Econometrics June 23, 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

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

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 statistics 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)

Constructing the knockoffs 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 $\Sigma_{jj} = \|\mathbf{X}_j\|_2^2 = 1$

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

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

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

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

$$\mathbf{X}_{i}^{\prime}\tilde{\mathbf{X}}_{k} = \mathbf{X}_{i}^{\prime}\mathbf{X}_{k}, \ \forall j \neq k$$

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

$$\mathbf{X}_{j}'\tilde{\mathbf{X}}_{j} = \Sigma_{jj} - s_{j} = 1 - s_{j}$$

To construct such knockoffs,

- Given a proper \mathbf{s} , if $n \ge 2p$, then

$$\tilde{\mathbf{X}} = \mathbf{X}(\mathbf{I} - \mathbf{\Sigma}^{-1} \text{diag} \{\mathbf{s}\}) + \tilde{\mathbf{U}}\mathbf{C}$$

where $\tilde{\mathbf{U}} \in \mathbb{R}^{n \times p}$ is an **orthonormal** matrix s.t. $\tilde{\mathbf{U}}'\mathbf{X} = \mathbf{0}$ and $\mathbf{C}'\mathbf{C} = 2\mathrm{diag}\{\mathbf{s}\} - \mathrm{diag}\{\mathbf{s}\} \Sigma^{-1}\mathrm{diag}\{\mathbf{s}\} \geq \mathbf{0}$

- A sufficient and necessary condition for $\tilde{\mathbf{X}}$ to exist: diag $\{\mathbf{s}\} \leq 2\Sigma$
- 2 types of knockoffs can be constructed, following these procedures
- T1 <u>Equi-correlated</u> knockoffs: set $s_j = 2\lambda_{\min}(\Sigma) \wedge 1$ for all j, then $\langle \mathbf{X}_j, \tilde{\mathbf{X}}_j \rangle = 1 2\lambda_{\min}(\Sigma) \wedge 1$ for all j. This is essentially minimizing $|\langle \mathbf{X}_j, \tilde{\mathbf{X}}_j \rangle|$
- T2 SDP knockoffs: solve the convex problem

$$\arg\min_{\mathbf{x}} \sum_{j} (1 - s_j) \qquad \qquad s.t.0 \le s_j \le 1, \operatorname{diag}\{\mathbf{s}\} \le 2\Sigma$$

which is essentially minimizing the average of $\langle \mathbf{X}_i, \tilde{\mathbf{X}}_i \rangle$

Calculate test statistics Define and calculate test statistics W_j for each $\beta_j \in \{1, \dots, p\}$ using $[\mathbf{X} \ \tilde{\mathbf{X}}]$:

• the test statistic W_j should be constructed s.t. large positive values are evidence against the null hypothesis $\beta_j = 0$, for example, consider a Lasso on $\begin{bmatrix} \mathbf{X} & \tilde{\mathbf{X}} \end{bmatrix}$

$$\hat{\beta}(\lambda) = \arg\min_{\mathbf{b}} \left\{ \frac{1}{2} \| \mathbf{y} - \begin{bmatrix} \mathbf{X} & \tilde{\mathbf{X}} \end{bmatrix} \mathbf{b} \|_{2}^{2} + \lambda \| \mathbf{b} \| \right\}_{1}$$

where λ is the point on the Lasso path at which the feature enters the model as

$$Z_j = \sup \{ \lambda : \hat{\beta}_j(\lambda) \neq 0 \}$$

and set
$$W_j = (Z_j \vee \tilde{Z}_j) \cdot \begin{cases} +1, & Z_j > \tilde{Z}_{j_1} \\ -1, & Z_j < \tilde{Z}_j \end{cases}$$

• In general, the statistics W should satisfy the **sufficient** property and **anti-symmetry** property:

¹Other choices of
$$W_j$$
 are $W_j = \left| \mathbf{X}_j' \mathbf{y} \right| - \left| \tilde{\mathbf{X}}_j' \mathbf{y} \right|$, or $\left| \hat{\beta}_j^{\mathrm{LS}} \right| - \left| \hat{\beta}_{j+p}^{\mathrm{LS}} \right|$

