Feature Selection via Detecting Ineffective Features

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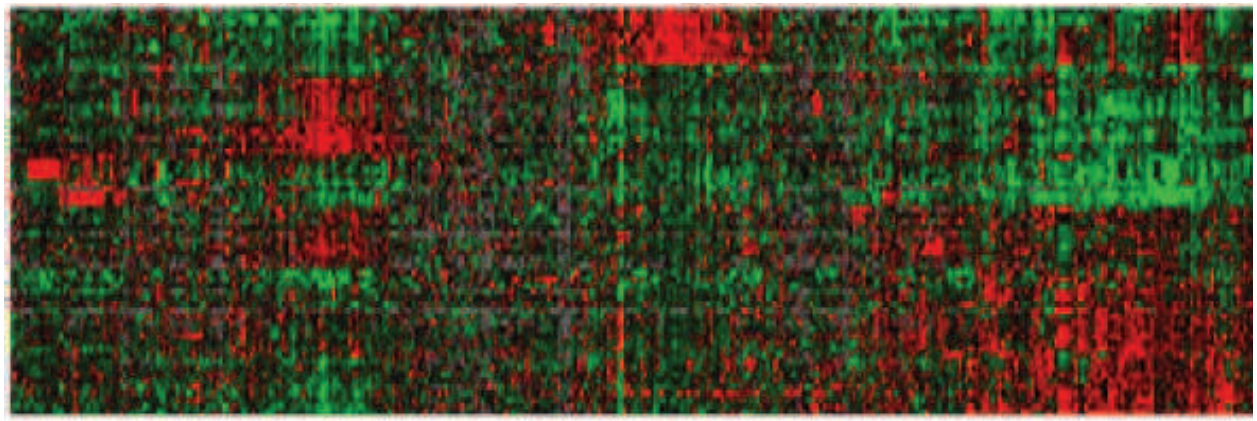
Outline

Outline

Problem description

Application & methods



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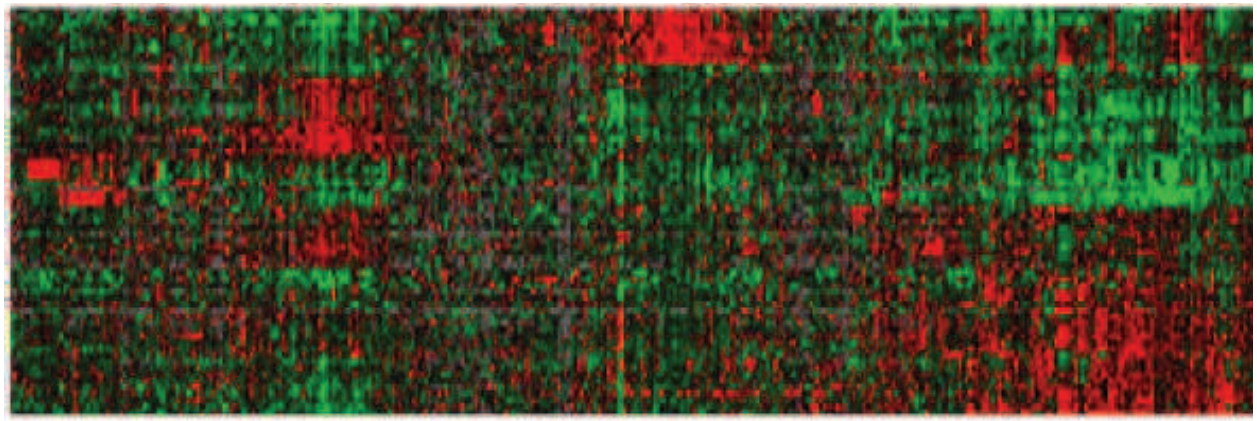
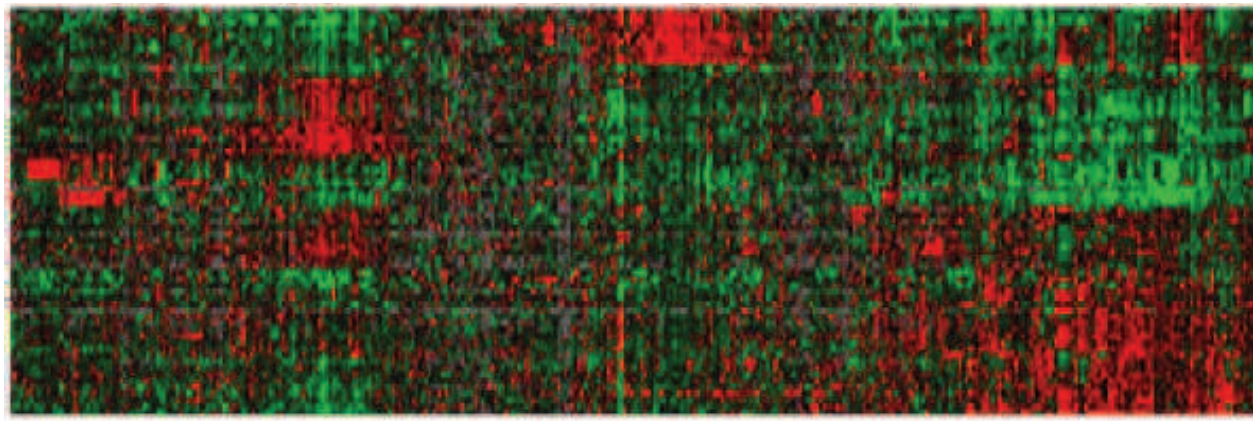


