

STAT/CSE 416: Intro to Machine Learning Hunter Schafer (slides by Emily Fox) University of Washington April 5, 2018

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## Generic linear regression model

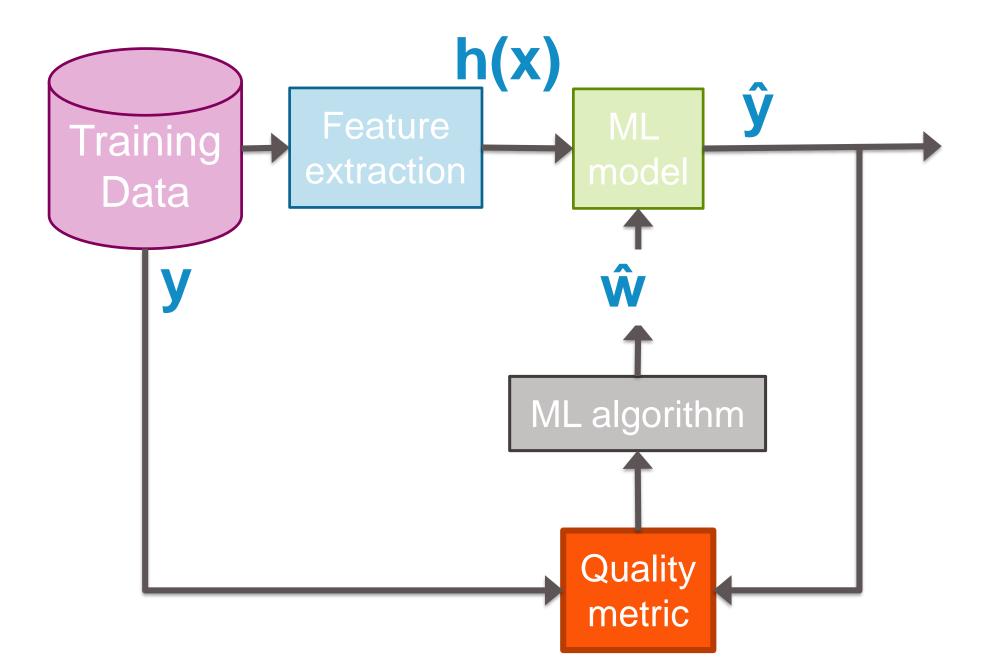
Model:  

$$y_{i} = \underset{D}{\mathbf{w}_{0}} h_{0}(\mathbf{x}_{i}) + \underset{1}{\mathbf{w}_{1}} h_{1}(\mathbf{x}_{i}) + \ldots + \underset{D}{\mathbf{w}_{D}} h_{D}(\mathbf{x}_{i}) + \varepsilon_{i}$$

$$= \sum_{j=0}^{D} \underset{j=0}{\mathbf{w}_{j}} h_{j}(\mathbf{x}_{i}) + \varepsilon_{i}$$

feature  $1 = h_0(x) \dots e.g., 1$ feature  $2 = h_1(x) \dots e.g., x[1] = sq.$  ft. feature  $3 = h_2(x) \dots e.g., x[2] = \#bath$ or, log(x[7]) x[2] = log(#bed) x #bath

feature  $D+1 = h_D(x) \dots$  some other function of x[1],..., x[d]



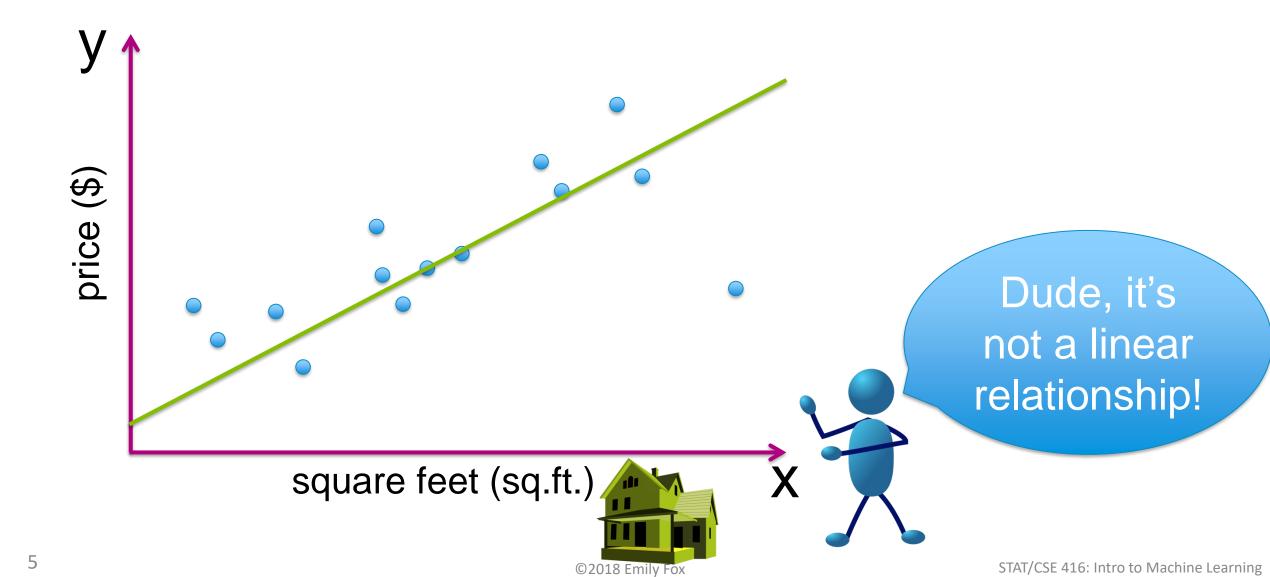
# Measuring loss

Loss function:  $L(y, f_{\hat{w}}(x))$ actual value  $\hat{f}(x) = \text{predicted value } \hat{y}$ 

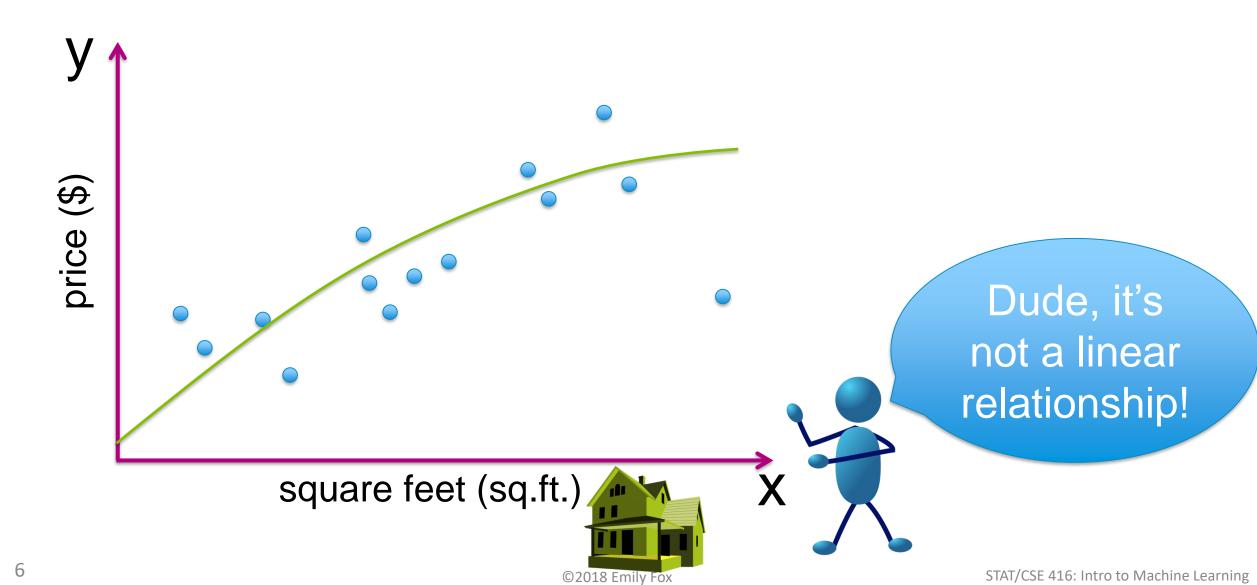
Cost of using ŵ at x when y is true

Examples: (assuming loss for underpredicting = overpredicting) Absolute error:  $L(y,f_{\hat{w}}(x)) = |y-f_{\hat{w}}(x)|$ Squared error:  $L(y,f_{\hat{w}}(x)) = (y-f_{\hat{w}}(x))^2$ 

