

A practical evaluation of recent methods in high-dimensional inference

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Problem and motivation

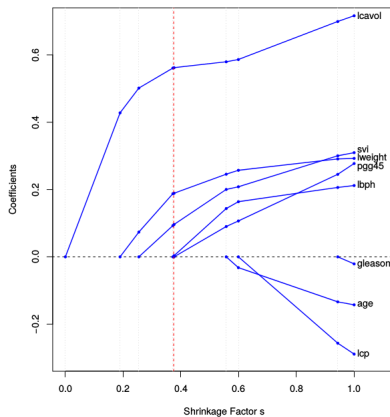
- $x \in \mathbb{R}^p, y \in \mathbb{R}$ have a joint distribution P where $y|x \sim N(x^T \beta, \sigma^2)$
- Observe $X = (x_1, \dots, x_n)^T$, $Y = (y_1, \dots, y_n)$ iid
- Problem: test $H_i : \beta_0 = i$ for $i = 1, \dots, p$
- Motivation: x are SNPs (mutations), y is phenotype

| | Control | $p > n$ |
|--|----------|---------|
| Classical inference (Pearson 1930) | Marginal | No |
| Debiased lasso (Javanmard et al. 2014) | Marginal | Yes |
| Knockoffs (Barber et al. 2014) | FDR | ? |
| Covariance test (Lockhart et al. 2014) | ?? | Yes |
| ... + FDR control (G'Sell et al. 2013) | FDR | Yes |
| | | |

The LASSO path

All three methods share an association with LASSO:

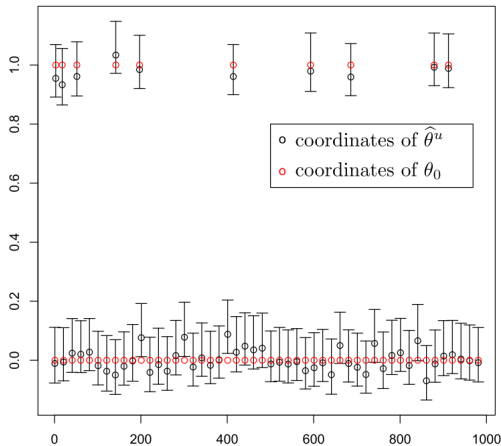
$$\hat{\beta}_{\lambda} = \operatorname{argmin}_{\beta} \frac{1}{2} \|X\beta - Y\|^2 + \lambda \|\beta\|_1$$



(Image credit: ??)

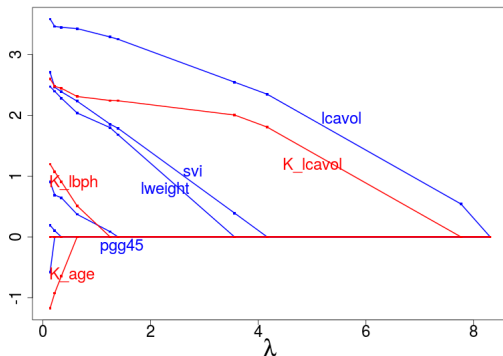
Debiased regularized M-estimators

- (2014) Javanmard and Montanari
- Standard assumptions + sparsity condition on β + large n and p asymptotics



Knockoff filter

- (2014) Barber and Candés
- *Finite sample* $Y \sim N(X\beta, \sigma^2 I)$, $n \leq p$, control FDR
- Extension to $p > n$, FWER control, etc. forthcoming...



| | |
|---------|---------|
| lweight | 22.5652 |
| lcavol | 20.5199 |
| svi | 4.4871 |
| lbph | 1.1865 |
| age | 0.0829 |
| gleason | 0.0387 |
| lcp | -0.2359 |
| pgg45 | -3.3742 |

Covariance test

- (2014) Lockhart, Taylor, Tibshirani ($\times 2$)
- Standard assumptions $Y \sim N(X\beta, \sigma^2 I) +$ large p asymptotics
- See *also* non-asymptotic exact test (Lee, Sun $\times 2$, Taylor 2015)
- What kind of Type I error does it control?

| Step | Predictor entered | Forward stepwise | Lasso |
|------|-------------------|------------------|-------|
| 1 | lcavol | 0.000 | 0.000 |
| 2 | lweight | 0.000 | 0.052 |
| 3 | svi | 0.041 | 0.174 |
| 4 | lbph | 0.045 | 0.929 |
| 5 | pgg45 | 0.226 | 0.353 |
| 6 | age | 0.191 | 0.650 |
| 7 | lcp | 0.065 | 0.051 |
| 8 | gleason | 0.883 | 0.978 |

