

From selective inference to adaptive data analysis

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Acknowledgement

My advisor:

- ▶ Jonathan Taylor

Other coauthors:

- ▶ Snigdha Panigrahi
- ▶ Jelena Markovic
- ▶ Nan Bi

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- ▶ Observe data (y, X) , $X \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$

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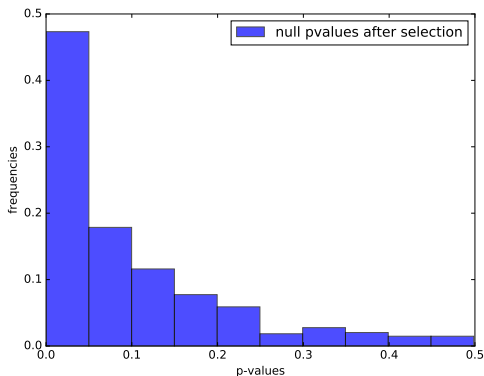
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- ▶ Problem: inflated significance
 1. Normal z-tests need adjustment
 2. Selection is biased towards “significance”

Inflated Significance

Setup:

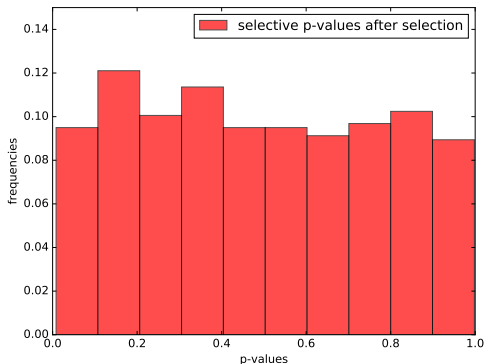
- ▶ $X \in \mathbb{R}^{100 \times 200}$ has i.i.d normal entries
- ▶ $y = X\beta + \epsilon$, $\epsilon \sim N(0, I)$
- ▶ $\beta = (\underbrace{5, \dots, 5}_{10}, 0, \dots, 0)$
- ▶ LASSO, nonzero coefficient set E
- ▶ z-test, null pvalues for $i \in E$, $i \notin \{1, \dots, 10\}$



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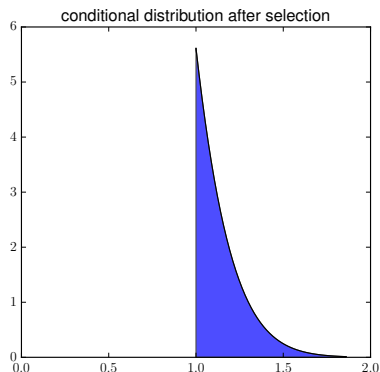
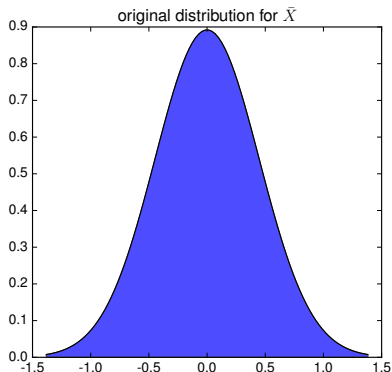
Selective inference: features and caveat

- ▶ Specific to particular selection procedures
- ▶ Exact post-selection test
- ▶ More powerful test

Selective inference: popping the hood

Consider the selection for “big effects”:

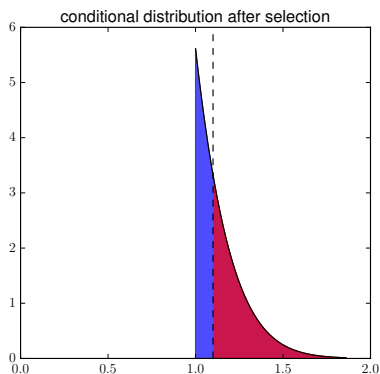
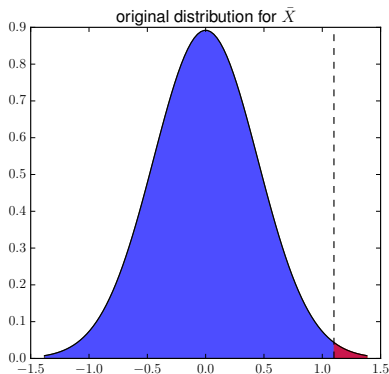
- ▶ $X_1, \dots, X_n \stackrel{i.i.d.}{\sim} N(0, 1)$, $\bar{X} = \frac{\sum_{i=1}^n X_i}{n}$
- ▶ Select for “big effects”, $\bar{X} > 1$
- ▶ Observation: $\bar{X}_{obs} = 1.1$, with $n = 5$
- ▶ Normal z-test v.s. selective test for $H_0 : \mu = 0$.



