MS&E 228: Prediction with High-Dimensional Linear Models

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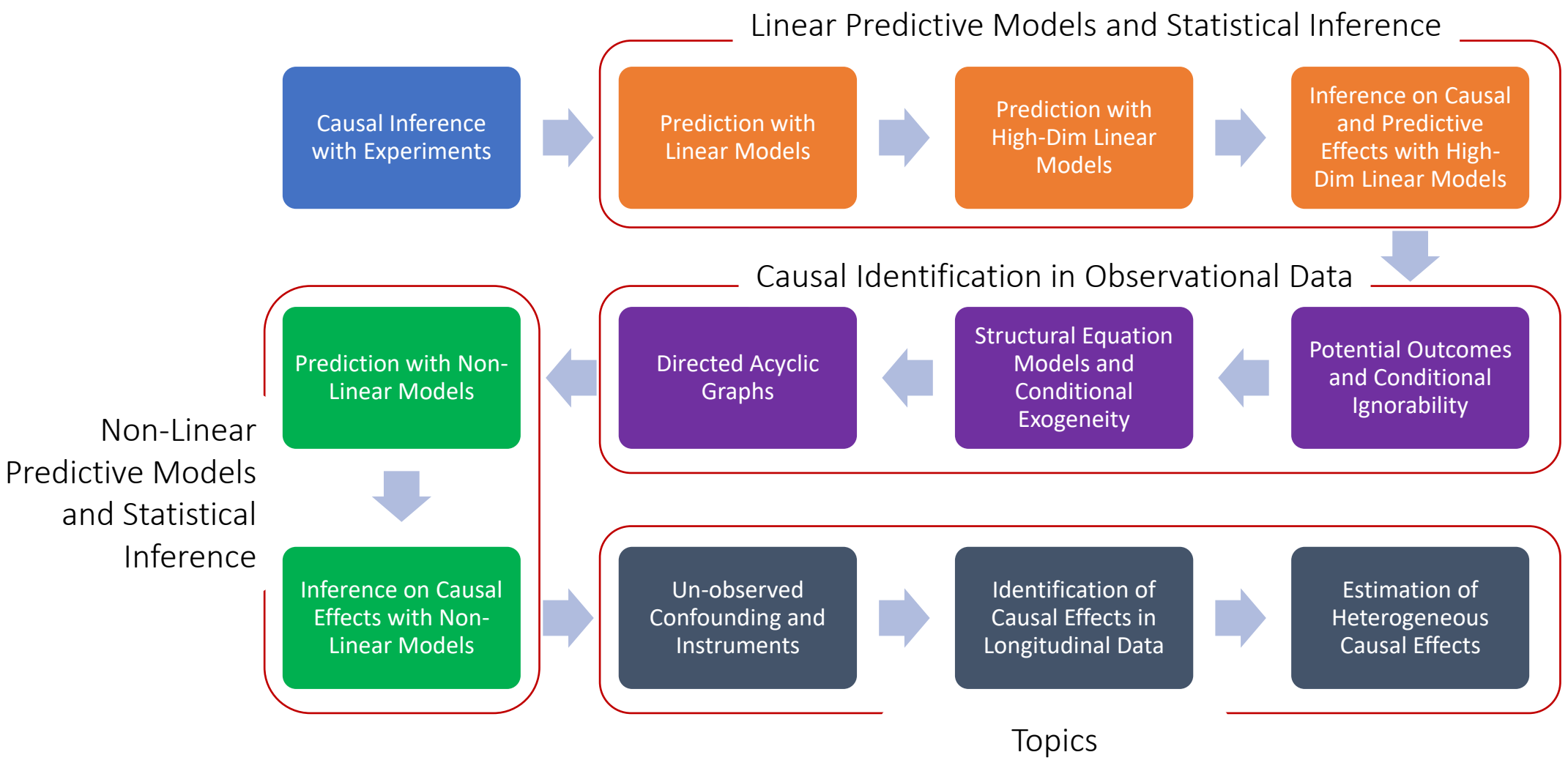
Linear Predictive Models and Statistical Inference
Causal Inference with Experiments
Prediction with Linear Models
Prediction with High-Dim Linear Models
Inference on Causal and Predictive Effects with High-Dim Linear Models
Causal Identification in Observational Data
