein, Su, Bogdan, Barber, Candès (2023, to appear in AOS)

Definition

A random variable Π is said to be ϵ-sparse if $\mathbb{E}\,\Pi^2 < \infty$ and $\mathbb{P}(\Pi \neq 0) = \epsilon$.

Theorem

Assume that $\epsilon/2 < \epsilon_{\mathsf{DT}}(\delta/2)$, where $\epsilon_{\mathsf{DT}}(\delta)$ is a point on the Donoho-Tanner transition curve. Then for any fixed $0 < \lambda_1 < \lambda_2, 0 < q < 1$, and any $\nu > 0$, there exists an ϵ-sparse prior Π and n' such that

$$\mathbb{P}\left(\inf_{\lambda_1 \le \lambda \le \lambda_2} (\lambda, \Pi, q, n, p) > 1 - \nu\right) \geq 1 - \nu$$

if $n \geq n'$.

How to pick λ

Given that

$$\hat{\beta}_i \sim \tau\eta_\alpha\left(\frac{\Pi}{\tau} + Z\right)$$

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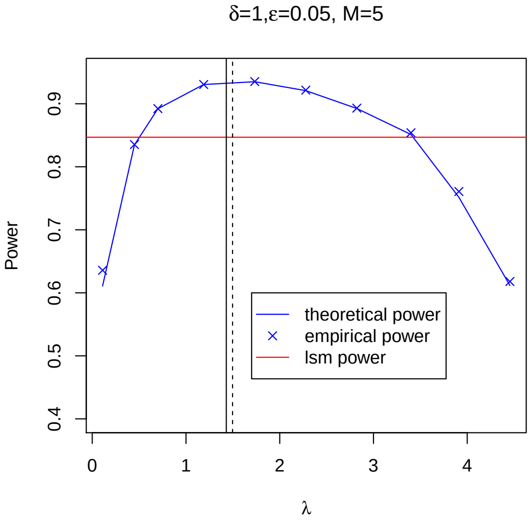
Thus minimizing τ corresponds to minimizing the prediction error.
Optimal τ can be identified through crossvalidation

Gain in power over LSM



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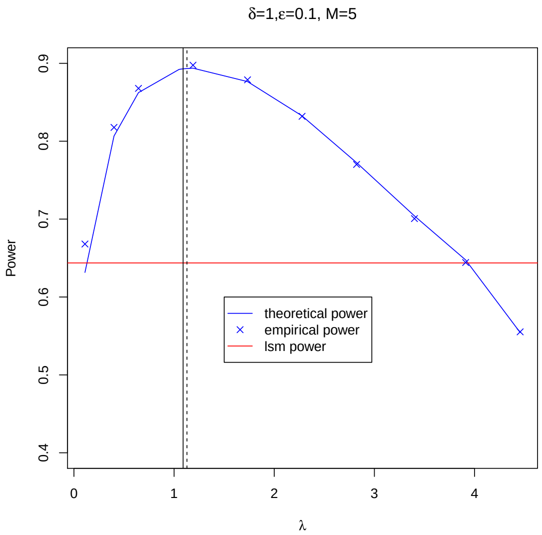

Other examples of applications of the AMP theory or the mean field asymptotics

G. Reeves, 2017, neural networks

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G. Reeves, 2017, neural networks

P.Sur and E.J.Candès, 2018, maximum likelihood estimators in logistic regression

The method relies on two de-randomizaton steps. First, the knockoff threshold value τ is calculated based on many knockoff test statistics:

$$W_{mj} = Z_{mj} - \tilde{Z}_{mj}, \qquad m = 1, 2, \cdots, M \text{ and } j = 1, 2, \cdots, p,$$

$$\tau = \min\left\{ t : \frac{1}{M} \sum_{m=1}^{M} \frac{\#\{j : W_{mj} \leq -t\} + c}{\#\{j : W_{mj} \geq t\} \vee 1} \leq q \right\} \tag{8}$$

with $c = \frac{1}{m}$.
In the second step for each $j = 1, 2, \cdots, p$ we calculate the median $med(W_j) = median(W_{mj})$ over $m = 1, \ldots, M$ and reject the j-th variable if $med(W_j) \geq \tau$.

Theorem

Consider the single knockoffs procedure, which rejects $H_{0j} : \beta_j = 0$ if the feature statistics W_j satisifes $W_j > t$ and let

$$FDR(t) = \mathbb{E}\left[\frac{\#\{j \in H_0 : W_j \geq t\}}{1 \vee \#\{j : W_j \geq t\}}\right] \quad . \tag{9}$$

If for each $i \in 1, \ldots, m$ it holds that the signs of the feature statistics W_{mj} , $j \in \{1, \ldots, p\}$ are i.i.d coin flips then we have:

$$\mathbb{E}\left(\frac{1}{M}\sum_{m=1}^{M}\frac{\#\{j : W_{mj} \leq -t\}}{\#\{j : W_{mj} \geq t\} \vee 1}\right) \geq FDR(t)$$