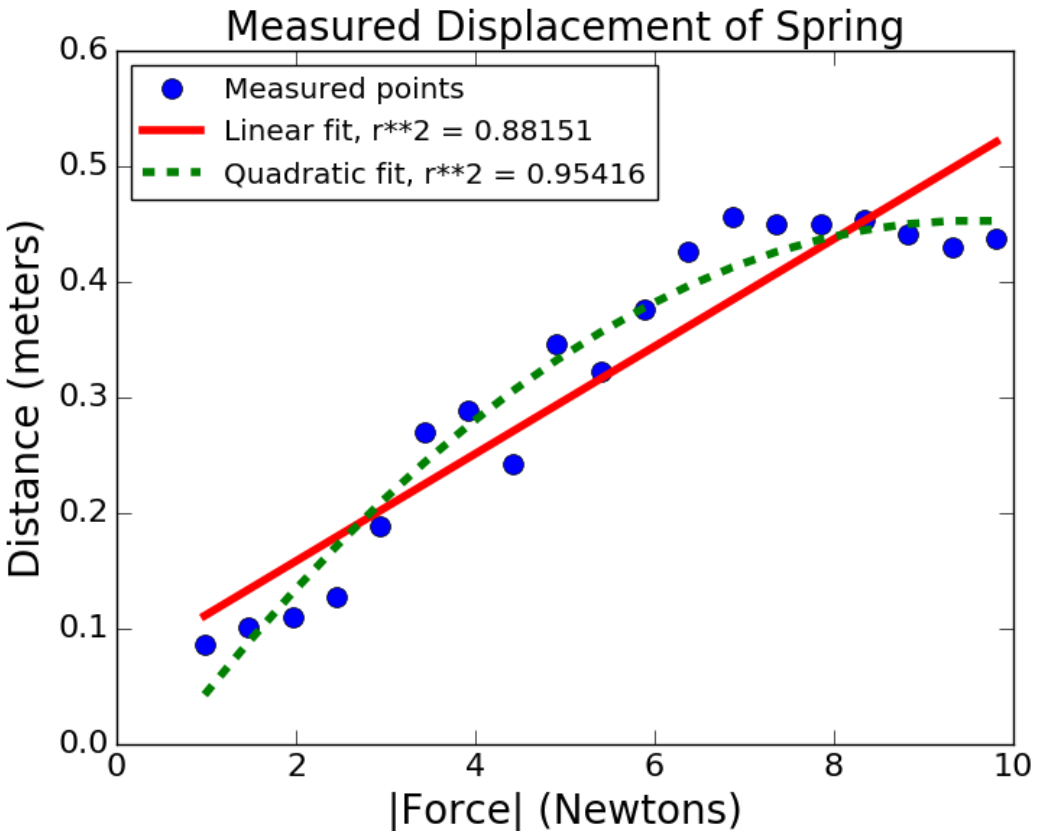
Understanding Experimental Data, cont.

The Take Home Message

- Choosing an overly-complex model leads to overfitting to the training data
- Increases the risk of a model that works poorly on data not included in the training set
- On the other hand choosing an insufficiently complex model has other problems
  - As we saw when we fit a line to data that was basically parabolic

Returning to Where We Started



Quartic fit tighter

But remember Hooke

Unless we believe theory is wrong, that should guide us

Holds up to elastic limit of spring

Should probably fit different models to different segments of data

Suppose We Don't Have a Solid Theory

- Use cross-validation results to guide the choice of model complexity
- If dataset small, use leave one-one-out cross validation
- If dataset large enough, use k-fold cross validation or repeated-random-sampling validation