Potential Outcomes and Conditional Ignorability
Structural Equation Models and Conditional Exogeneity
Directed Acyclic Graphs
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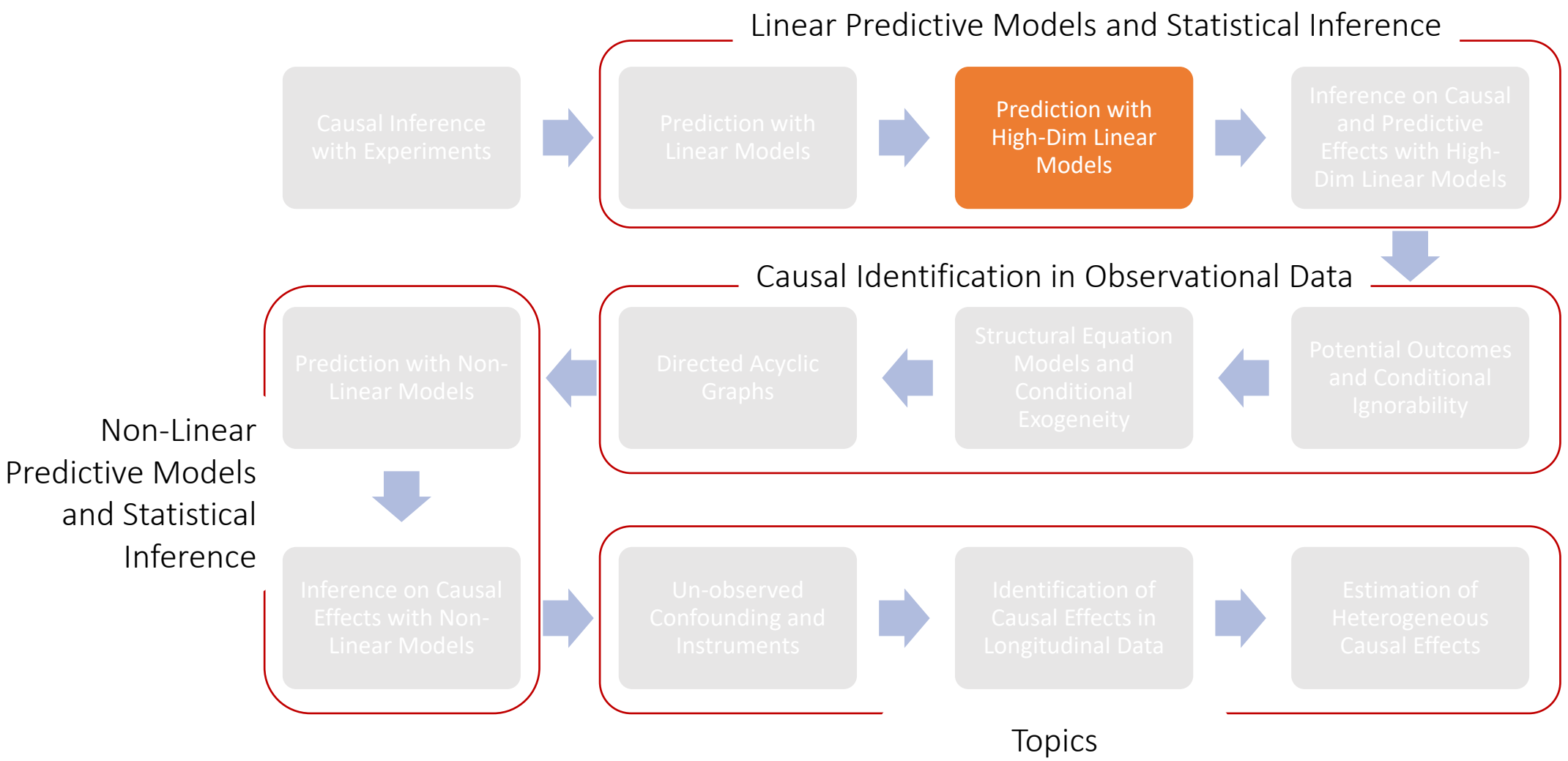
Un-observed Confounding and Instruments
Identification of Causal Effects in Longitudinal Data
Estimation of Heterogeneous Causal Effects
Topics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Recap of Previous Lecture

