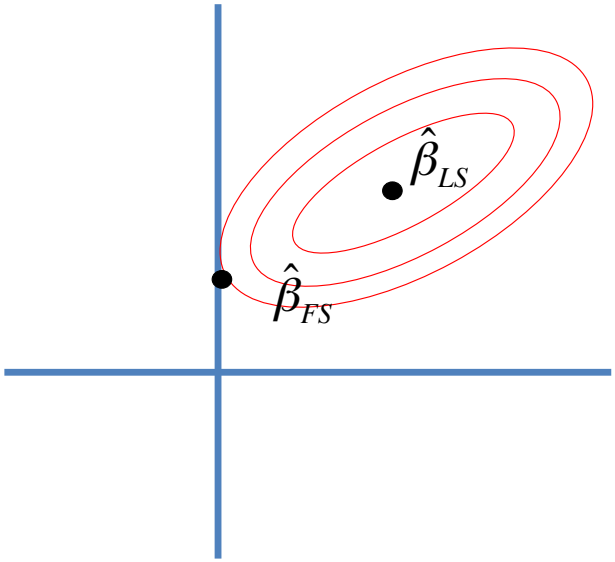
Outline: (Linear) Models in Large Feature Spaces
Traditional Feature Selection

(F. Chiaromonte)

Introduction to Statistical Learning

Chapter 6 Section 1, Lab 1



Traditional ("hard") feature selection: (most) **NON-CONVEX constrained optimization**

L0 norm counts non-0 coefficients, but size of each non-0 coefficient is unconstrained.

Much harder, previously not computationally viable; now *Mixed Integer Optimization*.

Some (non-traditional) references:

- Bertsimas D., King A., Mazumder R. (2016) Best subset selection via a modern optimization lens. AOS 44(2) 813-852.
- Kenney A., Chiaromonte F., Felici G. (2020) MIP-BOOST: Efficient and Effective L_0 Feature Selection for Linear Regression. JCGS.

$$\| \underline{Y} - \underline{X}\beta \|^2 = \min_{\beta \in R^p}$$

$$\sum_{j=1}^{p} Ind(\beta_j \neq 0) \leq c$$ size constraint

SIZE CONSTRAINT TUNED BY CROSS VALIDATION
… the traditional **Best Subset Selection** problem

Important: can also add further "integer" constraints to capture structure.

Back to traditional statistical approaches:

- **Feature (Subset) Selection**
  - Best Subset Selection
  - Step-wise (sequential) Selection

  Followed by LS fit of the (smaller) model comprising the selected features.

- **Dimension Reduction**
  - Principal Components (unsupervised reduction)
  - Sufficient Dimension Reduction (supervised reduction)

  Followed by LS fit of the (smaller) model comprising the selected linear combinations

Also these can be though of in the framework of constrained LS: *Linear constraints* to force β in a coordinate space, or a generic linear subspace, of R^p. ***BUT WE NEED AN ADDITIONAL "INGREDIENT"!***

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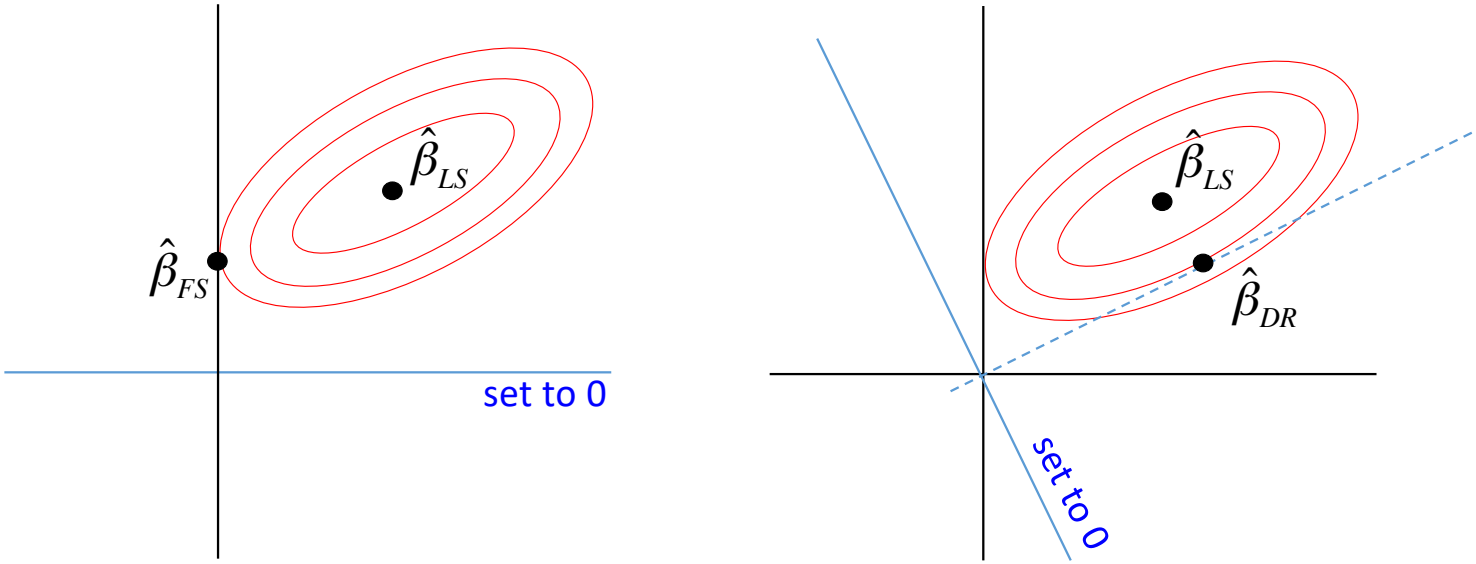
Dimension Reduction: ISLR also describes Partial Least Squares. But does not describe Sufficient Dimension Reduction techniques.

