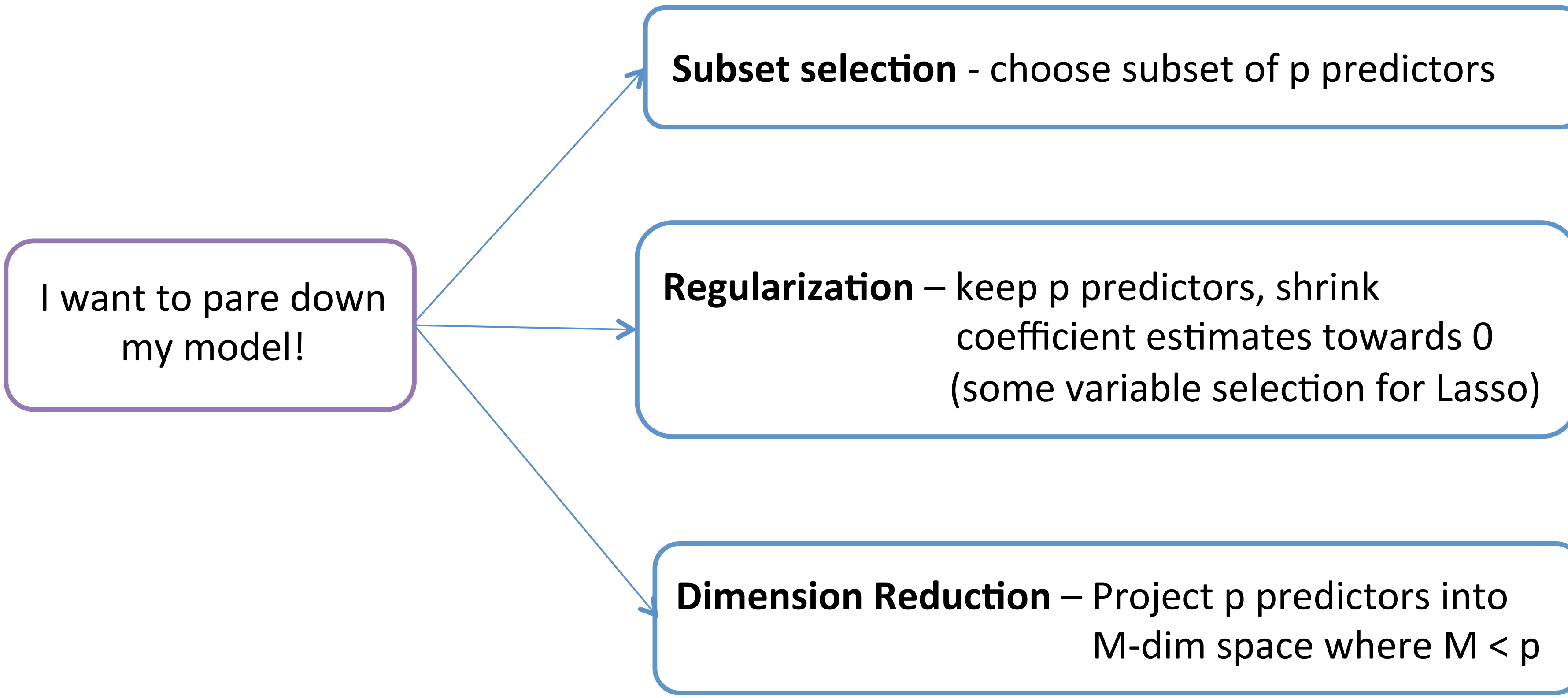
Cross-Validation

"Some of the figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani "

Overview

- Subset Selection of Predictors
- Cross-Validation
- K-fold Cross-Validation

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon$$



Subset Selection

- Best subset: Try every model. Every possible combination of *p* predictors
  - Computationally intensive, especially for *p* large
  - Also, huge search space. Higher chance of finding models that look good on training data but have little predictive power on future data

- Stepwise
  - In practice, commonly done
  - Forward, Backward, Forward + Backward

Subset Selection - Forward Stepwise

$M_0 \rightarrow M_1 \rightarrow M_2 \rightarrow \dots\dots \rightarrow M_p$

+1 predictor with smallest RSS $\Leftrightarrow$ largest R^2

+1 predictor with smallest RSS $\Leftrightarrow$ largest R^2

Now we have *p* candidate models

Are RSS and R^2 good ways to decide amongst the *p* candidates?