Find important genes

Application & methods



Find important genes

- LASSO (Tibshirani, 1996)
- Prediction Analysis for Microarrays (Tibshirani *et al.*, 2002)
- t-test (Chun & Wen, 2010)
- Variable selection via additive models (Antoniadis *et al.*, 2012)
- LARS (Efron *et al.*, 2004)
- ...

Application & methods (cont'd)

- Consider $(X_1, Y_1), \ldots, (X_n, Y_n)$ with $X_i \in \mathbb{R}^d$ and $Y_i \in \mathbb{R}$
- samples are i.i.d
- Model: $Y_i = \sum_{j=1}^{d} \beta_j X_i^{(j)} + \varepsilon_i \quad 1, \ldots, n$
- $\varepsilon_1, \ldots, \varepsilon_n$ are i.i.d. and independent of X_i
- $\mathbf{E}[\varepsilon_i \mid X_i] = 0$

LASSO

When $d > n$, standard LS estimator is not unique and will overfit data. Therefore, some kind of regularization is needed.

$$\hat{\beta} = \arg\min_{\beta} \|\mathbf{Y} - \mathbf{X}\beta\|_2^2/n + \lambda\|\beta\|_1$$

Some asymptotic theory for LASSO: $Y = X\beta + \varepsilon$ is correct

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1. Consistency prediction (Greenshtein & Ritov, 2004; Bartlett *et al.*, 2009): If
   - $\lambda = \lambda_n = O\big(\sqrt{\log(d)/n}\big)$
   - $\|\beta\|_1 = o\big((n/\log n)^{1/4}\big)$
   - then $(\hat{\beta} - \beta)^T \Sigma_X (\hat{\beta} - \beta) = o_P(1)$ as $n \to \infty$

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2. Consistency variable selection (Meinshausen & Bühlmann, 2006)
   - Let $\hat{S}(\lambda) = \{j : \hat{\beta}_j \neq 0, j = 1, \ldots, d\}$
   - if $\inf_{j \in S} |\beta_j| \gg \sqrt{(\mathrm{card}(S) \log d)/n}$ and $\lambda = \lambda_n \gg O\big(\sqrt{\log(d)/n}\big)$
   - Design matrix $\mathbf{X}$ is not *ill posed* and no strong linear dependence within sub-matrices
   - then $\mathbf{P}[\hat{S}(\lambda) = S] \to 1$ as $d \geq n \to \infty$

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λ is larger for variable selection than prediction

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Parameter selection for variable selection

- BIC, AIC, CV $\rightarrow$ no theoretical justification for variable selection
- CV: LASSO often selects too many variables
- λ close to zero $\rightarrow$ LARS until end of regularization path
- Other ways: stability selection, hypothesis testing

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Substantial relevant covariates (Bühlmann & van de Geer, 2011)

Let

$$S^{\text{relevant}(C)} = \{j : |\beta_j| \geq C, j = 1, \ldots, d\},$$

then for any fixed $0 < C < \infty$

$$\mathbf{P}[\hat{S}(\lambda) \supset S^{\text{relevant}(C)}] \rightarrow 1, \quad n \rightarrow \infty.$$

