Bias/Variance and Cross-Validation

Review: Linear Regression

Overfitting and Underfitting

The Bias/Variance Tradeoff

Cross-Validation

K-fold Cross-Validation

Subset Selection of Predictors

Bias and Variance

Bias and Variance

One Goal of Data Science: Make Future Predictions

One goal is to make accurate ***predictions*** on future (unseen) data.

1. Define a business goal.

   e.g. make Tesla cars the most dependable vehicles on the market

2. Collect training data.

   e.g. Tesla cars' event logs + historical record of parts replaced

3. Train a model.

   e.g. **features:** event statistics, **target:** time until failure

4. Deploy the model.

   e.g. monitor cars' events in real time, send mechanics to replace parts that will soon fail

Review: Linear Regression

We assume the world is built on linear relationships. Under that assumption, we can model the relationship between *features* and a *target* like this:

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

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

target
(aka, outcome)

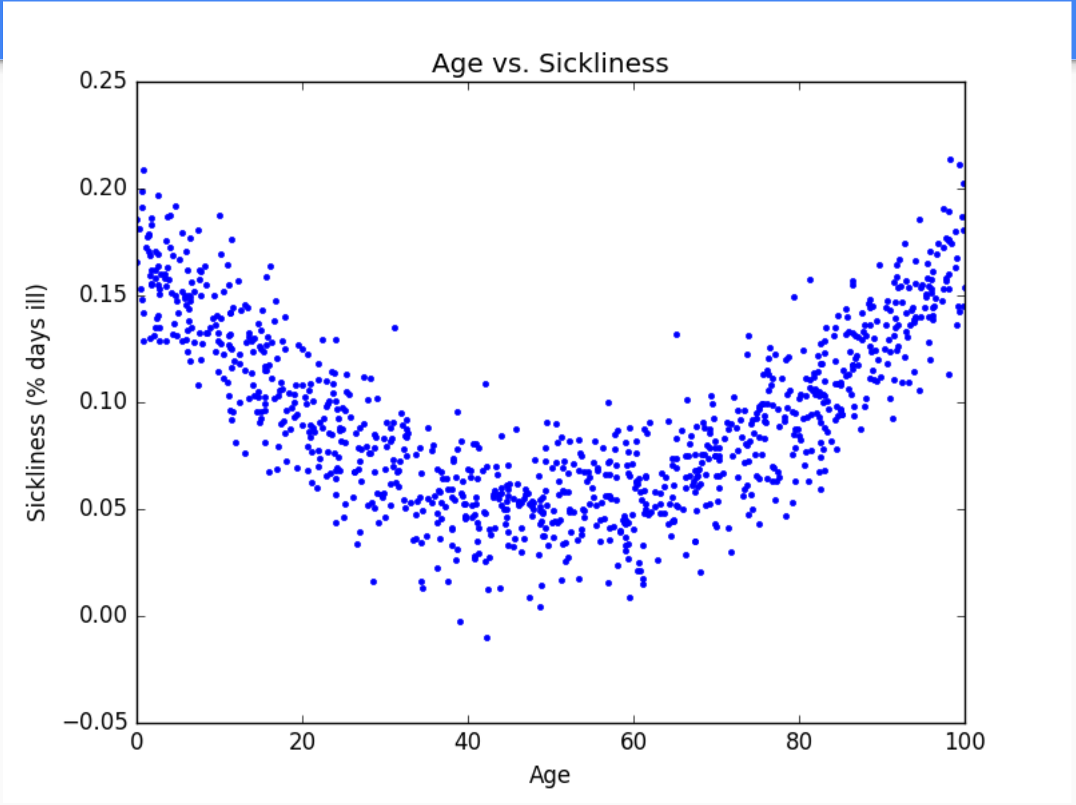
model parameters
(aka, coefficients)

features
(aka, predictors)

sampling error

Review: Linear Regression

We can make linear regression non-linear by inserting extra “interaction” features or higher-order features.



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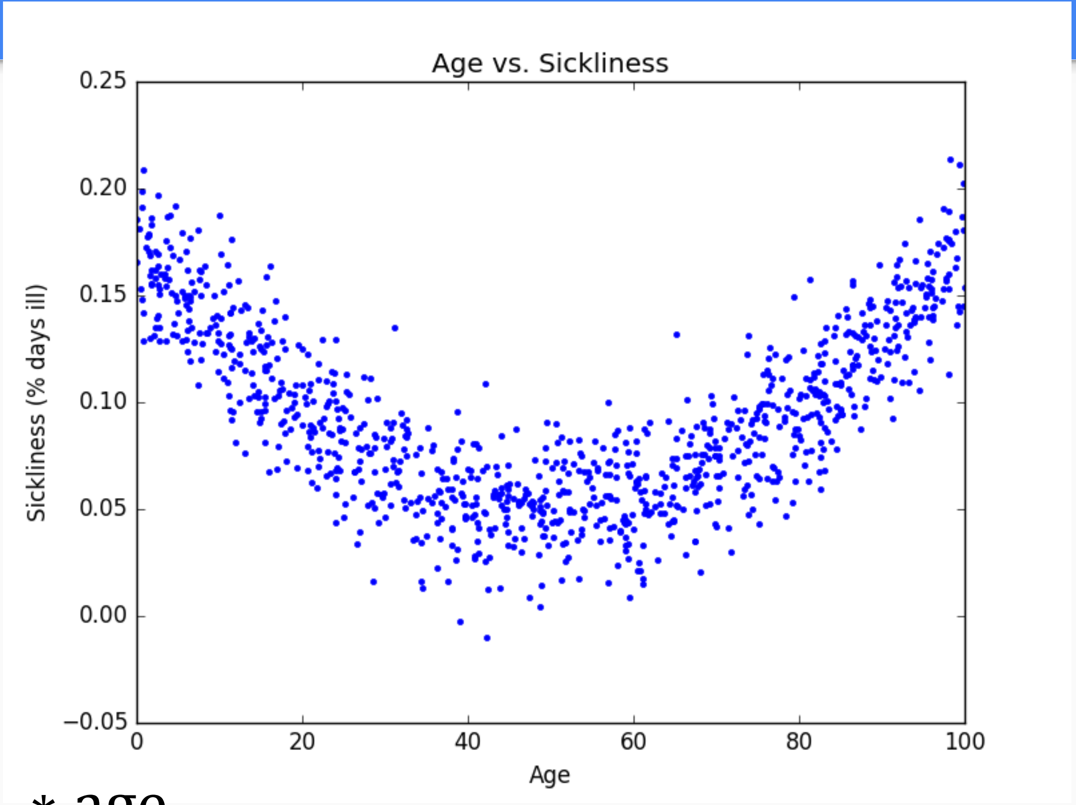


