The knockoff filter

Statistical Learning
CLAMSES - University of Milano-Bicocca

Aldo Solari

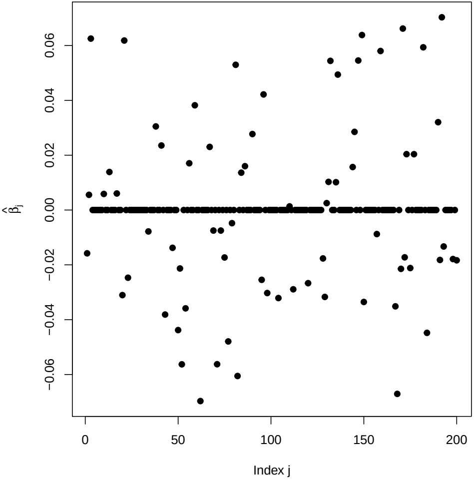
References

- Barber, Candès (2015) Controlling the False Discovery Rate via Knockoffs. Ann. Statist. 43:2504–2537
- Candès, Fan, Janson, Lv (2018). Panning for gold: model-X knockoffs for high dimensional controlled variable selection. JRSS-B 80:551–577.

There are two main approaches:

- *Fixed-X knockoffs*
  Requires that X is full rank with $n \geq 2p$
- *Model-X knockoffs*
  Requires assumptions on X but works with $p > n$

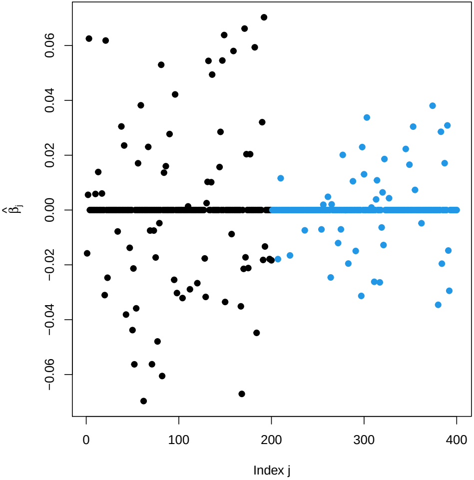
Fixed-X knockoffs



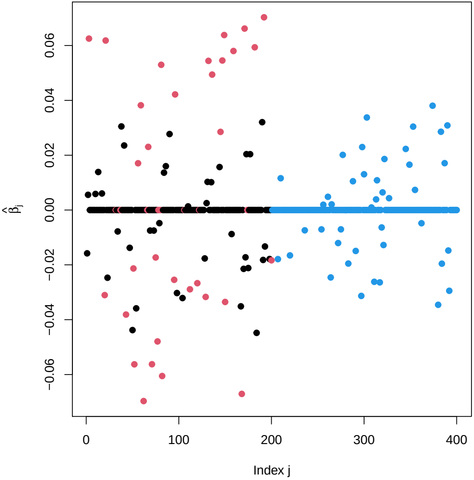
Lasso selects 67 features: $\mathrm{FDP}(\hat{S}) = ?/67$

Main idea

- For each feature X_j, construct a *knockoff* copy $\tilde{X}_j$
- Knockoffs $\tilde{X}_1, \ldots, \tilde{X}_p$ are independent of y and mimic the original variables $X_1, \ldots, X_p$ if they were null



Lasso selects 70 original and 43 knockoff: $\widehat{\mathrm{FDP}}(\hat{S}) \approx 43/70 \approx 61\%$



$$\text{True FDP}(\hat{S}) = 34/70 \approx 54\%$$

Knockoff construction

- Suppose without loss of generality that the features are centered and scaled such that $\|X_j\|_2^2 = 1$ for all j
- Let $\Sigma = X^t X$ be the correlation matrix of the features
- The method begins by augmenting the design matrix X with a second matrix $\tilde{X} \in \mathbb{R}^{n \times p}$ of knockoff variables, constructed to satisfy

$$\begin{aligned} G = [X \, \tilde{X}]^t [X \, \tilde{X}] &= \left[\begin{array}{cc} X^t X & X^t \tilde{X} \\ \tilde{X}^t X & \tilde{X}^t \tilde{X} \end{array} \right] \\ &= \left[\begin{array}{cc} \Sigma & \Sigma - D \\ \Sigma - D & \Sigma \end{array} \right] \end{aligned}$$

for some diagonal matrix $D = \mathrm{diag}(d_1, \ldots, d_p)$ such that G is positive definite