For $C_n > O(\text{card}(S)\sqrt{\log(d_n)/n})$ and $\lambda_n = O\big(\sqrt{\log(d_n)/n}\big)$: with high probability $\hat{S}(\lambda_n) \supset S^{\text{relevant}(C)} \rightarrow \hat{S}(\lambda_{CV}) \supset S^{\text{relevant}(C)}$

Summary LASSO: Pros vs. Cons

- Easy to implement
- Fast algorithms available (Matlab/R)
- Results are easy to interpret
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- Solid theoretical foundations (if model is correct)

- Model based
- Model restrictions are not necessarily met
- No theoretical results if model does not hold

Outline

Theoretical aspects

- Let $Y \in \mathbb{R}$ and $\mathbf{X} = (X_1, \ldots, X_d) \in \mathbb{R}^d$
- $L^\star := \mathbf{E}\{(Y - m(\mathbf{X}))^2\} = \min_f \mathbf{E}\{(Y - f(\mathbf{X}))^2\}$ be minimum MSE
- $L^\star = \mathbf{E}\{Y^2\} - \mathbf{E}\{m(\mathbf{X})^2\}$

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$$\Downarrow$$

$$\boxed{L_n^\star := \frac{1}{n}\sum_{i=1}^{n} Y_i^2 - \frac{1}{n}\sum_{i=1}^{n} Y_i Y_{i,1}}$$

- $Y_{i,1}$ is value of first nearest neighbor of $\mathbf{X}_i$ from $\mathbf{X}_1, \ldots, \mathbf{X}_{i-1}, \mathbf{X}_{i+1}, \ldots, \mathbf{X}_n$

Theoretical aspects (cont'd)

Theorem (Almost sure convergence & universal consistency)

Assume bounded Y*, then*

$$L_n^\star \to L^\star \quad a.s.$$

Moreover, if $\mathbf{E}\{Y^2\} < \infty$

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Theorem (Rate of convergence & consistency)

Assume X and Y bounded and the regression function m is Lipschitz continuous. Further, assume that ties occur with probability zero. Then, for $d \geq 2$

$$\mathbf{E}\{|L_n^\star - L^\star|\} \leq c_1 n^{-1/2} + c_2 n^{-2/d}.$$

Further, if $n \to \infty$ faster than d

$$\mathbf{E}\{|L_n^\star - L^\star|\} = o_p(1).$$

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- Under $\mathcal{H}_k$:

$$m(\mathbf{X}) := \mathbf{E}\{Y \mid \mathbf{X}\} = \mathbf{E}\{Y \mid \mathbf{X}^{(-k)}\} =: m^{(-k)}(\mathbf{X}^{(-k)}) \quad a.s.$$

Detection of inefficient features (cont'd)

- Data without k-th component:

$$D_n^{(-k)} = \{(\mathbf{X}_1^{(-k)}, Y_1), \ldots, (\mathbf{X}_n^{(-k)}, Y_n)\}$$

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$$L_n^{(-k)} - L_n = \frac{1}{n}\sum_{i=1}^{n} Y_i (Y_{i,1} - Y_{i,1}^{(-k)})$$

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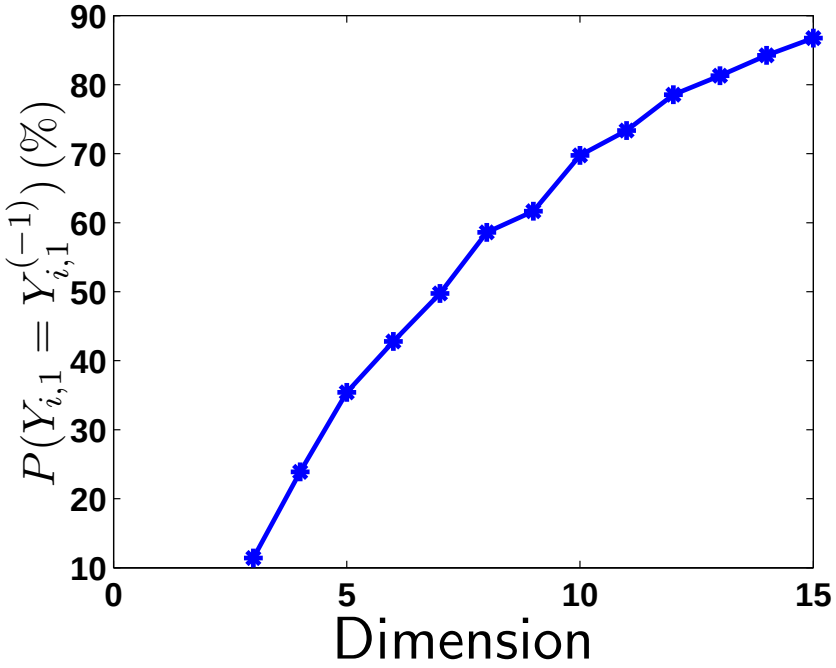

