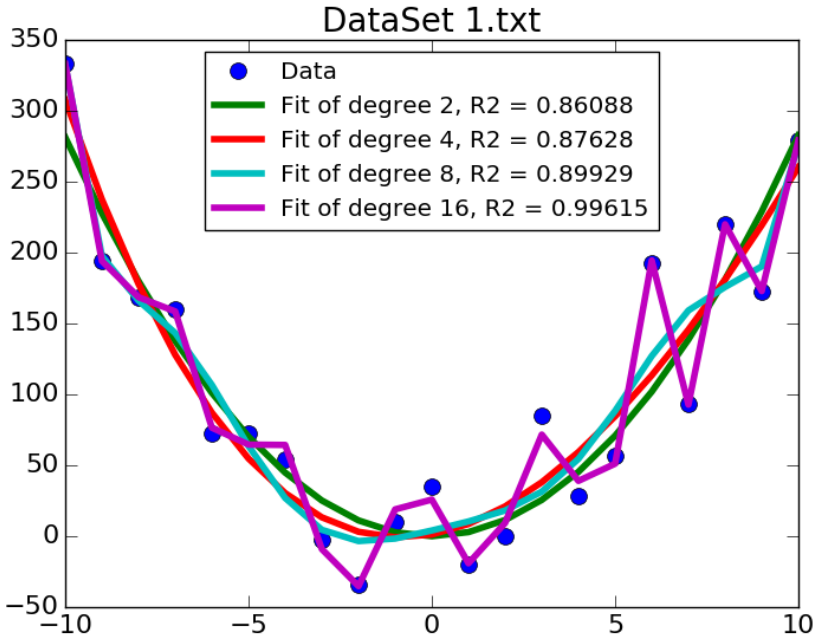
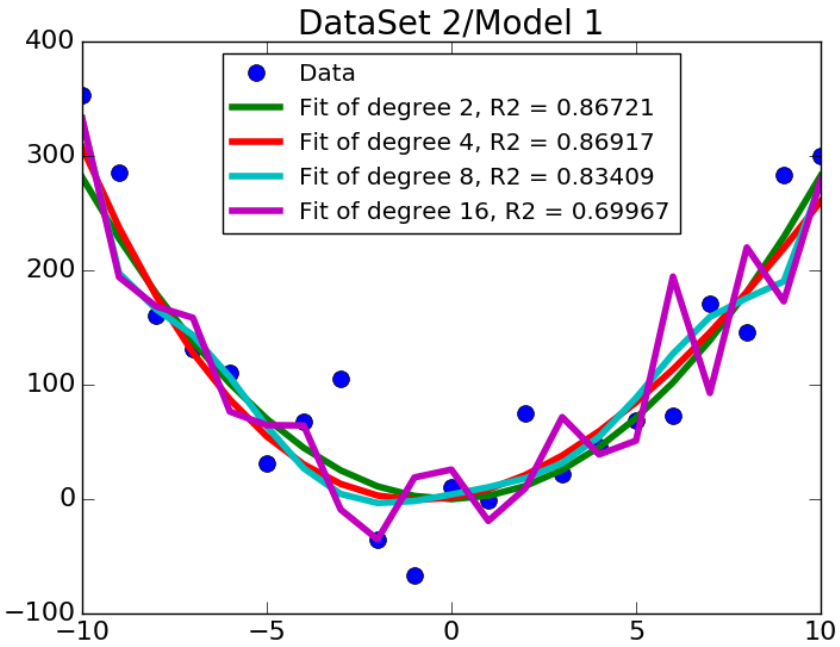
Understanding Experimental Data, cont.