Even if the relationship between outcome Y and covariates X is non-linear, we can always write:

$$Y = \beta' X + \epsilon, \qquad E[\epsilon X] = 0 \Leftrightarrow \epsilon \perp X$$

The function $\beta' X$ is the Best Linear Predictor (BLP) or equivalently the best linear approximation to the Conditional Expectation Function (CEF) $E[Y|X]$

Even if the relationship between outcome Y and covariates X is non-linear, we can always write:

$$Y_i = \hat{\beta}' X_i + \hat{\epsilon}_i, \qquad E_n[\hat{\epsilon} X] = 0$$

The function $\hat{\beta}' X$ is the Best Linear Predictor in sample and $\hat{\beta}$ are the sample regression coefficients

You should expect OLS to produce accurate predictions in the worst-case only if the number of variables is small compared to number of samples.

Its predictions converge to the predictions of the BLP in the population

Almost always measure predictive performance of your estimated model on a held-out sample

Predictive effect β_1 of *target variable* is the coefficient in a *simple one variable regression*

$$\begin{pmatrix}\text{part of outcome}\\ \text{un-explained by other}\end{pmatrix} \sim \begin{pmatrix}\text{part of target}\\ \text{un-explained by other}\end{pmatrix}$$

Coefficient of D in OLS(y~D,W) is mathematically equivalent in samples to

yres = y - OLS(y~W).predict(W)
Dres = D - OLS(D~W).predict(W)

Coefficient of Dres in OLS(yres~Dres)

If we want an interval that roughly contains the predictive effect with probability α, we can use

$$CI(\alpha) \coloneqq \left[\hat{\beta}_1 - z_{1-\frac{\alpha}{2}}\hat{\sigma}_n, \hat{\beta}_1 + z_{1-\frac{\alpha}{2}}\hat{\sigma}_n\right]$$

$$\hat{\sigma}_n \coloneqq \frac{1}{\sqrt{n}}\sqrt{\frac{E_n\left[\hat{\epsilon}^2\breve{D}^2\right]}{E_n\left[\breve{D}^2\right]^2}}$$

e.g. for 95% confidence interval, $z_{1-\frac{a}{2}} \approx 1.96$

The coefficient associated with treatment D in OLS with co-variate adjustment is always consistent for the treatment effect, when run on data from a randomized experiment, as-long-as covariates are de-meaned. The true relationship of outcome with covariates does not need to be linear.

High Dimensions: $p > n$

Best Linear Predictor

- We want to learn the BLP of Y using $X = \left(X_1, \dots, X_j, \dots, X_p\right)$

$$Y = \beta' X + \epsilon, \qquad E[\epsilon X] = 0 \Leftrightarrow \epsilon \perp X$$

- From n samples $\{(X_i, Y_i)\}_{i=1}^{n}$

- When number of variables p is larger than the number of samples n

When do we encounter $p > n$?

Inherent High-Dimensionality

Inherent High-Dimensional Data

- Rich datasets with many covariates
- Country characteristics in cross-country wealth analysis
- Housing characteristics in housing pricing/appraisal analysis
- Individual electronic health records and claims data
- Product characteristics at point of purchase in demand analysis
- Customer characteristics in operations management
- User characteristics and history in the digital economy

Fabricated High-Dimensionality

As a means for better real-world approximations

High-Dimensionality from Feature Engineering

- A purely linear model in the given features X can be a poor approximation to reality
- Recall that if we care about RMSE, then optimal is $E[Y|X]$

$$E[Y|X] = \text{argmin}_f E\left[\left(Y - f(X)\right)^2\right]$$

- By variance decomposition

$$E\left[(Y - b'X)^2\right] = E\left[(Y - E[Y|X])^2\right] + E\left[(E[Y|X] - b'X)^2\right]$$

- The BLP minimizes

$$\min_{b \in \mathbb{R}^p} E\left[(E[Y|X] - b'X)^2\right]$$

- The BLP is the **Best Linear Approximation (BLA) of the CEF**

High-Dimensionality from Feature Engineering

- If instead we first construct variables $P(X) = \left(P_1(X), \ldots, P_p(X)\right)$ that correspond to non-linear functions of the raw variables X
- Then the Best Linear Predictor using $P(X)$ can be a much better BLA

$$\min_b E\left[\left(E[Y|X] - b'P(X)\right)^2\right] \ll \min_b E\left[(E[Y|X] - b'X)^2\right]$$

