

1 Variable Selection

Let y be response variable and x be explanatory variables or covariates. Given i.i.d. samples $(x, y) \in \mathbb{R}^p \times \mathbb{R}$ from the joint distribution $p_{x,y}$, we are interested in asking the question

which of the many covariates x_1, \dots, x_p does the response y depend on?

assuming that the response does depend on a sparse set of variables. In general, we want to find a subset $\mathcal{S} \subset [p]$ such that \mathcal{S} retains the relevant information in x for making inference about y ,

$$\begin{aligned} & \text{maximize}_{\mathcal{S} \subset [p]} \quad \mathcal{Q}(\mathcal{S}) \\ & \text{subject to} \quad \|\mathcal{S}\|_0 \leq t \end{aligned}$$

where $\mathcal{Q}(\cdot)$ quantifies the relevance of a feature subset to response. The choice of $\mathcal{Q}(\cdot)$ should be 1) capable of detecting the desired functional dependence between the covariates and the response and 2) concentrated with respect to the underlying measure (generalize well to test data) [1]. Example of criteria $\mathcal{Q}(\cdot)$ include leave-one-out error bound of SVM, mutual information $I(x; y)$, and Hilbert Space-based estimator like Hilbert-Schmidt Independence Criterion (HSIC) [2].

$$\begin{aligned} & \text{maximize}_{\mathcal{S} \subset [p]} \quad I(x_{\mathcal{S}}; y) \\ & \text{subject to} \quad \|\mathcal{S}\|_0 \leq t \end{aligned}$$

2 Instance-wise Variable Selection

The goal of instance-wise variable selection is to find a subset $\mathcal{S}(x) \subset [p]$ most informative in making inference about y . Here $\mathcal{S} : \mathcal{X} \rightarrow \{0, 1\}^d$ is a function dependent on a particular covariates x , and there fore $\mathcal{S}(x)$ is a random variable. For example, L2X maximizes the lower bound of mutual information between response and selected features [3]

$$\begin{aligned} & \text{maximize}_{\mathcal{S}} \quad I(x_{\mathcal{S}(x)}; y) \\ & \text{subject to} \quad \|\mathcal{S}(x)\|_0 \leq t \end{aligned}$$

Similarly, INVASE finds \mathcal{S} such that $y \perp\!\!\!\perp x_{\mathcal{S}(x)} \mid x_{\mathcal{S}(x)}$ or that $p_{y|x}(\cdot|x) \stackrel{d}{=} p_{y|x_{\mathcal{S}(x)}}(\cdot|x_{\mathcal{S}(x)})$ [4],

$$\begin{aligned} & \text{minimize}_{\mathcal{S}} \quad KL \left(p_{y|x}(\cdot|x) \parallel p_{y|x_{\mathcal{S}(x)}}(\cdot|x_{\mathcal{S}(x)}) \right) \\ & \text{subject to} \quad \|\mathcal{S}(x)\|_0 \leq t \end{aligned}$$

3 Variable Selection as Finding Markov Blanket

In reality, we are interested in the causal relationship. However, quantifying causal effects requires interventions and not possible from purely observational data. A natural relaxation is to find covariates dependent (in a statistical sense) on the response, conditioned on all other observed features [5]. Formally, we want to find smallest $\mathcal{S} \subset [p]$ s.t.

$$y \perp\!\!\!\perp x_{\setminus \mathcal{S}} \mid x_{\mathcal{S}}$$

A natural interpretation is that the other variables $\mathbf{x}_{\setminus \mathcal{S}}$ do not provide additional information about y . If we think of \mathcal{G} as graph representing the joint distribution $p_{\mathbf{x}, y}$, then \mathcal{S} is the markov blanket for node y . Alternatively, we can interpretate $\mathbf{x}_{\mathcal{S}}$ as minimal sufficient statistics for predicting y . This connection exists in literature related to information bottleneck method. We can pose the problem of finding the Markov blanket of y as a multiple

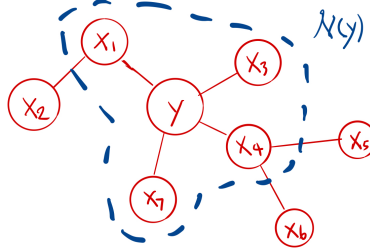


Figure 1: $\mathcal{S} = \{x_1, x_3, x_4, x_7\}$

(independent) binary hypothesis test

$$H_0^{(j)} : y \perp\!\!\!\perp x_j \mid \mathbf{x}_{\setminus \{j\}} \quad \text{for } j = 1, \dots, p \quad (1)$$