FDR control for covariance test

- G'Sell, Wager, Chouldechova, Tibshirani (2013)
- Two methods to control FDR for covariance test... but under a *different* definition of Type I error
- Type I error is defined according to the *incremental null* (next slide)

Formulations for hypothesis testing

- For a subset E of the variables, define $\beta^E = (X_E^T X_E)^{-1} X_E^T X \beta$

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- **The full model null.** Test multiple hypotheses $H_i : \beta_i = 0$
- **Selective inference.** Condition on a randomly selected subset E , test hypotheses $H_i : \beta_i^E = 0$ for all $i \in E$

Formulations for hypothesis testing

- For a subset E of the variables, define $\beta^E = (X_E^T X_E)^{-1} X_E^T X \beta$
- **The full model null.** Test multiple hypotheses $H_i : \beta_i = 0$
- **Incremental null.** (Informal explanation).
 - Test variables as they are added to the model
 - I make a mistake whenever I add a variable which *doesn't* improve the fit of the model
 - If a variable I added previously *becomes* redundant later, it doesn't count against me

Formulations for hypothesis testing

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- **The full model null.** Test multiple hypotheses $H_i : \beta_i = 0$
- In this talk, we define type I errors according to *full model null*...

There is yet another method which is commonly used for variable selection...!

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| Marginal screening | ??? | Yes |

Statistical Validation

- These procedures are derived under strong assumptions (linearity, gaussianity, homoscedasticity)
- How well do they work in real data where these assumptions are violated?
- We could validate inference procedures in real data if only we knew the 'true' β , (re)defined as

$$\beta = \mathbf{E}[\mathbf{x}\mathbf{x}^T]^{-1}\mathbf{E}[\mathbf{y}\mathbf{x}]$$

Statistical Validation

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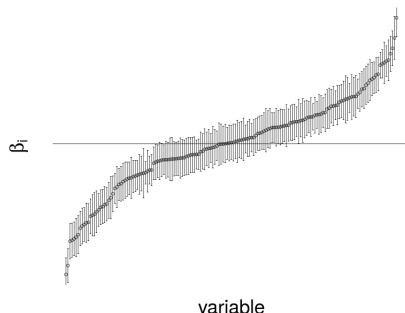
- Possibility: take a dataset with large p and *humongous* n , so we can get an extremely precise estimate of β using OLS. Then test the high-dimensional inference procedures on subsamples of size $n_0 \leq p < n$ of the data

Example: personality data

- Data with $p = 163$ survey questions from an online personality test, $n = 49086$ (after processing)
- Predict self-reported age of respondent, y , from their responses
- Is n large enough for us to confidently say which $\beta_i = 0$ (for use as ground truth?)

Example: personality data

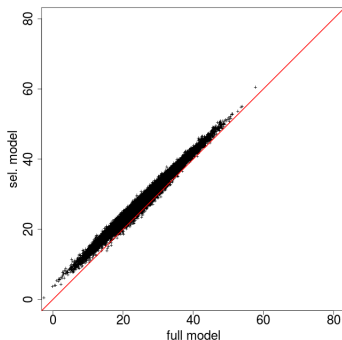
Coefficient estimates ± 3 sd



Consider declaring all variables whose intervals cross 0 to be null. Then $p_1 = 105$ (out of 163)

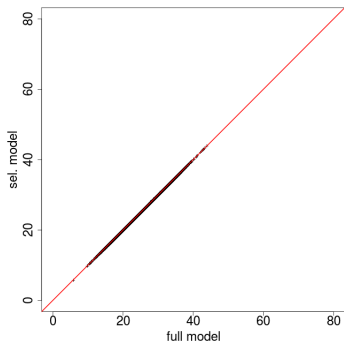
Example: personality data

- If n were large enough, then for the selected model S we should have $\hat{y} = \sum_{i=1}^p X_i \hat{\beta}_i$ close to $\hat{y}_S = \sum_{i \in S} X_i \hat{\beta}_i$
- But...



Example: personality data

- Here n is not large enough for $p = 163$
- If we reduce the dimensionality to 15 by subsampling columns, it looks more convincing that we selected the correct 10 variables



- It is by no means *impossible* to get large enough data to estimate high-dimensional β , with say, $p > 100$
- But if were *easy* to get such large n data... we wouldn't need these new inference techniques in the first place!

Why not use simulations?

- Simulations can be used to test robustness of the procedure
- In simulations, we can add all the nonlinearities, nongaussianity, etc. that we want

Why not use simulations?

