Using Probabilistic Knockoffs of Binary Variables to Control the False Discovery Rate

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Overview

1. Original Knockoffs: What They Do and Where They Fail
2. Making Knockoffs Work With GLMs
3. Random Binary Knockoffs: The Theory
4. Random Binary Knockoffs: Performance
5. Where to next?

Variable Selection in Linear Regression

Assume

$$\mathbf{y} = X\beta + \mathbf{z}$$

where $\mathbf{y} \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$, $\beta \in \mathbb{R}^p$, and $\mathbf{z}$ is Gaussian noise. Also, assume sparsity:

$$\beta_i = 0 \quad \forall i \notin S$$

How do we choose a model $\hat{S}$?

False Discovery Rate

A common goal for a method that generates $\hat{S}$ is to control the false discovery rate

$$\mathrm{FDR} = \mathrm{E}\left[\frac{|\{j : \beta_j = 0 \;\&\; j \in \hat{S}\}|}{\max\{|\hat{S}|, 1\}}\right]$$

In other words, control proportion of elements in $\hat{S}$ which aren't in S.

FDR is controlled at level q if $q \geq$FDR irrespective of true β.

Knockoff Features

Knockoff variables can be used to control FDR in linear regression.

- The idea is to create a forgery of each variable; if the forgeries seem about as good predictors as the originals, the originals are lousy predictors.
- For each variable X_i, create a knockoff feature $\tilde{X}_i$ such that, where $X^T X = G$, $\mathrm{diag}\{X^T X\} - s$ is small and

$$\tilde{X}^T \tilde{X} = G \quad \& \quad X^T \tilde{X} = G - \mathrm{diag}\{\mathbf{s}\}$$

- $\tilde{X}_i$ and X_i will have same correlation with other variables, but only low correlation with each other.
- For $\tilde{X}$ to exist, it must be the case that

$$G_L = [X\ \tilde{X}]^T [X\ \tilde{X}] = \begin{bmatrix} G & G - \mathrm{diag}\{\mathbf{s}\} \\ G - \mathrm{diag}\{\mathbf{s}\} & G \end{bmatrix} \succeq 0$$

- Given $\mathbf{s}$, $\tilde{X}$ can be generated via a rotation of X.

Knockoff Filter

These knockoffs can be used in the knockoff filter method.

- Fit full path of LASSO regression on $[\,X\,\tilde{X}\,] := X_L$.

$$\beta(\lambda) = \arg\min_{\mathbf{b}} \left\{ \frac{1}{2}\|\mathbf{y} - X_L\mathbf{b}\|_2^2 + \lambda\|\mathbf{b}\|_1 \right\}$$

- Z_i, $\tilde{Z}_i$ are the largest λ such that X_i, $\tilde{X}_i$ have nonzero coefficient.
- $W_i = Z_i$ if $Z_i > \tilde{Z}_i$, otherwise $W_i = -\tilde{Z}_i$.
- Since G_L & $[\,X\,\tilde{X}\,]^T\mathbf{y}$ are sufficient statistics for $\beta(\lambda)$, W_i symmetrically distributed around 0 when X_i null predictor.
- Thus, FDR controlled when $\hat{S} = \{i : W_i \geq T\}$ for

$$T = \min\left\{ t > 0 \;:\; \frac{|\{j : W_j \leq -t\}|}{\max\{|\{j : W_j \geq t\}|, 1\}} \leq q \right\}$$

Variable Selection in GLMs

Knockoffs work great for linear regression, but what about GLMs?

