Machine Learning

Week 2

Linear Regression

ECE
14/01/2019

Course overview

1. Introduction to Linear Regression

2. Simple Linear Regression

3. Multiple Linear Regression

4. Evaluation of a Linear Regression Model

5. Practical Work

What is Linear Regression ?

- <u>Goal:</u> predict real (continuous) valued outputs, by modeling how our observations that are associated with some features change as we change the values of theses features.

- Example: training set of housing prices

X= input, features, covariate, predictors

y= output, target

m= number of training examples

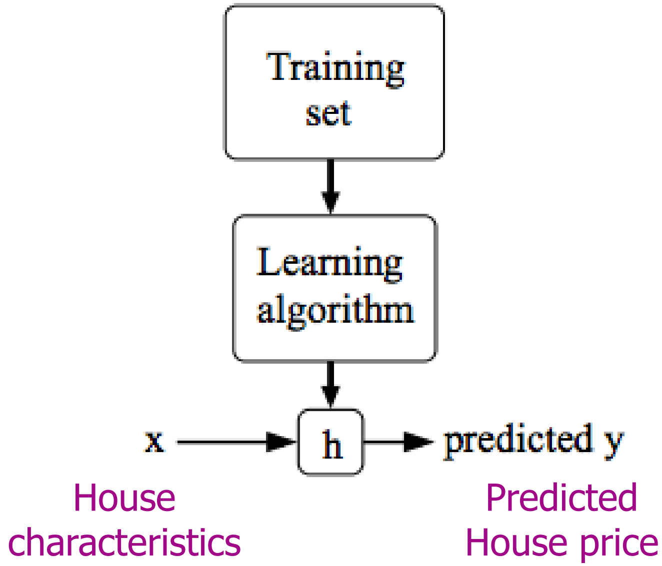
	Size (m2)	Built Year	Nb bathrooms	......	Sale price (k$)
$x^{(1)}$	200	2010	2	....	$y^{(1)}$ = 800
$x^{(2)}$	300	1995	2	.....	$y^{(2)}$ = 750
....	......	......	......	.....	......

- Regression is about learning the relationship between X and y, and using it to predict the house price of new data

	250	2005	3	.....	????????

Model Representation

- $x^{(i)}$ denotes the "input" variables (house characteristics)
- $y^{(i)}$ denotes the "output" or target variable that we are trying to predict (price)
- A pair $(x^{(i)}, y^{(i)})$ is called a training example
- A list of m training examples $(x^{(i)}, y^{(i)})$; i=1,...,m—is called a training set

