Cross-Validation & Regularized Regression

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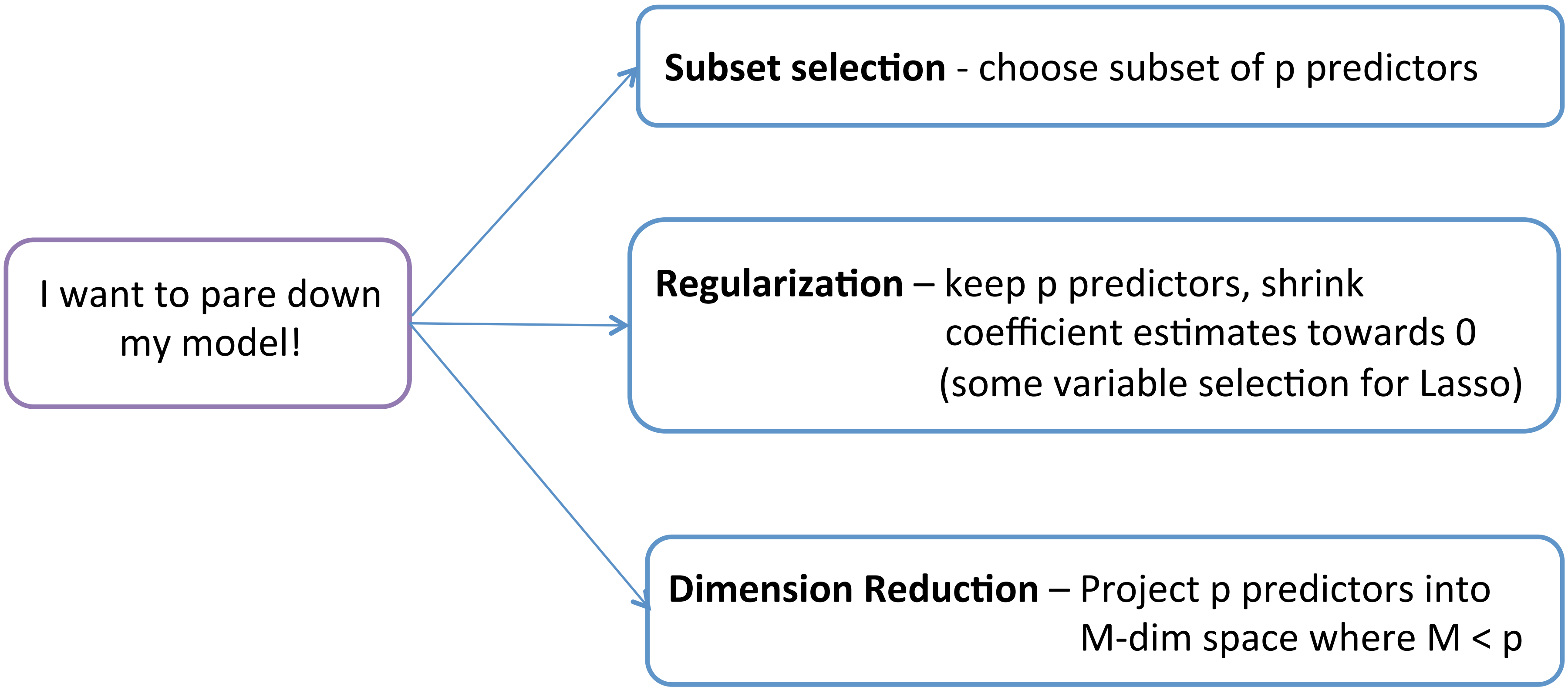
Overview

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

- Bias-Variance Tradeoff
- Regularized Regression
  - Lasso
  - Ridge

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



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

$M_0 \rightarrow M_1 \rightarrow M_2 \rightarrow .... \rightarrow M_p$

+1 predictor with smallest RSS ⇔ largest R^2

+1 predictor with smallest RSS ⇔ 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.
==============================================================================
```

Subset selection

Mallow's C_p:

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

where d is the total # of parameters used and $\hat{\sigma}^2$ is an estimate of the variance of the error ϵ associated with each response measurement.