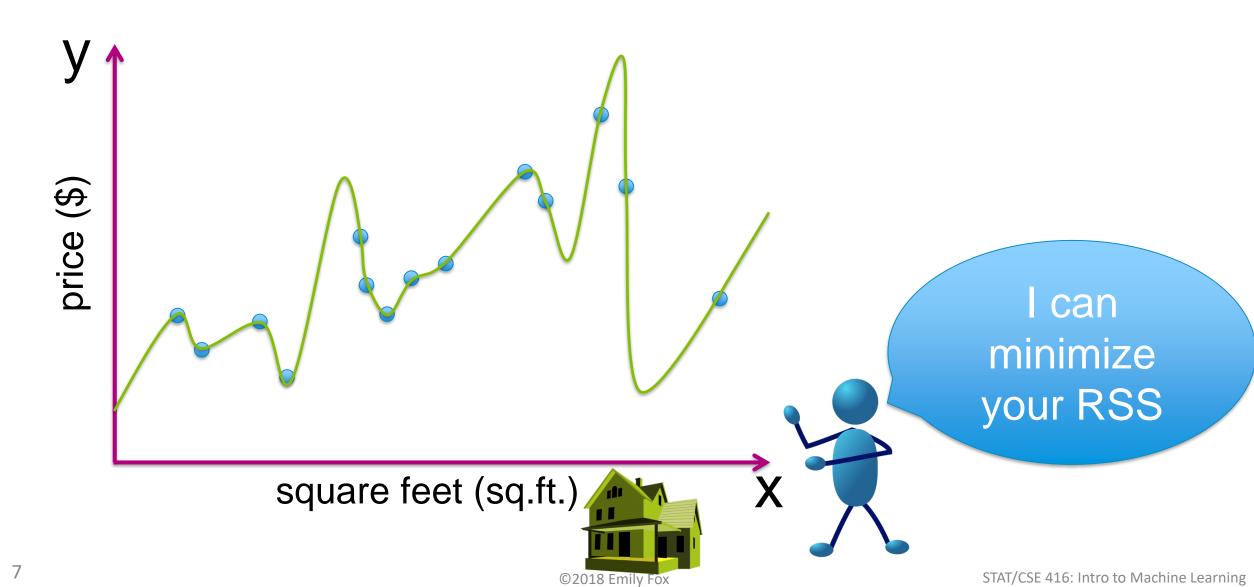
#### Fit data with a line or ... ?



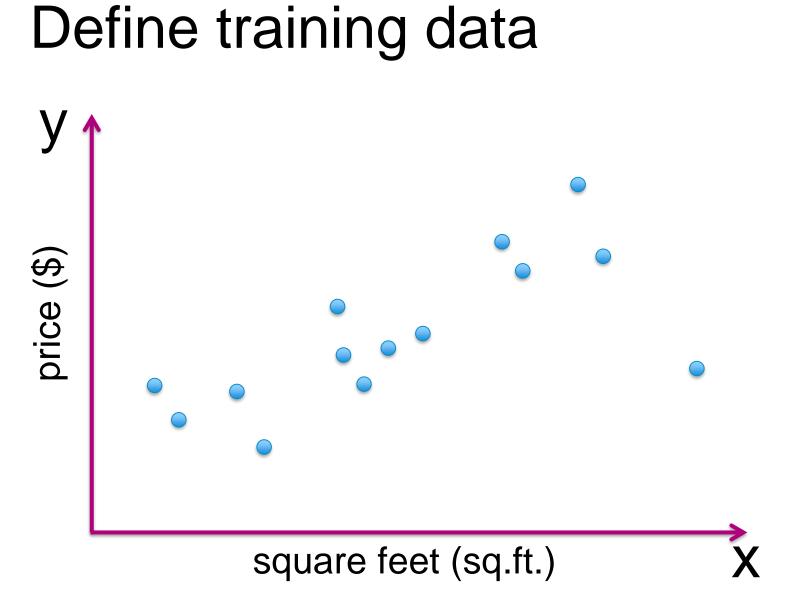
# What about a quadratic function?