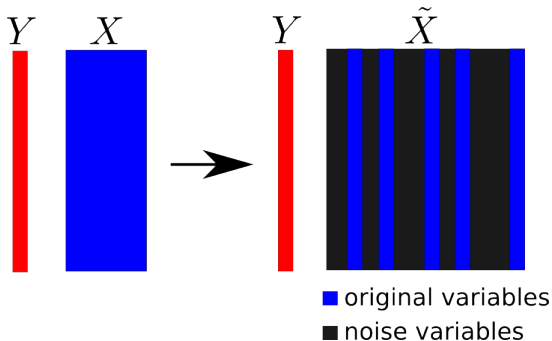
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- Advantage: In simulations, we not only know β , but exactly how the data is generated
- Advantage: We can vary simulation parameters and get a lot of insight about the procedure being tested
- **Disadvantage:** Are these simulations relevant? How can we tell the simulated models are realistic?

Idea

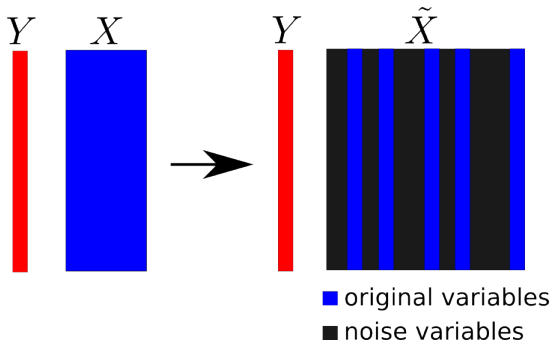
I give you real data *mixed in* with noise variables



- Can you identify the original columns from the noise columns?

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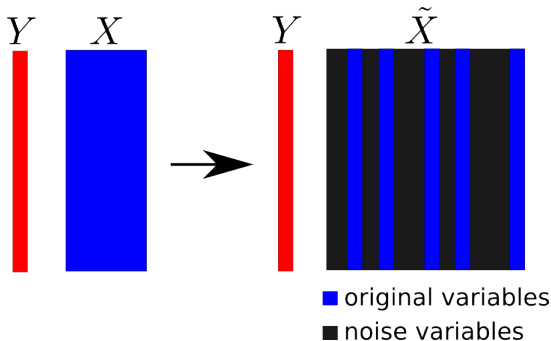
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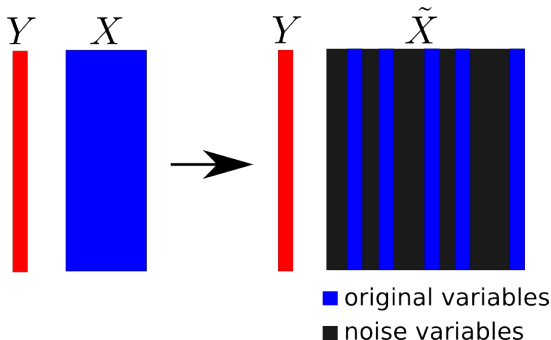
I give you real data *mixed in* with noise variables



- Can you identify the original columns from the noise columns?
- I can test your procedure this way, because I know the ground truth!
- **Caveat:** this test is unrealistically 'easy' (due to lack of correlations)

Synthetic Negative Controls

- Synthetic negative controls (SNCs) are artificial columns *which are correlated* to Y , yet still have zero (population) regression coefficients
- Suppose I give you real data + SNCs, then you apply high-dimensional inference. If you reject any SNCs, we know these are errors!
- This gives us some measure of performance on “real” data (maybe?)



Synthetic Negative Controls

- Given random vector $x \in \mathbb{R}^p$, let e be noise in \mathbb{R}^p independent of x .
- Let Γ be a fixed $p \times q$ matrix. *Define* synthetic negative controls $z \in \mathbb{R}^q$ by

$$z = x'\Gamma + e$$

and let $\tilde{x} = (x, z)$, so that

$$\tilde{x}_1 = x_1, \dots, \tilde{x}_p = x_p$$

$$\tilde{x}_{p+1} = z_1, \dots, \tilde{x}_{p+q} = z_q$$

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- Let

$$\beta = \mathbf{E}[xx^T]^{-1}\mathbf{E}[yx], \quad \tilde{\beta} = \mathbf{E}[\tilde{x}\tilde{x}^T]^{-1}\mathbf{E}[y\tilde{x}]$$

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$$\beta = \mathbf{E}[xx^T]^{-1}\mathbf{E}[yx], \quad \tilde{\beta} = \mathbf{E}[\tilde{x}\tilde{x}^T]^{-1}\mathbf{E}[y\tilde{x}]$$

- Then

$$\forall i \in \{1, \dots, p\} : \beta_i = \tilde{\beta}_i$$

$$\forall i \in \{p+1, \dots, p+q\} : \tilde{\beta}_i = 0$$

Why is this...?