These non-linear functions can involve

- Interactions of the raw features: $X_1 \cdot X_2$, $X_1 \cdot X_2 \cdot X_3$
- Polynomials of raw features: X_1^2, X_1^3, $X_1 \cdot X_2^2$
- Other non-linear transformations: $\log(X_1)$, $\exp(X_2)$

Coding Example

High-Dimensionality from Feature Engineering

- These larger feature vectors are always a good idea in population; if we had infinite data
- But when we have finite data, more features introduce more noise!
- Eventually, will lead to severe overfitting to the samples and poor out-of-sample performance
- Recall that error scales with p/n
- We can easily reach a high-dimensional regime!

Coding Example

Not imposing any restrictions or biases on the parameters can lead to un-stable estimation in finite samples

Solution: add penalty terms to your estimation that induce biases towards solutions we a prior believe are more probable

Sparsity and the Lasso

The Premise

- We might be willing to believe that most of the parameters β are roughly zero

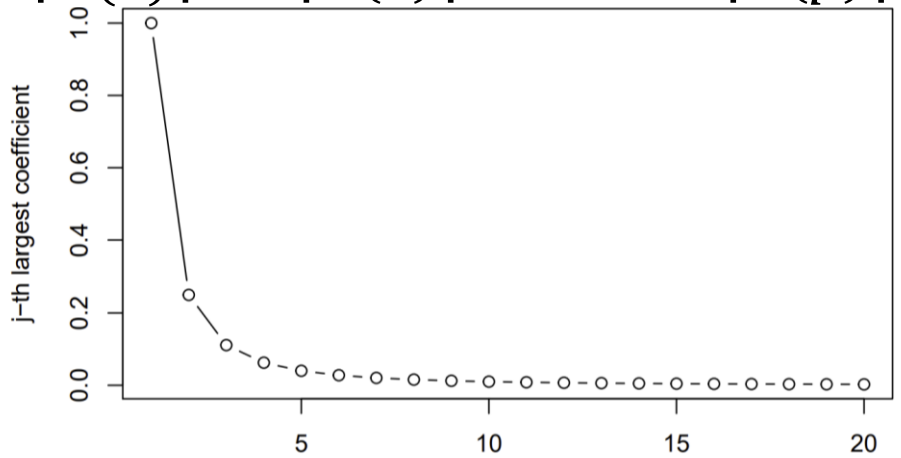
- In that case we should be penalizing finite sample solutions $\hat{\beta}$ that have many non-zero and large coefficients

- This can stabilize the finite sample solution while keeping it close to the true β

Approximate Sparsity

- If we order our coefficients in decreasing order of magnitude

$$|\beta_{(1)}| \geq |\beta_{(2)}| \geq \cdots \geq |\beta_{(p)}|$$



- We assume that for some constant A and for some constant a

$$|\beta_{(j)}| \leq \frac{A}{j^a}$$

Effective Dimension

- The effective dimension is

$$s = c \cdot A^{\frac{1}{a}} \cdot n^{\frac{1}{2a}}$$

- The number of coefficients that have magnitude larger than $\frac{1}{\sqrt{n}}$

$$\frac{A}{j^a} \gtrsim \frac{1}{\sqrt{n}} \Rightarrow j \lesssim A^{\frac{1}{a}} \cdot n^{\frac{1}{2a}}$$