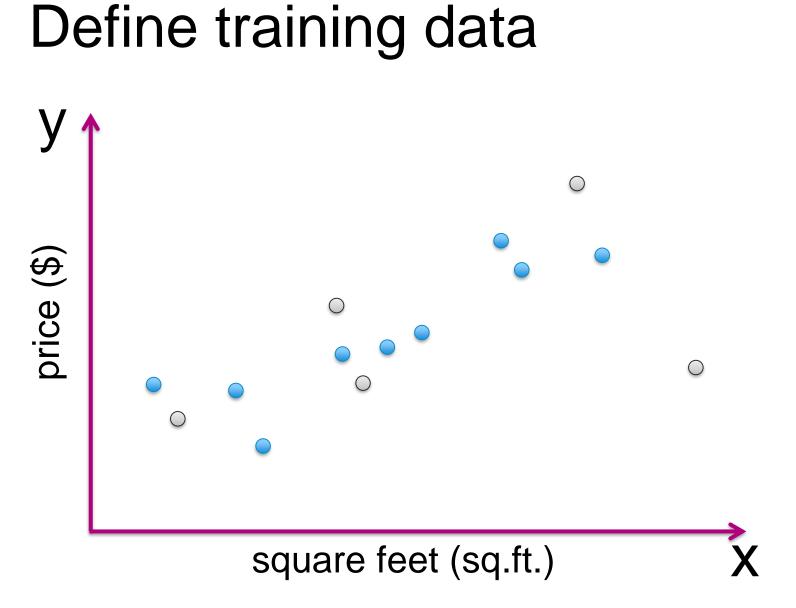


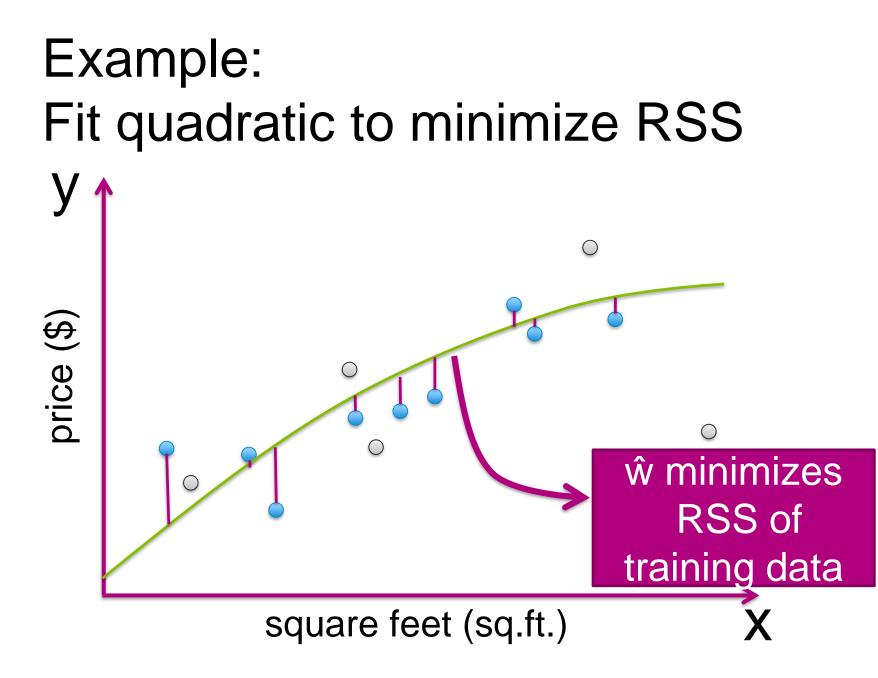
# Even higher order polynomial



#### Assessing the loss Part 1: Training error

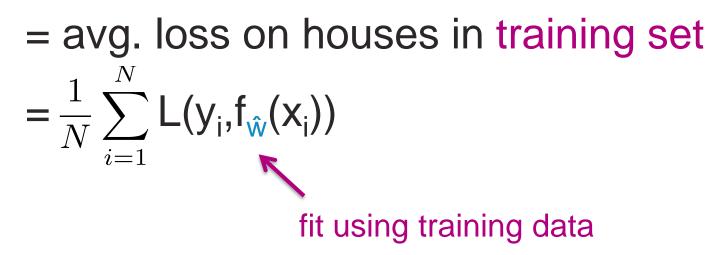


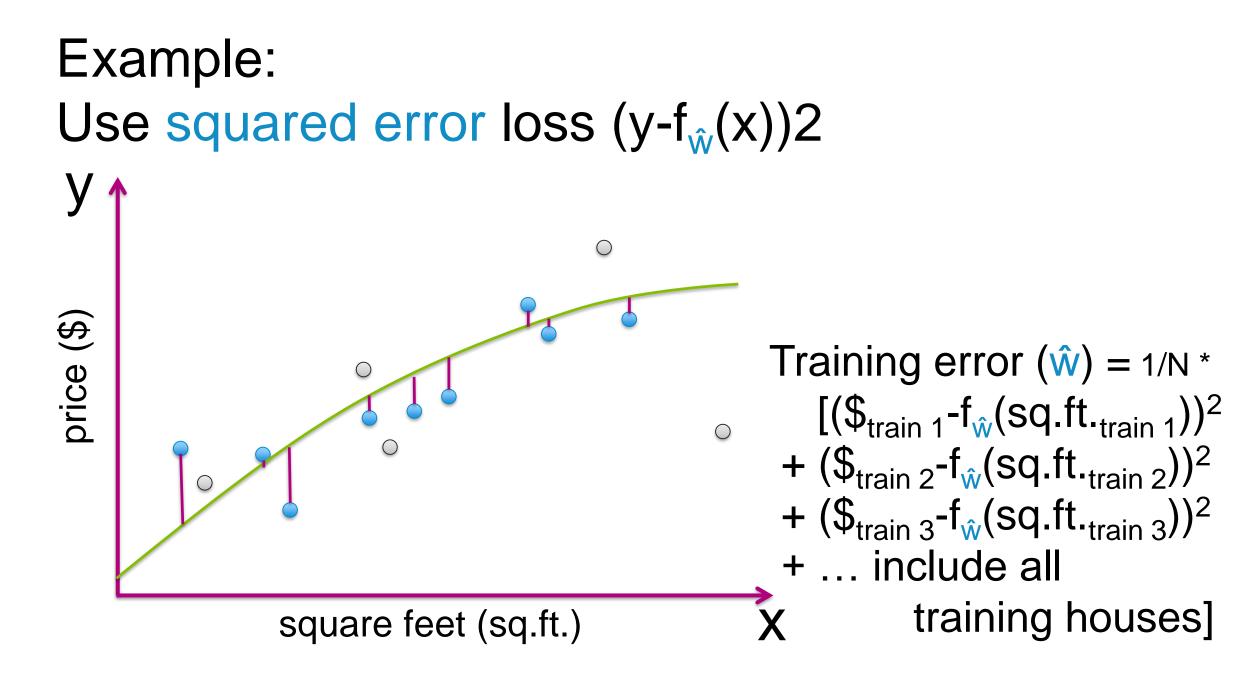


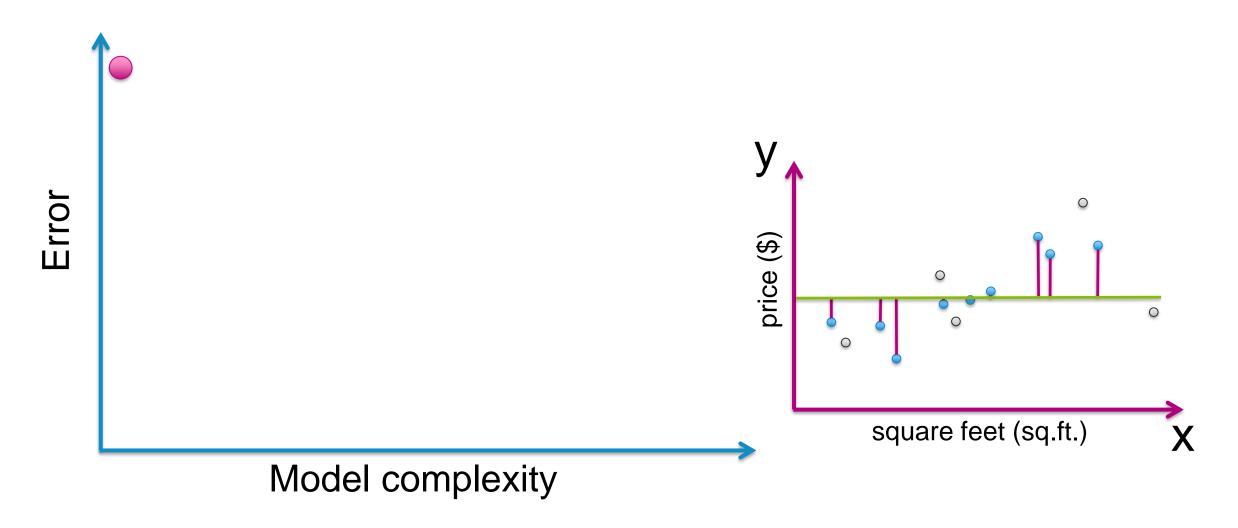


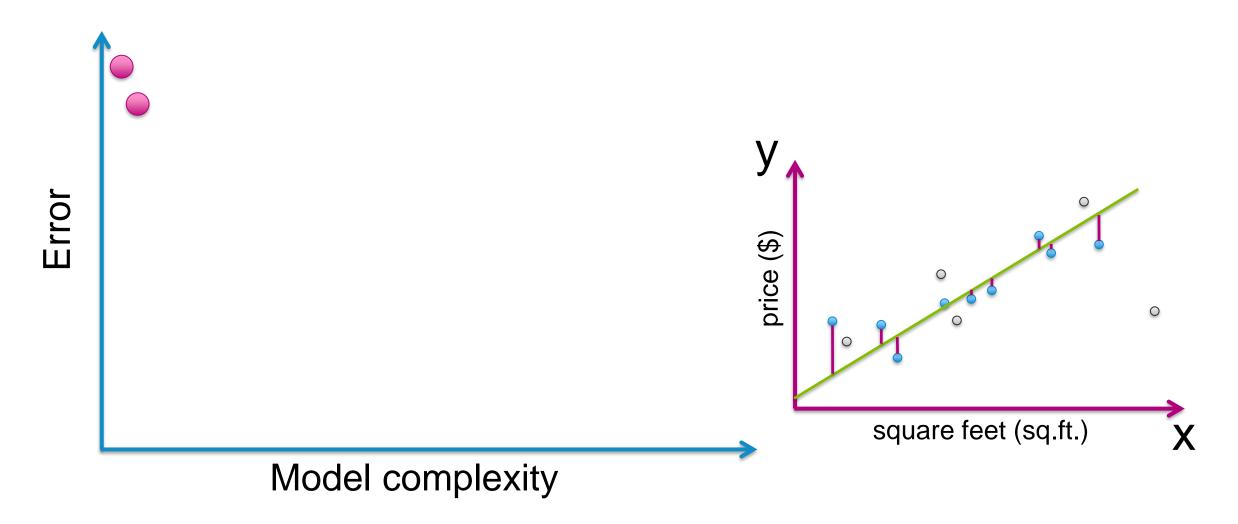
# Compute training error

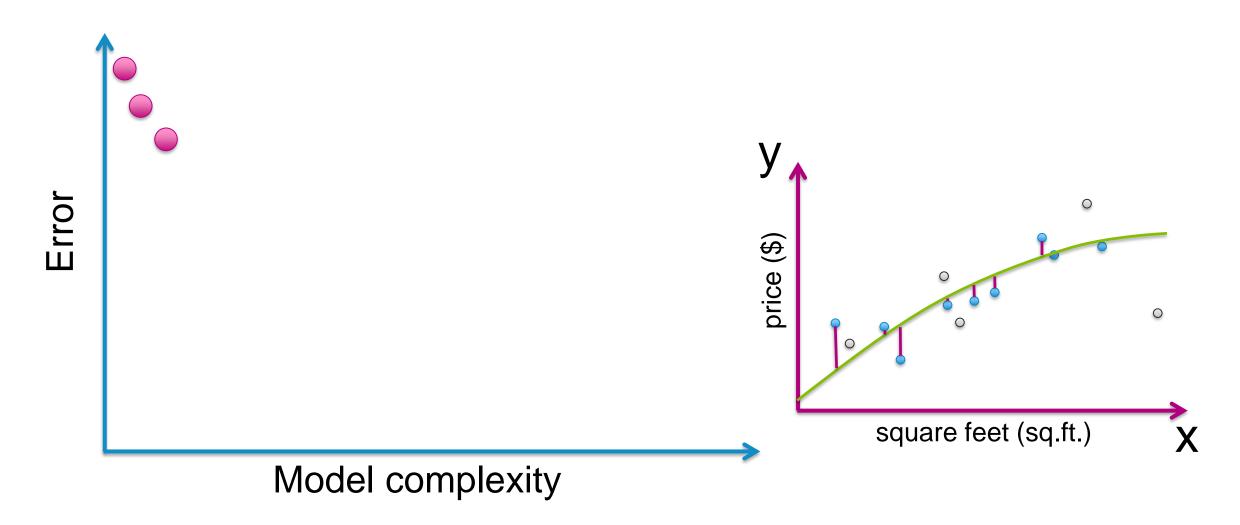
- 1. Define a loss function  $L(y, f_{\hat{w}}(x))$ 
  - E.g., squared error, absolute error,...
- 2. Training error