Definition 17.2.1: Property of Test Statistics W_i

The test statistic W_i is said to obey

the <u>sufficient</u> property if W depends <u>only</u> on the Gram matrix and on feature-response inner products, that is

$$\mathbf{W} = f\left(\begin{bmatrix} \mathbf{X} & \tilde{\mathbf{X}} \end{bmatrix}' \begin{bmatrix} \mathbf{X} & \tilde{\mathbf{X}} \end{bmatrix}, \begin{bmatrix} \mathbf{X} & \tilde{\mathbf{X}} \end{bmatrix}' \mathbf{y}\right)$$

- the **antisymmetry** property if swapping the original X_j and its knockoff \tilde{X}_j has the effect of **switching the sign** of W_j , that is

$$W_j(Z_j, \tilde{Z}_j) = -W_j(\tilde{Z}_j, Z_j)$$

Calculate a threshold for the test statistics After defining the test statistic, we then

• Let *q* be the target FDR, define the data-dependent threshold *T* as

$$T = \min \left\{ t \in \mathcal{W} : \frac{\# \{j : W_j \le -t\}}{\# \{j : W_j \ge t\} \lor 1} \le q \right\}$$

where $W = \{|W_j| : j = 1, \dots, p\} \setminus \{0\}$ is the set of unique non-zero values attained by $|W_j|$'s.

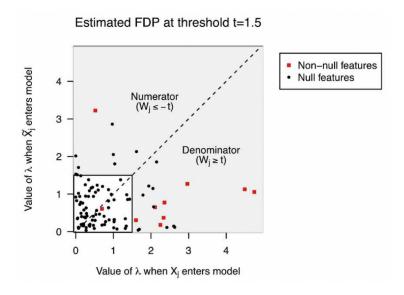


Figure 17.1: Visualizing Test Statistic Thresholding

Variable selection after building the threshold,

• for each $j = 1, \dots, p$, reject $H_{0,j} : \beta_j = 0$ if $W_j \ge T$, the knockoff filter selects the model

$$\hat{S} = \left\{ j : W_j \ge T \right\}$$

17.2.1 Intuition and Theory

Why knockoffs work?

- **W** is constructed (antisymmetry and sufficiency) such that the signs of the W_j 's are i.i.d. random for the null
- for any threshold *t* , we have

$$\#\{j: \beta_j = 0, W_j \ge t\} \stackrel{d}{=} \#\{j: \beta_j = 0, W_j \le -t\}$$

, and the false discovery proportion (FDP) can be estimated as

$$\frac{\#\{j: \beta_{j} = 0, W_{j} \ge t\}}{\max(\#\{j: W_{j} \ge t\}, 1)} \simeq \frac{\#\{j: \beta_{j} = 0, W_{j} \le -t\}}{\max(\#\{j: W_{j} \ge t\}, 1)}$$
$$\le \frac{\#\{j: W_{j} \le -t\}}{\max(\#\{j: W_{j} \ge t\}, 1)} := \widehat{FDP}(t)$$

then the knockoff procedure can be interpreted as finding a threshold via $T = \min \left\{ t \in \mathcal{W} : \widehat{\mathrm{FDR}}(t) \leq q \right\}$

The knockoff procedure essentially controls a quantity **nearly equal** to the FDR. To control the FDR **exactly**, we have, <u>textbfknockoff+</u>, a more conservative modification of the knockoff procedure, where the threshold is

$$T = \min \left\{ t \in \mathcal{W} : \frac{1 + \# \{ j : W_j \le -t \}}{\max (\# \{ j : W_j \ge t \}, 1)} \le q \right\}$$

the +1 part makes it harder to reject the null:

$$\begin{split} \text{FDP} &= \frac{\#\left\{j: \beta_{j} = 0, W_{j} \geq -T\right\}}{\#\left\{j: W_{j} \geq T\right\} \vee 1} \cdot \frac{1 + \#\left\{j: \beta_{j} = 0, W_{j} \leq -T\right\}}{1 + \#\left\{j: \beta_{j} = 0, W_{j} \leq -T\right\}} \\ &\leq \frac{1 + \#\left\{j: W_{j} \leq -T\right\}}{\#\left\{j: W_{j} \geq T\right\} \vee 1} \cdot \frac{\#\left\{j: \beta_{j} = 0, W_{j} \geq T\right\}}{1 + \#\left\{j: \beta_{j} = 0, W_{j} \leq -T\right\}} \\ &\leq q \cdot 1 \end{split}$$