- These are roughly the number of parameters we are estimating

Example: Exact Sparsity

- If only $k < p$ of the coefficients are non-zero and bounded by C
- Then for $j \leq k$, for any a:

$$\left|\beta_{(j)}\right| \leq C \left(\frac{k}{j}\right)^{a}$$

- For $j > k$, for any a:

$$\left|\beta_{(j)}\right| = 0 \leq C \left(\frac{k}{j}\right)^{a}$$

- Coefficient is $(C\ k^{a}, a)$-approximately sparse for $a \to \infty$:

$$s = c\ C^{\frac{1}{a}} \cdot k \cdot n^{\frac{1}{2a}} \approx k$$

The Method

- We want to penalize solutions that have many large coefficients
- One rough measure of the number of a vector that penalizes vectors with many large coefficients is the ℓ_1-norm

$$\|\beta\|_1 = |\beta_1| + \cdots + |\beta_p|$$

- So instead of minimizing the empirical RMSE, we will add a penalty

$$\min_b \frac{1}{2} E_n\left[(Y - b'X)^2\right] + \lambda\|b\|_1$$

Note: Standardization

- Note that as currently stated the lasso method is not invariant to re-scaling or centering the parameters
- It is always advisable to standardize the variables before passing them to the optimization method

$$\tilde{X} = \frac{(X - E_n[X])}{\sqrt{Var_n(X)}}$$

- This way we are equally penalizing all the variables
- Otherwise, variables with larger variance are given more priority as they need smaller coefficients to be included

Choosing the Penalty

- A typical way to choose the penalty λ in practice is via cross-validation

Cross-Validation

- Partition the data into K folds (typically $K = 5$)
- Leave one block out. Fit prediction rule on the other. Predict the outcome on the left-out block and record RMSE
- Repeat for each block
- Average the RMSE across repetitions
- Repeat these steps for many values of the penalty level and choose the value that minimizes Average RMSE

Coding Example

The Intuition

- The j-th component $\hat{\beta}_j$ in the Lasso solution is set to zero if

$$\underbrace{\left|\partial_{b_j} E_n\left[\left(Y-\hat{\beta}'X\right)^2\right]\right|}_{\text{Marginal benefit in prediction}} \leq \underbrace{\lambda}_{\text{Marginal increase in penalty}}$$

- Invoking the form of the gradient (Normal Equation)

$$\beta_j = 0 \; if \; \left|\hat{S}_j\right| = 0, \qquad \hat{S}_j \coloneqq E_n\left[\left(Y-\hat{\beta}'X\right)X_j\right]$$

Coding Example

The intuition

- At the true parameter β we know that for all j

$$E\left[(Y - \beta' X)X_j\right] = 0$$

- But in finite samples

$$S_j \coloneqq E_n\left[(Y - \beta' X)X_j\right]$$

- Might be non-zero. The amount of variation of this is called the noise of the problem; the noise of measuring the marginal predictive ability
- We need the penalty to be larger than this inherent noise
- Otherwise even good solutions, like the true β, will be ruled out

The intuition

- The S_j behave like a multi-variate normal distribution

$$\left(S_j\right)_{j=1}^{p} \sim \frac{\sigma}{\sqrt{n}}\left(N_j\right)_{j=1}^{p}, \qquad N_j \sim N(0,1)$$

- By union bound and symmetry

$$P\left(\max_j \left|N_j\right| > \Phi^{-1}\left(1-\frac{\alpha}{2p}\right)\right) \leq \alpha$$

- Thus we have our condition of λ dominating the noise, if we set:

$$\lambda = \frac{\sigma}{\sqrt{n}}\Phi^{-1}\left(1-\frac{\alpha}{2p}\right) \approx \sigma\sqrt{\frac{\log(p/\alpha)}{n}}$$

Coding Example

The Theory

Under approximate sparsity, *restricted isometry condition (RIP)* and other regularity conditions, with the theoretically driven penalty level λ, with probability approaching $1-\alpha$:

$$\sqrt{E_X\left[\left(\beta' X - \hat{\beta}' X\right)^2\right]} \leq const \cdot \sqrt{E[\epsilon^2]} \sqrt{\frac{s \log(p \vee n)}{n}}$$

where s is the effective dimension

$$s = const\ A^{\frac{1}{a}}\ n^{\frac{1}{2a}}$$

The number of regressors selected is at most $const \cdot s$

The Technical Assumption

- Restricted Isometry Condition
- For any subset Z of X of dimension $L = s\log(p \vee n)$
- The restricted co-variance matrix $E[ZZ']$ is well-posed and bounded

$$C_1 \preccurlyeq E[ZZ'] \preccurlyeq C_2$$

- The empirical co-variance converges to the population covariance in ℓ_∞ norm

$$\sup_{a:\, \|a\|_1 = 1} |a'(E_n[ZZ'] - E[ZZ'])a|$$

Post-Lasso OLS

- It could be beneficial in finite samples to attempt to remove the regularization bias, at least from the chosen coefficients
- We can do that by running an OLS step after the Lasso step on the subset of variables with a non-zero coefficient
- The method has the same worst-case guarantees as Lasso, so it cannot hurt