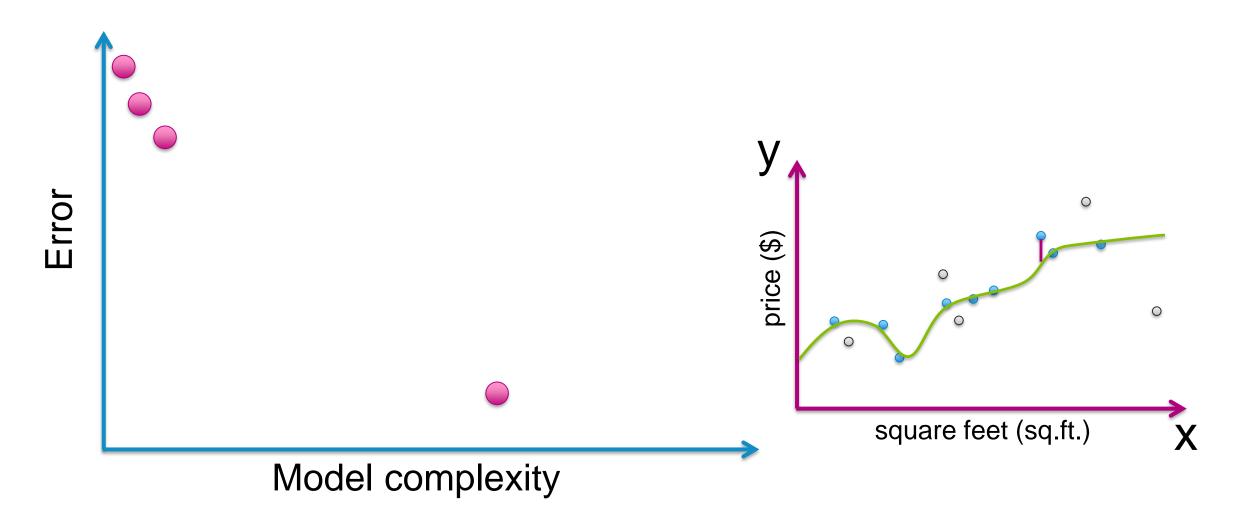


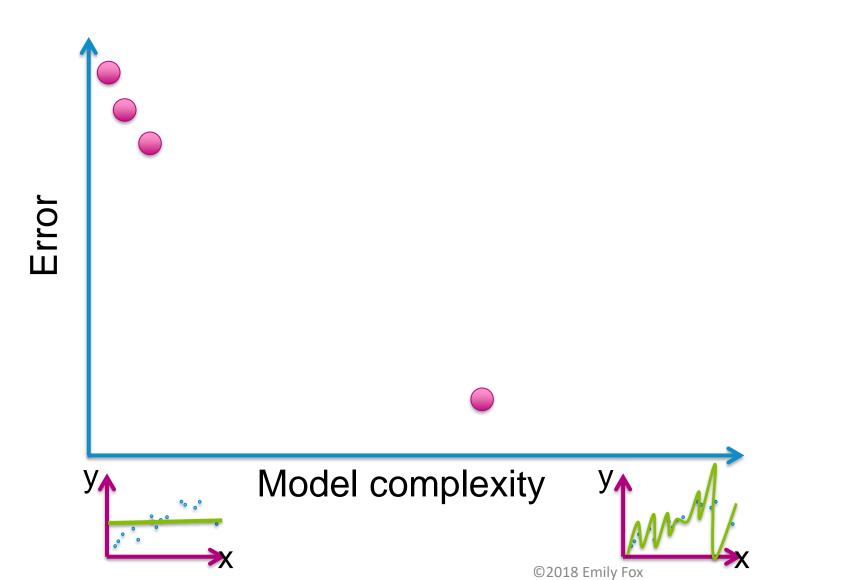










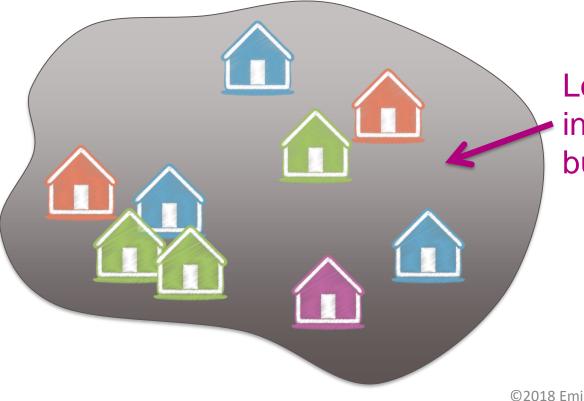


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#### Assessing the loss Part 2: Generalization (true) error

## Generalization error

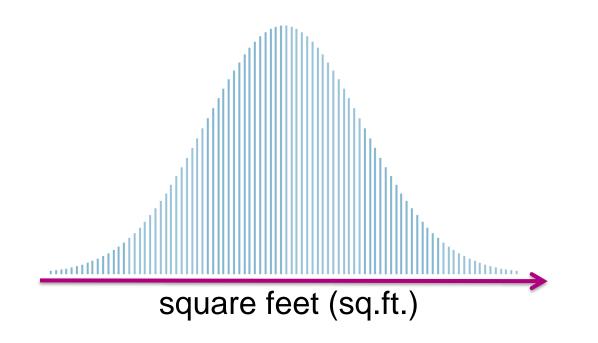
#### Really want estimate of loss over all possible (1,\$) pairs



Lots of houses in neighborhood, but not in dataset

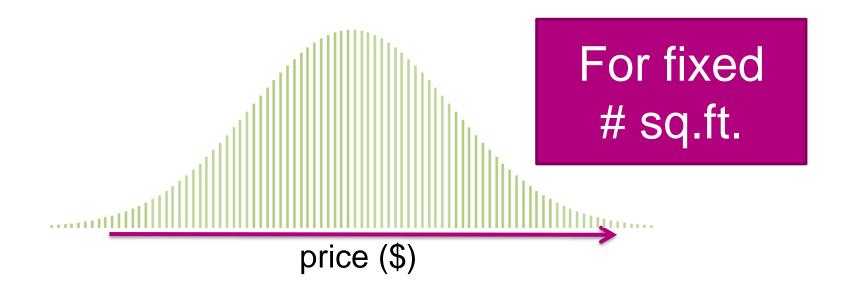
## **Distribution over houses**

# In our neighborhood, houses of what # sq.ft. (1) are we likely to see?



## Distribution over sales prices

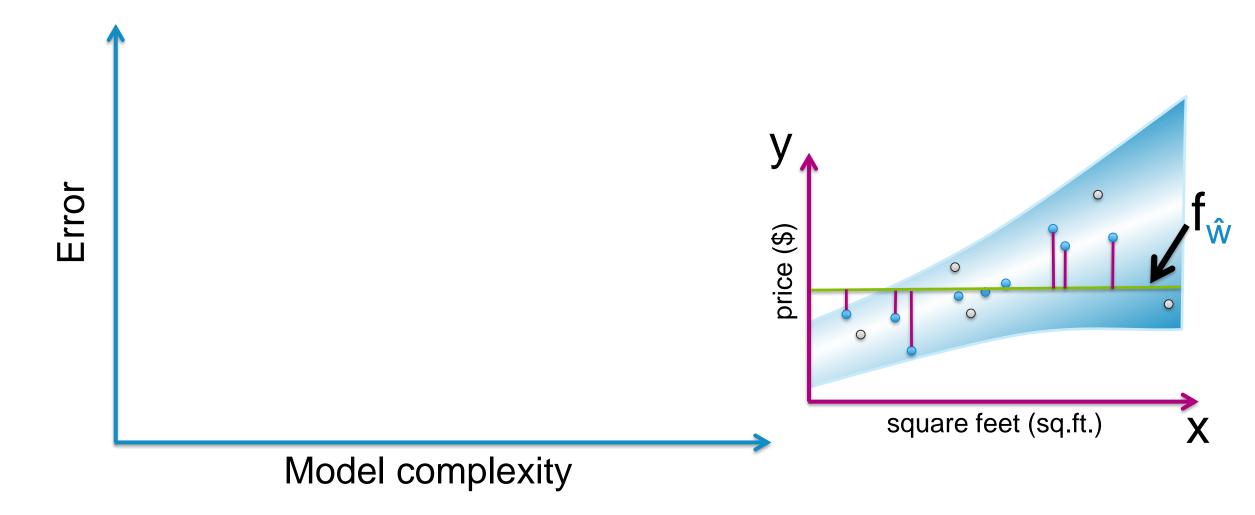
# For houses with a given # sq.ft. (1), what house prices \$ are we likely to see?