The *AIC* criterion is defined for a large class of models fit by maximum likelihood:

$$\text{AIC} = -2\log L + 2 \cdot d$$

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

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

Subset selection

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

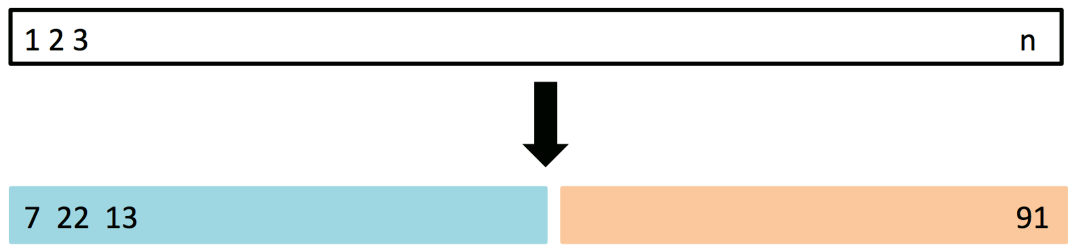
Notice that BIC replaces the $2d\hat{\sigma}^2$ used by C_p with a $\log(n)d\hat{\sigma}^2$ term, where n is the number of observations.

Since $\log n > 2$ for any $n > 7$, the BIC statistic generally places a heavier penalty on models with many variables

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

Unlike the R^2 statistic, the adjusted R^2 statistic *pays a price* for the inclusion of unnecessary variables in the model.

Cross-Validation



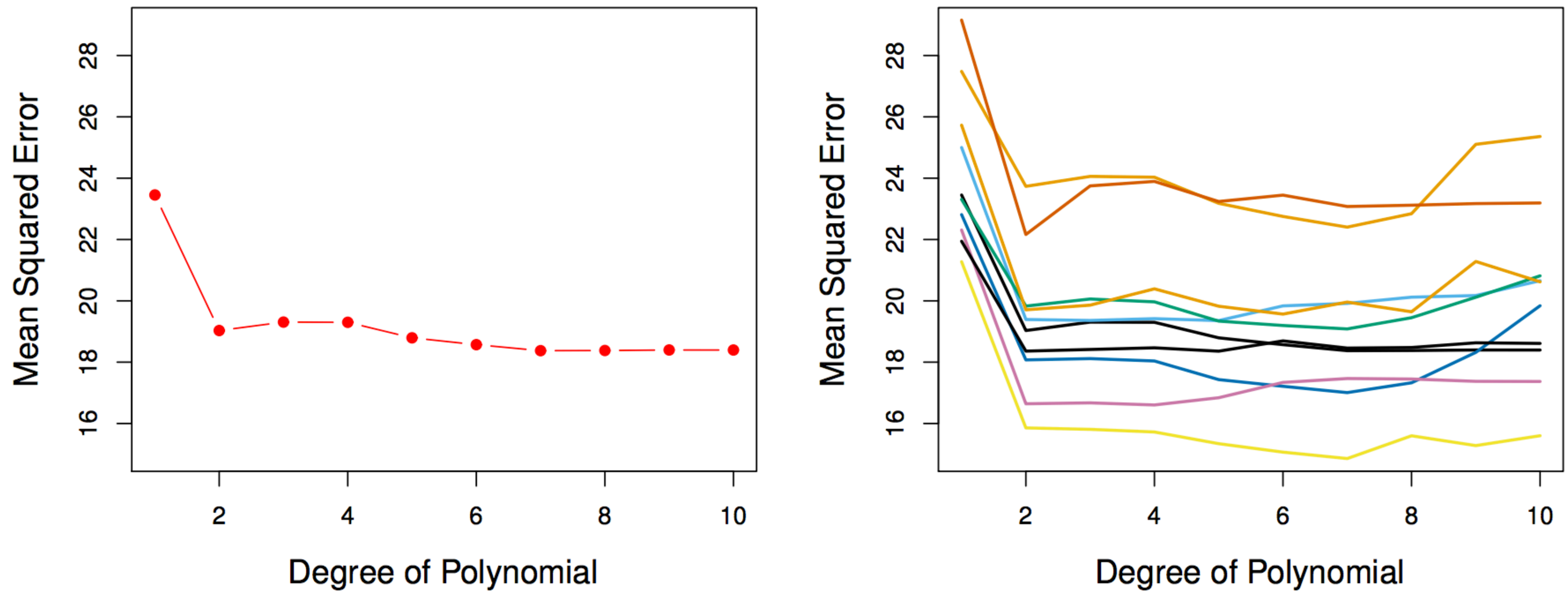
Randomly divide data into training set and validation set

- 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?