Examples:

$$\text{Sickliness} = \beta_0 + \beta_1 * \text{age}$$

$$\text{Sickliness} = \beta_0 + \beta_1 * \text{age} + \beta_1 * \text{age}^2$$

Is R^2 all that matters?

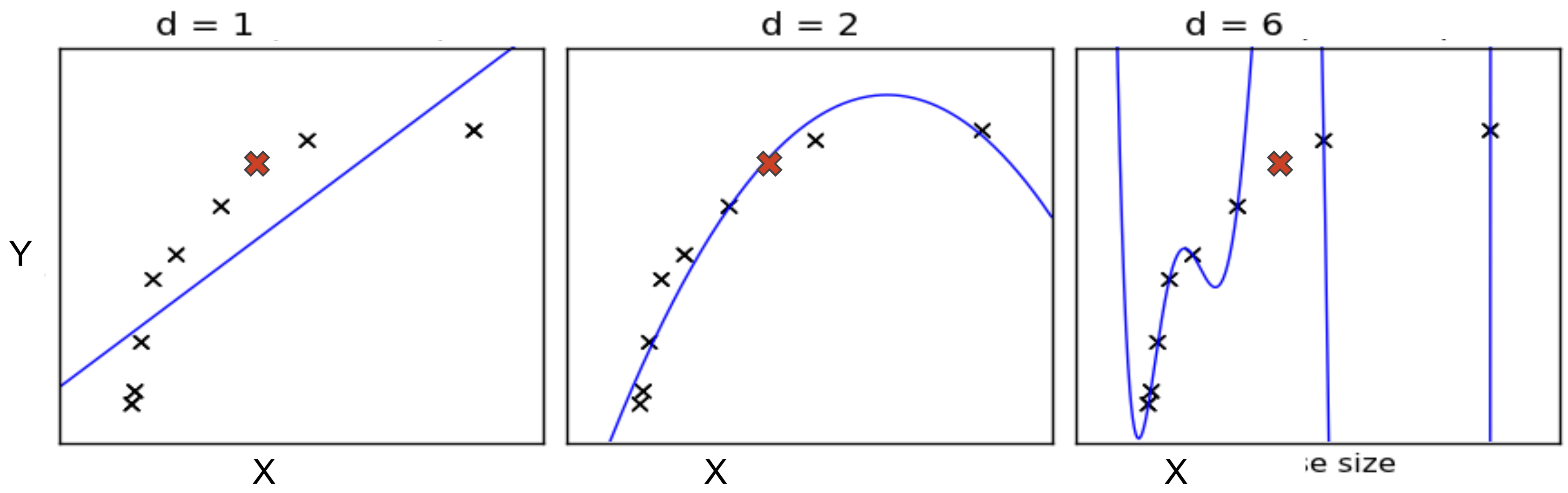
We *could* just keep inserting interaction features until $R^2 = 1$.

Boom. I solved data science. Here’s my idea:

```
def train_super_awesome_perfect_model(X, y):
    while True:
        model = LinearRegression()
        model.fit(X, y)
        if calculate_r2(model, X, y) >= 0.999:
            return model
        else:
            X = insert_random_interaction_feature(X)
```

Why is this a bad idea?

Oh the woes of overfitting...



Underfitting and Overfitting

Underfitting: The model doesn't fully capture the relationship between predictors and the target. The model has *not* learned the data's signal. The model is not flexible enough.

→ What should we do if our model underfits the data?

Overfitting: The model has tried to capture the sampling error. The model has learned the data's signal *and* the noise. I.e., the model attributes to signal that which is truly noise. The model is too flexible.

→ What should we do if our model overfits the data?