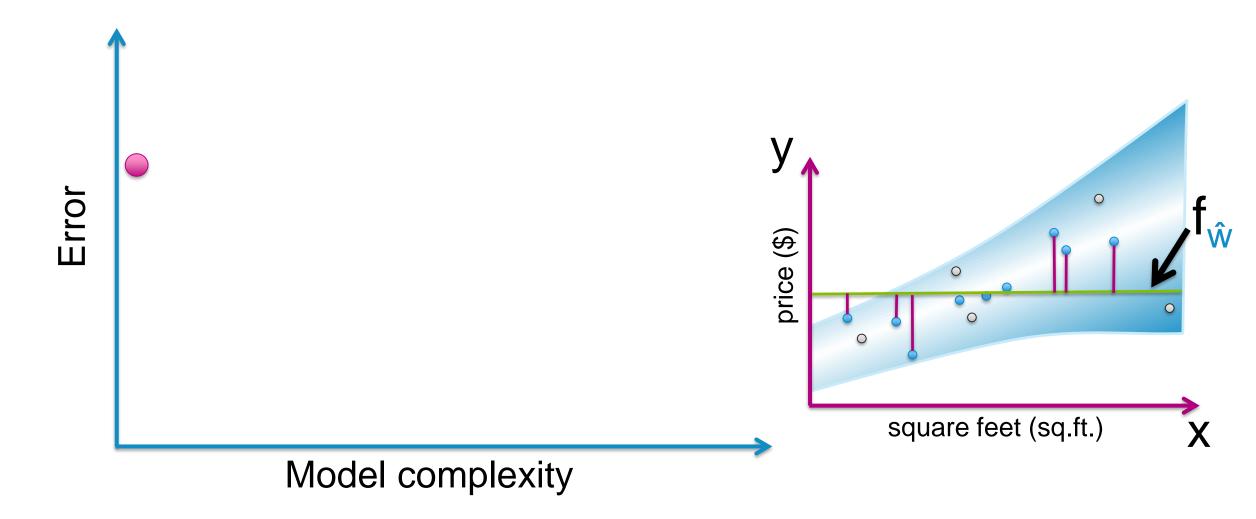


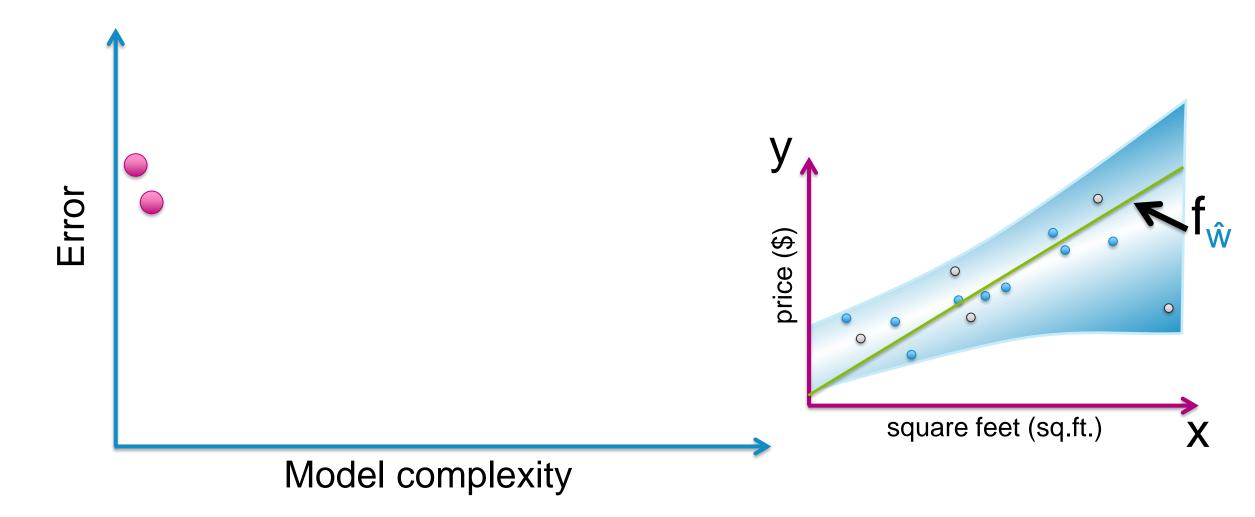
### Generalization error definition

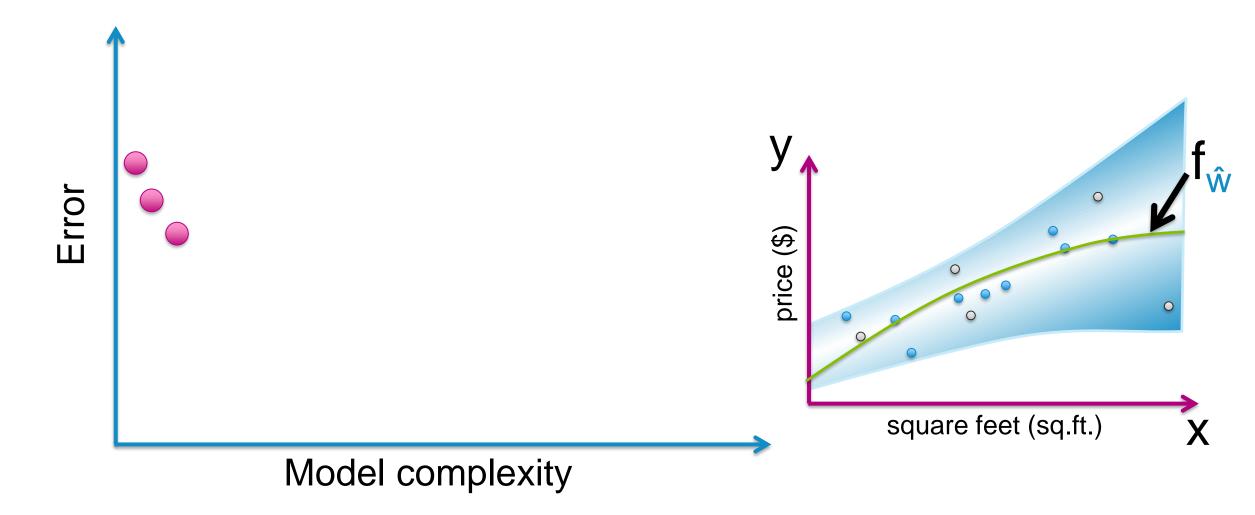
Really want estimate of loss over all possible (1,\$) pairs

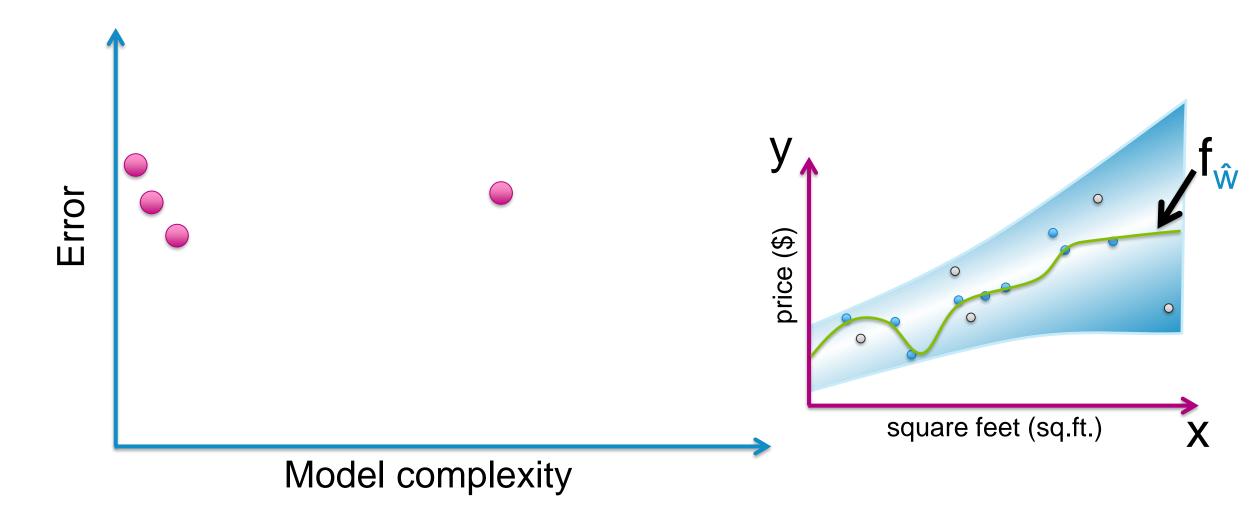
Formally: average over all possible (x,y) pairs weighted by how likely each is generalization error =  $E_{x,y}[L(y,f_{\hat{w}}(x))]$ fit using training data