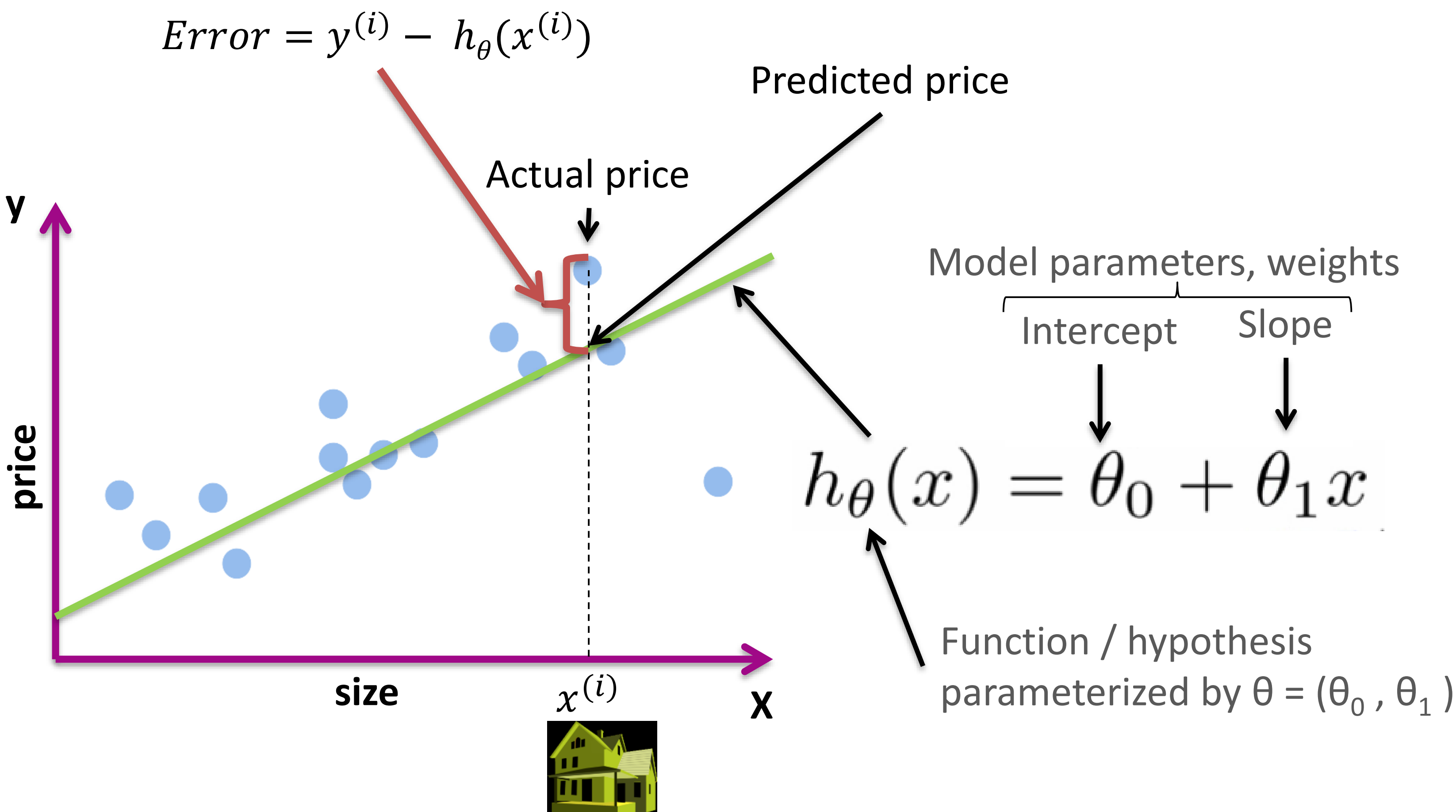


h: X → Y

Hypothesis or function that takes as input the house's characteristics to estimate its price.

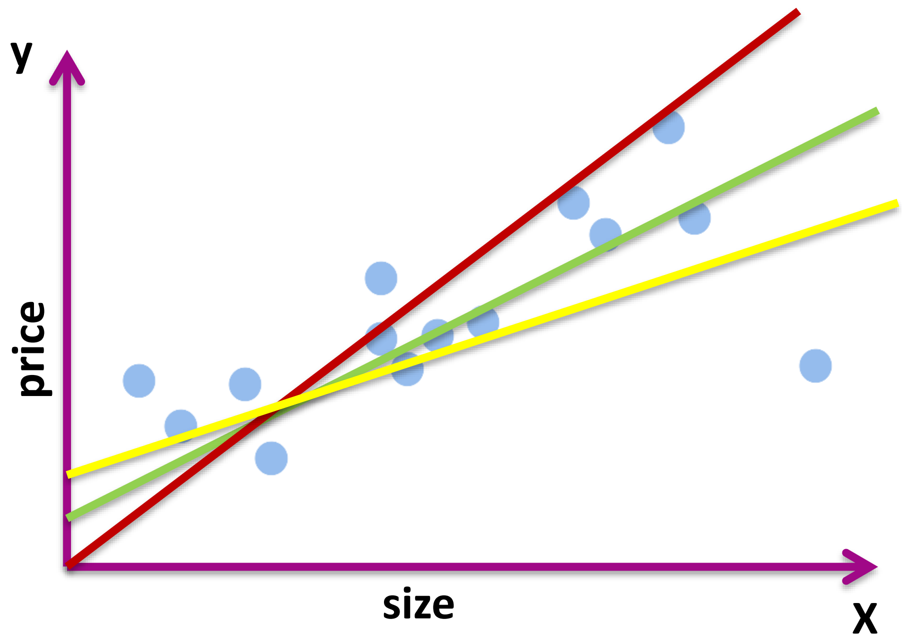
1.2
Simple/Univariate Linear Regression

Simple Linear Regression: Model



$$\boxed{y = \theta_0 + \theta_1 x + \varepsilon}$$

Simple Linear Regression: Model Evaluation



Each line has different parameters $\theta = (\theta_0 , \theta_1)$
➔ different errors