Cartoons with p=2 and c=1 (d=1)



$$\| \underline{Y} - \underline{X}\beta \|^2 = \min_{\beta \in R^p}$$

$$H_{FS}\beta = 0_{(p-c)}$$

linear constraints

$$\| \underline{Y} - \underline{X}\beta \|^2 = \min_{\beta \in R^p}$$

$$V_{DR}\beta = 0_{(p-d)}$$

THE (maximal) **COUNT** OF FEATURES *c* OR THE **DIMENSION** *d* IS FIXED… SO IS THE **(O.N.) BASIS** OF THE FEATURE SPACE FROM WHICH WE FORM THE (*p*-*c*) or (*p*-*d*) CONSTRAINTS.

Feature Selection: How do we produce a pxp matrix H expressing an O.N. basis in the feature space?

(we then focus on its last (*p*-*c*) rows to create the linear constraints with H_{FS})

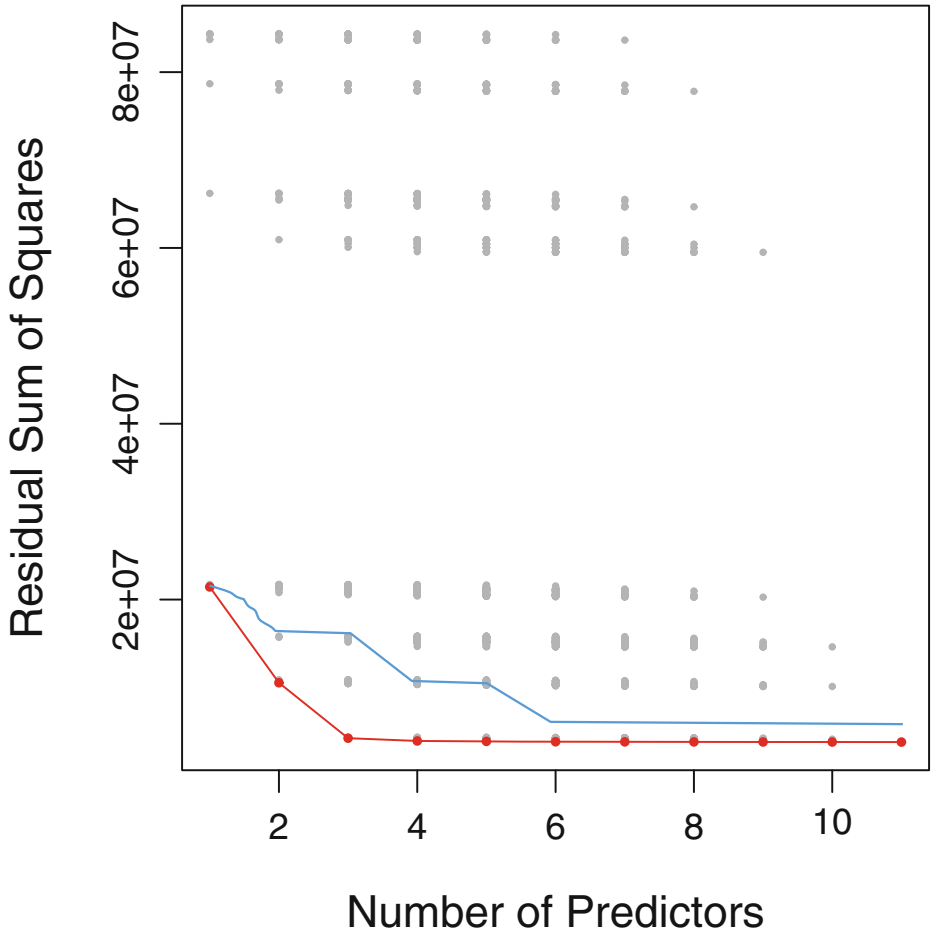
Feature (subset) Selection:

Make a sequence of nested subsets adding one feature at a time, i.e., make an ordering of the features.