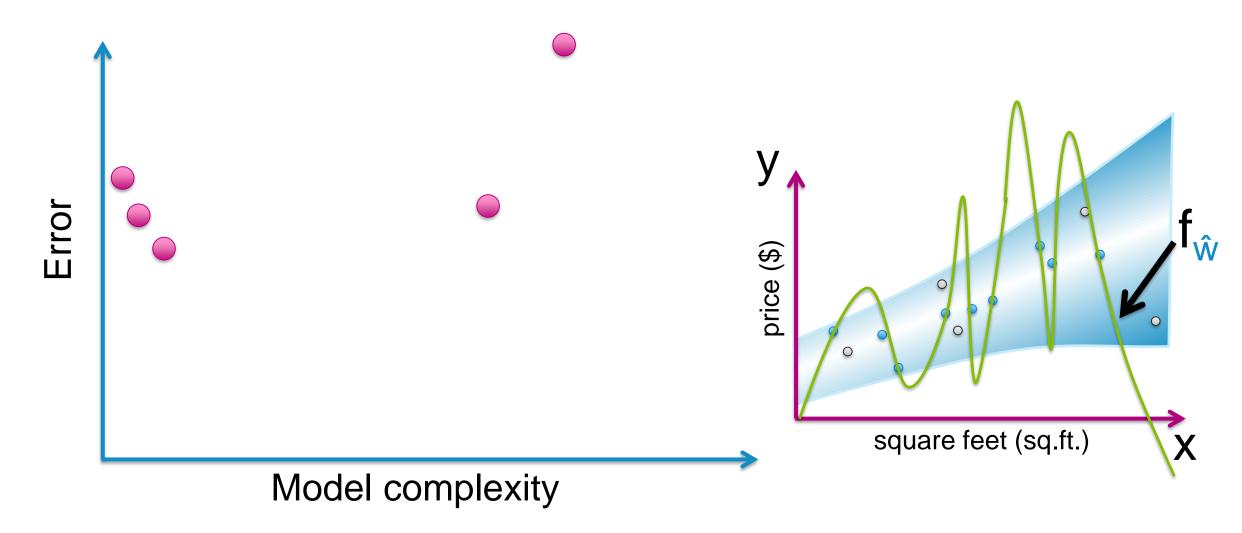


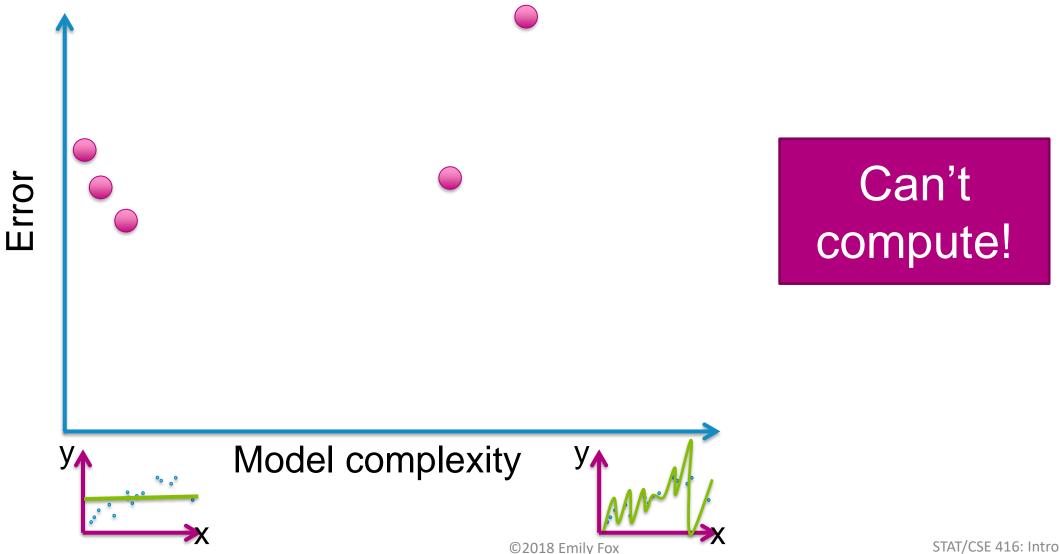












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#### Assessing the loss Part 3: Test error

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# Approximating generalization error

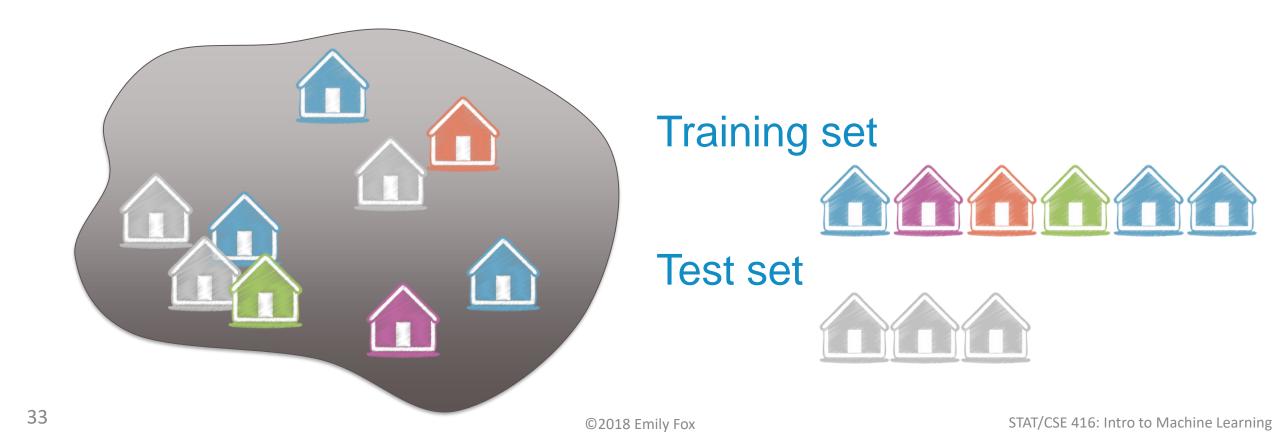
#### Wanted estimate of loss over all possible $(\widehat{\mathbf{n}}, \$)$ pairs



# Approximate by looking at houses not in training set

## Forming a test set

#### Hold out some ( $^{(n)}$ , $^{(n)}$ ) that are *not* used for fitting the model



## Forming a test set

#### Hold out some ( $\widehat{m}$ ) that are *not* used for fitting the model



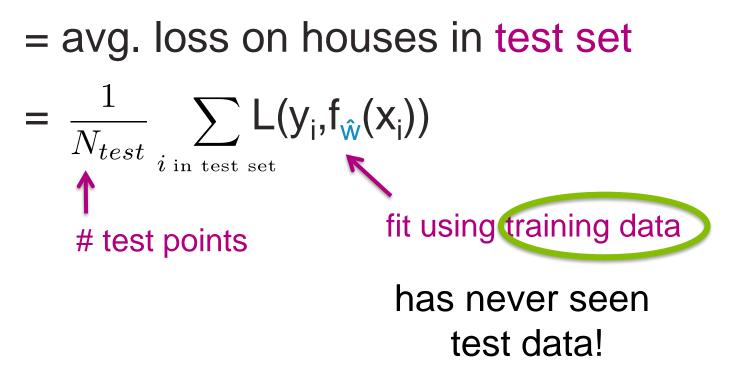
# Proxy for "everything you might see"