- Which line is the best fit ?
- what should a good function $h_\theta(x)$ minimize?
  - Sum error on all data points
  - Sum abs(error) on all data points
  - Sum error^2 on all data points

Simple Linear Regression: Model Evaluation

- Sum error on all data points

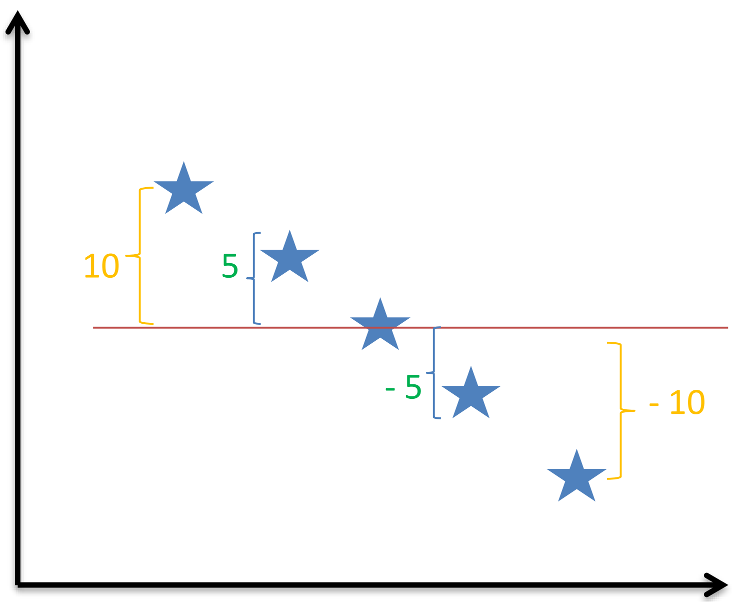
Sum error = 0 

- Sum abs(error) on all data points

Sum abs(error) > 0 

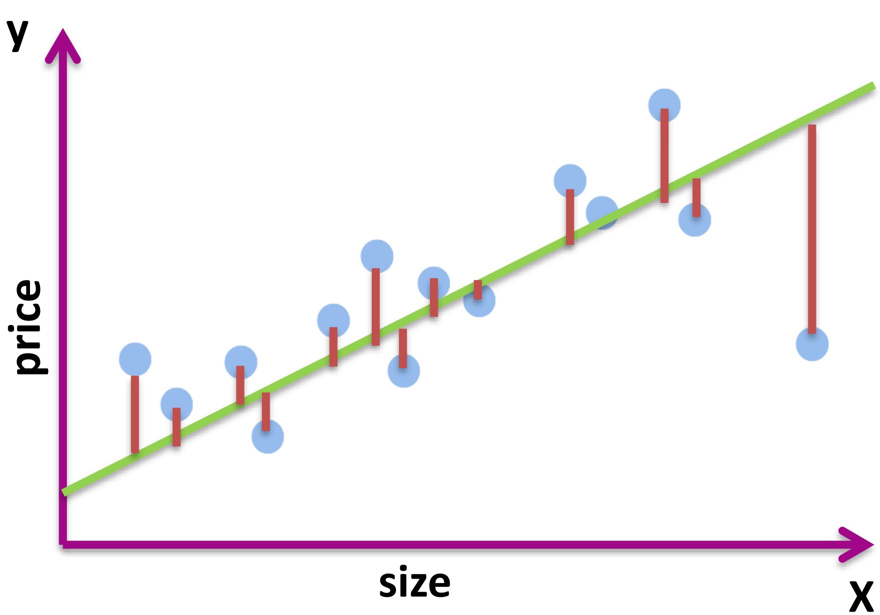
- Sum error^2 on all data points

Sum error^2 > 0  



Simple Linear Regression: Model Evaluation

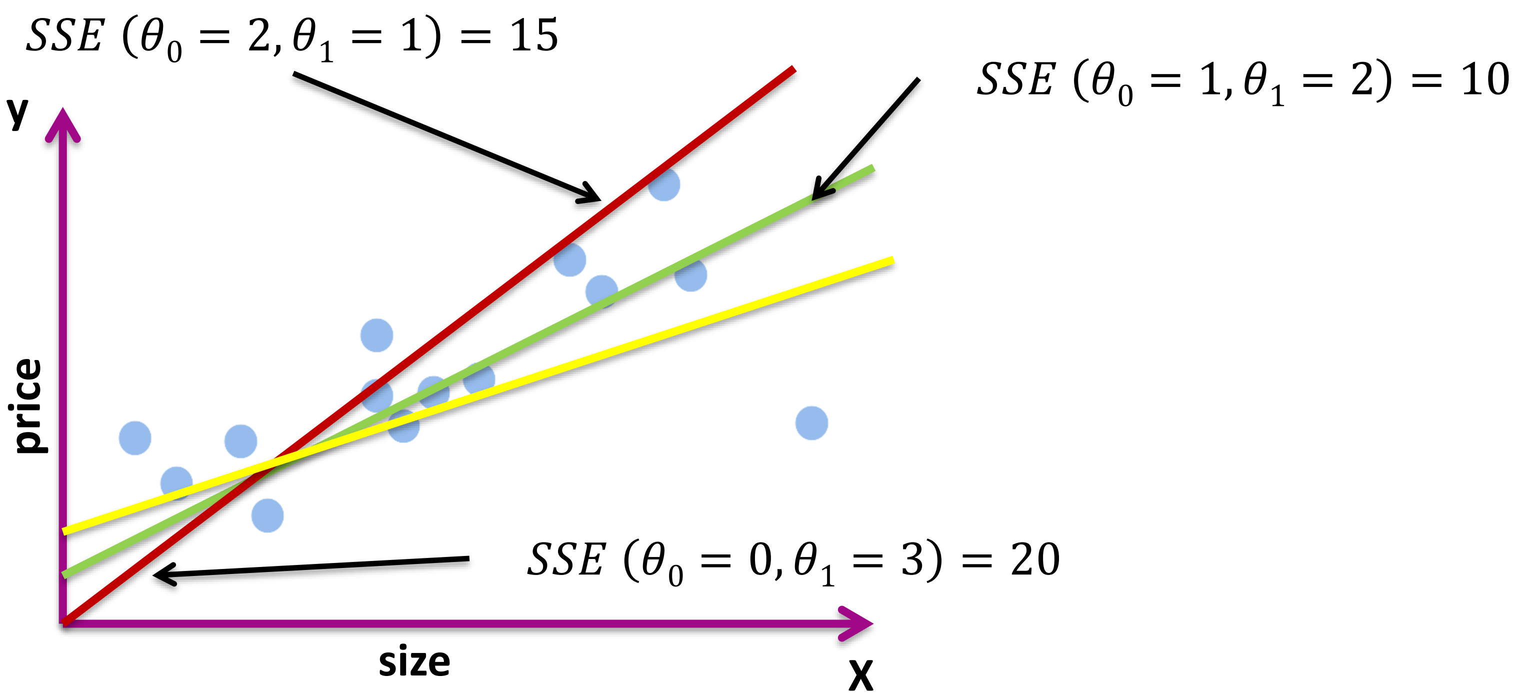
- The Sum of Squared Errors (SSE) is also called Residual Sum of Squares (RSS)



$$SSE\ (\theta_0, \theta_1) =$$

$$\left(y^{(1)} - (\theta_0 + \theta_1 * x^{(1)}) \right)^2 +$$
$$\left(y^{(2)} - (\theta_0 + \theta_1 * x^{(2)}) \right)^2 +$$
$$\ldots\ldots\ldots\ldots\ldots\ldots +$$
$$\left(y^{(m)} - (\theta_0 + \theta_1 * x^{(m)}) \right)^2$$

Simple Linear Regression: Model Evaluation



- The green line is a better fit
- Let's see how to find the best line automatically

Simple Linear Regression: Cost function

- The best hypothesis $h_\theta(x)$ is the one that minimizes the cost function

Sum over all data points

Actual

$$J(\theta_0, \theta_1) = \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Predicted

- 1/m - means we determine the average
- 1/2m, the 2 makes the math a bit easier, and doesn't change the weights θ we determine at all (i.e. half the smallest value is still the smallest value!)