- Recall that $\hat{\beta}_i$ is the *univariate regression* coefficient of Y on $X_{i|-i}$, where $X_{i|-i}$ is the *residual* of X_i after X_i is regressed on the other columns..
- Population version: $\beta_i = 0$ if the projection of X_i on the null space of the other covariates is uncorrelated with Y

Why is this...?

- Population version: $\beta_i = 0$ if the projection of X_i on the null space of the other covariates is uncorrelated with Y
- For $i = 1, \dots, q$, we have

$$\tilde{X}_{p+i} = x' \Gamma_i + E_i$$

where here \tilde{X}_{p+1} denotes the random variable (not the column of the design matrix)

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- The orthogonal projection P_X^\perp of \tilde{X}_{p+1} is

$$P_X^\perp \tilde{X} = P_X^\perp X \Gamma_i + P_X^\perp E_i = 0 + E_i$$

since $P_X^\perp X = 0$; meanwhile since $E_i \perp X$, $P_X^\perp E_i = E_i$.

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- Population version: $\beta_i = 0$ if the projection of X_i on the null space of the other covariates is uncorrelated with Y

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since $P_X^\perp X = 0$; meanwhile since $E_i \perp X$, $P_X^\perp E_i = E_i$.

- Since $E_i \perp y$, we have $\text{Cor}(P_X^\perp \tilde{X}_{p+i}, y) = 0$, hence $\tilde{\beta}_{p+i} = 0$

Why is this...?

- Population version: $\beta_i = 0$ if the projection of X_i on the null space of the other covariates is uncorrelated with Y
- Since $E_i \perp y$, we have $\text{Cor}(P_X^\perp \tilde{X}_{p+i}, y) = 0$, hence $\tilde{\beta}_{p+i} = 0$
- And since $\tilde{\beta}_j = 0$ for all the added variables $j = p+1, \dots, p+q$, it follows that $\tilde{\beta}_i$ is unchanged for $i = 1, \dots, p$.

Using SNCs to evaluate procedures

- Take low-dimensional real data mixed with SNCs (synthetic negative controls), apply inference procedure
- *Proxy for Type I error*: Rejected SNCs
- *Proxy for Power*: Rejected original variables

A step-by-step tutorial (in R)

1. Take the prostate data

```
> data(prostate)
> x <- prostate[, 1:8]
> y <- prostate[, 9]
> colnames(x)
[1] "lcavol" "lweight" "age"      "lbph"      "svi"
     "lcp"   "gleason" "pgg45"
> dim(x)
[1] 97 8
```

A step-by-step tutorial

2. Construct 20 synthetic negative controls

```
> GAMMA <- matrix(rnorm(8 * 20), 8, 20)
> E <- matrix(rnorm(97 * 20), 97, 20)
> sncs <- as.matrix(x) %*% GAMMA + 2 * E
> sncs <- data.frame(sncs)
> colnames(sncs)
[1] "X1"  "X2"  "X3"  "X4"  "X5"  "X6"  ...
[19] "X19" "X20"
```

3. Create combined design matrix

```
> x2 <- cbind(x, sncs)
```

A step-by-step tutorial

4. Try marginal screening

```
> cors <- cor(x2, y)
> cors[order(-abs(cors)), , drop = F]
      [,1]
lcavol  0.7344603
svi      0.5662182
lcp      0.5488132
X6       -0.4591506
X16      0.4482263
lweight  0.4333194
X4       -0.4326898
```


A step-by-step tutorial

5. Try covariance test

```
> library(covTest)
> covTest(lars(as.matrix(x2), y), as.matrix(x2), y)
$results
```

| Predictor_Number | Drop_in_covariance | P-value |
|------------------|--------------------|---------|
| 1 | 69.0292 | 0.0000 |
| 5 | 1.5390 | 0.2219 |
| 2 | 6.8094 | 0.0020 |
| 11 | 0.8559 | 0.4294 |

(Numbers 1, 5, 2 are original, 11 is a SNC)

A step-by-step tutorial

6. Try debiased lasso (code at <http://web.stanford.edu/~montanar/sslasso/>)

```
> res <- SSLasso(as.matrix(x2), y)
[1] "10% done"
...
[1] "90% done"
> rej <- (res$up < 0) | (res$low > 0)
> names(x2)[rej]
[1] "lcavol" "lweight" "svi"
```

A step-by-step tutorial

7. Try knockoffs

```
> library(knockoff)
```

```
> knockoff.filter(x2, y)
```

Call:

```
knockoff.filter(X = x2, y = y)
```

Selected variables:

| | |
|---------|----|
| lweight | X7 |
| 2 | 15 |

Disclaimer!