Now, assume, for some link function g and $y_1, \ldots, y_n$ from a exponential family distribution,

$$\mathrm{E}(\mathbf{y}) = g(X\beta)$$

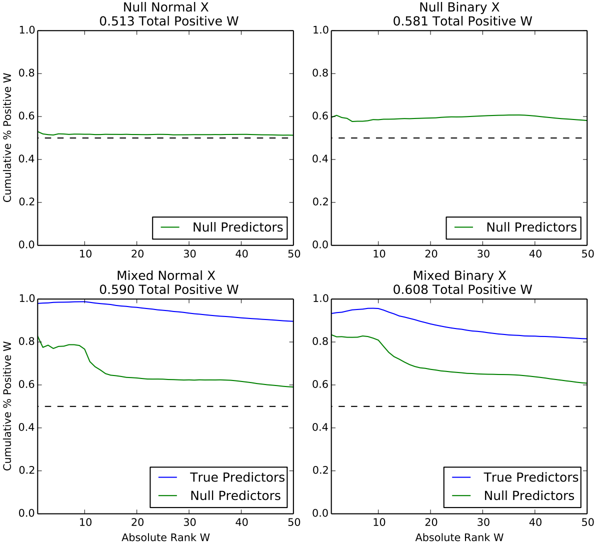
where $X \in \mathbb{R}^{n \times p}$ and $\beta \in \mathbb{R}^p$. Also, assume sparsity:

$$\beta_i = 0 \quad \forall i \notin S$$

How do we choose a model $\hat{S}$?

Where Knockoff Filter Fails

Knockoff filter doesn't work for other GLMs.



Can Knockoffs Be Fixed for GLMs?

- Other GLMs don't have the same sufficient statistics as linear regression.
- Original Knockoffs don't remotely have same distribution as X, so "look" different than real variables.
- Knockoffs will likely work better if they have the same marginal distribution as originals.
- For X_i with arbitrary distribution, unclear how this might be accomplished.

Random Binary Notation

- Binary data is common in data analysis and a much more manageable family of distributions for X.
- We can think of observations in X as observations of random binary vector $\mathbf{x} \in \{0,1\}^p$.
- The full family for $\mathbf{x}$ is multinomial on 2^p outcomes.
- Can summarize with the first two moments:

$$\mathrm{E}(\mathbf{x}\mathbf{x}^T) = M \in [0,1]^{p \times p} \quad \& \quad \mathrm{diag}\{M\} = \mathrm{E}(\mathbf{x}) = \mathbf{m} \in [0,1]^p$$

- For arbitrary M to correspond to a random binary vector, must be case that $M - \mathbf{m}\mathbf{m}^T = \Sigma \succeq 0$

$$\max\{0, m_i + m_j - 1\} \leq M_{ij} \leq \min\{m_i, m_j\}$$

Random Binary Knockoffs

- Integer programing is NP-hard, making finding $\tilde{X} \in \{0,1\}^{n \times p}$ to fit correlations optimally difficult.
- Instead, introduce a relaxed problem where $\tilde{X} \mid X$ is drawn randomly such that, where $\Sigma = \mathrm{Cov}(\mathbf{x})$

$$\mathrm{Cov}(\tilde{\mathbf{x}}, \mathbf{x}) = \Sigma - \mathrm{diag}\{\mathbf{s}\} \quad \& \quad \mathrm{Cov}(\tilde{\mathbf{x}}) = \Sigma$$

- For this to correspond to a random binary vector, must be the case

$$\Sigma_L = \mathrm{Cov}([\,\mathbf{x}\,\tilde{\mathbf{x}}\,]) = \begin{bmatrix} \Sigma & \Sigma - \mathrm{diag}\{\mathbf{s}\} \\ \Sigma - \mathrm{diag}\{\mathbf{s}\} & \Sigma \end{bmatrix} \succeq 0$$

- Almost same correlation condition as before, but only holds in expectation.
- Switch from Gramian matrix to correlation matrix makes moment condition less likely to be violated.