- The learning algorithm should find $\theta^* = (\theta_0^*, \theta_1^*)$ that minimizes this cost
- Several algorithms:
  - Gradient descent
  - Ordinary least square (OLS): Used in the linear regression in python (sklearn)

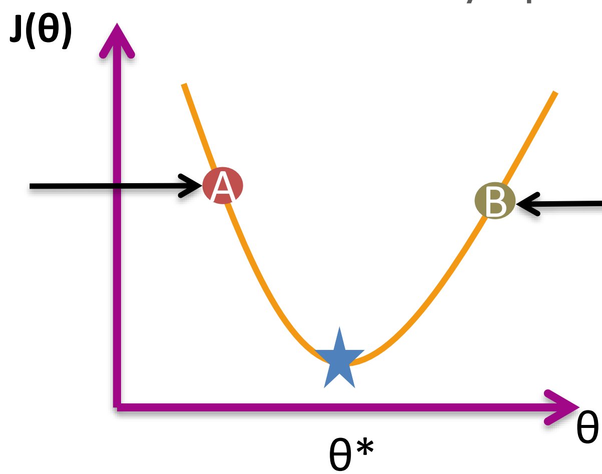
Gradient Descent Algorithm: Intuition

- Let's assume that we have one parameter θ, and that we want to minimize J(θ)

$$h_\theta(x) = \theta x$$

- GD starts by a random initial θ and iteratively update it to get towards θ*.

In this case, the derivative (gradient) ∂J(θ) / ∂θ < 0 .
θ^A - α*∂J(θ) / ∂θ > θ^A
θ^A is moving to the right
θ is increasing



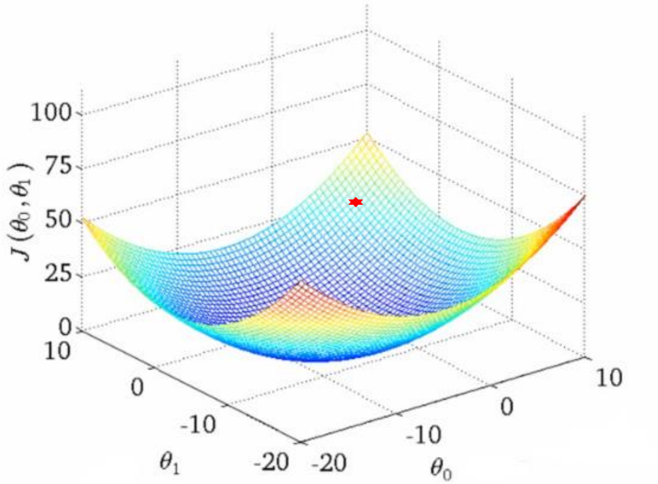
In this case, the derivative (gradient) ∂J(θ) / ∂θ > 0 .
θ^B - α* ∂J(θ) / ∂θ < θ^B
θ^B is moving to the left
θ is decreasing

- α is called the learning rate or the step size
  - Too small
    - Take baby steps ➔ Take too long to converge
  - Too large
    - Can overshoot the minimum ➔ fail to converge

Simple Linear regression with GD

- Repeat until convergence :

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \qquad (\text{for } j = 0 \text{ and } j = 1)$$



- If we calculate the derivatives, the expression becomes:

$$\boxed{h_\theta(x) = \theta_0 + \theta_1 x}$$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \qquad \theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x^{(i)}$$

- Convergence means either:
  - The cost function is no longer changing by more than ε.
  - The number of iterations is reached

- Go further

Ordinary Least Square Algorithm

- The Ordinary least square (OLS) approach chooses θ_0, θ_1 to minimize SSE

$$SSE = \sum_{i=1}^{m} (y^{(i)} - \theta_0 - \theta_1 * x^{(i)})^2$$

- In this method, we will minimize SSE by explicitly taking its derivatives with respect to the θ_0, θ_1, and setting them to zero.