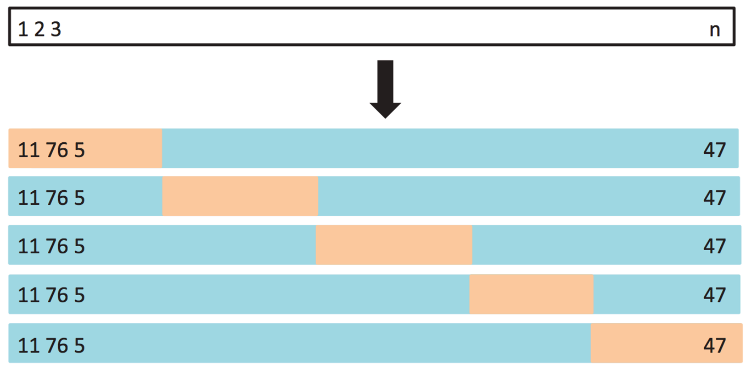
Cross-Validation



- 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 test-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

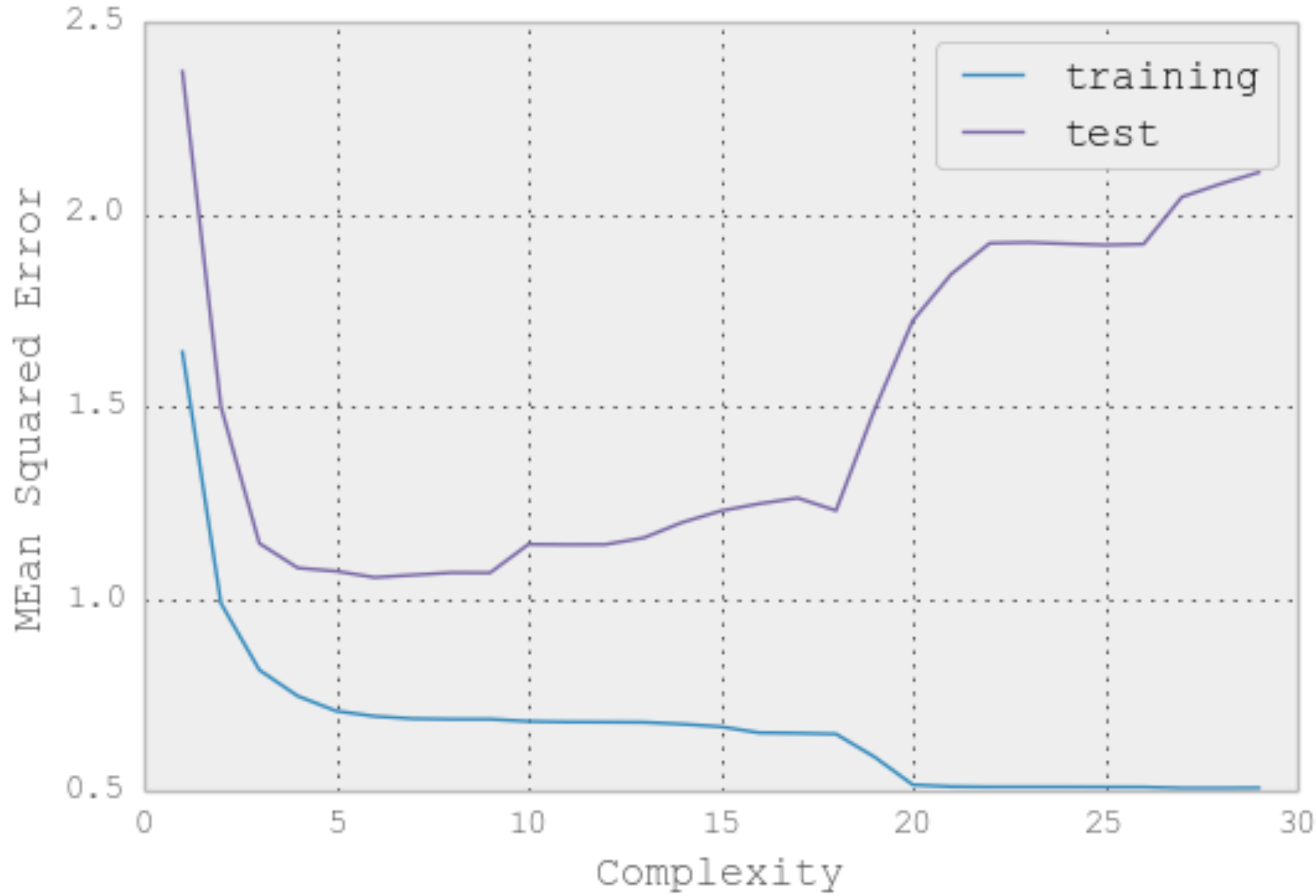
$$\rightarrow \mathrm{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k} \mathrm{MSE}_i$$

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
0.5
1.0
1.5
2.0
2.5
0
5
10
15
20
25
30

Bias-Variance Tradeoff

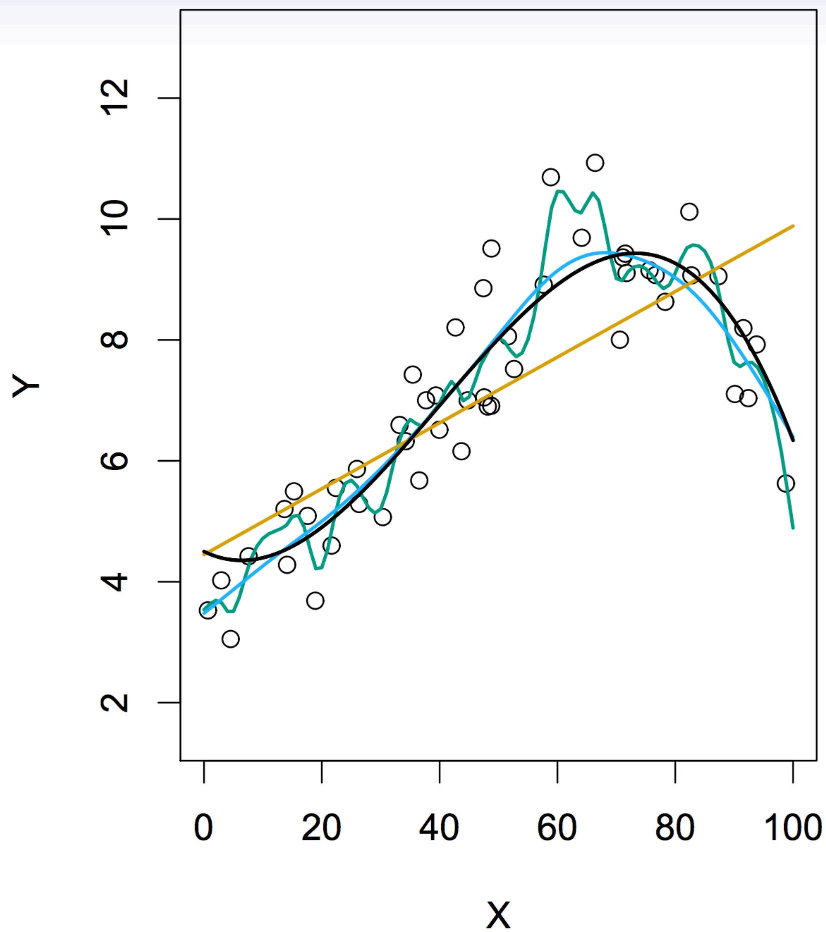
Suppose we have fit a model $\hat{f}(x)$ to some training data Tr, and let (x_0, y_0) be a test observation drawn from the population. If the true model is $Y = f(X) + \epsilon$ (with $f(x) = E(Y|X = x)$), then

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \mathrm{Var}(\hat{f}(x_0)) + [\mathrm{Bias}(\hat{f}(x_0))]^2 + \mathrm{Var}(\epsilon).$$

Ok….what is going on here?

- Applies to modeling in general, beyond Linear Regression
- Want your model to minimize the expected test MSE on LHS. But how?
  - Var(ε), or "Irreducible Error". Can't do anything about that!