- I am *not* proposing SNCs as a methodology for *inference*
- There is a danger of inferring *that Type I error has been controlled* from lack of rejection of SNCs. There are no formal guarantees of this!
- One should interpret results from experiments with SNCs in the same way one interprets simulation results with purely synthetic data

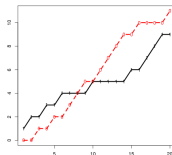
More Experiments!

| Data | n | p_1 | Linear? | Gaussian? | Constant σ^2 ? |
|-------------|------|-------|---------|-----------|-----------------------|
| Personality | 3000 | 163 | No | No | No |
| fMRI | 1750 | 53 | No | OK | No |
| HIV | 842 | 207 | No | Yes? | OK? |
| Galaxy | 323 | 4 | No | OK | No |

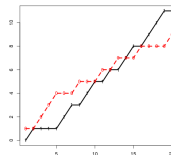
- We add $n/2 - p_1$ synthetic negative controls
- X is scaled, Γ is a gaussian matrix, $Var(E)$ is chosen to yield 'interesting' results
- Personality data is subsampled

Marginal Screening

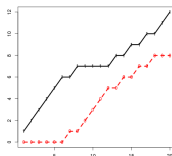
Personality



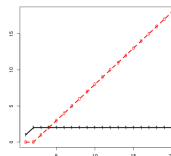
fMRI



HIV



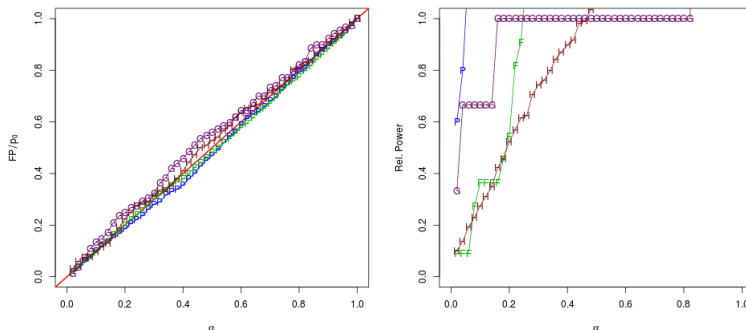
Galaxy



Legend: 0 = False positives, 1 = True positives

Ordinary Least Squares

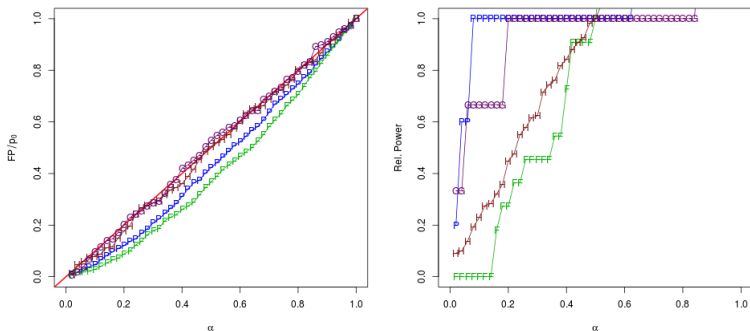
“Rel. power” = $TP / (\text{max number of TPs at } \alpha = 0.5 \text{ for any method})$



Legend: **P** = Personality, **F** = fMRI, **H** = HIV, **G** = Galaxy

Debiased Lasso

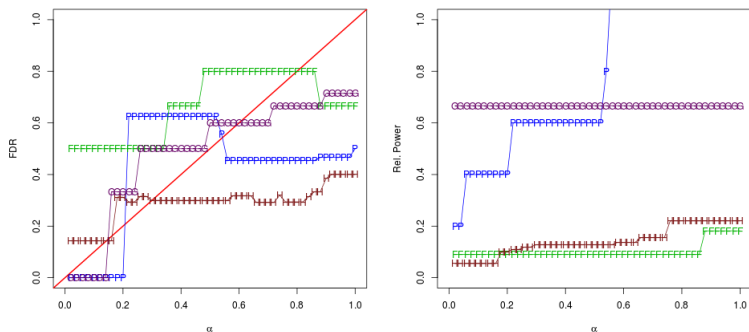
Can you spot the difference from the previous slide?