Quadratic Programing

- Simplest approach to is to draw the entries of $\tilde{X}$ independently based on probabilities $P \in [0,1]^{n \times p}$.
- P should satisfy

$$\begin{array}{rl} \text{minimize} & \|X^T P - (M - \mathrm{diag}\{s\})\|_{fro}^2 + \sum_{i \neq j} (P_i^T P_j - M_{ij})^2 \\ \text{subject to} & \mathbf{1}^T P = \mathbf{m} \\ & 0 \leq P \leq 1 \end{array}$$

- Can be formulated as a quadratic program with slack variables

$$\begin{array}{rl} \text{minimize} & \|W\|_{fro}^2 + \|V\|_{fro}^2 \\ \text{subject to} & -W \leq X^T P - (M - \mathrm{diag}\{s\}) \leq W \\ & -V_{ij} \leq P_i^T P_j - M_{ij} \leq V_{ij} \quad \forall i \neq j \\ & \mathbf{1}^T P = \mathbf{m} \\ & 0 \leq P \leq 1 \end{array}$$

- Huge optimization problem, likely computationally difficult.

Ising Model

- Alternatively, find a random binary vector variable $\mathbf{x}_L$ that has cross-moments M_L corresponding to Σ_L.
- The Ising model can match any proper M_L. If A is a lower triangular matrix and L the logistic link function

$$\mathrm{P}(\mathbf{x} = \gamma) \propto L(\gamma^T A \gamma)$$

- The Ising model binary analog of normal distribution; maximum entropy for given covariance matrix.
- Very easy to draw successive entries

$$\mathrm{P}(x_i = 1 \mid x_1, ..., x_{i-1}) = L\left(A_{ii} + \sum_{k=1}^{i-1} A_{ik} x_i\right)$$

- Once fit, can draw $\tilde{\mathbf{x}} \mid \mathbf{x}$ easily.

Fitting Ising Model

- If we were just trying to fit A to X, we could do so via successive logistic regression to fit row $\mathbf{a}_i$.
- Instead, simulate $\mathbf{m}_i = f(\mathbf{a}_i)$ and fit via Newton-Raphson.
- Draw K samples $\mathbf{x}_{-i}^{(k)} \sim \mathbf{x}_{-i}$. Then

$$f(\mathbf{a}_i) \approx \frac{1}{K} \sum_{k=1}^{K} L\left(\mathbf{a}_i^T \begin{bmatrix} \mathbf{x}_{-i}^{(k)} \\ 1 \end{bmatrix}\right) \begin{bmatrix} \mathbf{x}_{-i}^{(k)} \\ 1 \end{bmatrix}$$

$$J(\mathbf{a}_i) \approx \frac{1}{K} \sum_{k=1}^{K} L'\left(\mathbf{a}_i^T \begin{bmatrix} \mathbf{x}_{-i}^{(k)} \\ 1 \end{bmatrix}\right) \begin{bmatrix} \mathbf{x}_{-i}^{(k)} \\ 1 \end{bmatrix} \begin{bmatrix} [x_{-i}^{(k)}]^T & 1 \end{bmatrix}$$

- Make successive updates

$$\mathbf{a}_i^{(k+1)} = \mathbf{a}_i^{(k)} - \left[J\left(\mathbf{a}_i^{(k)}\right)\right]^{-1} \left[f\left(\mathbf{a}_i^{(k)}\right) - \mathbf{m}_i\right]$$