Training and Testing Errors



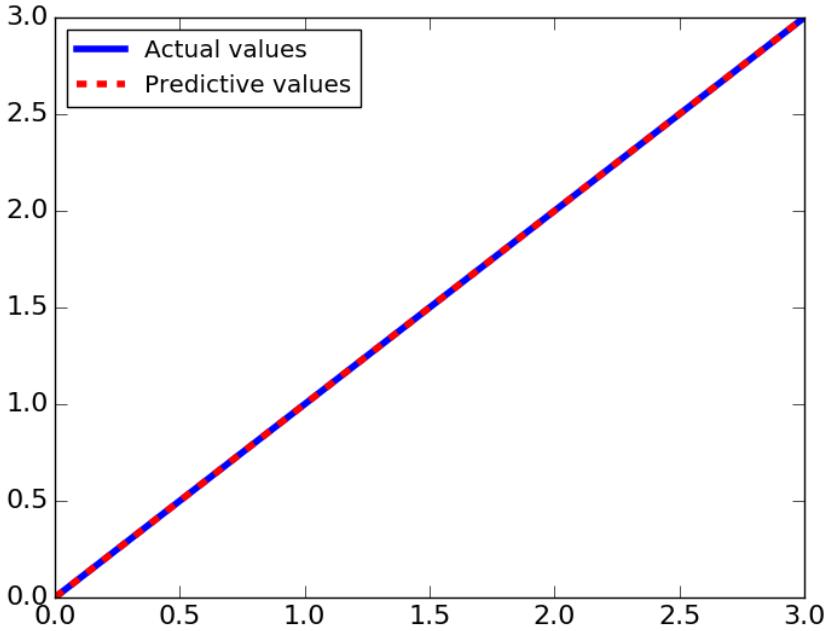


Increasing the Complexity

- What happens when we increase order of polynomial?
  - Can we get a worse fit to training data?
- If extra term is useless, coefficient will merely be zero
- But if data is noisy, can fit the noise rather than the underlying pattern in the data

Fitting a Quadratic to a Perfect Line

```
xVals = (0,1,2,3)
yVals = xVals
pylab.plot(xVals, yVals, label = 'Actual values')
a,b,c = pylab.polyfit(xVals, yVals, 2)
print('a =', round(a, 4), 'b =', round(b, 4),
        'c =', round(c, 4))
estYVals = pylab.polyval((a,b,c), xVals)
pylab.plot(xVals, estYVals, 'r--', label ='Predictive values')
print('R-squared = ', rSquared(yVals, estYVals))
```