- The knockoffs have the same correlation structure as the original features

$$\tilde{X}^t\tilde{X} = X^tX = \Sigma$$

- The correlation between $\tilde{X}_k$ and X_j is

$$\tilde{X}_j^t X_k = X_j^t X_k \quad \forall\, k \neq j$$

- The correlation between $\tilde{X}_j$ and X_j is

$$\tilde{X}_j^t X_j = 1 - d_j$$

  with d_j as close to 1 as possible

Equi-correlated knockoffs

Suppose we require $d_j = d$ for all j. Define

$$\tilde{X} = X(I_p - d\Sigma^{-1}) + UC$$

where

- $U \in \mathrm{R}^{n \times p}$ is an orthonormal matrix such that $U^t X = 0$
- $C \in \mathrm{R}^{p \times p}$ from the Cholesky decomposition of

$$C^t C = 4((d/2)I_p - (d/2)^2 \Sigma^{-1})$$

This approach corresponds to `method="equi"` in the `knockoff` package. A semidefinite programming approach is used to determine the values that minimize $\sum_{j=1}^{p}(1 - d_j)$ subject to the constraints (`method="sdp"`)

The knockoff statistics

- Fit the lasso to the augmented design matrix $[X\ \tilde{X}]$ for $\lambda \in \Lambda$
- Let $[\hat{\beta}(\lambda)\ \ \tilde{\beta}(\lambda)]$, $\lambda \in \Lambda$ denote the coefficient estimates
- Compute

$$\begin{aligned} Z_j &= \sup\{\lambda \in \Lambda : \hat{\beta}_j(\lambda) \neq 0\} = \text{ first time } X_j \text{ enters the lasso path} \\ \tilde{Z}_j &= \sup\{\lambda \in \Lambda : \tilde{\beta}_j(\lambda) \neq 0\} = \text{ first time } \tilde{X}_j \text{ enters the lasso path} \end{aligned}$$

- Then define the statistics

$$W_j = \max(Z_j, \tilde{Z}_j) \cdot \mathrm{sign}(Z_j - \tilde{Z}_j) = \begin{cases} Z_j & \text{if } X_j \text{ enters first } (Z_j > \tilde{Z}_j) \\ 0 & \text{if } Z_j = \tilde{Z}_j \\ -\tilde{Z}_j & \text{if } \tilde{X}_j \text{ enters first } (Z_j < \tilde{Z}_j) \end{cases}$$

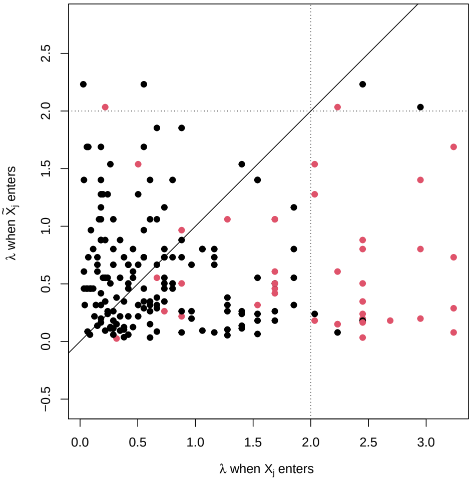
FDP estimate

- For some threshold $\tau \geq 0$, select

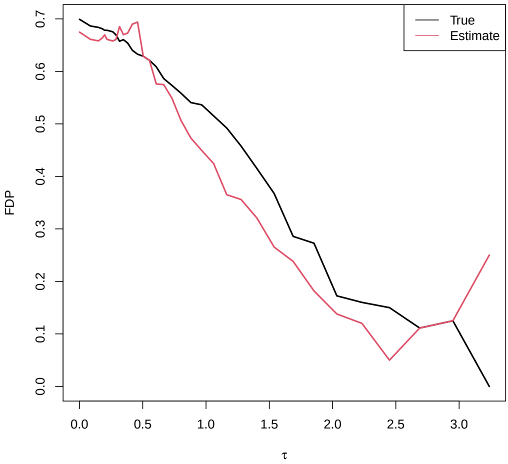
$$\hat{S}_\tau = \{j \in \{1, \ldots, p\} : W_j \geq \tau\}$$

- The knockoff estimate of the FDP is

$$\begin{aligned} \mathrm{FDP}(\hat{S}_\tau) &= \frac{\#\{j \in N : W_j \geq t\}}{\#\{j : W_j \geq t\}} \\ &\approx \frac{\#\{j \in N : W_j \leq -t\}}{\#\{j : W_j \geq t\}} \\ &\leq \frac{1 + \#\{j : W_j \leq -t\}}{\#\{j : W_j \geq t\}} = \widehat{\mathrm{FDP}}(\hat{S}_\tau) \end{aligned}$$



For $\tau = 2$, $|\hat{S}_\tau| = 29$ with $\widehat{\mathrm{FDP}}(\hat{S}_\tau) = 4/29$ and $\mathrm{FDP}(\hat{S}_\tau) = 5/29$


True
Estimate
FDP
τ
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.0
0.5
1.0
1.5
2.0
2.5
3.0

The knockoff procedure chooses a data-dependent threshold

$$\hat{\tau} = \min\left\{\tau > 0 : \widehat{\mathrm{FDP}}(\hat{S}_\tau) \leq \alpha\right\}$$

with $\hat{\tau} = +\infty$ if no such τ exists.