Let $\mathcal{H}_0 = \{j \mid H_0^{(j)} \text{ holds}\}$ be the set of truly irrelevant covariates. In general, we are interested in maximizing true positives while controlling the number of false positives. Sometimes, a global threshold for p-values of each tests is overly conservative for large p , an alternative approach is to maximize *power* while control *false discovery rate* (FDR) [6].

$$\text{maximize}_{\mathcal{S} \subset [p]} \quad \mathbb{E} \left[\frac{|\mathcal{S} \setminus \mathcal{H}_0|}{|\mathcal{S}|} \right] \quad (2)$$

$$\text{subject to} \quad \text{FDR} := \mathbb{E} \left[\frac{|\mathcal{S} \cap \mathcal{H}_0|}{\max\{|\mathcal{S}|, 1\}} \right] \leq q \quad (3)$$

where expectation is take w.r.t. randomness in \mathbf{x} and y . If $p_{y|\mathbf{x}}(\cdot|x)$ assumes a parametric generalized linear model form,

$$\mathbb{E}[y|\mathbf{x}] = g^{-1}(\eta) \quad \eta = \beta_1 x_1 + \dots + \beta_p x_p$$

Then by [7], testing for conditional independence (1) is equivalent to the following test,

$$H_0^{(j)} : \beta_j = 0 \quad \text{for } j = 1, \dots, p$$

4 Model-X Knockoff

Traditionally, $p_{y|\mathbf{x}}$ is chosen to be in some parametric family, e.g. GLM, and variable selection with FDR control is performed by computing & plugging p-values into the BHq procedure [6]. Recently, [8, 7] designed a *knockoff* framework for performing variable selection on high-dimensional nonparametric models with finite sample guarantees over the constraints in (3). The framework requires significant knowledge of $p_{\mathbf{x}}$ and assumes nothing about the $p_{y|\mathbf{x}}$. This might give way to performing reproducible and robust variable selection where the $p_{y|\mathbf{x}}$ is parameterized by highly complex mappings, e.g. neural networks. In

addition, modeling $p_{\mathbf{x}}$ might be a suitable task for problems where we have large amount of unsupervised data, or we know a priori some structure about $p_{\mathbf{x}}$, which are often the case for large scale machine learning applications.

Definition. $\tilde{\mathbf{x}}$ is a model- X knockoff for \mathbf{x} if

$$\tilde{\mathbf{x}} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{x} \quad (4)$$

$$(\mathbf{x}, \tilde{\mathbf{x}})_{\text{swap}(\mathcal{S})} \stackrel{d}{=} (\mathbf{x}, \tilde{\mathbf{x}}) \quad \text{for any} \quad \mathcal{S} \subset [p] \quad (5)$$

where $(\cdot)_{\text{swap}(\mathcal{S})}$ swaps coordinates for all $j \in \mathcal{S}$ with coordinate $j + p$ and leaves other coordinate unchanged. Note (5) is equivalent to below

$$(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_p, \tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_j, \dots, \tilde{\mathbf{x}}) \stackrel{d}{=} (\mathbf{x}_1, \dots, \tilde{\mathbf{x}}_j, \dots, \mathbf{x}_p, \tilde{\mathbf{x}}_1, \dots, \mathbf{x}_j, \dots, \tilde{\mathbf{x}}) \quad (6)$$

for any $j = 1, \dots, p$. (4) is guaranteed if $\tilde{\mathbf{x}}$ is constructed without knowledge of \mathbf{y} .

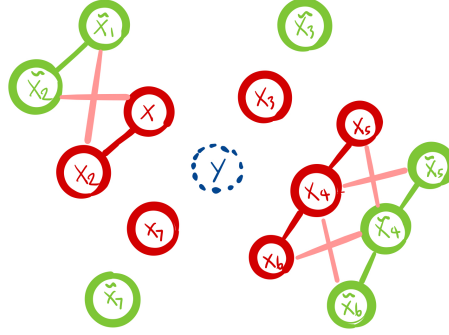


Figure 2: \mathcal{G} represents $p_{\mathbf{x}, \tilde{\mathbf{x}}}$. (4) implies $\tilde{\mathbf{x}}$ is not in the Markov blanket of node \mathbf{y} for a graph representing joint distribution $p_{\mathbf{x}, \tilde{\mathbf{x}}}$. (5) implies that the $\mathbf{x}, \tilde{\mathbf{x}}$ are pairwise exchangeable, i.e. taking any subset of (green) variables and swap them with their (red) knockoff creates an isomorphism of \mathcal{G} , i.e. edges preserved from the perspective of swapped variables. In practice, we want $\mathbf{x}_j, \tilde{\mathbf{x}}_j$ be as independent as possible, i.e. no edge connecting $\mathbf{x}_j, \tilde{\mathbf{x}}_j$ for all $j \in [p]$

Intuitively, *knockoffs* mimics the dependence structure as the original covariates \mathbf{x} , while being invariant to $\text{swap}(\cdot)$ operation, and is independent of the response \mathbf{y} . It serves as a control for evaluating how much of dependence on the response is due to dependence structure of other variables and how much of it is due to dependence with response \mathbf{y} .