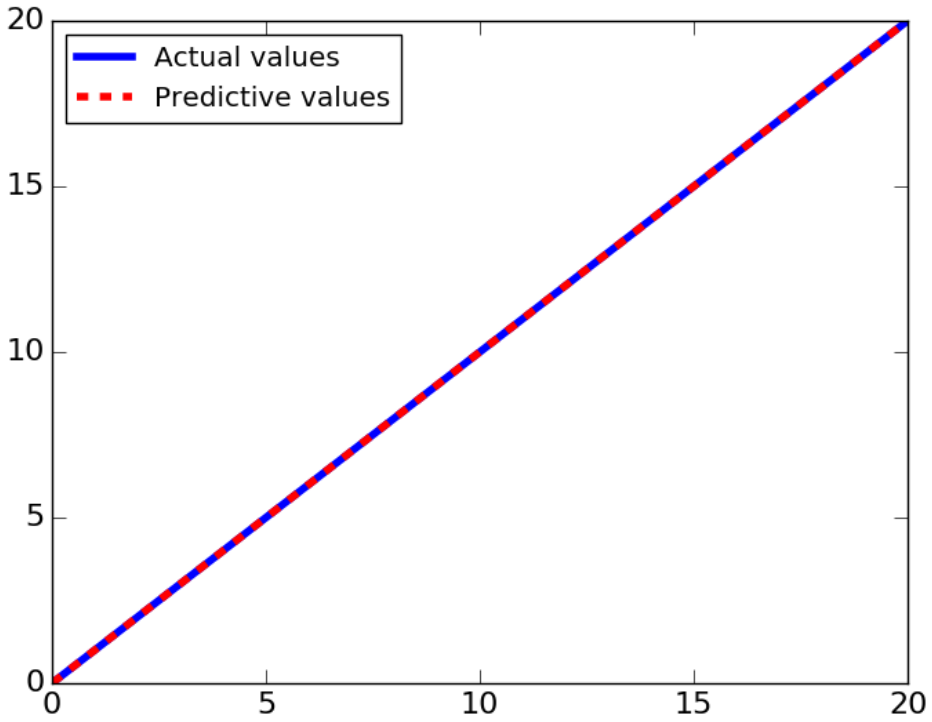
$$y = ax^2 + bx + c$$

$$y = 0x^2 + 1x + 0$$

$$y = x$$

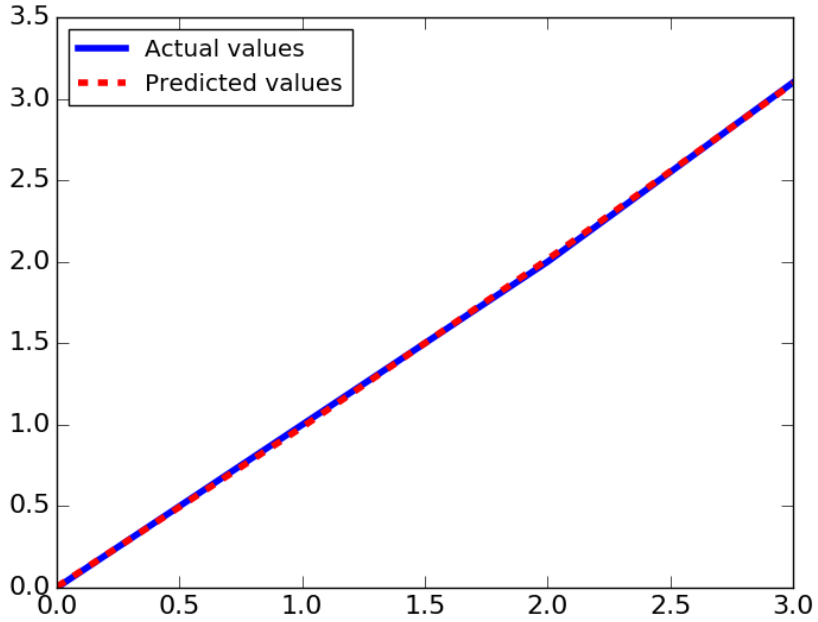
Predict Another Point Using Same Model

```
xVals = xVals + (20,)
yVals = xVals
pylab.plot(xVals, yVals, label = 'Actual values')
estYVals = pylab.polyval((a,b,c), xVals)
pylab.plot(xVals, estYVals, 'r--', label = 'Predictive values')
print('R-squared = ', rSquared(yVals, estYVals))
```



Simulate a Small Measurement Error

```
xVals = (0,1,2,3)
yVals = (0,1,2,3.1)
pylab.plot(xVals, yVals, label = 'Actual values')
model = pylab.polyfit(xVals, yVals, 2)
print(model)
estYVals = pylab.polyval(model, xVals)
pylab.plot(xVals, estYVals, 'r--', label = 'Predicted values')
print('R-squared = ', rSquared(yVals, estYVals))
```