Leave-one-out Cross Validation

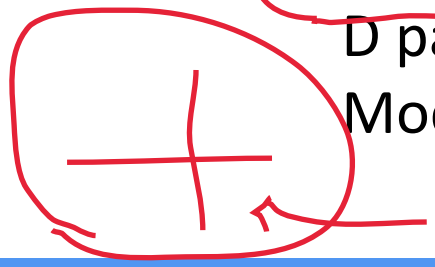
```
Let D be the original data set

testResults = []
for i in range(len(D)):
    training = D[:].pop(i)
    model = buildModel(training)
    testResults.append(test(model, D[i]))

Average testResults
```

train on all other example,
test the one left out

see which degree is better

do this on each item
to all degrees of polynomials

- K-fold very similar
- D partitioned into k equal size sets
- Model trained on k-1, and tested on remaining



leave one part out

Repeated Random Sampling

```
Let D be the original data set
    n be the number of random samples

testResults = []
for i in range(n):
    randomly partition D into two sets:
       training and test
    model = buildModel(training)
    testResults.append(test(model, test))

Average testResults
```

An Example, Temperature By Year

- Task: Model how the mean daily high temperature in the U.S. varied from 1961 through 2015
- Get means for each year and plot them
- Randomly divide data in half n times
  - For each dimensionality to be tried
    - Train on one half of data
    - Test on other half
    - Record r-squared on test data
- Report mean r-squared for each dimensionality

A Boring Class

```
class tempDatum(object):
    def __init__(self, s):
        info = s.split(',')
        self.high = float(info[1])
        self.year = int(info[2][0:4])
    def getHigh(self):
        return self.high
    def getYear(self):
        return self.year
```

Read Data

```
def getTempData():
    inFile = open('temperatures.csv')
    data = []
    for l in inFile:
        data.append(tempDatum(l))
    return data
```

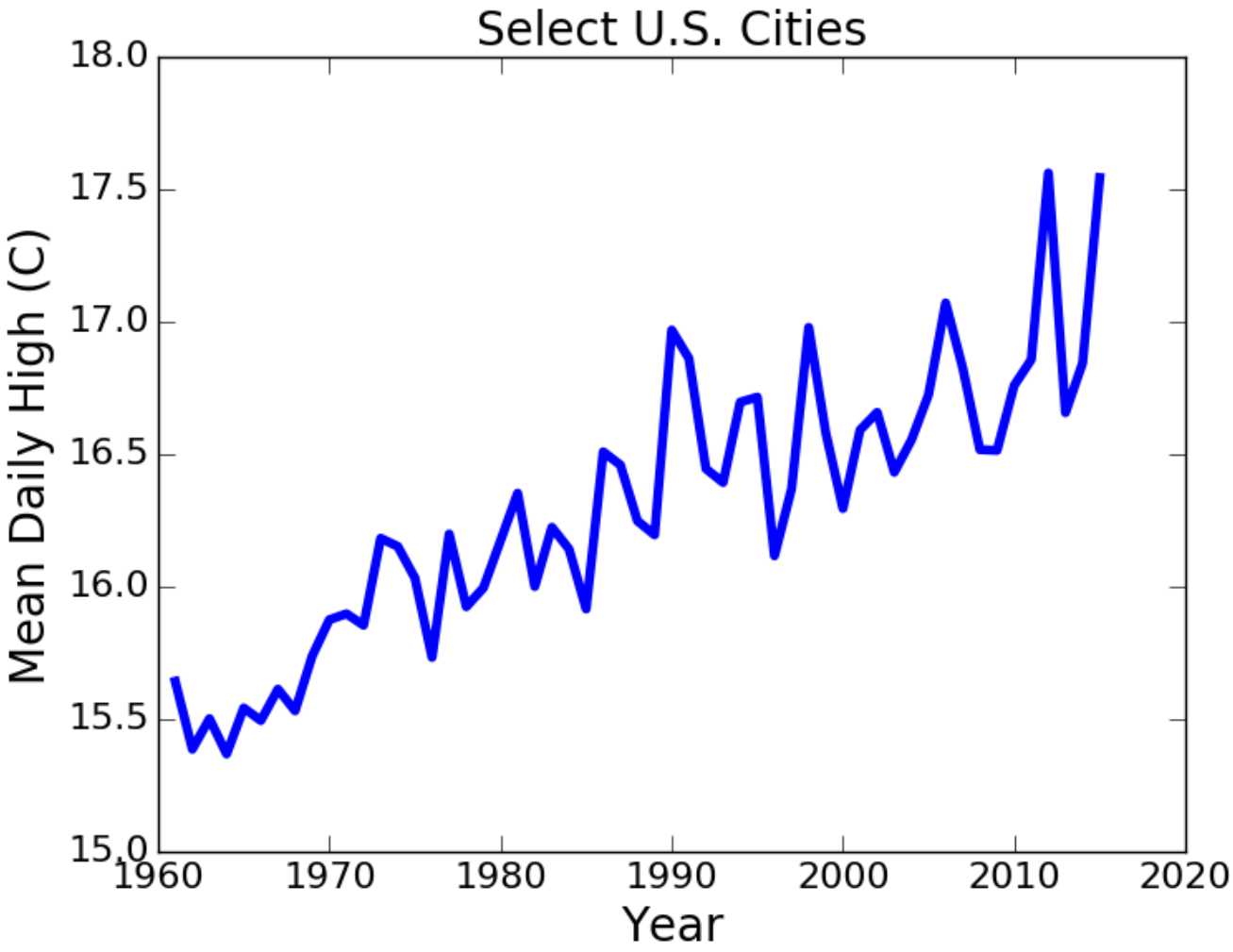
Get Means

```
def getYearlyMeans(data):
    years = {}
    for d in data:
        try:
            years[d.getYear()].append(d.getHigh())
        except:
            years[d.getYear()] = [d.getHigh()]
    for y in years:
        years[y] = sum(years[y])/len(years[y])
    return years
```