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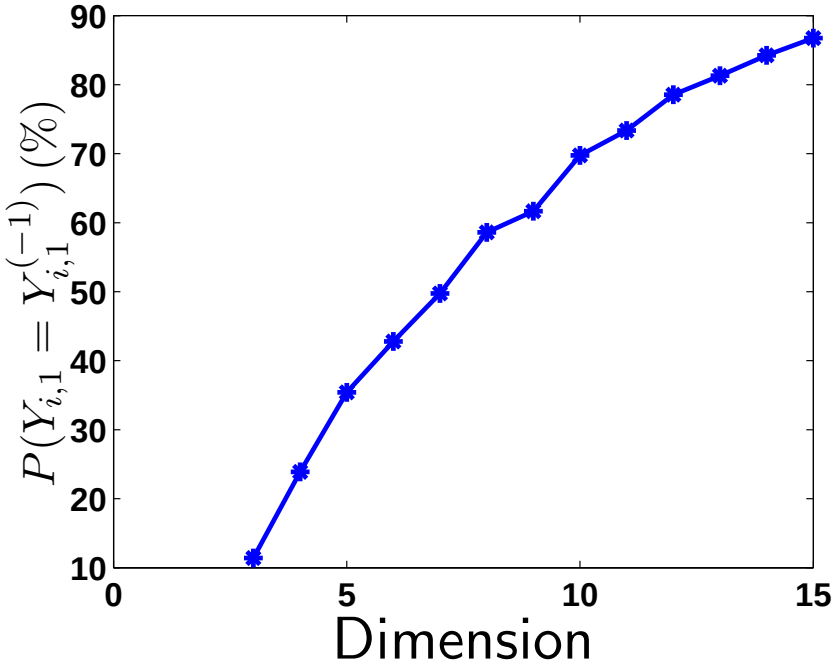