Subset selection

Choosing among *p* candidate models…

- Cross-validation - always a great standby
- Mallow's C_p
- AIC
- BIC
- Adjusted R^2

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                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.933
Model:                            OLS   Adj. R-squared:                  0.928
Method:                 Least Squares   F-statistic:                     211.8
Date:                Mon, 03 Nov 2014   Prob (F-statistic):           6.30e-27
Time:                        14:45:06   Log-Likelihood:                -34.438
No. Observations:                  50   AIC:                             76.88
Df Residuals:                      46   BIC:                             84.52
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [95.0% Conf. Int.]
------------------------------------------------------------------------------
x1             0.4687      0.026     17.751      0.000         0.416     0.522
x2             0.4836      0.104      4.659      0.000         0.275     0.693
x3            -0.0174      0.002     -7.507      0.000        -0.022    -0.013
const          5.2058      0.171     30.405      0.000         4.861     5.550
==============================================================================
Omnibus:                        0.655   Durbin-Watson:                   2.896
Prob(Omnibus):                  0.721   Jarque-Bera (JB):                0.360
Skew:                           0.207   Prob(JB):                        0.835
Kurtosis:                       3.026   Cond. No.                         221.
==============================================================================
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Subset selection

$$C_p = \frac{1}{n}(RSS + 2\underline{p}\hat{\sigma}^2)$$

Mallow's Cp
p is the total # of parameters
$\hat{\sigma}^2$ is an estimate of the variance of the error, ε

$$AIC = -2logL + 2 \cdot \underline{p}$$

L is the maximized value of the likelihood function for the model estimated

$$BIC = \frac{1}{n}(RSS + log(n)\underline{p}\hat{\sigma}^2)$$

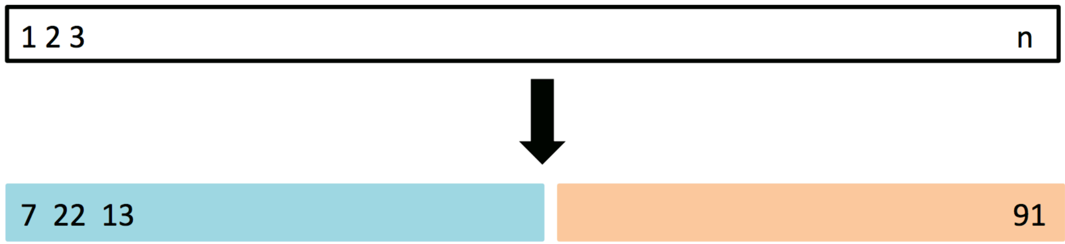
This is Cp, except 2 is replaced by log(n). log(n) > 2 for n>7, so BIC generally exacts a heavier penalty for more variables

$$Adjusted\ R^2 = 1 - \frac{RSS/(n - \underline{p} - 1)}{TSS/(n - 1)}$$

Similar to R^2, but pays price for more variables

Side Note: Can show AIC and Mallow's Cp are equivalent for linear case

Cross-Validation



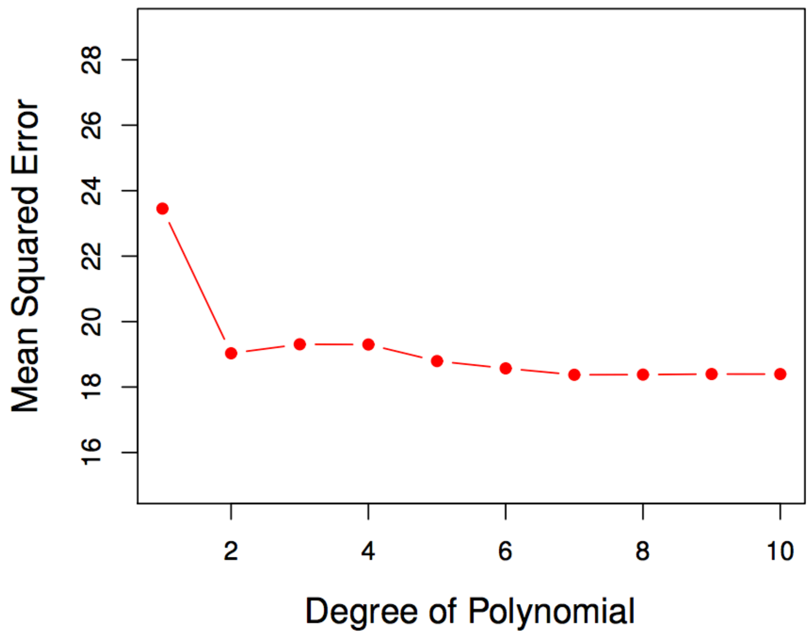
Randomly divide data into training set and validation set