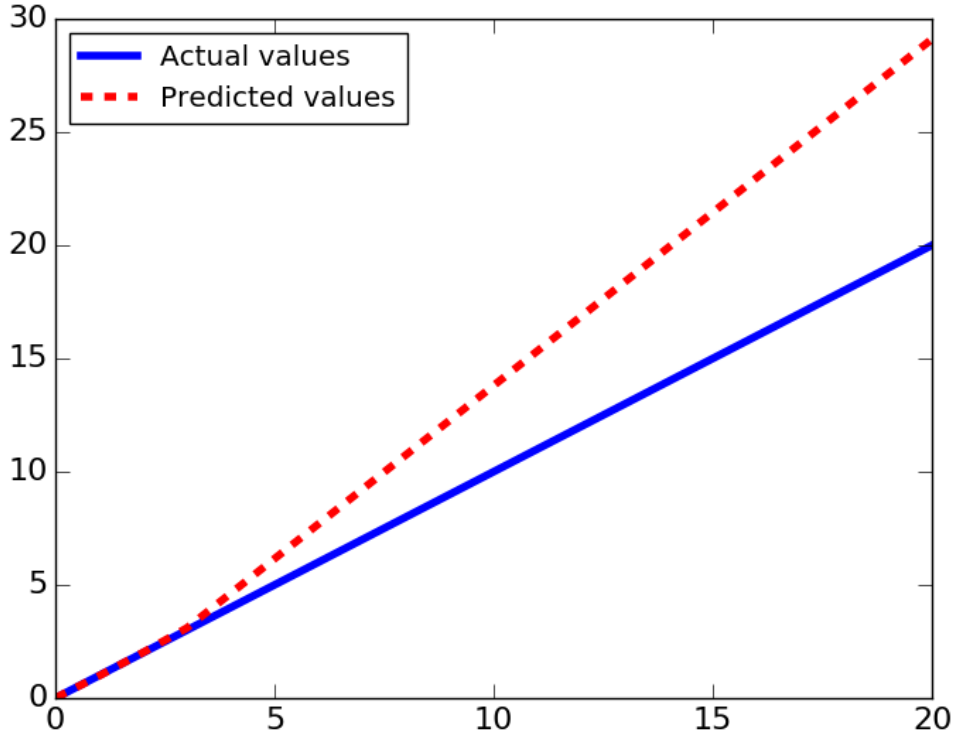
$$y = ax^2 + bx + c$$

$$y = .025x^2 + .955x + .005$$

R-squared = 0.9994

Predict Another Point Using Same Model

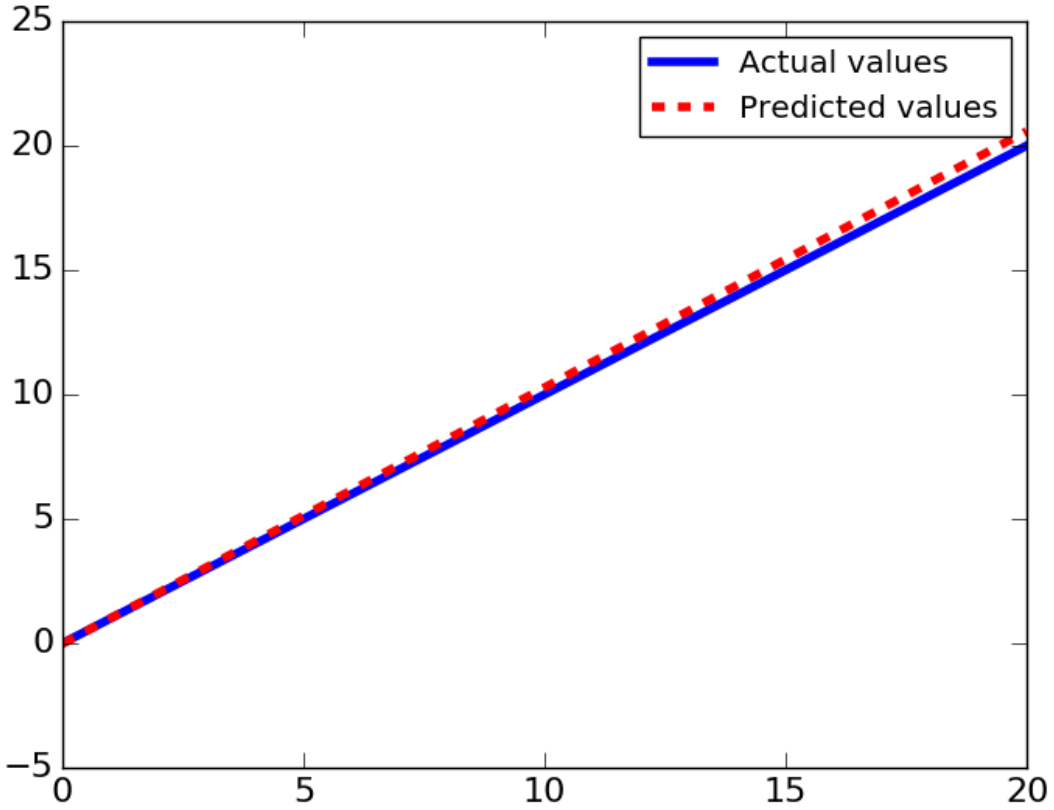
```
xVals = xVals + (20,)
yVals = xVals
estYVals = pylab.polyval(model, xVals)
print('R-squared = ', rSquared(yVals, estYVals))
pylab.figure()
pylab.plot(xVals, estYVals)
```



R-squared = 0.7026

Suppose We Had Used a First-degree Fit

- model = pylab.polyfit(xVals, yVals, 1)



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