This corresponds to a permutation of the elements of the Canonical O.N. basis $\{e_1,... e_p\}$, and provides

H (a permutation matrix)

Rigorous for feature selection implemented through **stepwise (sequential) methods**, not for **best subset methods** which find the best subset of each size – in principle such subsets may not be nested (but the intuition still works).



The RSS of 2^p possible models (subsets of features).

For each size c, there are $\binom{p}{c}$ possible models.

On the lower boundary (red) are the best models of each size; best subsets. May or may not be a nested sequence.

The blue path represents a nested sequence of "good" models obtained stepwise. May depart from the lower boundary.

Algorithm 6.1 *Best subset selection*

1. Let $\mathcal{M}_0$ denote the *null model*, which contains no predictors. This model simply predicts the sample mean for each observation.
2. For $k = 1, 2, \ldots p$:
   (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors.
   (b) Pick the best among these $\binom{p}{k}$ models, and call it $\mathcal{M}_k$. Here *best* is defined as having the smallest RSS, or equivalently largest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

Best Subset approach requires fitting ALL possible models ("brute" enumeration).

Algorithm 6.2 *Forward stepwise selection*

1. Let $\mathcal{M}_0$ denote the *null* model, which contains no predictors.
2. For $k = 0, \ldots, p-1$:
   (a) Consider all $p-k$ models that augment the predictors in $\mathcal{M}_k$ with one additional predictor.
   (b) Choose the *best* among these $p-k$ models, and call it $\mathcal{M}_{k+1}$. Here *best* is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

Stepwise (sequential) approaches do not; they explore fewer models. Computationally leaner.

Hybrid stepwise approaches mix forward and backward progression.

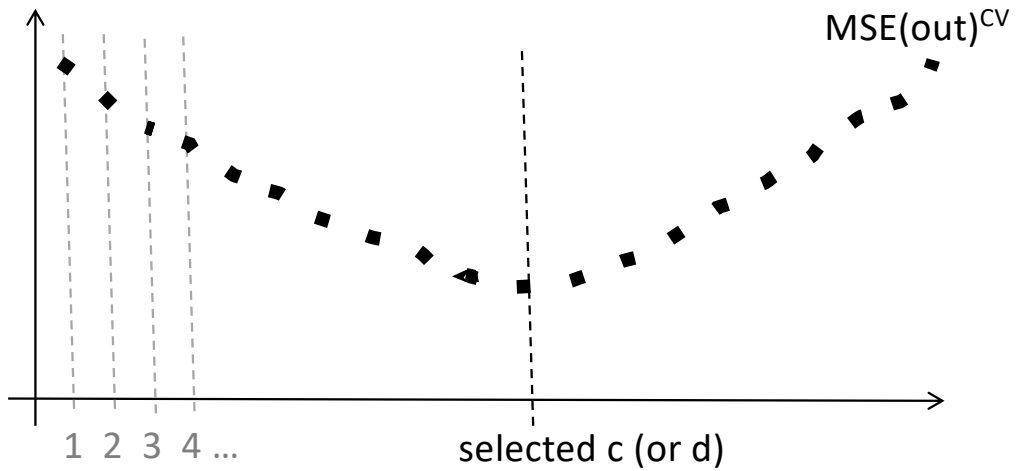
Algorithm 6.3 *Backward stepwise selection*

1. Let $\mathcal{M}_p$ denote the *full* model, which contains all p predictors.
2. For $k = p, p-1, \ldots, 1$:
   (a) Consider all k models that contain all but one of the predictors in $\mathcal{M}_k$, for a total of $k-1$ predictors.
   (b) Choose the *best* among these k models, and call it $\mathcal{M}_{k-1}$. Here *best* is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

(Step 3 in each algorithm; next…)

How do we select the (maximal) count c, or dimension d, along an ordered sequence of features or linear combinations?

Of course, once H (or V) are fixed we could perform the selection estimating the out-of-sample MSE associated to each value of *c* or *d*, e.g., by cross-validation (same as for the penalty parameter in Ridge or LASSO).



Historically though other (non-computation based) approaches and criteria have been used.