Then, we have the following theorem

Theorem 17.2.2: Property of the Knockoff Method

For any $q \in [0, 1]$, the **knockoff** method satisfies

$$\mathbb{E}\left[\frac{\#\{j: \beta_{j} = 0, j \in \hat{S}\}}{\#\{j: j \in \hat{S}\} + q^{-1}}\right] \le q$$

and the **knockoff+** method satisfies

$$\mathbb{E}\left[\frac{\#\left\{j:\beta_{j}=0,j\in\hat{S}\right\}}{\#\left\{j:j\in\hat{S}\right\}}\right]\leq q$$

in both cases, teh expectation is taken over the Gaussian noise in the model, while treating original variables X and knockoffs \tilde{X} as fixed

17.3 Candes et al. (2018)

Another way of constructing knockoffs, introduced by Candès et al. (2018), is by a swapping method:

Constructing the knockoffs for the family of random variables $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_p)$ are a new family of random variables $\tilde{\mathbf{X}} = (\tilde{\mathbf{X}}_1, \dots, \tilde{\mathbf{X}}_p)$ constructed with the following 2 properties

• for any subset $S \subset \{1, \dots, p\}$,

$$(\mathbf{X}, \tilde{\mathbf{X}})_{\text{swap}(S)} \stackrel{\text{d}}{=} (\mathbf{X}, \tilde{\mathbf{X}})$$

• $\tilde{X} \perp \!\!\! \perp Y \mid X$ if there is a response Y

Suppose $\mathbf{X} \sim \mathcal{N}(0, \Sigma)$, then $(\mathbf{X}, \tilde{\mathbf{X}})_{\text{swap}(S)}$ satisfies $(\mathbf{X}, \tilde{\mathbf{X}})_{\text{swap}(S)} \stackrel{\text{d}}{=} (\mathbf{X}, \tilde{\mathbf{X}})$ if

$$(\mathbf{X}, \tilde{\mathbf{X}})_{\text{swap}(S)} \stackrel{\text{d}}{=} (\mathbf{X}, \tilde{\mathbf{X}}) \sim \mathcal{N}(0, \mathbf{G}),$$
 where $\mathbf{G} = \begin{pmatrix} \mathbf{\Sigma} & \mathbf{\Sigma} - \text{diag}(s) \\ \mathbf{\Sigma} - \text{diag}(s) & \mathbf{\Sigma} \end{pmatrix}$

where diag(s) is any **diagonal matrix** s.t. G is **positive semidefinite**. The knockoffs constructed this way are named **MX knockoffs**. For **P**, the permutation matrix encoding the swap,

$$PGP = G$$

then we can sample the knockoff vector $\tilde{\mathbf{X}}$ from the conditional distribution

$$\tilde{\mathbf{X}} \mid \mathbf{X} \stackrel{\mathrm{d}}{=} \mathcal{N}(\mu, \mathbf{V})$$

where

$$\mu = \mathbf{X} - \mathbf{X}\mathbf{\Sigma}^{-1} \operatorname{diag}(s)$$

$$\mathbf{V} = 2\operatorname{diag}(s) - \operatorname{diag}(s)\mathbf{\Sigma}^{-1} \operatorname{diag}(s)$$

An important lemma is

Lemma 17.3.1: MX Knockoff Construction

For MX knockoffs, swapping null covariates with their knockoffs would not change the joint distribution of the original covariate X and their knockoffs \tilde{X} , conditional on the repsonse Y: Take any subset $S \subset \mathcal{H}_0$ of nulls, then

$$(\mathbf{X}, \tilde{\mathbf{X}}) \mid \mathbf{y} \stackrel{\mathrm{d}}{=} (\mathbf{X}, \tilde{\mathbf{X}})_{\mathrm{swap}(S)} \mid \mathbf{y}$$