Theorem

For any $\alpha \in (0, 1)$, the knockoff procedure selects

$$\hat{S}_{\hat{\tau}} = \{j \in \{1, \ldots, p\} : W_j \geq \hat{\tau}\}$$

with the guarantee that

$$\mathrm{FDR}(\hat{S}_{\hat{\tau}}) = \mathbb{E}\left(\frac{|N \cap \hat{S}_{\hat{\tau}}|}{|\hat{S}_{\hat{\tau}}|}\right) \leq \alpha$$

where the expectation is taken over ε in the Gaussian linear model $y = X\beta + \varepsilon$ while treating X and $\tilde{X}$ as fixed.

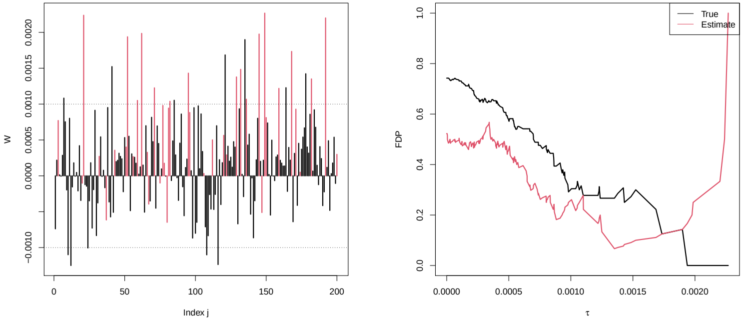
Variable importance statistics

- Fit the Random Forest to the augmented design matrix $[X \; \tilde{X}]$
- Compute

$$
\begin{aligned}
Z_j &= \text{VariableImportance}(X_j) \\
\tilde{Z}_j &= \text{VariableImportance}(\tilde{X}_j)
\end{aligned}
$$

  The importance of a variable is measured as the total decrease in node impurities from splitting on that variable, averaged over all trees
- Then define the statistics

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



$$\text{For } \tau = 0.001,\ |\hat{S}_\tau| = 23 \text{ with } \widehat{\mathrm{FDP}}(\hat{S}_\tau) = 4/23 \text{ and } \mathrm{FDP}(\hat{S}_\tau) = 7/23$$

Model-X knockoff

Modeling X

- X is treated as a random matrix with i.i.d. rows x_i
- (x_i, y_i), $i = 1, \ldots, n$ are i.i.d. from some unknown distribution
- Assume we know the *marginal distribution* of x_i, e.g.

$$x_i = (x_{i1}, \ldots, x_{ip}) \sim N_p(\mu, \Sigma)$$

- Null features given by *conditional independence*

$$N = \{j \in \{1, \ldots, p\} : y \perp\!\!\!\perp x_j | x_{-j}\}$$

where $x_{-j} = \{x_1, \ldots, x_p\} \setminus \{x_j\}$

Knockoffs in the Gaussian case

- The joint distribution of original features and knockoff copies satisfies

$$[x\ \tilde{x}] \sim N(M, V) \quad \text{with } M = \begin{bmatrix} \mu \\ \mu \end{bmatrix}, \quad V = \begin{bmatrix} \Sigma & \Sigma - D \\ \Sigma - D & \Sigma \end{bmatrix}$$

  where $D = \text{diag}(d_1, \ldots, d_p)$ such that V is positive definite

- Draw a random $\tilde{x}_i$ from the conditional distribution $\tilde{x}_i | x_i$, which is normal with

$$\begin{aligned} \mathbb{E}(\tilde{x}_i | x_i) &= \mu + (\Sigma - D)\Sigma^{-1}(x_i - \mu) \\ \mathbb{V}\text{ar}(\tilde{x}_i | x_i) &= \Sigma - (\Sigma - D)\Sigma^{-1}(\Sigma - D) \end{aligned}$$

- If μ and Σ are unknown, replace by estimates $\hat{\mu}$ and $\hat{\Sigma}$