Legend: **P** = Personality, **F** = fMRI, **H** = HIV, **G** = Galaxy

Covariance Test

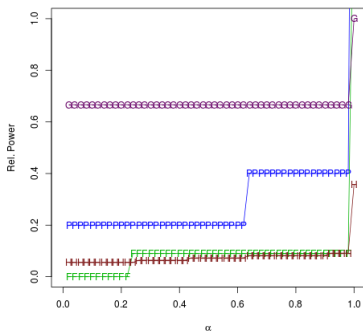
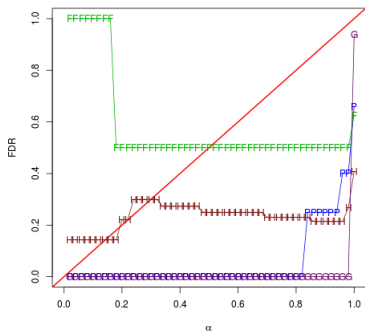
Forward Stop: reject first \hat{k} , where $-\frac{1}{\hat{k}} \sum_{i=1}^{\hat{k}} \log(1 - p_i) \leq \alpha$



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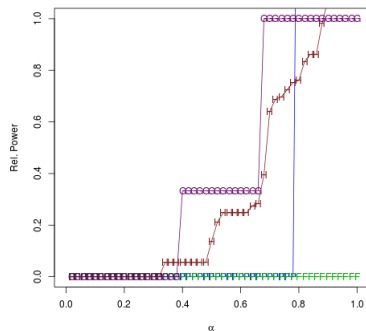
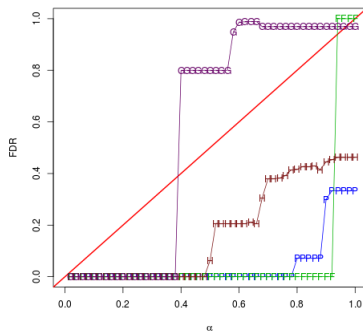
Strong Stop: reject first \hat{k} , where $\frac{m}{\hat{k}} e^{\sum_{j=\hat{k}}^p \log(p_j)/j} \leq \alpha$



Legend: **P** = Personality, **F** = fMRI, **H** = HIV, **G** = Galaxy

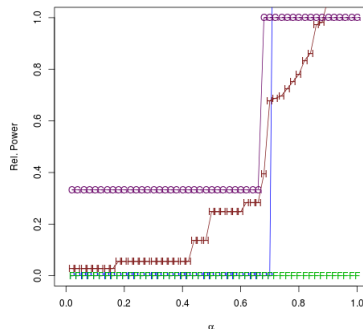
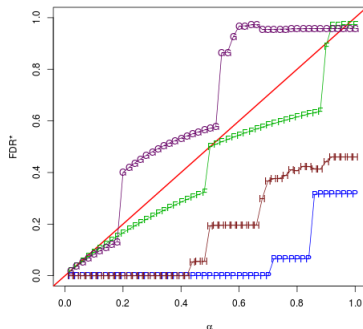
Knockoffs

Using Knockoff+ threshold



Legend: **P** = Personality, **F** = fMRI, **H** = HIV, **G** = Galaxy

Note: $FDR^* = \mathbf{E}[FP/(FP + TP + 1/\alpha)]$

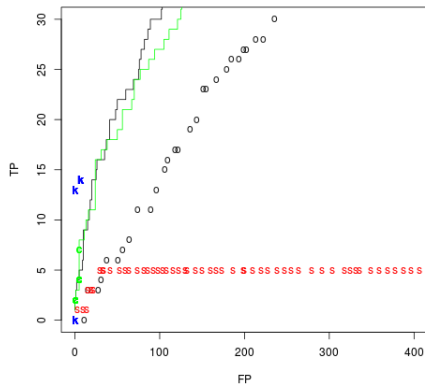


Legend: P = Personality, F = fMRI, H = HIV, G = Galaxy

Variable Ranking Criteria

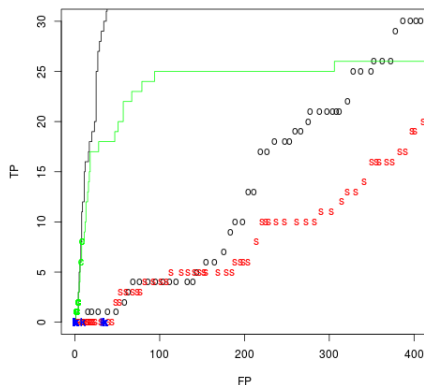
- Forget about Type I error for a second...
- Use procedures to *rank* variables by p-value
- Easy to compare procedures with different Type I criteria and also non-inference variable selection
- (Optional) score by Area Under Curve (AUC), etc.

