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Topic 17: False Discovery Rate (FDR) and Knockoffs

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Key points: Constructing knockoff variables to control FDR when estimating regression coefficients.

Disclaimer: The note is built on Prof. Jinchi Lv's lectures of the course at USC, DSO 607, High-Dimensional Statistics and Big Data Problems.

17.1 Motivation

Consider the classical linear regression setting

$$y = X\beta + \epsilon$$

where $\beta \in \mathbb{R}^p$ is the unknown vector of coefficients and $\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$. In a high-dimensional problem, we would like to just select a subset of all variables $\hat{S} \subset \{1, \cdots, p\}$ s.t. conditional on $\{\mathbf{X}_j\}_{j \in \hat{S}}$, \mathbf{y} is **independent** of all other variables, we can define the **False Discovery Rate** (FDR) in can be defined as

Definition 17.1.1: False Discovery Rate (FDR)

$$FDR = \mathbb{E}(FDP) = \mathbb{E}\left[\frac{|\hat{S} \cap \mathcal{H}_0|}{|\hat{S}|} = \frac{\#\{j : j \in \hat{S} \setminus S\}}{\#\{j : j \in \hat{S}\}}\right]$$

where $\mathcal{H}_0 \subset \{1, \dots, p\}$ is the set of **null** variables: \mathbf{X}_j is **null** iff \mathbf{Y} is independent of \mathbf{X}_j conditional on the other variables $\mathbf{X}_{-j} = \{\mathbf{X}_1, \dots, \mathbf{X}_p\} \setminus \{\mathbf{X}_j\}$.

In this note, we consider a series of knockoff-based methods to control FDR. They all follow a common procedure:

- Step 1: Construct Knockoffs
- Step 2: Calculate test satistics for both original and knockoff variables
- Step 3: Calculate a threshold for the test statistics, controlling for a desired FDR level
- Step 4: Select variables that pass the threshold

17.2 Barber and Candes (2015)

Barber and Candes (2015) construct the knockoffs by the following procedure

• Calculate the Gram matrix $\Sigma = \mathbf{X}'\mathbf{X}$ for the normalized original variables, where $\Sigma_{jj} = \left\|\mathbf{X}_{j}\right\|_{2}^{2} = 1$

 \bullet Construct the knockoffs \tilde{X} s.t.

$$\tilde{\mathbf{X}}'\tilde{\mathbf{X}} = \mathbf{X}'\tilde{\mathbf{X}} = -\operatorname{diag}\left\{s\right\}$$

and

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References

Rina Foygel Barber and Emmanuel J. Candes. Controlling the false discovery rate via knockoffs. *Annals of Statistics*, 43(5):2055–2085, 2015.