The Bias/Variance Tradeoff

We assume the true predictor/target relationship is given by an unknown function plus some sampling error:

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

We estimate the true (unknown) function by fitting a model over the training set.

$$\hat{Y} = \hat{f}(X)$$

Let's evaluate this model using a test observation **(x_0, y_0)** drawn from the population. What is the model's expected squared prediction error on this test observation?

$$E[(y_o - \hat{f}(x_0))^2] = \ldots$$

The Bias/Variance Tradeoff

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The Bias/Variance Tradeoff

Our model's expected squared prediction error will depend on (1) the variability of $\mathbf{y_0}$ and (2) the variability of the training set used to train our model. We can break this into three pieces:

$$E[(y_o - \hat{f}(x_0))^2] = \ldots = \mathrm{Var}(\hat{f}(x_0)) + \mathrm{Bias}^2(\hat{f}(x_0)) + \mathrm{Var}(\epsilon)$$

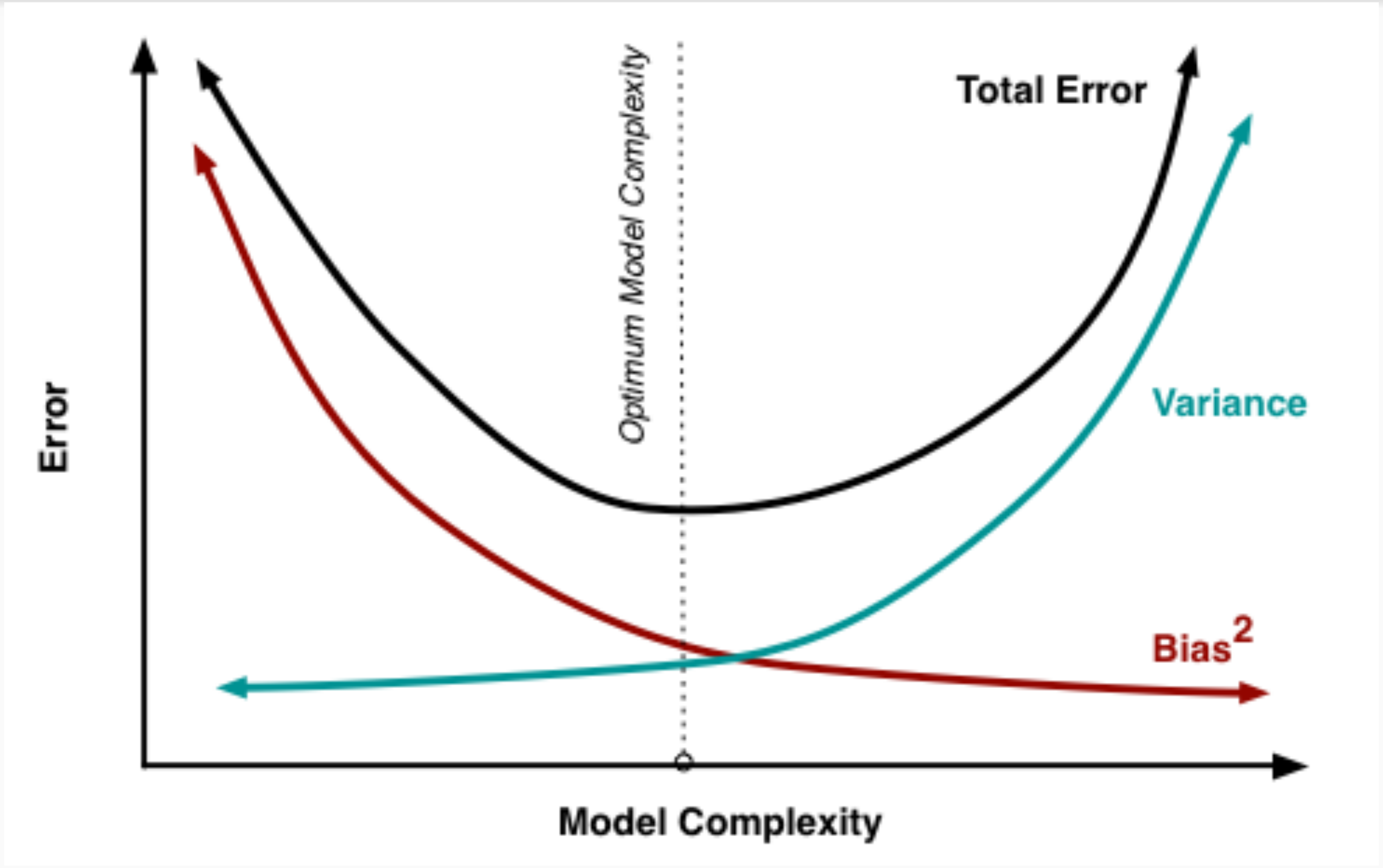
The variance of our model's prediction of $\mathbf{x_0}$ over all possible training sets

The difference between the true prediction and our model's average prediction over all possible training sets

The variance of the irreducible error.

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

The Bias/Variance Tradeoff



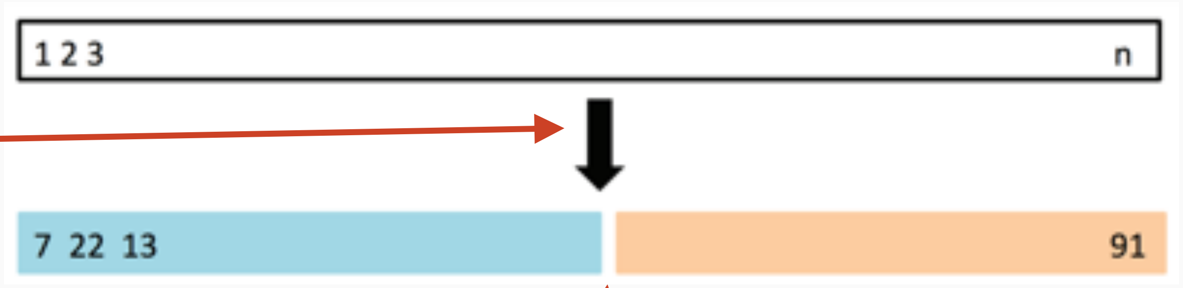
How is the **bias/variance tradeoff** related to **underfitting** and **overfitting**?