Coding Example

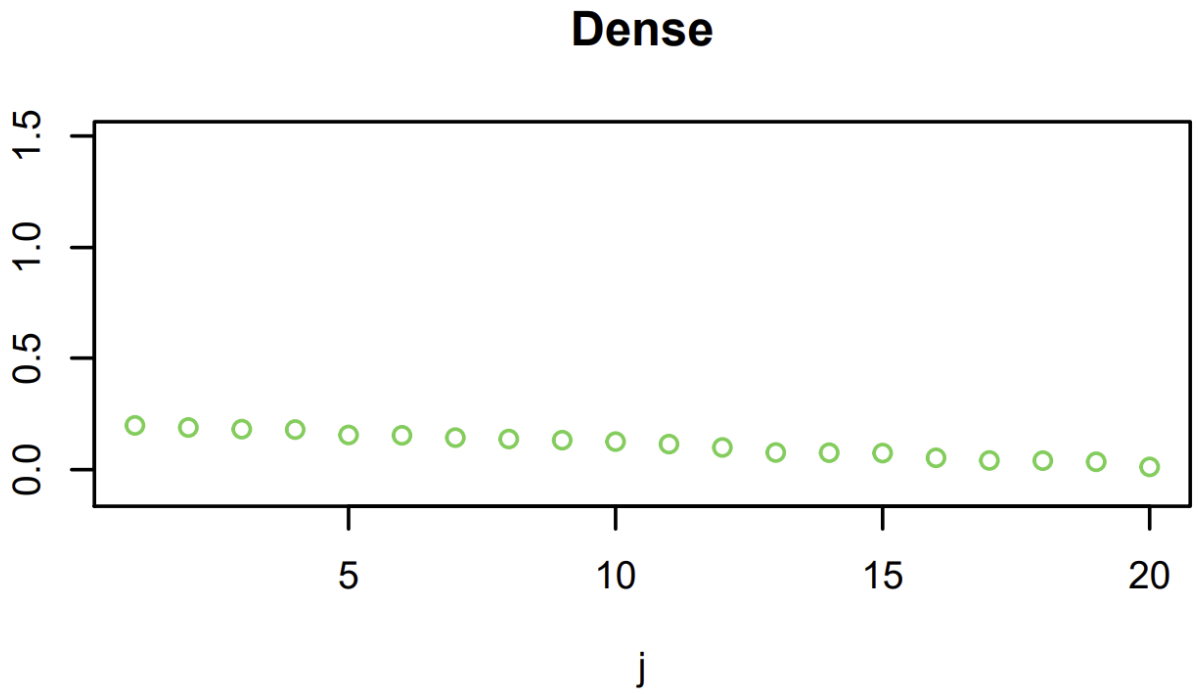
Watch out with regularizing Post Lasso OLS

Post (Lasso-CV) OLS ≠ (Post Lasso OLS)-CV

- Either choose theoretically driven penalty
- Or run cross-validation for the overall Post Lasso OLS procedure
- LassoCV tends to choose too many non-zero coefficients than optimal
- Adding an OLS step to such a large model can lead to overfitting
- CV'ing the overall process enforces a large penalty more appropriate for the Post Lasso OLS procedure