CRITERIA FOR FEATURE (SUBSET) SELECTION

The number of features c (**= d** if formulae below) is selected optimizing a criterion that approximates an estimate of the out-of-sample performance – but indirectly, not directly as in cross-validation; no intensive computation required. For instance:

$$\text{Adjusted } R^2 = 1 - \frac{\text{RSS}/(n-d-1)}{\text{TSS}/(n-1)}.$$

Adjusted R-squared provides the simplest solution, each sum of squares is divided by its degrees of freedom.

$$C_p = \frac{1}{n}\left(\text{RSS} + 2d\hat{\sigma}^2\right)$$

Mallow's C_p formula in the book, proportional to original formula. If $\hat{\sigma}^2$ is an unbiased estimate of the error variance, C_p is an unbiased estimate of the out-of-sample MSE (can take the s^2 estimate from the full model, least likely to carry bias.

Strike a balance between RSS (error on the training data) and d (size, complexity of the model)

Akaike and Bayes Information Criteria can be used for model selection whenever models are fitted by Maximum Likelihood.

For linear models with additive Gaussian errors their expressions become:

$$\mathrm{AIC} = \frac{1}{n\hat{\sigma}^2}\left(\mathrm{RSS} + 2d\hat{\sigma}^2\right)$$

Behaves exactly like C_p here!

$$\mathrm{BIC} = \frac{1}{n}\left(\mathrm{RSS} + \log(n)d\hat{\sigma}^2\right)$$

The weight of the adjustment uses log(n), depending on the sample size, instead of 2. For n>7 BIC has a steeper penalty than AIC (C_p); it favors smaller models.

General equations for Information Criteria:

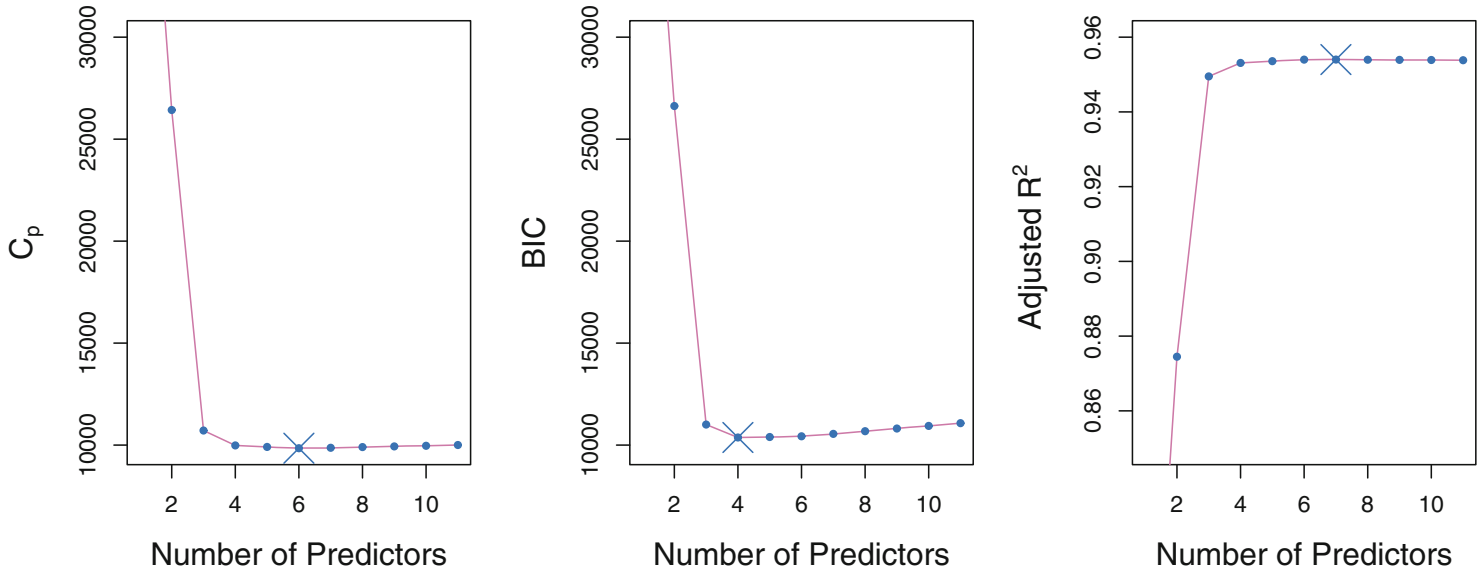
$$AIC = -2\log L(\hat{\vartheta}_{ML}) + 2d$$

$$BIC = -2\log L(\hat{\vartheta}_{ML}) + \log(n)d$$

$L(\hat{\vartheta}_{ML})$ = optimal likelihood value on MLE of parameter vector

d = # of free parameters being estimated

HOW DO THE TRADITIONAL CRITERIA LOOK IN PRACTICE?



This behavior is rather common; even though the criteria are NOT monotone and ought to have a minimum/maximum, in many applications they do not clearly discriminate unambiguously the number of features (the model) to be used – rather flat ranges.

Would you pick 3 instead of the “technical” optima, which btw differ across criteria?