Variable Ranking: Personality



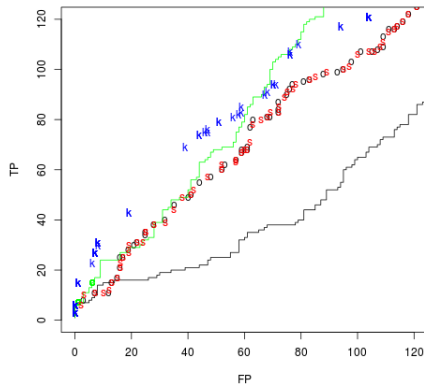
Legend: o = OLS, c = covariance test, k = knockoff, s = debiased lasso, (line) = marginal screening, (line) = lasso path

Variable Ranking: fMRI



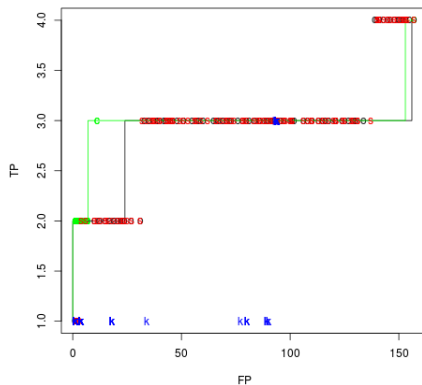
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Variable Ranking: HIV



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Variable Ranking: Galaxy

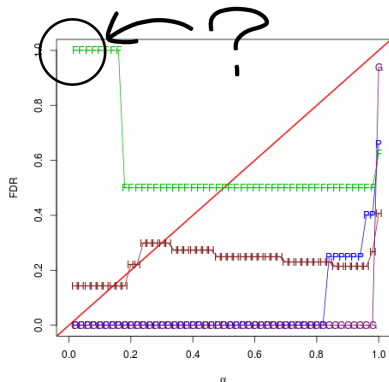


Legend: o = OLS, c = covariance test, k = knockoff, s = debiased lasso, (line) = marginal screening, (line) = lasso path

- We should not conclude too much from four experiments with rather arbitrary generation parameters...
- Debiased lasso similar to OLS but more conservative, less powerful
- Knockoffs vs covariance test:
 - Knockoffs may control FDR more robustly than Covariance test (especially at small α)
 - Knockoffs and covariance are similar in power overall but have different case-by-case behavior
- Knockoffs tend to be conservative, but have good variable ranking in some cases (Personality, fMRI)
- Marginal screening remains annoyingly effective...

Another look at covTest

Strong stop type I error

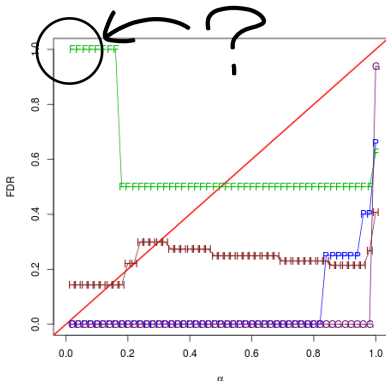


- Why did this negative control get rejected in the fMRI data at such a low α ?

(thanks to Stefan!)

Another look at covTest

Strong stop type I error

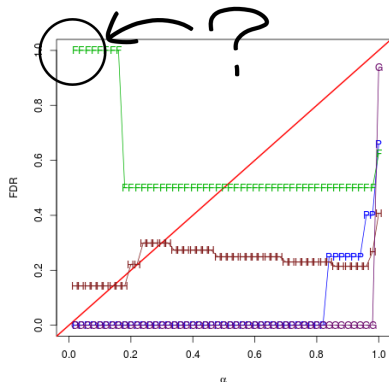


- According to the *incremental null*, the negative control was not a mistake... it is the best single predictor by far!
- The particular negative control took an *average* of the original columns

(thanks to Stefan!)

Another look at covTest

Strong stop type I error



- It is true that $\beta_i = 0$ for the rejected variable... but should we really disregard such strong "proxy" variables?