Beyond Sparsity

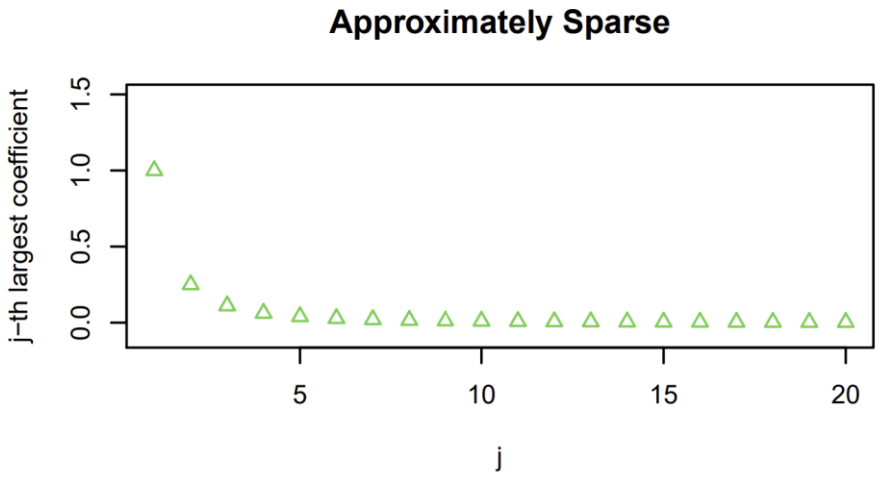
Small Dense Coefficients and Ridge

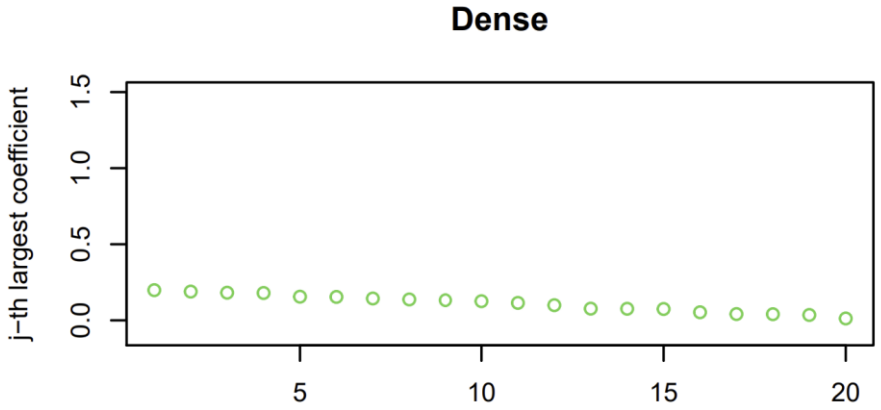


$$\min_b \frac{1}{2} E_n\left[(Y - b'X)^2\right] + \lambda \|\beta\|_2^2$$

$$\|\beta\|_2^2 = \beta_1^2 + \cdots + \beta_p^2$$

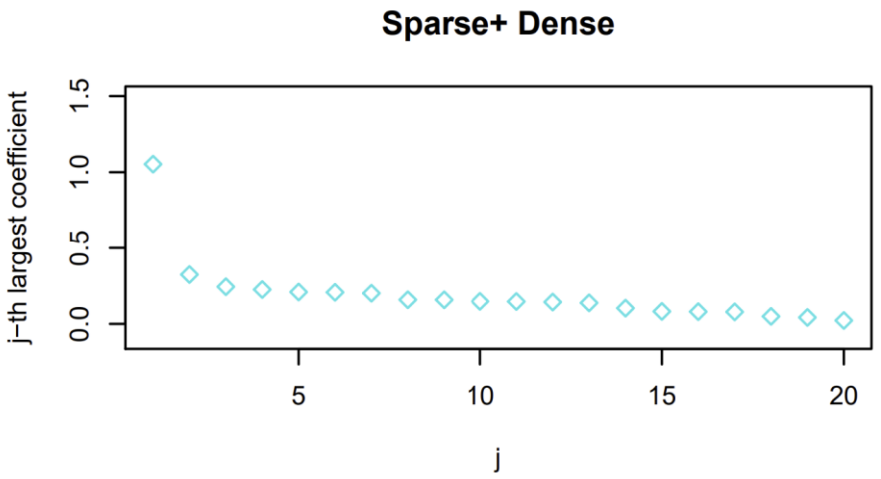
Dense or Sparse and ElasticNet





$$\min_b \frac{1}{2} E_n\left[(Y - b'X)^2\right] + \lambda\left((1-\alpha)\|b\|_2^2 + \alpha\|b\|_1\right)$$

Dense + Sparse and LAVA



$$\min_{b=\gamma+\delta} \frac{1}{2} E_n\left[(Y - b'X)^2\right] + \lambda_1 \|\gamma\|_2^2 + \lambda_2 \|\delta\|_1$$

Coding Example