How can we find the best tradeoff point? I.e. The optimum model complexity

Cross-Validation

Main idea: **Don't use all your data for training.**

Instead: **Split your data into a "training set" and a "validation set".**



randomize!
(why?)

training set

where to split?

validation set

Cross-Validation

1. Split your data into training/validation sets.

   70/30 or 90/10 splits are commonly used

2. Use the training set to train several models of varying complexity.

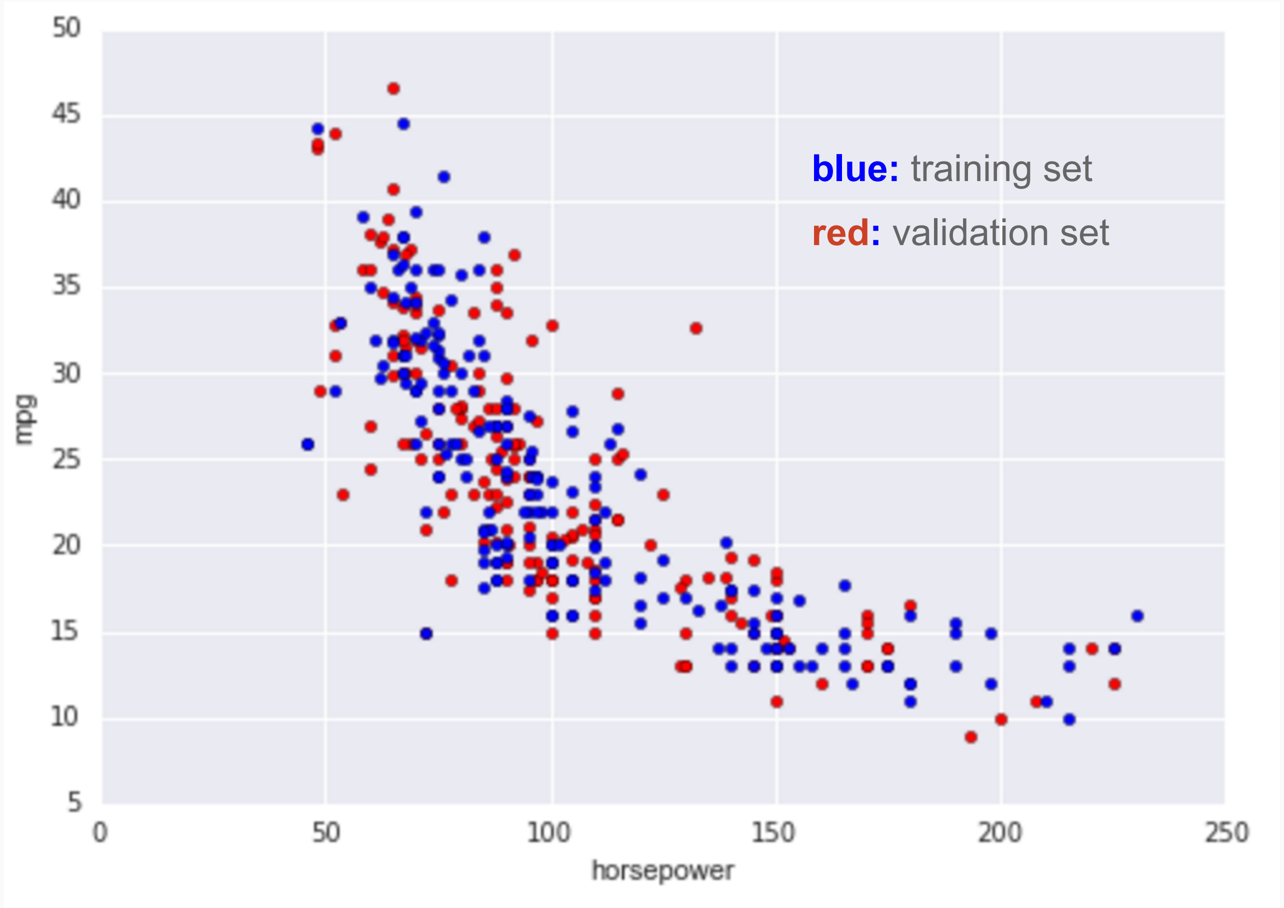
   e.g. linear regression (w/ and w/out interaction features), neural nets, decision trees, etc.
   (we'll talk about hyperparameter tuning, grid search, and feature engineering later)