4.1 Knockoff Procedure for LASSO

Consider a linear Gaussian model $\mathbf{y} = \beta^T \mathbf{x} + \epsilon$ where $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and $\epsilon \sim \mathcal{N}(0, 1)$. Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ be any design matrix with $n > p$. The knockoff filtering procedure for computing variable selection with controlled FDR is given by

1. (**Generate Knockoffs**) To ensure exchangeability property (5), it must be

$$\begin{pmatrix} \mathbf{x} \\ \tilde{\mathbf{x}} \end{pmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma} & \boldsymbol{\Sigma} - \text{diag}\{\mathbf{s}\} \\ \boldsymbol{\Sigma} - \text{diag}\{\mathbf{s}\} & \boldsymbol{\Sigma} \end{bmatrix} \right)$$

One way to construct knockoff is to sample \tilde{x} from the conditional distribution [7, 5],

$$\begin{aligned}\tilde{x} \mid (x = x) &\sim \mathcal{N}\left(\mu_{\tilde{x}|x}(x), \Sigma_{\tilde{x}|x}(x)\right) \\ \mu_{\tilde{x}|x}(x) &= (I - \text{diag}\{\mathbf{s}\} \Sigma^{-1}) x + \text{diag}\{\mathbf{s}\} \Sigma^{-1} \mu \\ \Sigma_{\tilde{x}|x}(x) &= 2 \text{diag}\{\mathbf{s}\} - \text{diag}\{\mathbf{s}\} \Sigma^{-1} \text{diag}\{\mathbf{s}\}\end{aligned}$$

Alternatively, we can match empirical first and second moment [8] and construct design for knockoff as

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

where $\tilde{\mathbf{U}} \in \mathbb{R}^{n \times p}$ is orthonormal matrix whose column is orthogonal to \mathbf{X} and $\mathbf{C}^T \mathbf{C} = 2 \text{diag}\{\mathbf{s}\} - \text{diag}\{\mathbf{s}\} \Sigma^{-1} \text{diag}\{\mathbf{s}\}$ is a Cholesky decomposition.

2. **(Compute Pairwise Statistics)** Compute Lasso for the coefficients

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^{2p}} \frac{1}{2} \left\| \mathbf{y} - [\mathbf{X}, \tilde{\mathbf{X}}] \beta \right\|_2^2 + \lambda \|\beta\|_1$$

Now we compute statistics w for each pair of original and knockoff variables

$$w_j := w_j(\mathbf{X}, \tilde{\mathbf{X}}, \mathbf{y}) = |\hat{\beta}_j| - |\hat{\beta}_{j+p}| \quad \text{for } j = 1, \dots, p$$

which satisfy the coin-flip property. One important consequence is that for any $j \in \mathcal{H}_0$, w_j is a symmetric distribution about the origin [8, 7].

3. **(Compute Threshold for Statistics)** Given $q > 0$ be target FDR, then let

$$\tau_+ = \min \left\{ t > 0 \mid \widehat{\text{FDP}}(t) \leq q \right\} \quad \text{where} \quad \widehat{\text{FDP}} = \frac{1 + \#\{j \mid w_j \leq -t\}}{\#\{j \mid w_j \geq t\}}$$

4. **(Perform Test)** with threshold τ_+ ,

$$\mathcal{S} = \{j \mid w_j \geq \tau_+\}$$

ensures that $\text{FDR} \leq q$

4.2 Current Problems

1. Generating knockoffs is a hard problem, there has been work to sample knockoffs using MCMC [9], with generative model [10], in particular with GAN [11] and with latent variable models [5].
2. There has been a few papers that tries to analyze power of the knockoff framework assuming Gaussian data [12]
3. There has been some preliminary work on adopting multiple hypothesis testing and FDR control when $p_{y|x}$ is parameterized by neural networks, e.g. by MLP [13]. The challenge here seems that it is not easy to maintain power of tests.
4. It seems that currently, experimental datasets is either simulated or small in size of n, p . I have not found any attempts that tried this method on image datasets. Might be interesting to see how this fairs.