Here, the main assumption of model-X knockoffs is assuming **known** joint distribution of covariates, and this leads to

Proposition 17.3.2: Conditional Exchangeability of MX Knockoffs

The random variables $(\tilde{\mathbf{X}}_1, \dots, \tilde{\mathbf{X}}_p)$ are **MX knockoffs** for $(\mathbf{X}_1, \dots, \mathbf{X}_p)$ if and only if for any $j \in \{1, \dots, p\}$, the pair $(\mathbf{X}_j, \tilde{\mathbf{X}}_j)$ is **exchangeable** conditional on all the other variables and their knockoffs.

under Prop.17.3.2, we can use the following algorithm to construct the MX Knockoffs

Algorithm 17.3.3: Sequential Conditional Independent Pairs

```
while j \le p do
    sample \tilde{\mathbf{X}}_j from \mathcal{L}(\mathbf{X}_j \mid \mathbf{X}_{-j}, \tilde{\mathbf{X}}_{1:j-1})
     <sup>a</sup>Example with p = 3
```

- j = 1: sample $\tilde{\mathbf{X}}_1'$ from $\mathcal{L}(\mathbf{X}_1 \mid \mathbf{X}_{2:3})$ j = 2: sample $\tilde{\mathbf{X}}_2$ from $\mathcal{L}(\mathbf{X}_2 \mid \mathbf{X}_1, \mathbf{X}_3, \tilde{\mathbf{X}}_1)$
- j = 3: sample $\tilde{\mathbf{X}}_3$ from $\mathcal{L}(\mathbf{X}_3 \mid \mathbf{X}_{1:2}, \tilde{\mathbf{X}}_{1:2})$

And an approximate construction can be achieved via matching the first 2 moments of $(X, \tilde{X})_{\text{SWad}(S)}$ and $(\mathbf{X}, \tilde{\mathbf{X}}),$

$$cov(X, \tilde{X}) = G$$

$$G = \begin{pmatrix} \Sigma & \Sigma - diag(s) \\ \Sigma - diag(s) & \Sigma \end{pmatrix}$$

which can be achieved through 2 ways:

• equicorrelated construction

$$s_j^{\text{EQ}} = 2\lambda_{\min}(\mathbf{\Sigma}) \wedge 1, \ \forall j$$

minimizing the correlation between variable knockoff pairs subject to the constraint that all such pairs must have the same correlation.

ISSUE with large $p: \lambda_{\min}(\Sigma)$ tends to be extremely small: computationally easy, but **low power** of s_i^{EQ}

semidefinite programme construction

minimize
$$\sum_j \left|1-s_j^{\rm SDP}\right|$$
 subject to
$$s_j^{\rm SDP} \geq 0, \; {\rm diag}\left(s^{\rm SDP}\right) \leq 2\Sigma$$

minimizing the **sum of the absolute values** of variable knockoff correlations between *all* suitable *s* **ISSUE** with large p: SDP (a convex problem) is computationally expensive

Hence, in high-dimensional situation, follow a 2-step procedure to combine both

• Step 1: choose an **approximation** Σ_{approx} of Σ and solve

minimize
$$\sum_{j}\left|1-\hat{s}_{j}\right|$$
 subject to
$$\hat{s}_{j}\geq0,\ \mathrm{diag}\left(\hat{s}_{j}\right)\leq2\Sigma_{\mathrm{approx}}$$

• Step 2: solve

maximize
$$\gamma$$
 subject to $\mathrm{diag}\left(\gamma \hat{s}\right) \leq 2\Sigma$

and set $s^{ASDP} = \gamma \hat{s}$

It's easy to see that this 2-step procedure can be reduced to equicorrelated or semidefinite programme

- equicorrelated: $\Sigma = \mathbf{I} \Rightarrow \hat{s}_j = 1, \gamma = 2 \times \lambda_{\min} \Sigma \wedge 1$
- semidefinite programme: $\Sigma = \Sigma$, $\hat{s}_i = s^{\text{SDP}}$, $\gamma = 1$