3. Evaluate each model using the validation set.

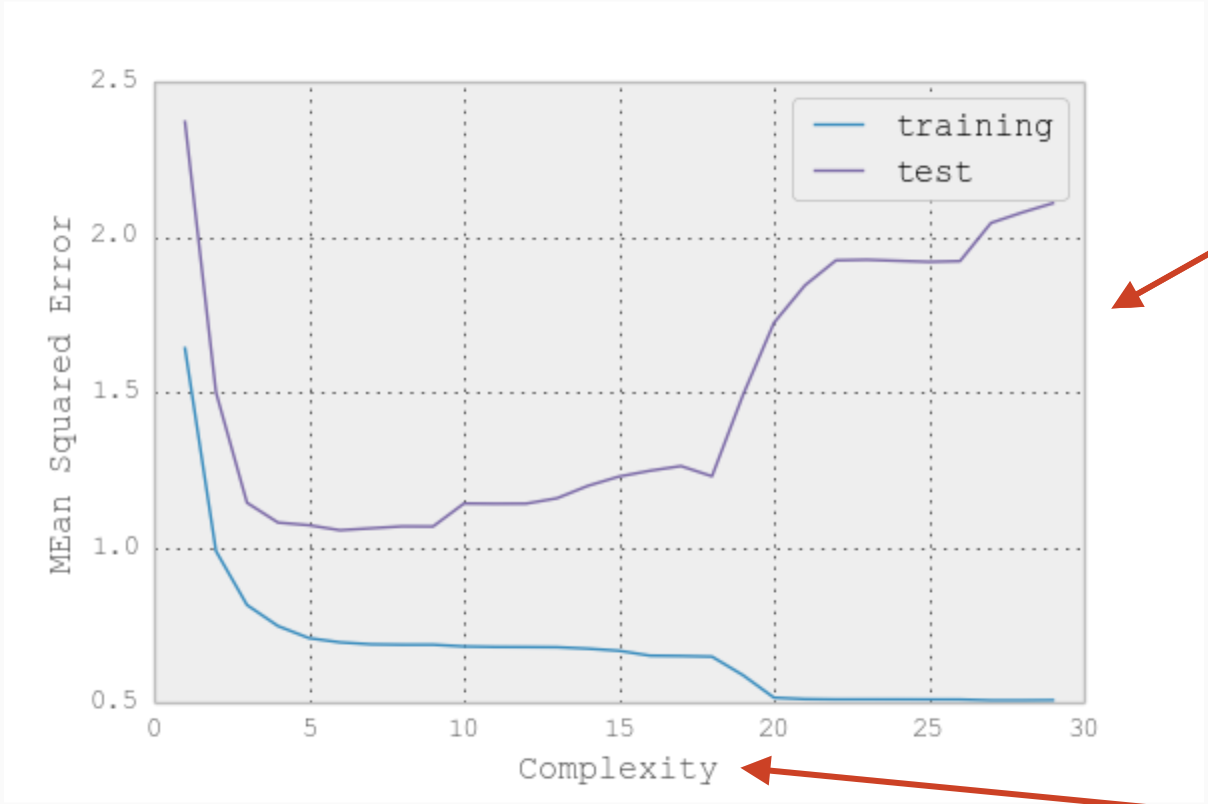
   calculate R^2, MSE, accuracy, or whatever you think is best

4. Keep the model that performs best over the validation set.

Let’s predict MPG from horsepower



Cross-Validation Example



You will see this shape all the time!

You will wrestle with the bias/variance tradeoff constantly...

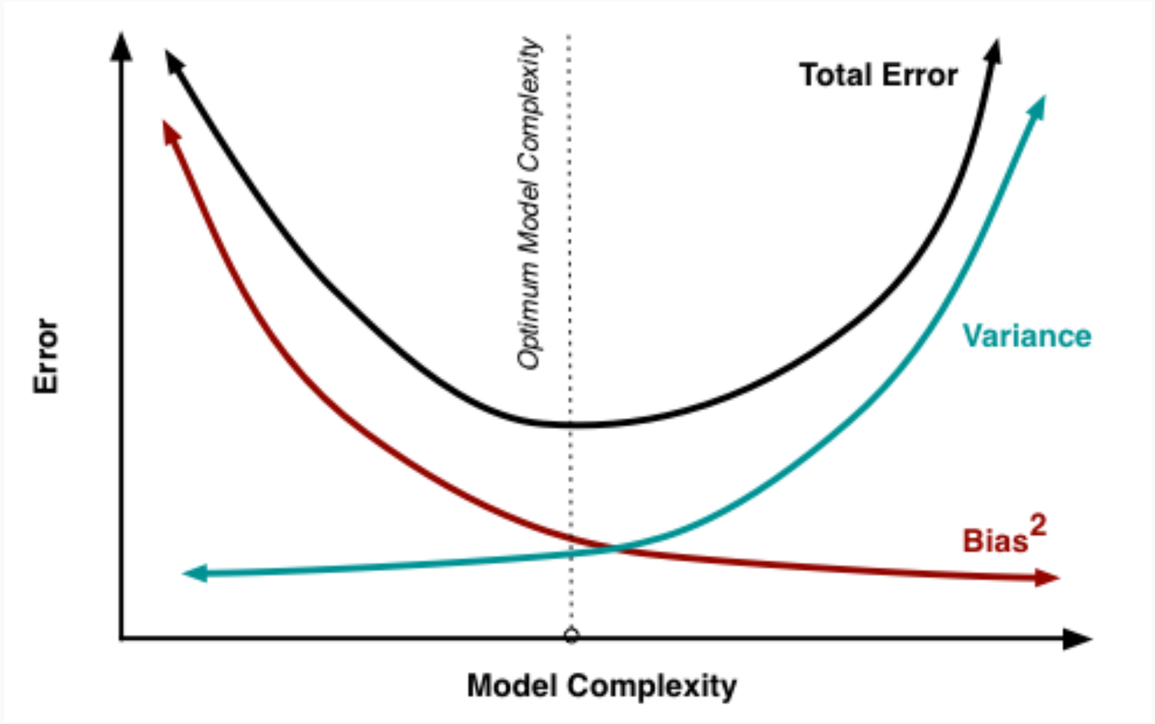
E.g. linear regression w/ varying degree of polynomial

Recall our goal: Making accurate future predictions

Fitting the training set perfectly is *easy*.
How?