References

- [1] Le Song et al. “Feature Selection via Dependence Maximization”. In: *Journal of Machine Learning Research* 13.47 (2012), pp. 1393–1434. URL: <http://jmlr.org/papers/v13/song12a.html> (visited on 04/24/2020).
- [2] Arthur Gretton et al. “Measuring Statistical Dependence with Hilbert-Schmidt Norms”. In: *Algorithmic Learning Theory*. Ed. by Sanjay Jain, Hans Ulrich Simon, and Etsuji Tomita. Red. by David Hutchison et al. Vol. 3734. Series Title: Lecture Notes in Computer Science. Berlin, Heidelberg: Springer Berlin Heidelberg, 2005, pp. 63–77. ISBN: 978-3-540-29242-5 978-3-540-31696-1. DOI: [10.1007/11564089_7](https://doi.org/10.1007/11564089_7). URL: http://link.springer.com/10.1007/11564089_7 (visited on 04/24/2020).
- [3] Pieter-Jan Kindermans et al. “Learning how to explain neural networks: PatternNet and PatternAttribution”. In: *arXiv:1705.05598 [cs, stat]* (Oct. 24, 2017). arXiv: [1705.05598](https://arxiv.org/abs/1705.05598). URL: <http://arxiv.org/abs/1705.05598> (visited on 01/16/2020).
- [4] Jinsung Yoon, James Jordon, and Mihaela van der Schaar. “INVASE: Instance-wise Variable Selection using Neural Networks”. In: International Conference on Learning Representations. Sept. 27, 2018. URL: <https://openreview.net/forum?id=BJg-roAcK7> (visited on 04/26/2020).
- [5] Jaime Roquero Gimenez, Amirata Ghorbani, and James Zou. “Knockoffs for the mass: new feature importance statistics with false discovery guarantees”. In: *arXiv:1807.06214 [cs, stat]* (May 28, 2019). arXiv: [1807.06214](https://arxiv.org/abs/1807.06214). URL: <http://arxiv.org/abs/1807.06214> (visited on 04/17/2020).
- [6] Yoav Benjamini and Yosef Hochberg. “Controlling The False Discovery Rate - A Practical And Powerful Approach To Multiple Testing”. In: *J. Royal Statist. Soc., Series B* 57 (Nov. 30, 1995), pp. 289–300. DOI: [10.2307/2346101](https://doi.org/10.2307/2346101).
- [7] Emmanuel Candes et al. “Panning for Gold: Model-X Knockoffs for High-dimensional Controlled Variable Selection”. In: *arXiv:1610.02351 [math, stat]* (Dec. 12, 2017). arXiv: [1610.02351](https://arxiv.org/abs/1610.02351). URL: <http://arxiv.org/abs/1610.02351> (visited on 02/03/2020).
- [8] Rina Foygel Barber and Emmanuel J. Candès. “Controlling the false discovery rate via knockoffs”. In: *The Annals of Statistics* 43.5 (Oct. 2015), pp. 2055–2085. ISSN: 0090-5364. DOI: [10.1214/15-AOS1337](https://doi.org/10.1214/15-AOS1337). arXiv: [1404.5609](https://arxiv.org/abs/1404.5609). URL: <http://arxiv.org/abs/1404.5609> (visited on 04/14/2020).
- [9] Stephen Bates et al. “Metropolized Knockoff Sampling”. In: *arXiv:1903.00434 [stat]* (Mar. 1, 2019). arXiv: [1903.00434](https://arxiv.org/abs/1903.00434). URL: <http://arxiv.org/abs/1903.00434> (visited on 04/18/2020).
- [10] Yaniv Romano, Matteo Sesia, and Emmanuel J. Candès. “Deep Knockoffs”. In: *arXiv:1811.06687 [math, stat]* (Nov. 16, 2018). arXiv: [1811.06687](https://arxiv.org/abs/1811.06687). URL: <http://arxiv.org/abs/1811.06687> (visited on 02/26/2020).
- [11] James Jordon, Jinsung Yoon, and Mihaela van der Schaar. “KnockoffGAN: Generating Knockoffs for Feature Selection using Generative Adversarial Networks”. In: International Conference on Learning Representations. Sept. 27, 2018. URL: https://openreview.net/forum?id=ByeZ5jC5YQ&source=post_page----- (visited on 04/17/2020).

- [12] Jingbo Liu and Philippe Rigollet. “Power analysis of knockoff filters for correlated designs”. In: *arXiv:1910.12428 [cs, math, stat]* (Jan. 9, 2020). arXiv: [1910.12428](https://arxiv.org/abs/1910.12428). URL: [http://arxiv.org/abs/1910.12428](https://arxiv.org/abs/1910.12428) (visited on 04/17/2020).
- [13] Yang Lu et al. “DeepPINK: reproducible feature selection in deep neural networks”. In: *Advances in Neural Information Processing Systems 31*. Ed. by S. Bengio et al. Curran Associates, Inc., 2018, pp. 8676–8686. URL: <http://papers.nips.cc/paper/8085-deeppink-reproducible-feature-selection-in-deep-neural-networks.pdf> (visited on 02/03/2020).