Calculate test statistics After constructing the knockoffs, we can construct the feature importance statistics by imposing a **flip sign** property: swapping the *j*th variable with its knockoff has the effect of changing the sign of W_i

$$w_{j}\left\{(\mathbf{X}, \tilde{\mathbf{X}})_{\text{swap}(S)}, \mathbf{y}\right\} = \begin{cases} w_{j}\left\{(\mathbf{X}, \tilde{\mathbf{X}}), \mathbf{y}\right\}, & j \notin S \\ -w_{j}\left\{(\mathbf{X}, \tilde{\mathbf{X}}), \mathbf{y}\right\}, & j \in S \end{cases}$$

consider a statistic T for each original and knockoff variable

$$\mathbf{T} \stackrel{\Delta}{=} (\mathbf{Z}, \tilde{\mathbf{Z}}) = (Z_1, \cdots, Z_p, \tilde{Z}_1, \cdots, \tilde{Z}_p) = t \{ (\mathbf{X}, \tilde{\mathbf{X}}), \mathbf{y} \}$$

if the components of T are switched in the same way:

$$(\mathbf{Z}, \tilde{\mathbf{Z}})_{\text{swap}(S)} = t \{ (\mathbf{X}, \tilde{\mathbf{X}})_{\text{swap}(S)}, \mathbf{y} \}$$

then the flip sign property can be achieved by setting

$$W_j = f_j(Z_j, \tilde{Z}_j)$$

where f_i is any **antisymmetric** function f(v, u) = -f(u, v)

Lemma 17.3.4: Feature Statistics: Lasso Coefficient Difference (LCD)

Consider the Lasso augmented with knockoffs

$$\min_{b \in \mathbb{R}^{2p}} \frac{1}{2} \| y - (\mathbf{X}, \tilde{\mathbf{X}}) b \|_{2}^{2} + \lambda \| b \|_{1}$$

which has solution $\hat{b}(\lambda) = (\hat{b}_1(\lambda), \dots, \hat{b}_p(\lambda), \hat{b}_{p+1}(\lambda), \dots, \hat{b}_{2p}(\lambda))$, then the statistic can be constructed as

$$W_j = Z_j - \tilde{Z}_j = |\hat{b}_j(\lambda)| - |\hat{b}_{j+p}(\lambda)|$$

and conditional on $(|W_1|, \dots, |W_p|)$, the sign of the null W_j s $(j \in \mathcal{H}_0)$ are i.i.d. coin flips^a.

- flip sign property: $W_{\text{swap}(S)} \stackrel{\Delta}{=} w \left\{ (\mathbf{X}, \tilde{\mathbf{X}})_{\text{swap}(S)}, \mathbf{y} \right\} \stackrel{d}{=} \epsilon \odot W = (\epsilon_1 W 1, \dots, \epsilon_p W_p)$
- Lemma 17.3.1: $W_{\text{swap}(S)} \stackrel{\text{d}}{=} W$ which establishes $W \stackrel{\text{d}}{=} \varepsilon \odot W$
- a large positive value of W_i provides some evidence that the distribution of Y depends on X_i
- value of λ can be chosen in any data-dependent fashion for a pair of \mathbf{y} and $(\mathbf{X}, \tilde{\mathbf{X}})$

Why i.i.d. coin flips? the null W_i s are symmetric

$$\#\{j: W_j \le -t, j \in \mathcal{H}_0\} \stackrel{d}{=} \#\{j: W_j \ge t, j \in \mathcal{H}_0\}$$

^aProof: for a sequence independent random variables $\epsilon = (\epsilon_1, \dots, \epsilon_p)$ s.t. $\epsilon_j = \pm 1$ with probability $\frac{1}{2}$ if $j \in \mathcal{H}_0$, and $\epsilon_j = 1$ otherwise, put $S = \{j : \epsilon_j = -1\} \subset \mathcal{H}_0$

and for any fixed threshold t > 0

$$\#\{j: W_j \le -t\} \ge \#\{j: W_j \le -t, j \in \mathcal{H}_0\}$$

so for the false discovery proportion (FDP)

$$FDP(t) = \frac{\# \{ j : W_j \ge t, j \in \mathcal{H}_0 \}}{\# \{ j : W_j \ge t \}}$$

an upward-biased estimate is

$$\widehat{\text{FDP}}(t) = \frac{\#\left\{j: W_j \leq -t\right\}}{\#\left\{j: W_j \geq t\right\}}$$

then Theorem 17.2.2 applies.