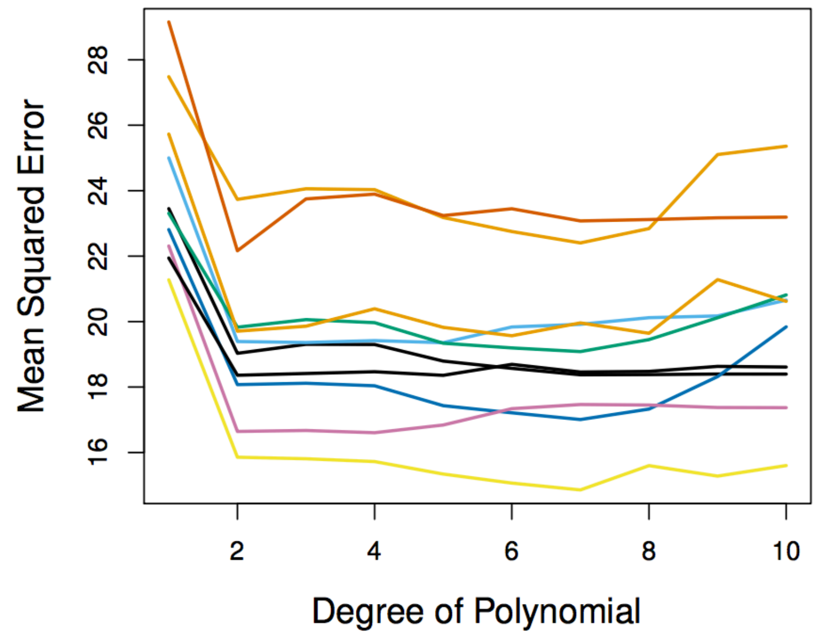
– 50/50, 60/40, 70/30, 80/20, no rule…

1. Fit model on training set
2. Use fitted model in 1. to predict responses for validation set
3. Compute validation-set error
   - Quantitative Response: Typically MSE
   - Qualitative Response: Typically Misclassification Rate

Why might validation-set error rate underestimate test-set error rate?

Cross-Validation

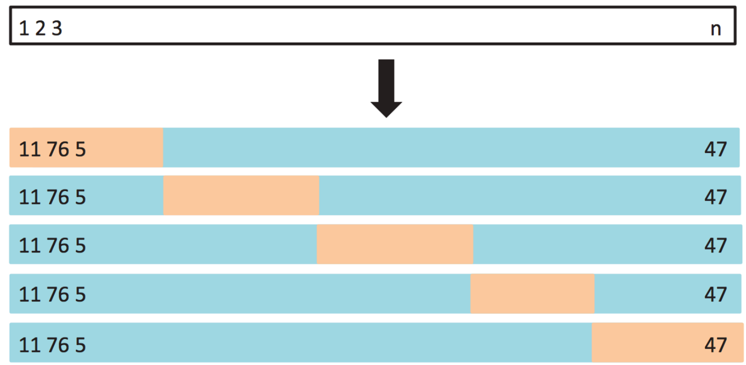




- Fitting MPG (Y) from Horsepower (X)
- Try different polynomial fits
  - Y~X+X^2
  - Y~X+X^2+X^3
  - Y~X+X^2+X^3+X^4

- Validation error can be highly variable depending on random split

K-Fold Cross-Validation



Randomly divide data into K=5 folds. Typically choose K=5 or 10.