Fitting future (unseen) data is *not easy*.

Cross validation helps us choose a model that performs well on unseen data.

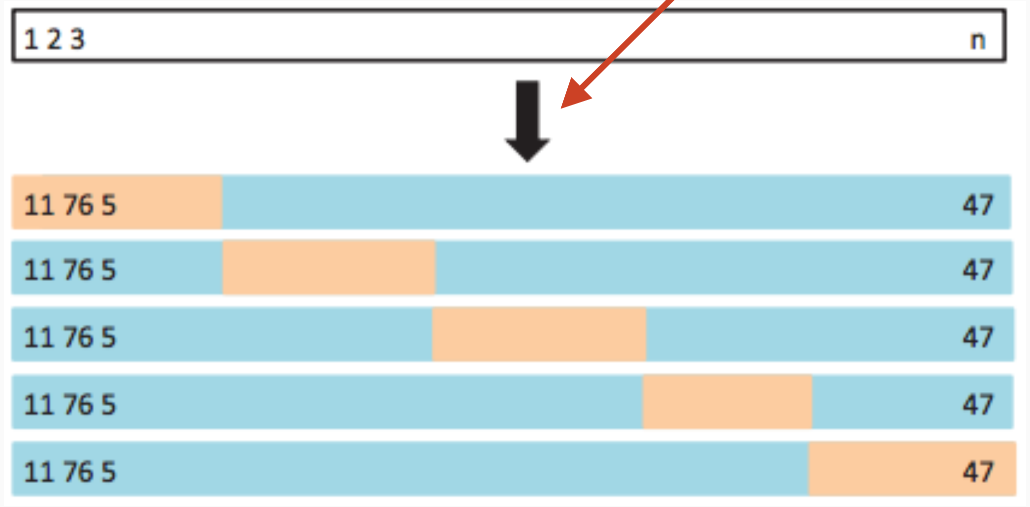


k-Fold Cross-Validation

1. Split the dataset into k "folds".
2. Train using (k-1) folds. Validate using the one left-out fold. Record a validation metric such as RSS or accuracy.
3. Train *k* models, leaving out a different fold for each one.
4. Average the validation results.

Commonly, k=5 or k=10

randomize!

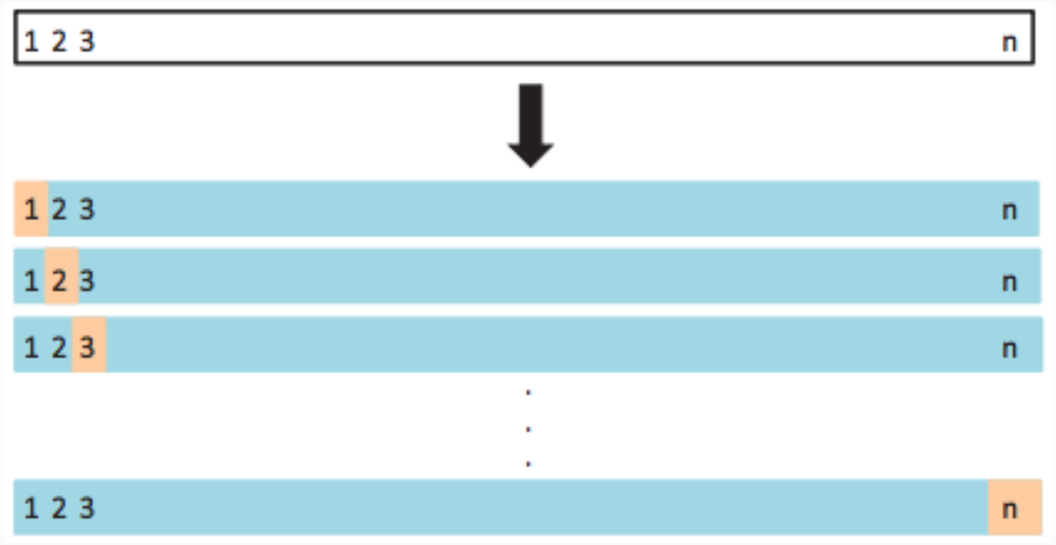


Leave-one-out Cross-Validation

Assume we have *n* training examples.

A special case of k-fold CV is when k=n. This is called *leave-one-out cross-validation*.