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Selective inference: in a nutshell

- ▶ Selection, e.g. $\bar{X} > 1$.
- ▶ Change of the reference measure
 - ▶ the conditional distribution, e.g. $N(\mu, \frac{1}{n})$, truncated at 1.
- ▶ Target of inference may depend on the outcome of selection
 - ▶ Example: selection by LASSO

What is the “selected” model?

Suppose a set of variables E are suggested by the data for further investigation.

- ▶ Selected model by [Fithian et al. \(2014\)](#):

$$\mathcal{M}_E = \{N(X_E \beta_E, \sigma_E^2 I), \beta_E \in \mathbb{R}^{|E|}, \sigma_E^2 > 0\}.$$

Target is β_E .

- ▶ Full model by [Lee et al. \(2016\)](#), [Berk et al. \(2013\)](#):

$$\mathcal{M} = \{N(\mu, \sigma^2 I), \mu \in \mathbb{R}^n\}.$$

Target is $\beta_E(\mu) = X_E^\dagger \mu$.

- ▶ Nonparametric model:

$$\mathcal{M} = \{\otimes^n F : (X, Y) \sim F\}.$$

Target is $\beta_E(F) = \mathbb{E}_F[X_E^T X_E]^{-1} \mathbb{E}_F[X_E \cdot Y]$.

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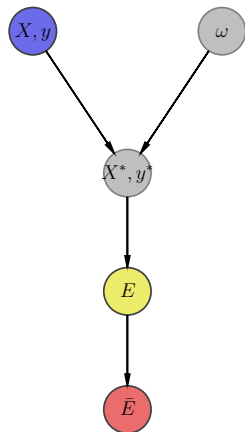
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A tool for valid inference after exploratory data analysis.

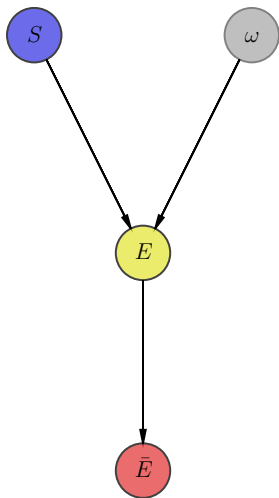
Selective inference on a DAG



- ▶ Incorporate randomness through ω
 1. $(X^*, y^*) = (X, y)$
 2. $(X^*, y^*) = (X_1, y_1)$
 3. $(X^*, y^*) = (X, y + \omega)$
- ▶ Reference measure conditioning on E , the yellow node.
- ▶ Target of inference can be \bar{E}
 1. Not E , but depends on the data through E
 2. “Liberating” target of inference from selection
 3. \bar{E} incorporate knowledge from previous literature.

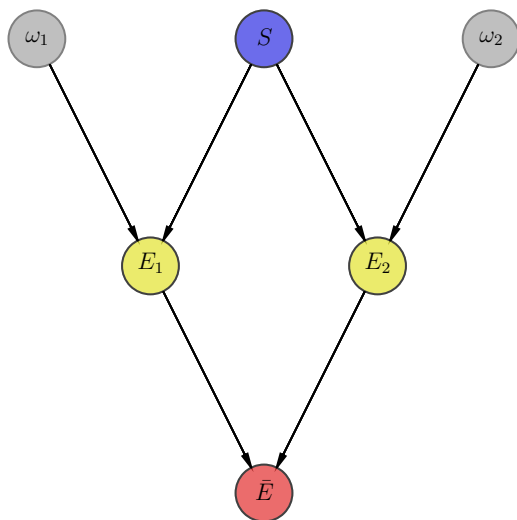
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Reference measure after selection

- ▶ Given any point null F_0 , use the conditional distribution F_0^* as reference measure,

$$\frac{dF_0^*}{dF_0}(S) = \ell_F(S).$$

- ▶ ℓ_F is called the **selective likelihood ratio**. Depends on the selection algorithm and the randomization distribution $\omega \sim G$.
- ▶ Tests of the form $H_0 : \theta(F) = \theta_0$ can be reduced to testing point nulls, e.g.
 - ▶ Score test
 - ▶ Conditioning in exponential families

Computing the reference measure after selection

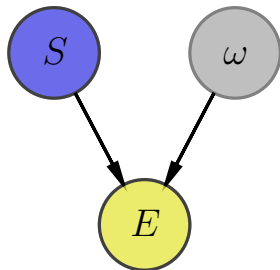
- ▶ **Selection map** \hat{Q} results from an optimization problem,

$$\hat{\beta}(S, \omega) = \arg \min_{\beta} \ell(S; \beta) + \mathcal{P}(\beta) + \omega^T \beta.$$

E is the active set of $\hat{\beta}$.