Run K times

1. Fit model on training set, using (K-1) folds
2. Use fitted model in 1. to predict responses for validation set, 1 of the folds
3. Compute validation-set error
   - Quantitative Response: Typically MSE
   - Qualitative Response: Typically Misclassification Rate

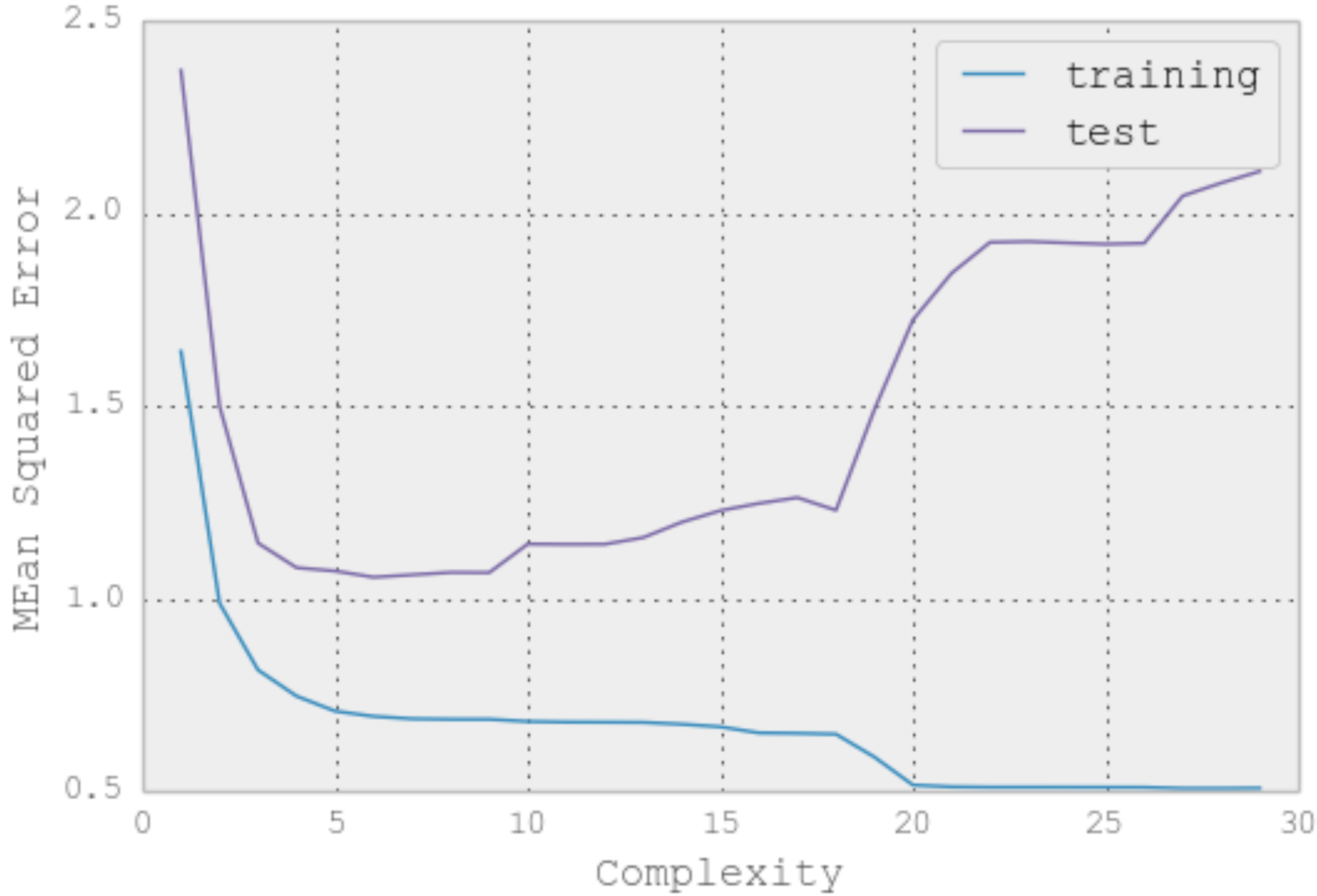
$$\mathrm{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k} \mathrm{MSE}_i$$

K-Fold Cross-Validation

TRY STUFF
- tune parameter 1
- tune parameter 2
- feature engineering
- feature selection
- scale factors 1 way
- scale factors another way
- etc. etc.

Test Set

Don't touch until end for final evaluation.
Gives best estimate of future error.



training
test
MEan Squared Error
Complexity
2.5
2.0
1.5
1.0
0.5
0
5
10
15
20
25
30