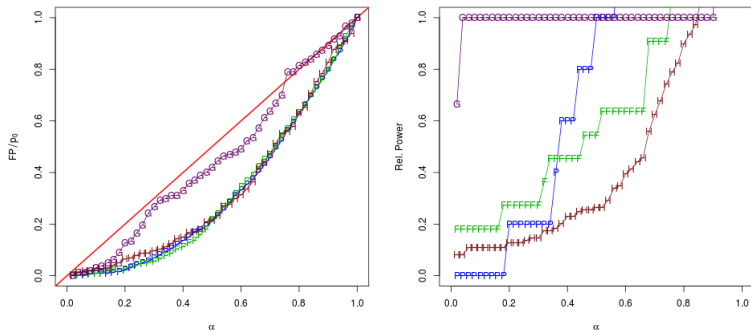
(thanks to Stefan!)

Low sample size

| Data | n | p | p_1 | Linear? | Gaussian? | Constant σ^2 ? |
|-------------|-----|------|-------|---------|-----------|-----------------------|
| Personality | 100 | 1500 | 163 | No | No | No |
| fMRI | 100 | 875 | 53 | No | OK | No |
| HIV | 100 | 421 | 207 | No | Yes? | OK? |
| Galaxy | 100 | 161 | 4 | No | OK | No |

- Reduce the sample size to 100, so that $p \gg n$
- Same number of negative controls, but larger added noise (easier)
- Covariance test requires estimate $\hat{\sigma}$: “cheat” by using OLS estimate from *original* data

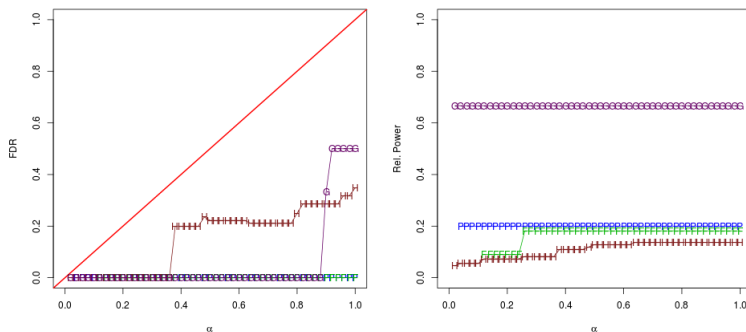
Debiased Lasso



Legend: **P** = Personality, **F** = fMRI, **H** = HIV, **G** = Galaxy

Covariance Test

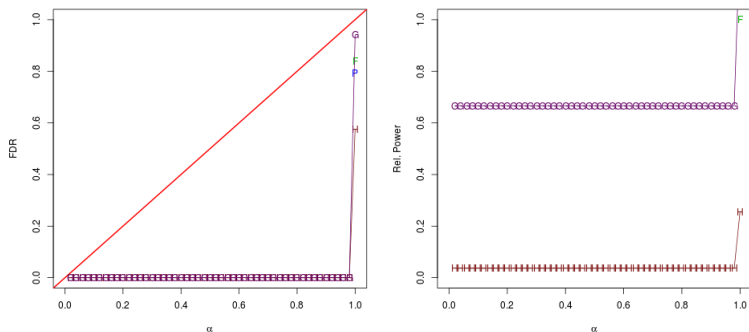
Forward Stop: reject first \hat{k} , where $-\frac{1}{\hat{k}} \sum_{i=1}^{\hat{k}} \log(1 - p_i) \leq \alpha$



Legend: **P** = Personality, **F** = fMRI, **H** = HIV, **G** = Galaxy

Covariance Test

Strong Stop: reject first \hat{k} , where $\frac{m}{\hat{k}} e^{\sum_{j=\hat{k}}^p \log(p_j)/j} \leq \alpha$



Legend: P = Personality, F = fMRI, H = HIV, G = Galaxy

- Debiased lasso and Covariance test + forward stop continue to control Type I error while finding true positives
- Covariance test + strong stop appears too conservative

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- But how do we know that β is really sparse?
- Even more importantly, how do we know that inferring coefficients of the *full model* β are a meaningful objective? E.g. should we consider the covariance test to have made a mistake in the fMRI data?
- How can we decide between the *full model null*, the *incremental null*, or an entirely different framework altogether?
- *Feedback from the practitioner* is the only way we can tell if we have the right formulation for any particular application

Questions to consider

- Why is OLS more powerful than lasso in some of these experiments even when β is sparse? Look at covariance conditions in the theory of LASSO...
- Why do knockoffs or lasso beat marginal screening/OLS in the HIV data? Was it due to how we generated the SNCs or is due to something special about the data itself?
- Suppose we wanted to validate selective inference or the incremental null. How can we do this with synthetic negative controls (other than pure noise?)

“ Both the client and the statistician... must base their thinking on a recognition that their assumptions will always require review and reappraisal... ”

– John Tukey

Acknowledgements

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