- ▶ Selection region $A(S) = \{\omega : \hat{Q}(S, \omega) = E\}$, $\omega \sim G$

$$\frac{dF_0^*}{dF_0}(S) = \int_{A(S)} dG(\omega).$$



$\{\hat{Q}(S, \omega) = E\}$ is difficult to describe.

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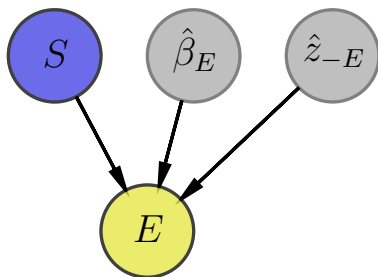
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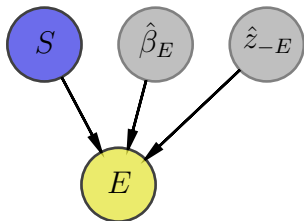
Let $\hat{z}(S, \omega)$ be the subgradient of the optimization problem.



$\{(\hat{\beta}_E, \hat{z}_{-E}) \in \mathcal{B}\}$, \mathcal{B} depends only on the penalty \mathcal{P} .

Monte-Carlo sampler for the conditional distribution

Suppose F_0 has density f_0 and G has density g ,



$$\begin{aligned} & \frac{dF_0^*}{dF_0}(S) \\ &= \int_{\mathcal{B}} g(\psi(S, \hat{\beta}_E, \hat{z}_{-E})) d\hat{\beta}_E d\hat{z}_{-E}, \end{aligned}$$

where $\omega = \psi(S, \hat{\beta}_E, \hat{z}_{-E})$.

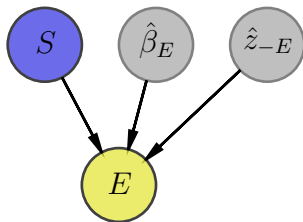
- ▶ The reparametrization map ψ is easy to compute, [Harris et al. \(2016\)](#)
- ▶ In simulation, we jointly sample $(S, \hat{\beta}_E, \hat{z}_{-E})$ from the density below,

$$f_0(S)g(\psi(S, \hat{\beta}_E, \hat{z}_{-E}))\mathbf{1}_{\mathcal{B}}.$$

Samples of S can be used as reference measure for selective inference.

Interactive Data Analysis

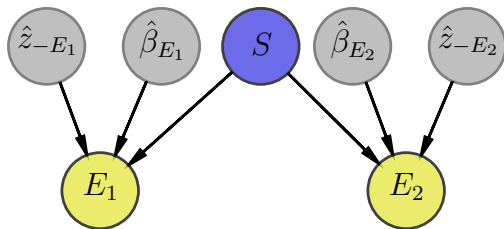
Easily generalizable in a sequential/interactive fashion.



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Interactive Data Analysis

Easily generalizable in a sequential/interactive fashion.



$$f_0(S)g(\psi_1(S, \hat{\beta}_{E_1}, \hat{z}_{-E_1}))\mathbf{1}_{B_1} \cdot g(\psi_2(S, \hat{\beta}_{E_2}, \hat{z}_{-E_2}))\mathbf{1}_{B_2}.$$

- ▶ Flexible framework. Any selection procedure resulting from a “Loss + Penalty” convex problem.
- ▶ Examples such as Lasso, logistic Lasso, marginal screening, forward stepwise, graphical Lasso, group Lasso, are considered in Harris et al. (2016).
- ▶ Many more is possible.

Summary

- ▶ Selective inference on a DAG
- ▶ Selection: more than one shot
- ▶ Feasible implementation of the selective tests
<https://github.com/selective-inference/Python-software>

Thank you!

Berk, R., Brown, L., Buja, A., Zhang, K. & Zhao, L. (2013), 'Valid post-selection inference', *The Annals of Statistics* **41**(2), 802–837.

URL: <http://projecteuclid.org/euclid.aos/1369836961>

Fithian, W., Sun, D. & Taylor, J. (2014), 'Optimal Inference After Model Selection', *arXiv preprint arXiv:1410.2597* . arXiv: 1410.2597.

URL: <http://arxiv.org/abs/1410.2597>

Harris, X. T., Panigrahi, S., Markovic, J., Bi, N. & Taylor, J. (2016), 'Selective sampling after solving a convex problem', *arXiv preprint arXiv:1609.05609* .

Lee, J. D., Sun, D. L., Sun, Y. & Taylor, J. E. (2016), 'Exact post-selection inference with the lasso', *The Annals of Statistics* **44**(3), 907–927.

URL: <http://projecteuclid.org/euclid.aos/1460381681>