  - Can reduce Variance
  - Can reduce Bias

Bias-Variance Tradeoff



$$\mathrm{Var}(\hat{f}(x_0))$$

Amount by which $\hat{f}$ would change if estimated it using a different training dataset

$$\mathrm{Bias}(\hat{f}(x_0))] = E[\hat{f}(x_0)] - f(x_0)$$

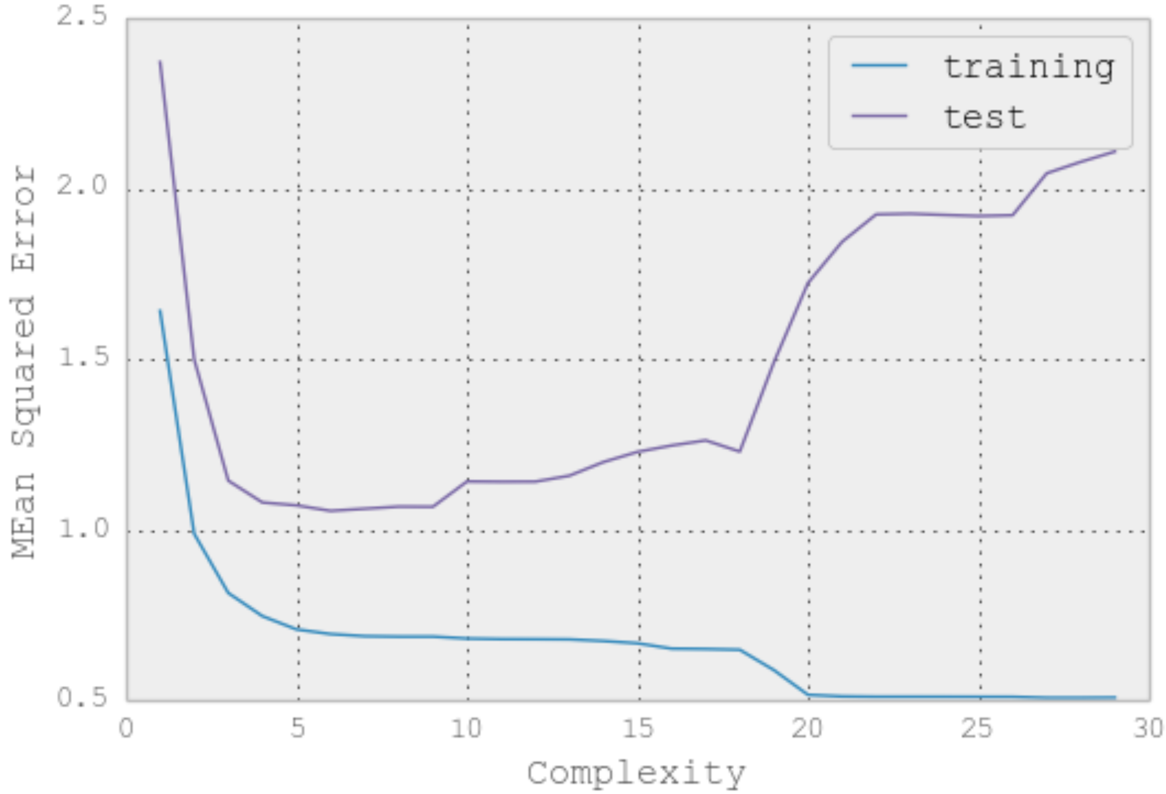
Difference between expected prediction of our model and correct value we are trying to predict

$$\mathrm{Var}(\epsilon)$$

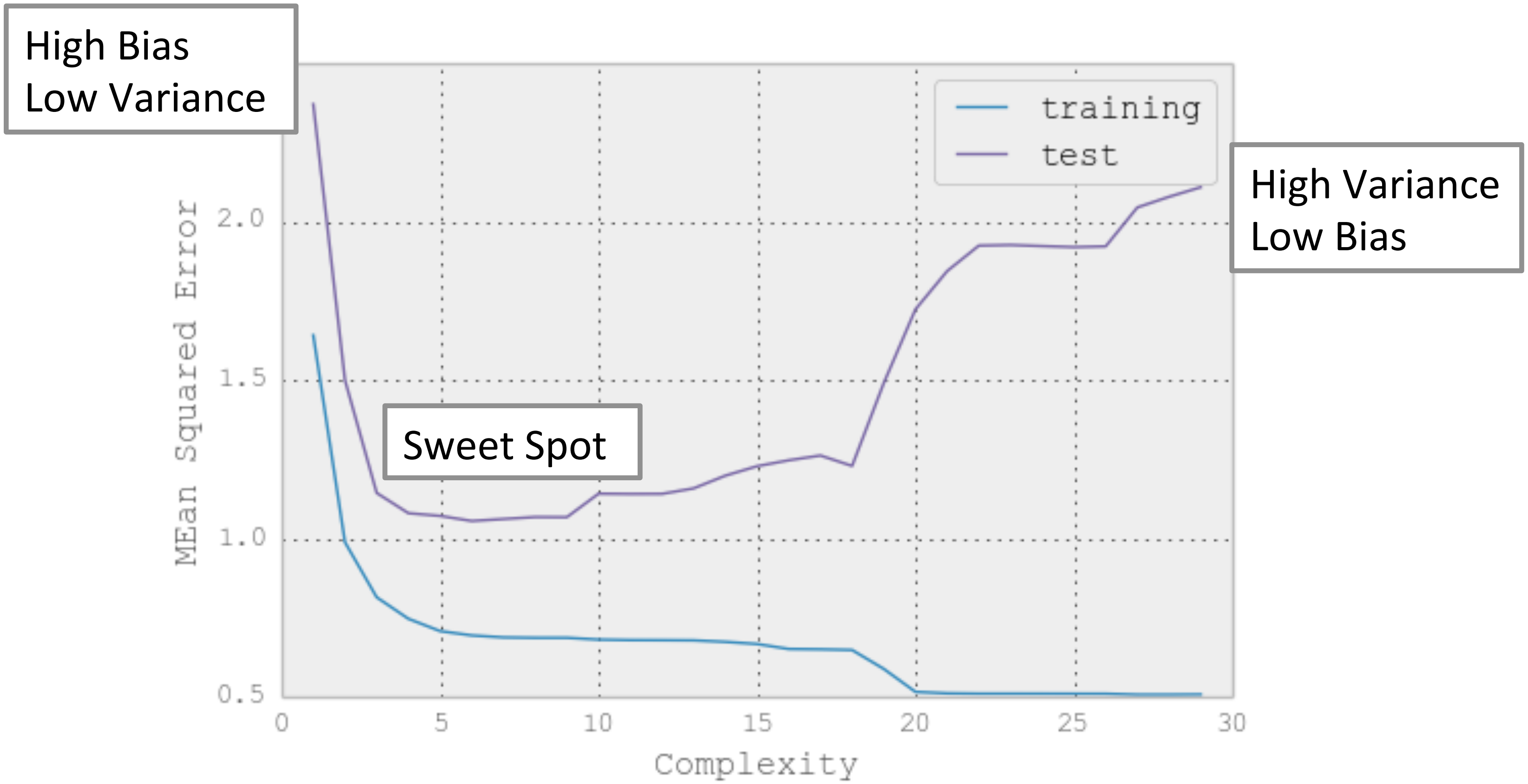
Simply because $Y = f(X) + \epsilon$

Generally speaking, the *more flexible* the model, the *greater the variance*.

Model Framework - Evaluation



Model Framework - Evaluation



- Can break this complexity tradeoff into what we call "bias" and "variance"

Managing the Bias-Variance Tradeoff with Linear Regression

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

I want to pare down my model, reducing the variance!

Subset selection - choose subset of p predictors