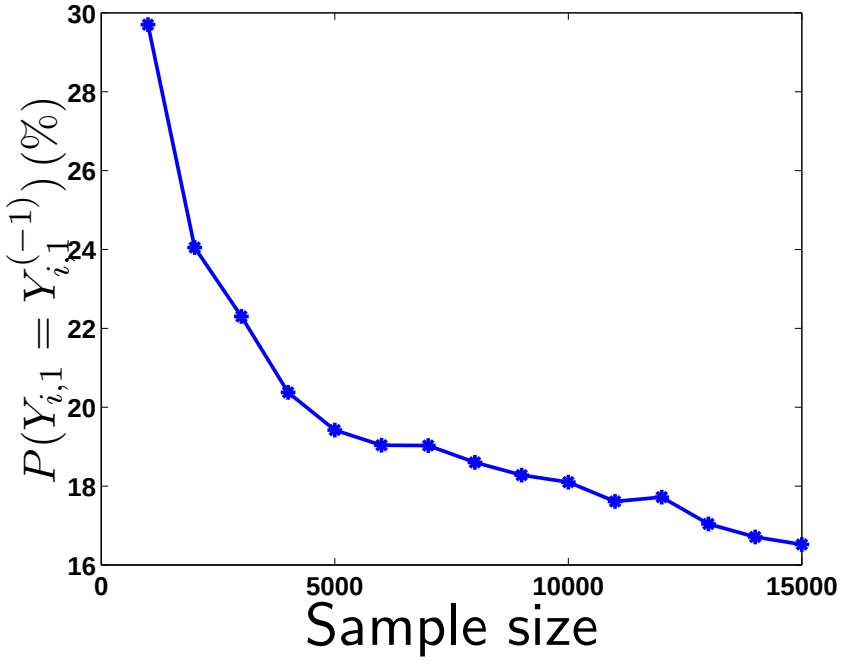

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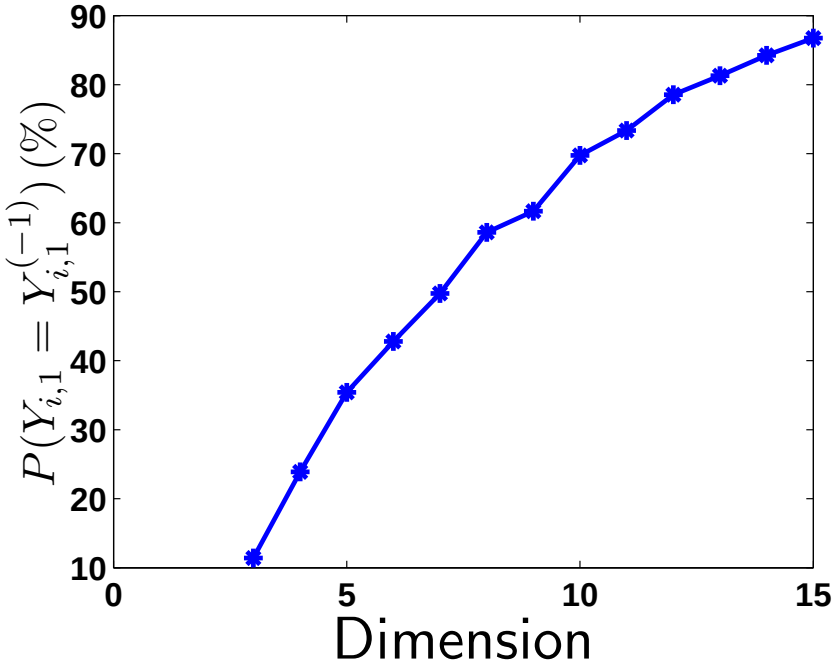

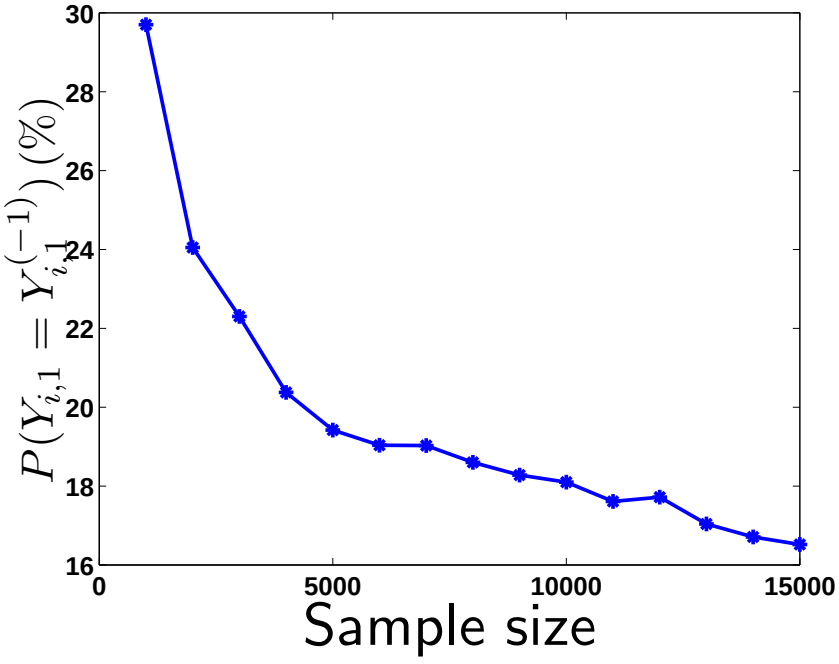

Modification of test statistic needed

Modification of test statistic

- Modify test statistic such that

$$(\hat{Y}_{i,1}, \hat{Y}_{i,1}^{(-k)}) = \begin{cases} (Y_{i,1}, Y_{i,1}^{(-k)}) & \text{if} \quad Y_{i,1} \neq Y_{i,1}^{(-k)} \\ \\ I_i(Y_{i,2}, Y_{i,1}^{(-k)}) + (1 - I_i)(Y_{i,1}, Y_{i,2}^{(-k)}) & \text{otherwise,} \end{cases}$$

with

$$I_i = \begin{cases} 0 & \text{with probability } 1/2, \\ 1 & \text{with probability } 1/2, \end{cases}$$

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Definition (Exchangeable random variables)

A triangular array $V_{n,i}, n = 1, \ldots,$ and $i = 1, \ldots, n$ is called (row-wise) exchangeable if for any fixed n and for any permutation $\rho(1), \ldots, \rho(n)$ of $1, \ldots, n$, the distributions of

$$(V_{n,1}, \ldots, V_{n,n})$$

and

$$(V_{n,\rho(1)}, \ldots, V_{n,\rho(n)})$$

are equal.