#### Test set



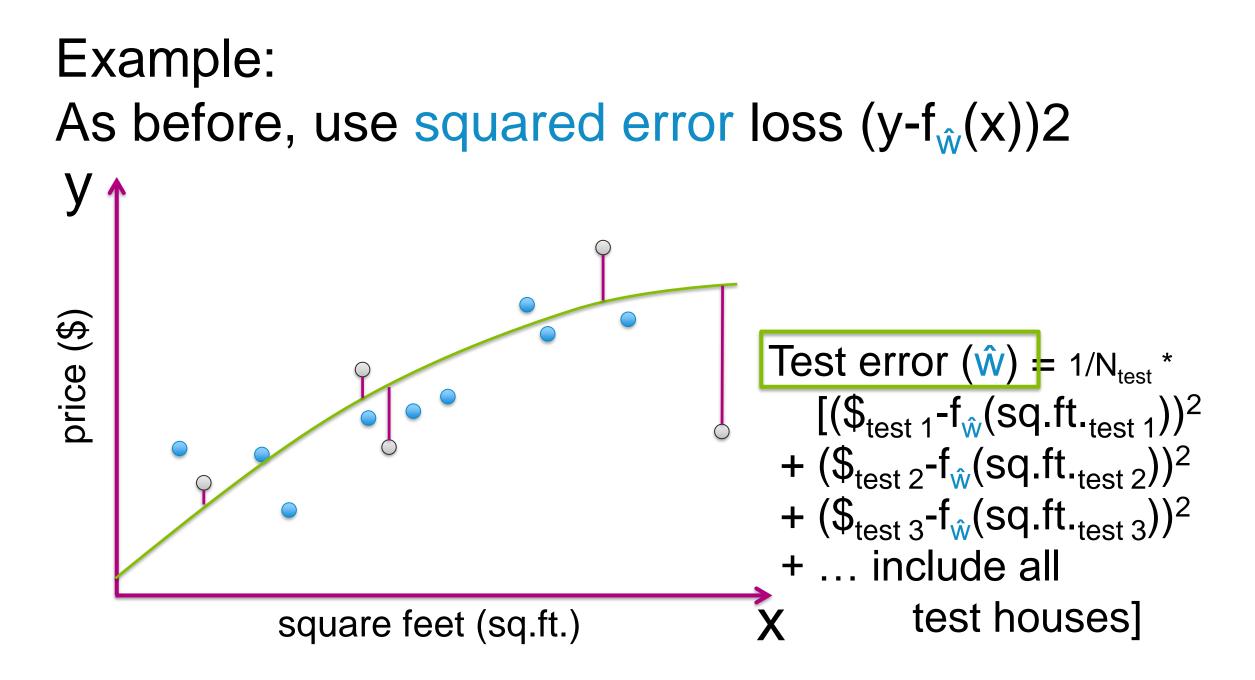
## Compute test error

#### Test error

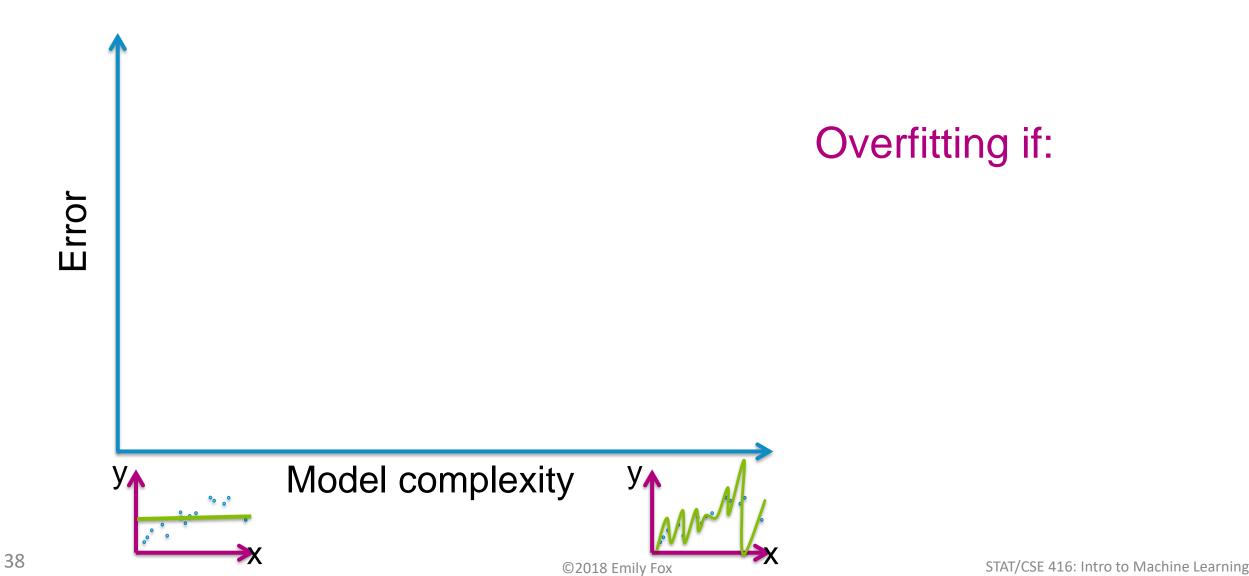


# Example: As before, fit quadratic to training data y $\bigcirc$ price (\$) $\bigcirc$ ŵ minimizes RSS of training data

square feet (sq.ft.)

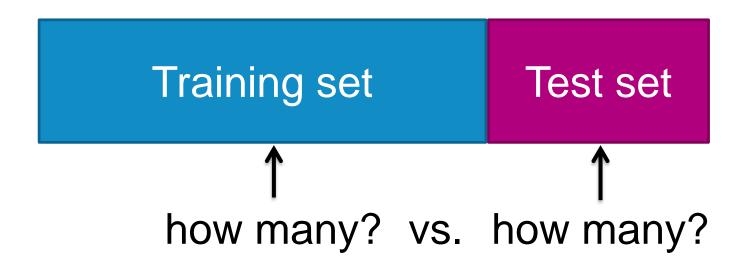


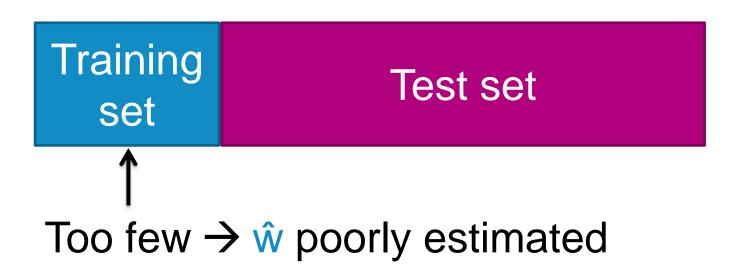
#### Training, true, & test error vs. model complexity

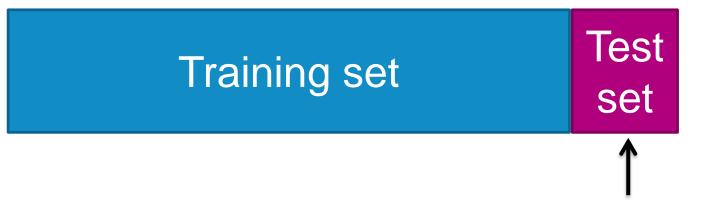


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Too few  $\rightarrow$  test error bad approximation of true error



Typically, just enough test points to form a reasonable estimate of true error

If this leaves too few for training, other methods like cross validation (will see later...)

#### 3 sources of error + the bias-variance tradeoff

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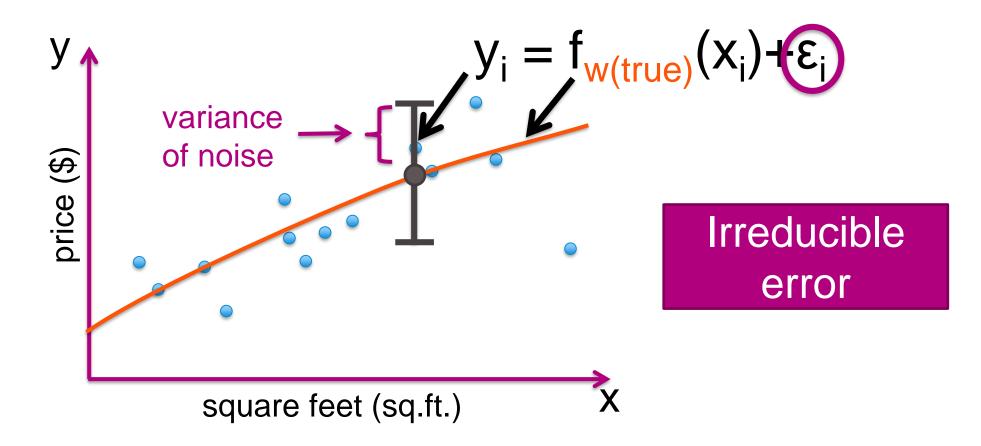
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#### 3 sources of error

In forming predictions, there are 3 sources of error:

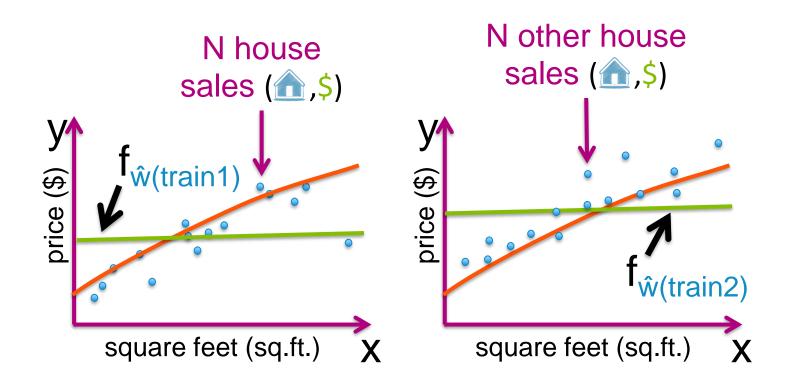
- 1. Noise
- 2. Bias
- 3. Variance

### Data inherently noisy



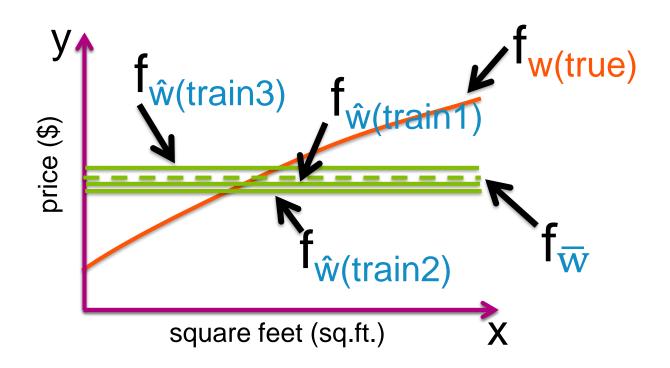
#### **Bias** contribution

#### Assume we fit a constant function



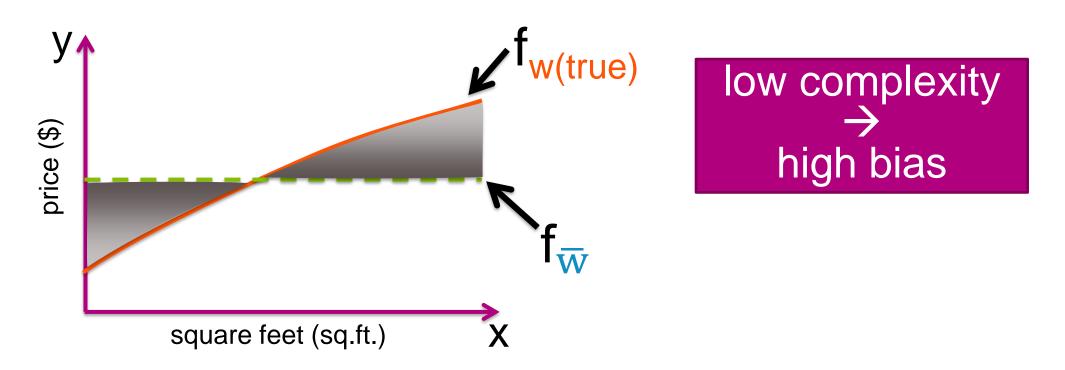
#### **Bias** contribution

Over all possible size N training sets, what do I expect my fit to be?