Regularization – keep p predictors, shrink coefficient estimates towards 0 (some variable selection for Lasso)

Dimension Reduction – Project p predictors into M-dim space where M < p

Regularization – Ridge regression

- Recall that the least squares fitting procedure estimates $\beta_0, \beta_1, \ldots, \beta_p$ using the values that minimize

$$\mathrm{RSS} = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 .$$

- In contrast, the ridge regression coefficient estimates $\hat{\beta}^R$ are the values that minimize

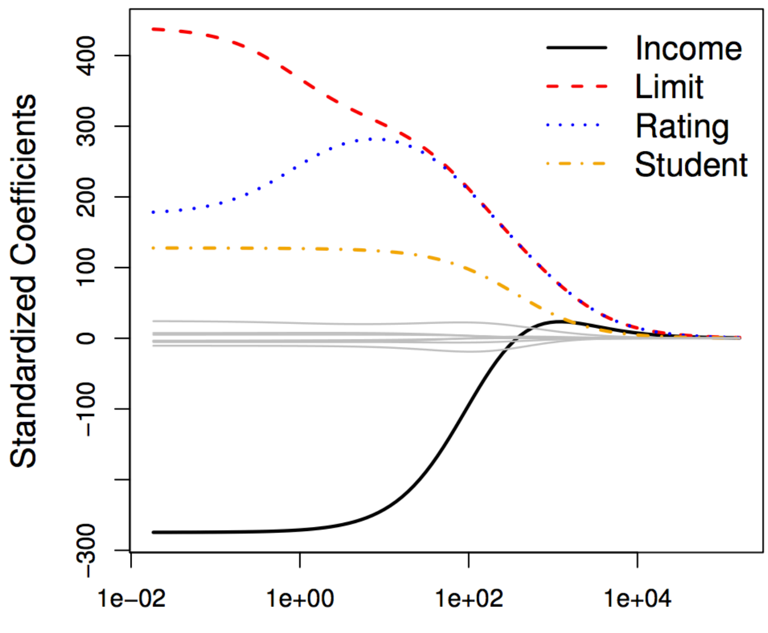
$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = \mathrm{RSS} + \boxed{\lambda \sum_{j=1}^{p} \beta_j^2,}$$

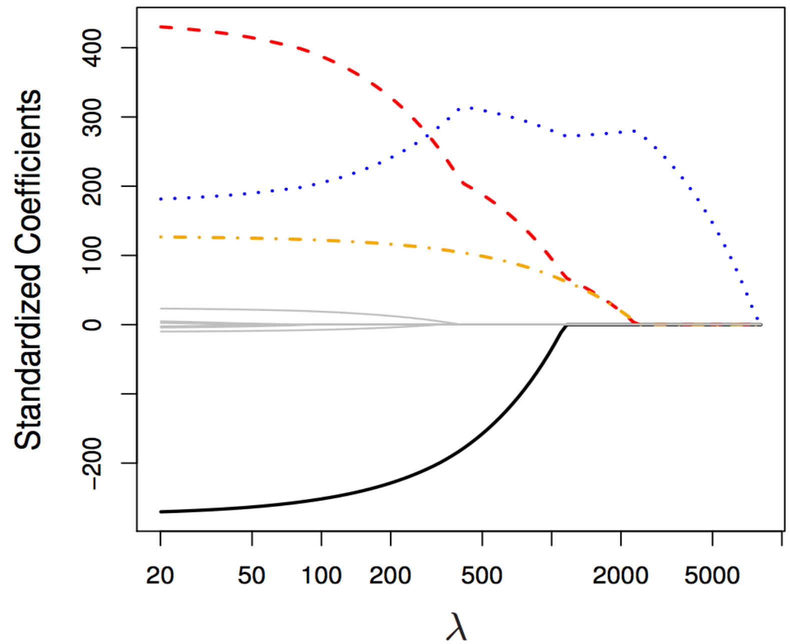
where $\lambda \geq 0$ is a *tuning parameter*, to be determined separately.

Regularization – Lasso regression

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| = \mathrm{RSS} + \boxed{\lambda\sum_{j=1}^{p}|\beta_j|}$$

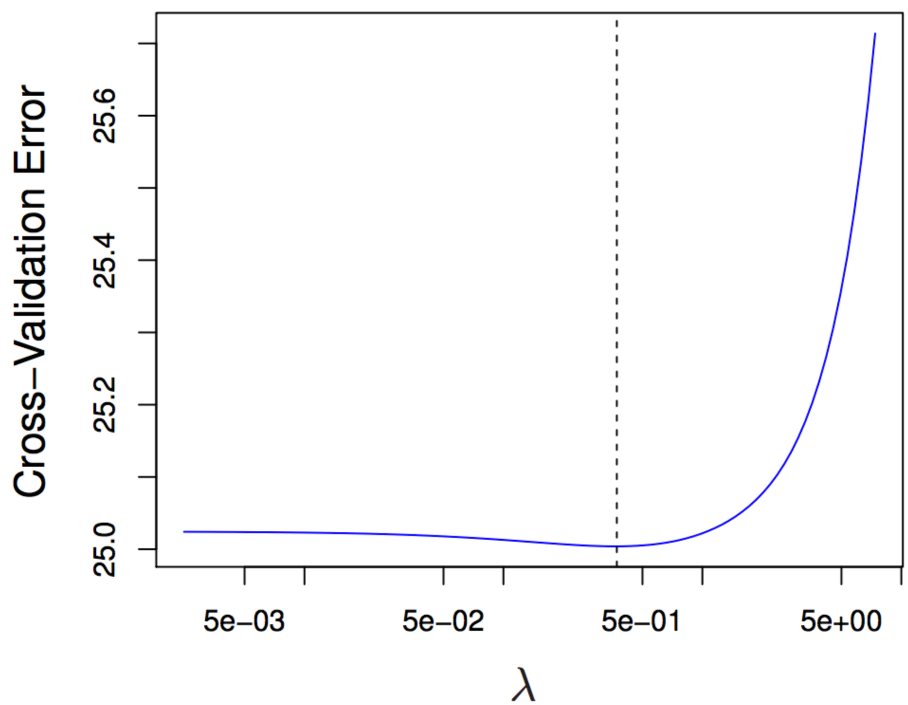
Ridge vs. Lasso

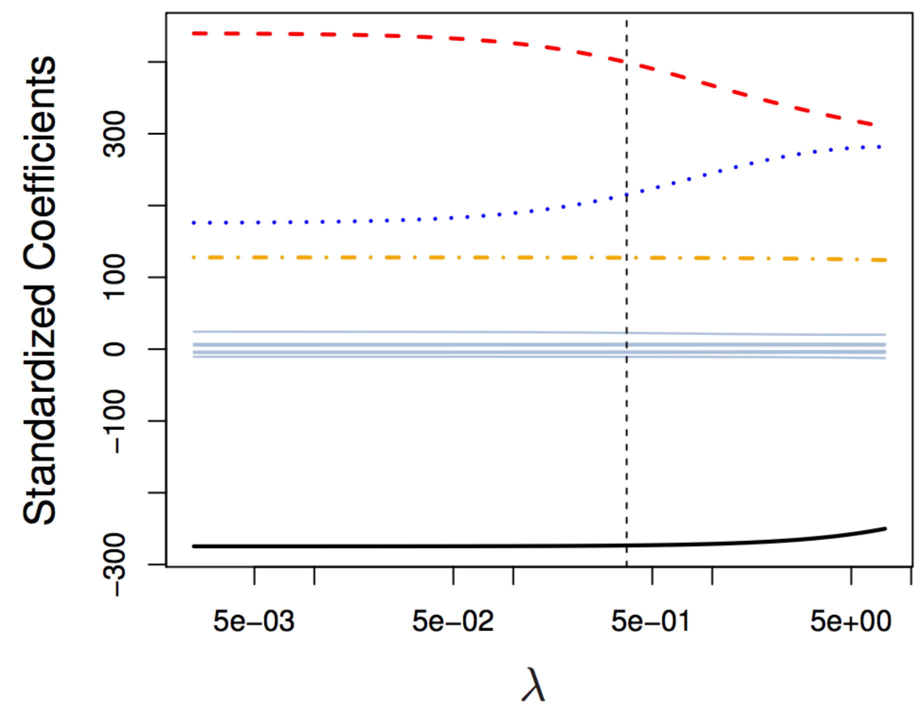