Limit distribution of the test statistic (cont'd)

Theorem (Blum *et al.* (1958), De Brabanter & Györfi (2012))

Let

$$V_{n,i} = \frac{Y_i(Y_{i,1} - Y_{i,1}^{(-k)}) - \mathbf{E}\{Y_i(Y_{i,1} - Y_{i,1}^{(-k)})\}}{\sqrt{\mathbf{Var}(Y_i(Y_{i,1} - Y_{i,1}^{(-k)}))}}.$$

Then for

- $\mathbf{E}\{V_{n,1}V_{n,2}\} = o(1/n)$
- $\lim_{n\to\infty} \mathbf{E}\{V_{n,1}^2 V_{n,2}^2\} = 1$
- $\mathbf{E}\{|V_{n,1}|^3\} = o(\sqrt{n})$,

it follows that

$$\sqrt{n}(L_n^{(-k)} - L_n) \xrightarrow{d} N(0, 2L^\star \, \mathbf{E}\{Y^2\})$$

under $\mathcal{H}_k$.

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!Smoothness of regression function and dimension do not count under $\mathcal{H}_k$!

Empirical verification of the theorem

- $Y = \sum_{i=1}^{5} c_i X^{(i)} + \varepsilon$, $c_1 = 0$ and $c_i = 1$ for $i = 2, \ldots, 5$.
- $\mathbf{X}$ uniform on $[0,1]^5$ and $\varepsilon \sim N(0, 0.05^2)$.
- Bootstrap (10,000 replications)

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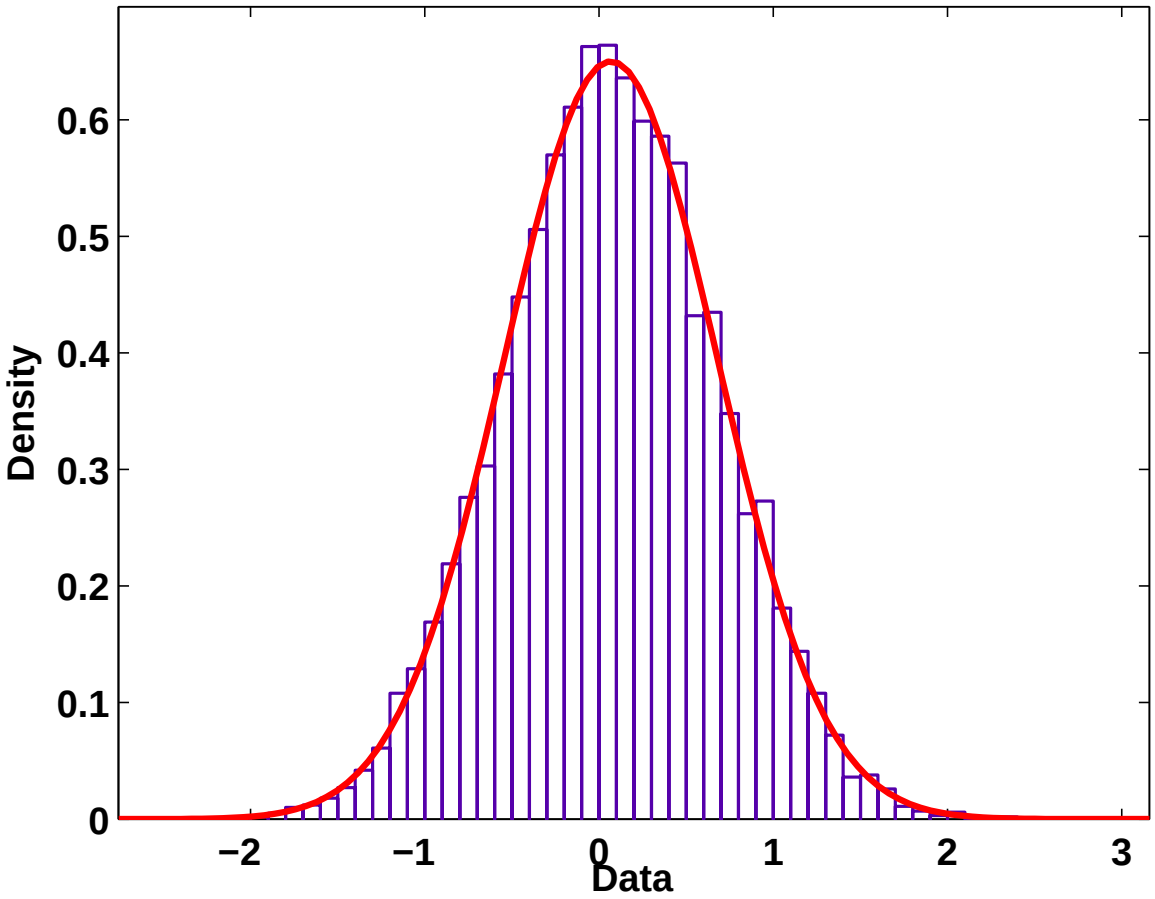