Computational Issues

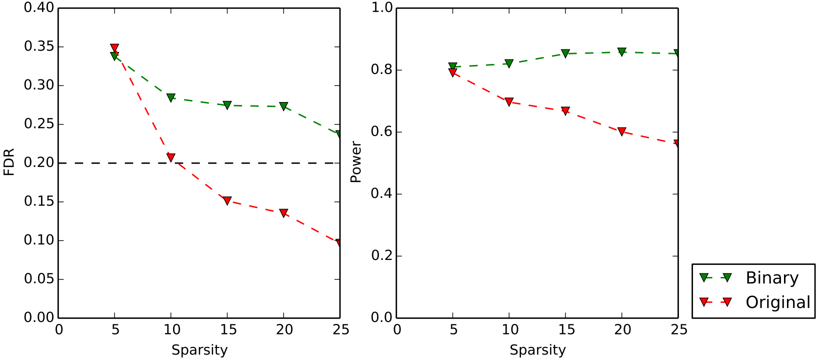
- K must be very large for big p and high correlation.
- This makes $J(\mathbf{a}_i)$ and even $f(\mathbf{a}_i)$ very expensive to calculate.
- This makes quasi-Newtonian methods, where $J(\mathbf{a}_i)$ is approximated, appealing.
- In particular, Anderson Mixing, where f approximated with secant hyperplane through $\mathbf{a}_i^k, \ldots, \mathbf{a}_i^{(k-h+1)}$ works well
- When K too small, can instead solve relaxed problem

$$\mathbf{m}_i^*(\tau) = (1-\tau)\mathbf{m}_i + \tau \begin{bmatrix} 0 & \ldots & 0 & M_{ii} \end{bmatrix}^T$$

- n doesn't matter, but this method is also fairly impractical for large p.

Random Binary Knockoffs in Linear Regression

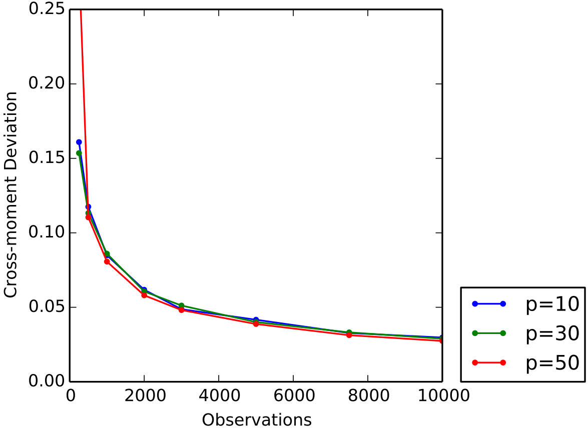
Random binary Knockoffs only provide approximate FDR control for linear regression.



They select too many variables, causing higher power at the expense of FDR control.

Distortion from M_L

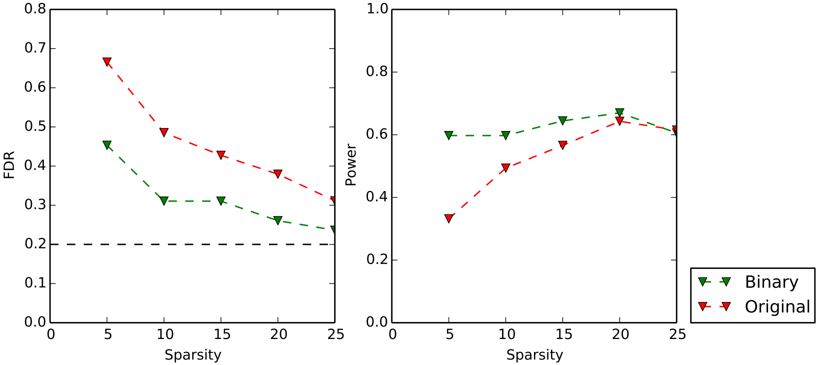
Since $\tilde{X}$ is randomly generated, $\frac{1}{n}X_L^T X_L$ deviates from M_L.



As n increases, this effect diminishes.

Random Binary Knockoffs in Logistic Regression

Random Binary Knockoffs perform much better than original knockoffs in logistic regression.



They have lower FDR and higher power.

Discussion

- Random Binary Knockoffs seem to offer promise as a useful technique, but have outstanding issues.
- Seem to offer a method to extend Knockoffs for one type of variable to GLMs.
- Computational complexity prohibitive; simpler method, perhaps by good approximation of P, would be helpful.
- Random distortion from desired cross-moments might be compensated for by ensemble method based on multiple $\tilde{X}$.
- Might build higher order interactions into Ising model to allow for nasty data.