Econometrics **June 15, 2023**

Topic 17: False Discovery Rate (FDR) and Knockoffs

by Sai Zhang

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

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where $\boldsymbol{\beta} \in \mathbb{R}^p$ is the unknown vector of coefficients and $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$. 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)

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

where $\mathcal{H}_0 \subset \{1, \cdots, p\}$ 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 $\mathbf{X}_{-j} = \{\mathbf{X}_1, \cdots, \mathbf{X}_p\} \setminus \{\mathbf{X}_j\}$.

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, controling 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 $\mathbf{\Sigma} = \mathbf{X}'\mathbf{X}$ for the normalized original variables, where $\Sigma_{jj} = \left\|\mathbf{X}_j\right\|_2^2 = 1$

- Construct the knockoffs $\tilde{\mathbf{X}}$ s.t.

$$\tilde{\mathbf{X}}'\tilde{\mathbf{X}} = \mathbf{\Sigma} \qquad \mathbf{X}'\tilde{\mathbf{X}} = \mathbf{\Sigma} - \mathrm{diag}\left\{\mathbf{s}\right\}$$

  where $\mathbf{s} \in \mathbb{R}_+^p$ is a p-dimensional non-negative vector (larger s_j indicates higher power) and

  - $\tilde{\mathbf{X}}$ exhibits the **same** covariance structrue as the original design $\mathbf{X}$
  - The correlation between distinct original variables and knockoffs are the same as between the originals:

$$\mathbf{X}_j'\tilde{\mathbf{X}}_k = \mathbf{X}_j'\mathbf{X}_k, \ \forall j \neq k$$

  - The correlation between the original variables and their own knockoffs is **less than 1**

$$\mathbf{X}_j'\tilde{\mathbf{X}}_j = \Sigma_{jj} - s_j = 1 - s_j$$

References

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