17.4 Fan et al. (2020)

The model-X knockoff (Candès et al., 2018) can accomodate an arbitrarily large p, but assumes **known** joint distribution of covariates. Fan et al. (2020) introduced a data-splitting procedure to separately estimate the unknown covariate distribution and then globally construct the knockoff variables.

- the components of ϵ are i.i.d. with sub-Gaussian distribution
- $\min_{j \in \mathcal{S}_n} \left| \beta_{0,j} \right| \ge k_n \left(\log(p)/n \right)^{1/2}$ for some slowly diverging sequence $k_n \xrightarrow{n \to \infty} \infty$: Lasso solution does not miss many important features
- $\exists c \in \left(\frac{2}{qs}, 1\right)$ s.t. with asymptotic probability $1, |\hat{S}| \ge cs$ for $\hat{S} = \{1 \le j \le p : W_j \ge T\}$: lower bound on the size of the sparse model

then we have

Theorem 17.4.1: Oracle Property of the MX Knockoff Procedure

Under the 3 conditions, all eigenvalues of Ω_0 are bounded away from 0 and ∞ , the smallest eigenvalue of $2\text{diag}(s) - \text{diag}(s)\Omega_0\text{diag}(s) > 0$ is bounded away from 0, $\lambda = C\sqrt{\log p/n}$ with C > 0. Then, the oracle MX knockoffs procedure satisfies that with probability at least $1 - c_3 p^{-c_3}$:

$$\operatorname{Power}(\hat{\mathcal{S}}) = \mathbb{E}\left[\frac{\left|\hat{\mathcal{S}} \cap \mathcal{S}_{0}\right|}{\left|\mathcal{S}_{0}\right|}\right] \geq 1 - C_{l_{1}}C_{\lambda}(\phi + 1)k_{n}^{-1} - c_{3}p^{-c_{3}} + o(k_{n}^{-1}) \xrightarrow{n \to \infty} 1$$

where ϕ is the golden ratio and C_{l_1} is some positive constant.

The oracle MX knockoffs procedure in knowing the true precision matrix Ω_0 for the covariate distribution can indeed have asymptotic power one.

RANK inference procedure The RANK inference procedure is

S1 Randomly split data (X, y) into two folds each of sample size n/2

- S2 Use $(\mathbf{X}^{(1)},\mathbf{y}^{(1)})$ to obtain $\hat{\mathbf{\Omega}}$ and a reduced model with support $\tilde{\mathcal{S}}$
- S3 Construct knockoffs matrix $\hat{\mathbf{X}} = \mathbf{X}^{(2)}(C^{\hat{\Omega}})' + ZB^{\hat{\Omega}}$ with Z an $\frac{n}{2} \times p$ matrix with i.i.d. $\mathcal{N}(0,1)$ components
- S4 Construct $W_j = W_j(\mathbf{y}^{(2)}, \mathbf{X}^{(2)}_{\tilde{S}}, \mathbf{X}_{\tilde{S}})$ for $j \in \tilde{S}$
- S5 Apply knockoff inference procedure to W_j 's to obtain final set of features \hat{S}

Implementing this modified procedure, we limit ourselves to sparse models \tilde{S} with size bounded by some positive integer K_n that diverges with n.

References

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

Emmanuel J Candès, Jianqing Fan, Lucas Janson, and Jinchi Lv. Panning for gold: 'model-x' knockoffs for high dimensional controlled variable selection. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 80(3):551–577, 2018.

Yingying Fan, Emre Demirkaya, Gaorong Li, and Jinchi Lv. Rank: Large-scale inference with graphical nonlinear knockoffs. *Journal of the American Statistical Association*, 115(529):362–379, 2020.