# **Linear Methods for Regression: Subset Selection**

Statistical methods for data analysis – Machine learning

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#### Motivation

## Possible problems of Least Squares Estimation (LSE):

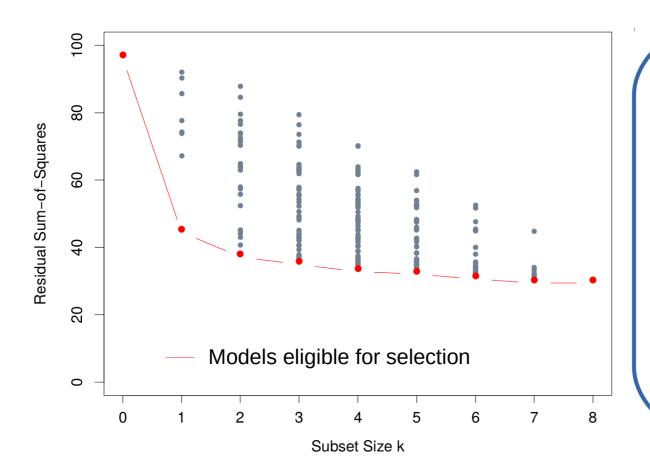
- Prediction accuracy:
  - Low bias, large variance
  - Can sometimes be improved by shrinking. Sacrifice a bit of bias but reduce variance
- Interpretation:
  - Identification of a small subset of variables with the strongest effect

#### Solution: Model selection

- Here we describe different strategies to variable subset selection with linear regression.
- In next lectures **shrinkage** and **dimension-reduction** approaches for controlling variance.

#### Best-subset selection

- Finds for each  $k=\{0,1,2,...,p\}$  the subset of size k that gives **smaller** Residual Sum of Squares.
- **Leaps and bounds** procedure (Furnival and Wilson, 1974): feasible for p as large as 30 or 40.
- RSSs of all subset models for the prostate cancer example:



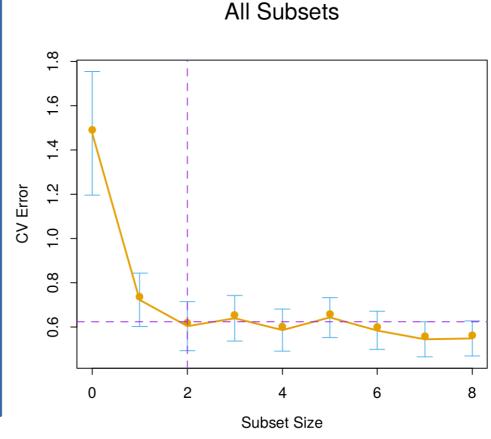
- Best subset of size 2 need not include the variables in the best subset of size 1
- Best-subset curve is necessary decreasing. It cannot be used to select the subset size k

#### General idea of best-subset selection

Use the training data to produce a sequence of models varying in complexity and indexed by a single parameter.

Cross-validation and the AIC criterion (presented in next lectures)
can be used to estimate the best parameter k.

Term	LS	Best Subset
Intercept	2.465	2.477
lcavol	0.680	0.740
lweight	0.263	0.316
age	-0.141	
lbph	0.210	
svi	0.305	
lcp	-0.288	
gleason	-0.021	
pgg45	0.267	
Test Error	0.521	0.492
Std Error	0.179	0.143



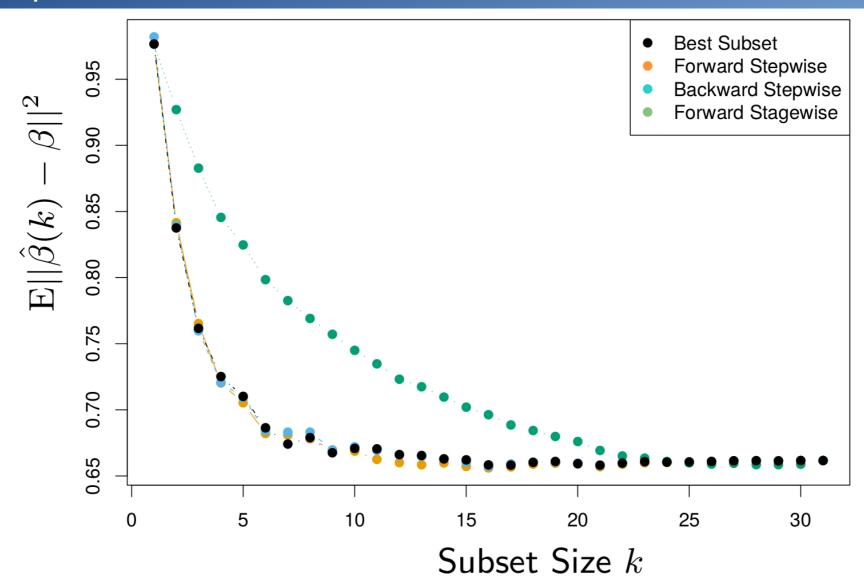
## Forward-Stepwise Selection

- Search all possible subsets is infeasible for large p, hence we seek a good path through them.
- Forward-stepwise selection:
  - starts with the intercept
  - sequentially adds into the model the predictor that most improve the fit
  - produces a sequence of models indexed by k, the subset size
  - is a greedy algorithm, producing a nested sequence of models
  - is **suboptimal** compared to best-subset selection
  - is applicable with large p
  - has lower variance but perhaps higher bias

## Backward-Stepwise Selection

- Backward-stepwise selection:
  - starts with the full model
  - sequentially deletes the predictor that has the least impact on the fit
  - the candidate for dropping is the variable with the smallest Zscore
  - can only be used when N > p
  - produces a sequence of models indexed by k, the subset size
  - is a greedy algorithm, producing a nested sequence of models
  - is **suboptimal** compared to best-subset selection
  - is applicable with large p
  - has lower variance but perhaps higher bias

## Comparison



On the prostate cancer example, best-subset, forward and backward selection all gave exactly the same sequence of terms.

# Hybrid stepwise selection strategies

- Hybrid stepwise-selection strategies consider both forward and backward moves at each step, and select the "best" of the two.
- The R function called *step* uses the Akaike (**AIC**) criterion for weighting the choices, i.e., at each step an add or drop is performed that minimizes the AIC score.
- Notice that standard errors of coefficients in non-full models are not valid since they do not account for the search process.
  - Bootstrap techniques (presented in next lectures) can be used to solve this problem



See text of Exercise 3

## References

[Hastie 2009] Trevor Hastie, Robert Tibshirani, Jerome Friedman. The Elements of Statistical Learning: Data Mining, Inference, and Prediction (second edition). Springer. 2009.