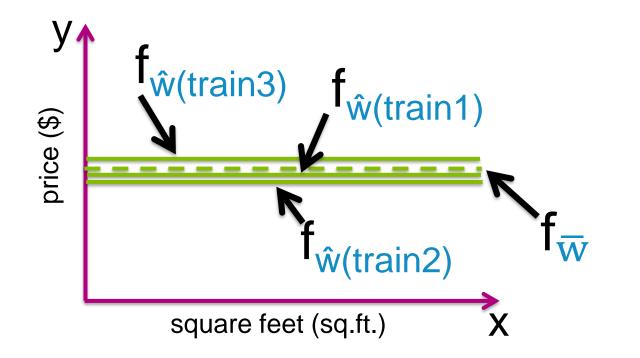
#### **Bias** contribution

 $Bias(x) = f_{w(true)}(x) - f_{\overline{w}}(x) \leftarrow Is our approach flexible enough to capture f_{w(true)}?$ If not, error in predictions.



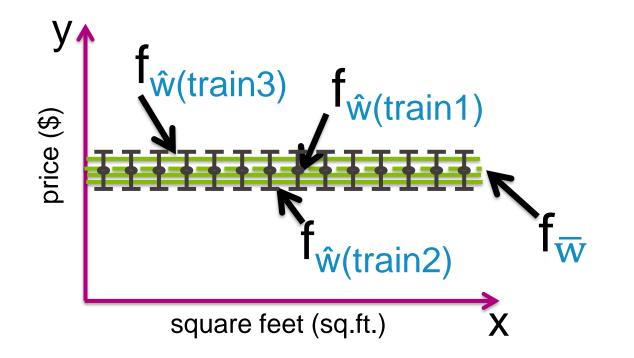
#### Variance contribution

How much do specific fits vary from the expected fit?



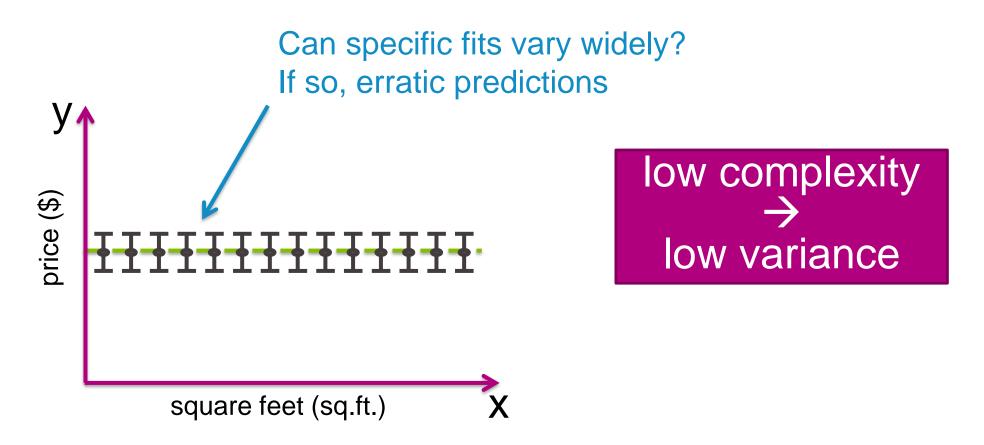
#### Variance contribution

How much do specific fits vary from the expected fit?



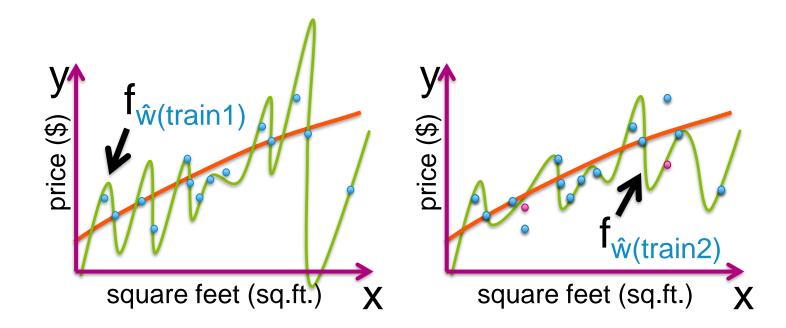
# Variance contribution

How much do specific fits vary from the expected fit?



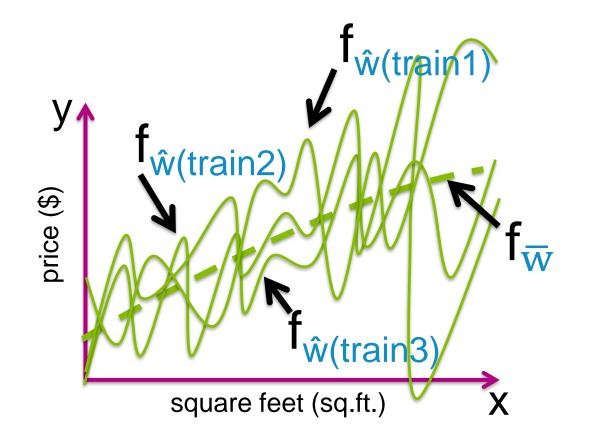
# Variance of high-complexity models

Assume we fit a high-order polynomial

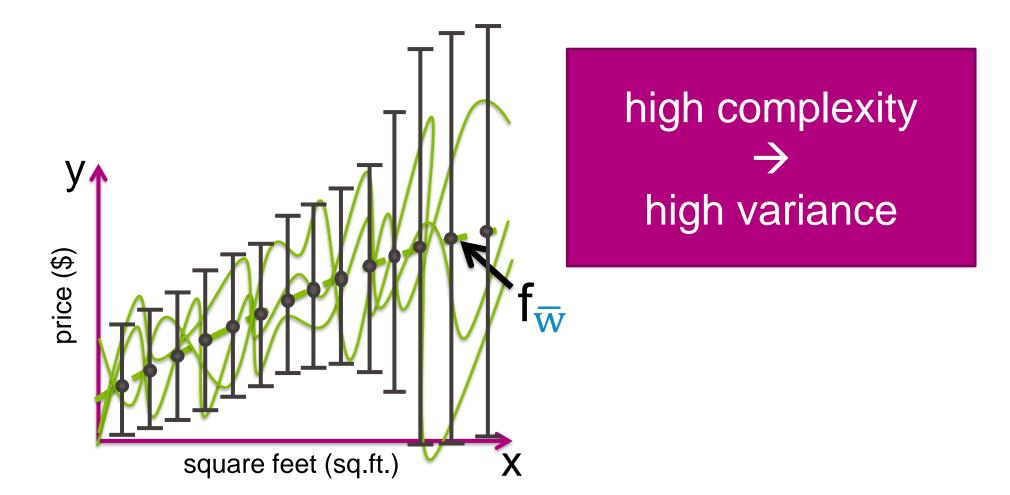


# Variance of high-complexity models

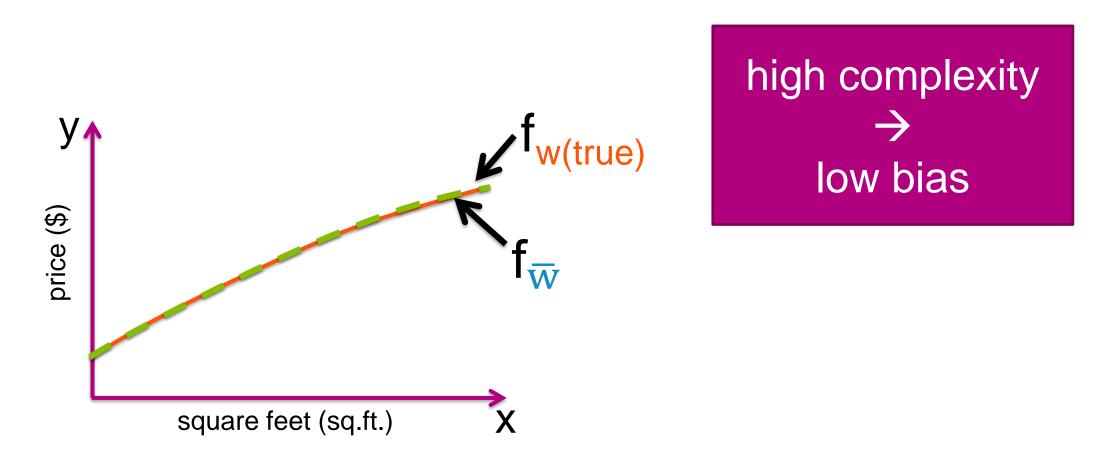
Assume we fit a high-order polynomial



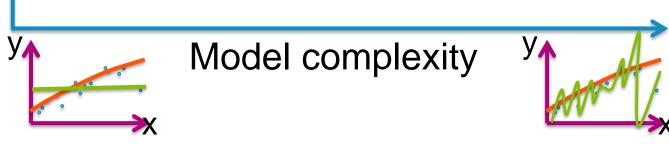
# Variance of high-complexity models



# **Bias** of high-complexity models



#### **Bias-variance** tradeoff



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#### Error vs. amount of data



# data points in training set

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# Summary of assessing performance

# What you can do now...

- Describe what a loss function is and give examples
- Contrast training and test error
- Compute training and test error given a loss function
- Discuss issue of assessing performance on training set
- Describe tradeoffs in forming training/test splits
- List and interpret the 3 sources of avg. prediction error
  - Irreducible error, bias, and variance