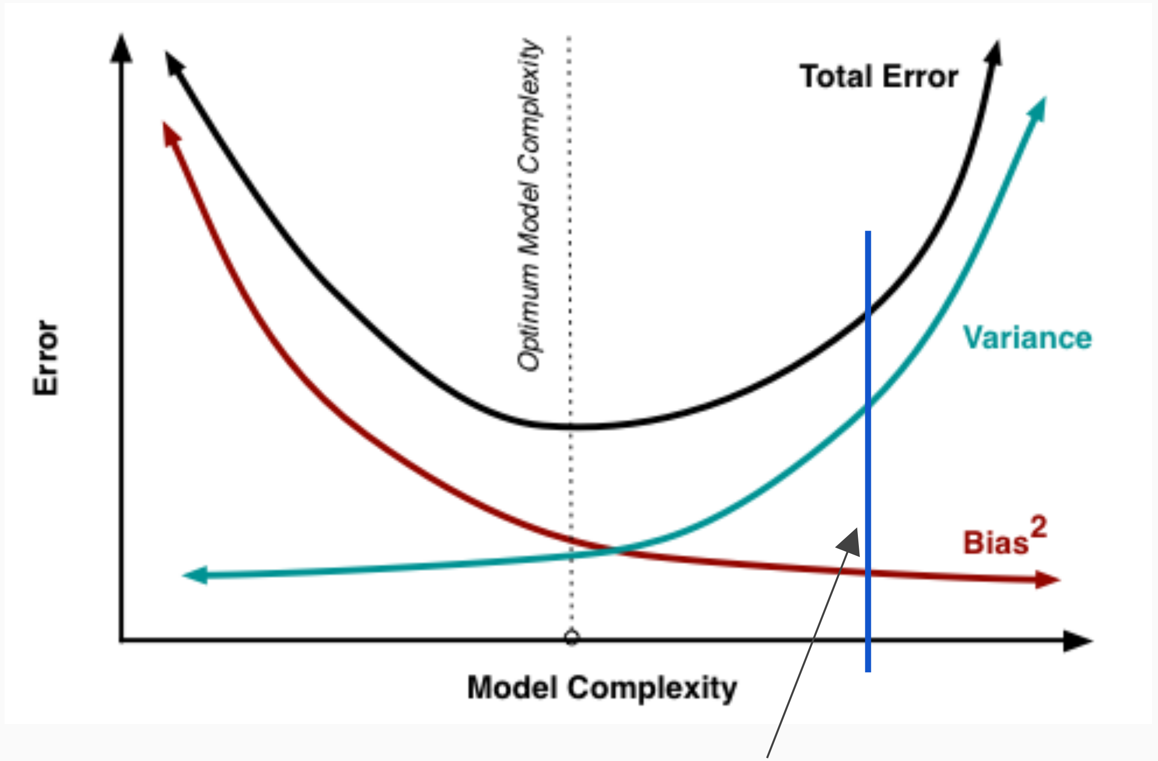
Useful (only) if you have a tiny dataset where you can't afford a large validation set.



Overfitting in high dimensions is easy, even with simple models.

If our data has high dimensionality (many many predictors), then it becomes easy to overfit the data.

Even linear regression might be too complex of a model for high dimensional data (and the smaller the dataset, the worse this problem is).



Linear regression in high dimensions

“HELP, my model is overfitting!”

You have a few options.

1. **Get more data:** not always possible/practical
2. $\boxed{\textbf{Subset Selection:}}$ keep only a subset of your predictors (i.e, dimensions)
3. **Regularization:** restrict your model’s parameter space
4. **Dimensionality Reduction:** project the data into a lower dimensional space

Subset Selection

Best subset: Try every model. Every possible combination of *p* predictors

Computationally intensive. 2^p possible subsets of *p* predictors

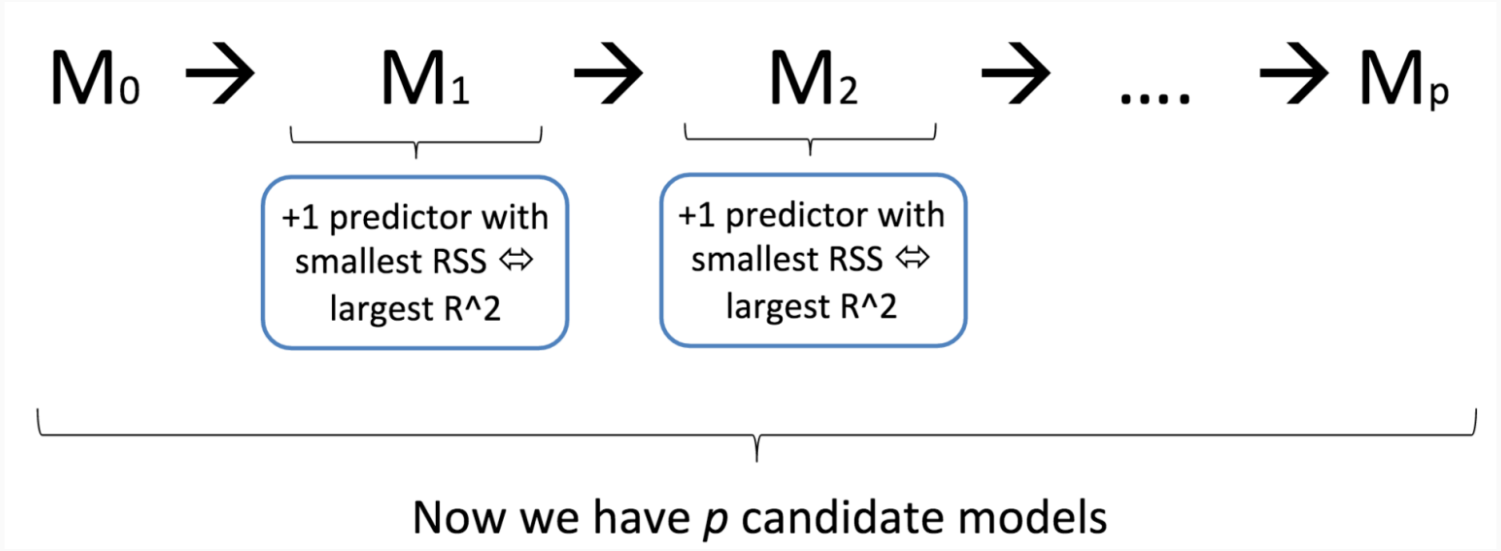
High chance of finding a “good” model by random chance.