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Toy example

- $Y = \sin(\pi X^{(1)}) \cos(\pi X^{(4)}) + \varepsilon$ with $\varepsilon \sim N(0, 0.1^2)$.
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- $n = 1000$
- 1000 repetitions, significance level $\alpha = 0.05$

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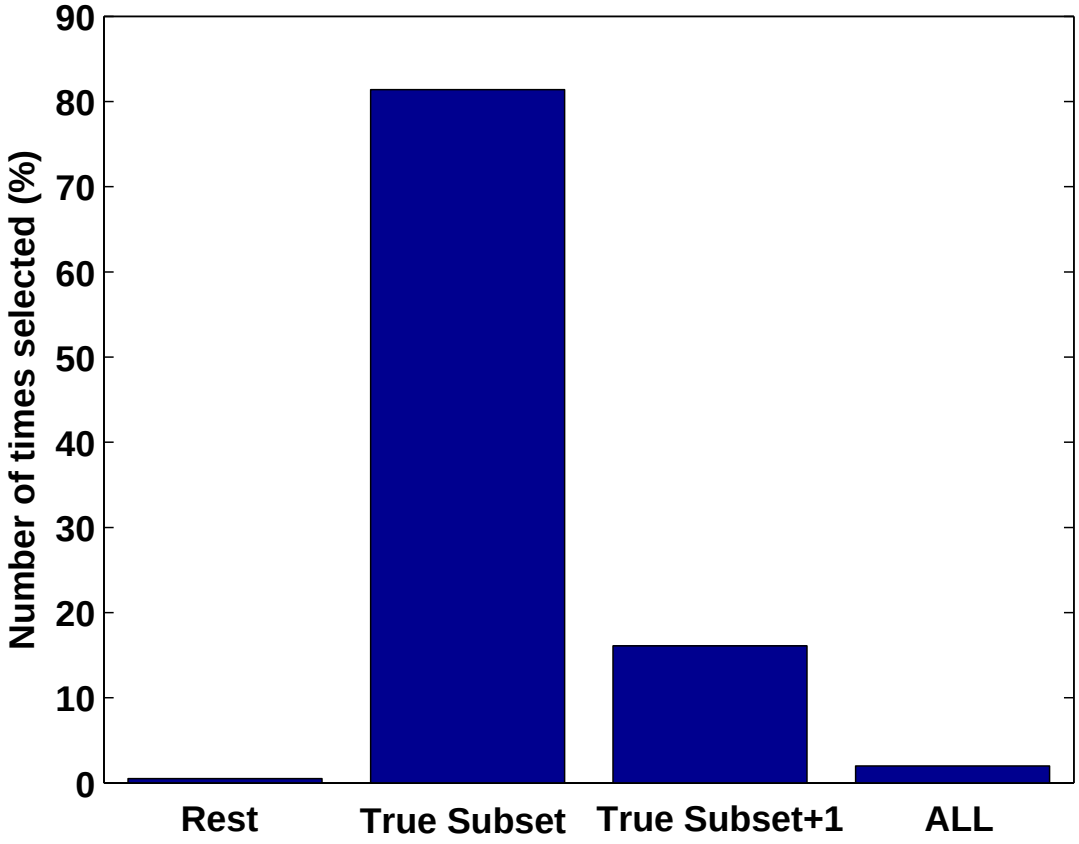

Bosting housing data

- Data set: $n = 506$, $d = 13$
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Variable	description
1	per capita crime rate by town
2	proportion of residential land zoned for lots over $25,000$ sq.ft
3	proportion of non-retail business acres per town
4	Charles River dummy variable
5	nitric oxides concentration
6	average number of rooms per dwelling
7	proportion of owner-occupied units built prior to 1940
8	weighted distances to five Boston employment centres
9	index of accessibility to radial highways
10	full-value property-tax rate per USD
11	pupil-teacher ratio by town
12	proportion of African-Americans by town
13	percentage of lower status of the population

