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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 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}\{\mathbf{s}\}\$ 

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  $\mathbf{C}'\mathbf{C} = 2\mathrm{diag}\left\{\mathbf{s}\right\} - \mathrm{diag}\left\{\mathbf{s}\right\} \sum_{i=1}^{n} \mathrm{diag}\left\{\mathbf{s}\right\} \geq \mathbf{0}$ 

- 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  $\lambda$  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:

<sup>1</sup>Other choices of 
$$W_j$$
 are  $W_j = \left| \mathbf{X}_j' \mathbf{y} \right| - \left| \mathbf{\tilde{X}}_j' \mathbf{y} \right|$ , 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

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

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

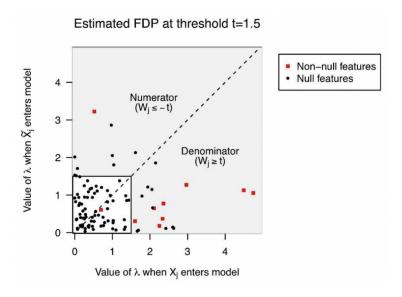


Figure 17.1: Visualizing Test Statistic Thresholding

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

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

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

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

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  $s_i^{\text{EQ}}$ 

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**  $\Sigma_{approx}$  of  $\Sigma$  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

$$W_i = f_i(Z_i, \tilde{Z}_i)$$

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<sup>a</sup>.

- 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  $\lambda$  can be chosen in any data-dependent fashion for a pair of  $\mathbf{v}$  and  $(\mathbf{X}, \tilde{\mathbf{X}})$

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

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

<sup>&</sup>lt;sup>a</sup>Proof: 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

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

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.

#### 

- ullet the components of  $\epsilon$  are i.i.d. with sub-Gaussian distribution
- $\min_{j \in S_n} |\beta_{0,j}| \ge k_n \left(\log(p)/n\right)^{1/2}$  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  $\Omega_0$  are bounded away from 0 and  $\infty$ 

# References

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