… A sort-of monkeys-Shakespeare situation …

Stepwise: Iteratively pick predictors to be in/out of the final model.

Forward, backward, forward-backward strategies

Forward Stepwise Selection


$M_0 \rightarrow M_1 \rightarrow M_2 \rightarrow \dots \rightarrow M_p$
+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 resulting *p* candidates?

Answer: Don't use RSS or R^2 for this part.
Use Mallow's C_p, or AIC, or BIC, or Adjusted R^2.

… or just use cross-validation with any error measurement.

Subset Selection: Comparing models of varying number of predictors...

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

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

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

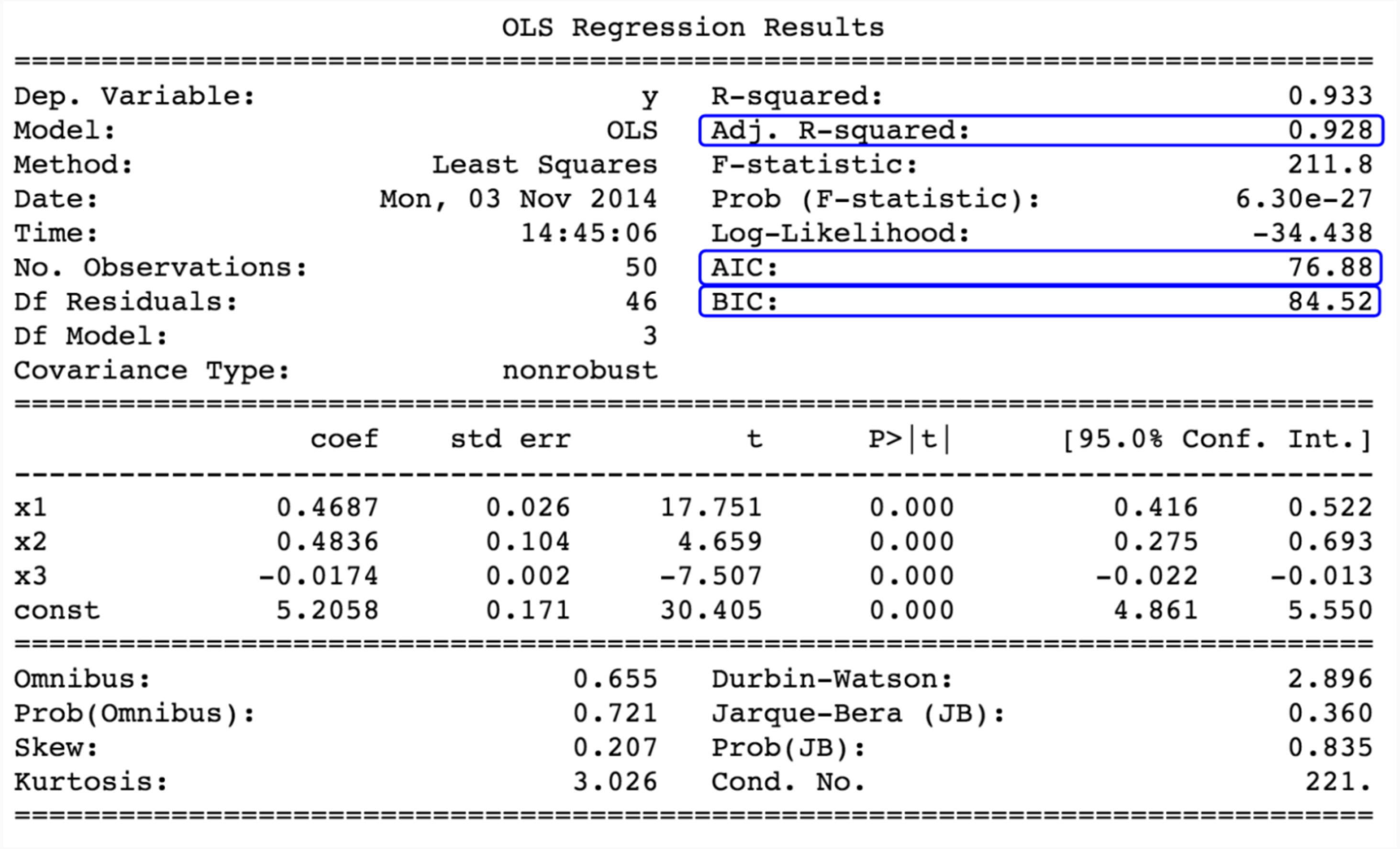
This is Cp, except 2 is replaced by log(n). log(n) > 2 for n>7, so BIC generally exacts a heavier penalty for more variables

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

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

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

Subset Selection: Comparing models of varying number of predictors...



```
                            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.
==============================================================================
```