- When λ = 0, we simply have linear models.
- As λ increases, both models become less flexible, reducing variance, but increasing bias.
- Lasso has the advantage of variable selection as well (especially nice when *p* is large)
- Neither universally dominate, but in general one might expect Lasso to do better when response is function of relatively few predictors.
  - Of course you never actually know this, so use your friend, cross-validation!

Choosing λ





- Just increment λ along, fit a large number of models (1 per increment), and choose λ which minimizes cross-validated error, and voila! You have your corresponding optimized model for Ridge Regression.

Don't forget....

- The standard least squares coefficient estimates are *scale equivariant*: multiplying X_j by a constant c simply leads to a scaling of the least squares coefficient estimates by a factor of $1/c$. In other words, regardless of how the jth predictor is scaled, $X_j\hat{\beta}_j$ will remain the same.
- In contrast, the ridge regression coefficient estimates can change *substantially* when multiplying a given predictor by a constant, due to the sum of squared coefficients term in the penalty part of the ridge regression objective function.
- Therefore, it is best to apply ridge regression after *standardizing the predictors*, using the formula

$$\tilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \overline{x}_j)^2}}$$

Questions

- What is training error? validation error? test error?
- What are the steps to cross-validation?
  - How would you use it to compare say ***p*** different models?
- Same question as above, except with K-fold cross-validation
- What is the Bias-Variance tradeoff?
  - What happens with Bias and Variance at **low** levels of complexity?
  - What happens with Bias and Variance at **high** levels of complexity?
- How do Ridge and Lasso attempt to win at the Bias-Variance tradeoff?
  - What's being penalized exactly?