Get and Plot Data

```
data = getTempData()
years = getYearlyMeans(data)
xVals, yVals = [], []
for e in years:
    xVals.append(e)
    yVals.append(years[e])
pylab.plot(xVals, yVals)
pylab.xlabel('Year')
pylab.ylabel('Mean Daily High (C)')
pylab.title('Select U.S. Cities')
```

The Whole Data Set



Initialize Things

```
numSubsets = 10
dimensions = (1, 2, 3)
rSquares = {}
for d in dimensions:
    rSquares[d] = []
```

Split Data

```
def splitData(xVals, yVals):
    toTrain = random.sample(range(len(xVals)),
                            len(xVals)//2)
    trainX, trainY, testX, testY = [],[],[],[]
    for i in range(len(xVals)):
        if i in toTrain:
            trainX.append(xVals[i])
            trainY.append(yVals[i])
        else:
            testX.append(xVals[i])
            testY.append(yVals[i])
    return trainX, trainY, testX, testY
```

list

generate index

-> num of eg

Train, Test, and Report

```
for f in range(numSubsets):
    trainX,trainY,testX,testY = splitData(xVals, yVals)
    for d in dimensions:
        model = pylab.polyfit(trainX, trainY, d)
        estYVals = pylab.polyval(model, trainX)
        estYVals = pylab.polyval(model, testX)
        rSquares[d].append(rSquared(testY, estYVals))

print('Mean R-squares for test data')
for d in dimensions:
    mean = round(sum(rSquares[d])/len(rSquares[d]), 4)
    sd = round(numpy.std(rSquares[d]), 4)
    print('For dimensionality', d, 'mean =', mean,
          'Std =', sd)
```

Results

```
Mean R-squares for test data
For dimensionality 1 mean = 0.7535 Std = 0.0656
For dimensionality 2 mean = 0.7291 Std = 0.0744
For dimensionality 3 mean = 0.7039 Std = 0.0684
```

- Line seems to be the winner
  - Highest average r-squared
  - Simplest model

Wrapping Up Curve Fitting

- We can use linear regression to fit a curve to data
  - Mapping from independent values to dependent values
- That curve is a model of the data that can be used to predict the value associated with independent values we haven't seen (out of sample data)
- R-squared used to evaluate model
  - Higher not always "better" because of risk of over fitting
- Choose complexity of model based on
  - Theory about structure of data
  - Cross validation
  - Simplicity