Boston housing data (cont'd)

- Repeated over 500 times
- Split random in training and test samples (80/20)
- $\text{MSE}_{\text{full}} = 0.22$ and $\text{MSE}_{\text{reduced}} = 0.21$

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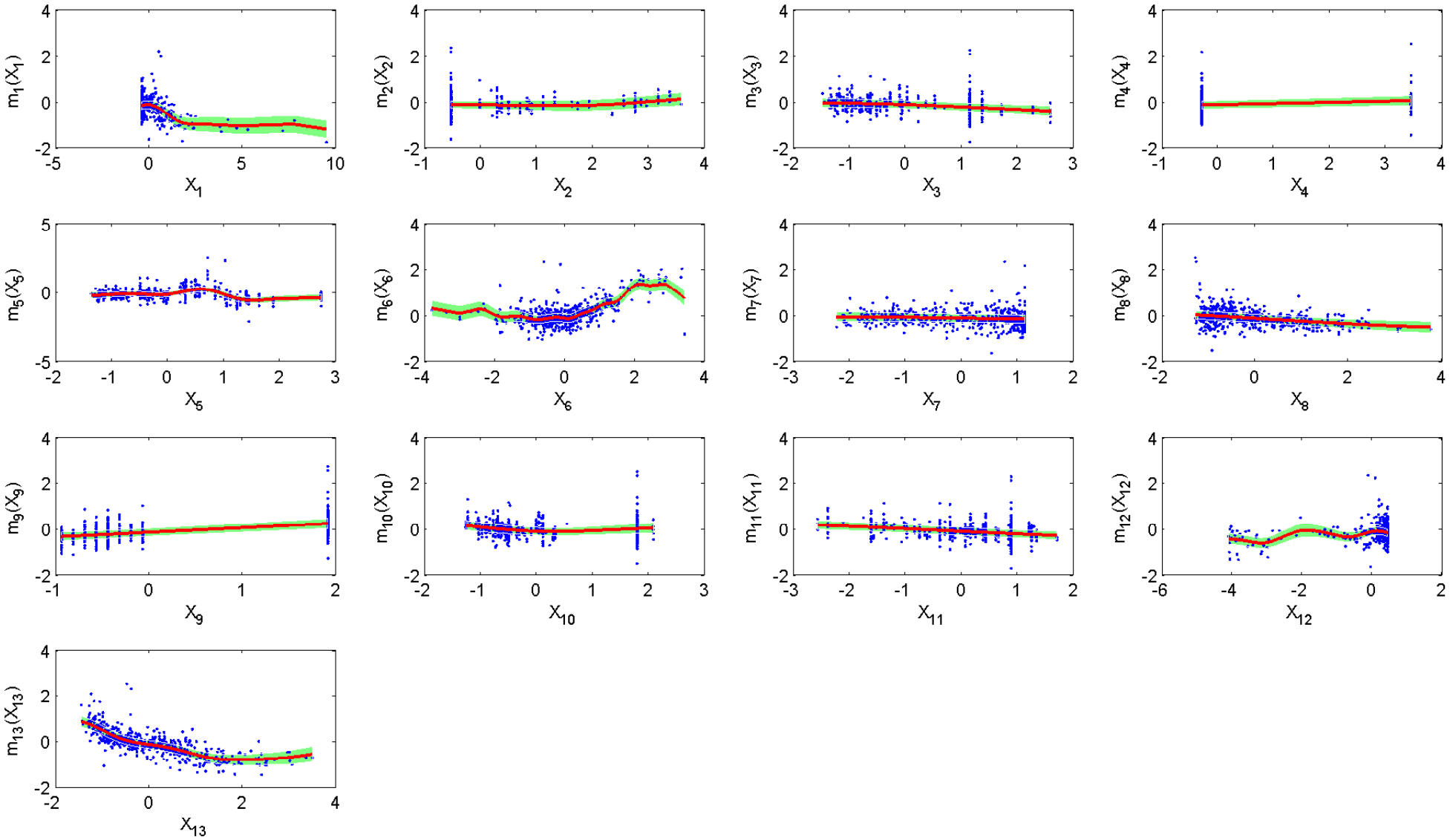

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- No theoretical result if d grows faster than n due to the model-free character

Thank you for your attention

Any questions...?

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