- The minimizing values can be shown to be:

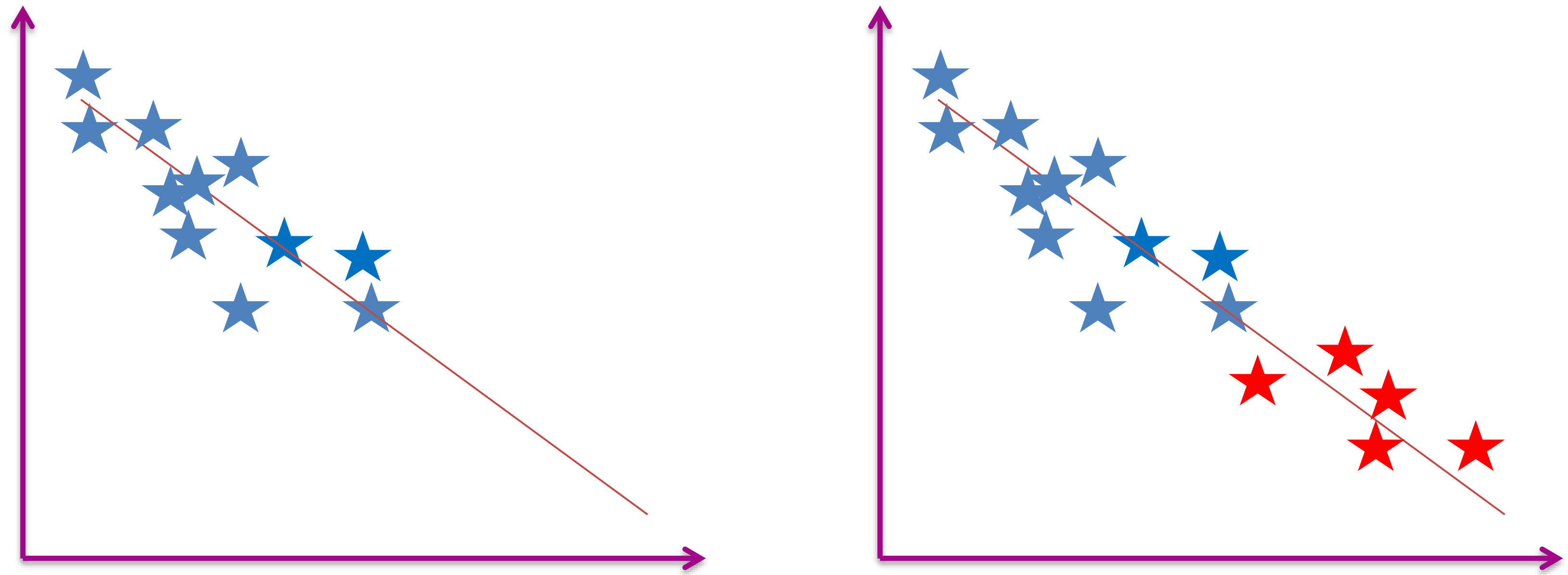
$$\widehat{\theta_1} = \frac{\sum_{i=1}^{m} (x^{(i)} - \bar{x}) (y^{(i)} - \bar{y})}{\sum_{i=1}^{m} (x^{(i)} - \bar{x})^2}$$

$$\widehat{\theta_0} = \bar{y} - \widehat{\theta_1} * \bar{x}$$

- Where $\bar{y} = \frac{1}{m} \sum_{i=1}^{m} y^{(i)}$, $\bar{x} = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}$ are the sample means

SSE is not perfect

- Which fit has larger SSE?



- Larger SSE doesn't necessarily mean worst fit ➔ Need an other metric

R^2 Statistic

- R^2 Answers the questions: **"how much of variability in the output (y) is explained by the change in the input (x)"**

- To calculate R^2, we use the formula:

$$R^2 = \frac{TSS - SSE}{TSS} = 1 - \frac{SSE}{TSS} \qquad TSS = \sum_{i=1}^{m} \left(y^{(i)} - \bar{y}\right)^2$$

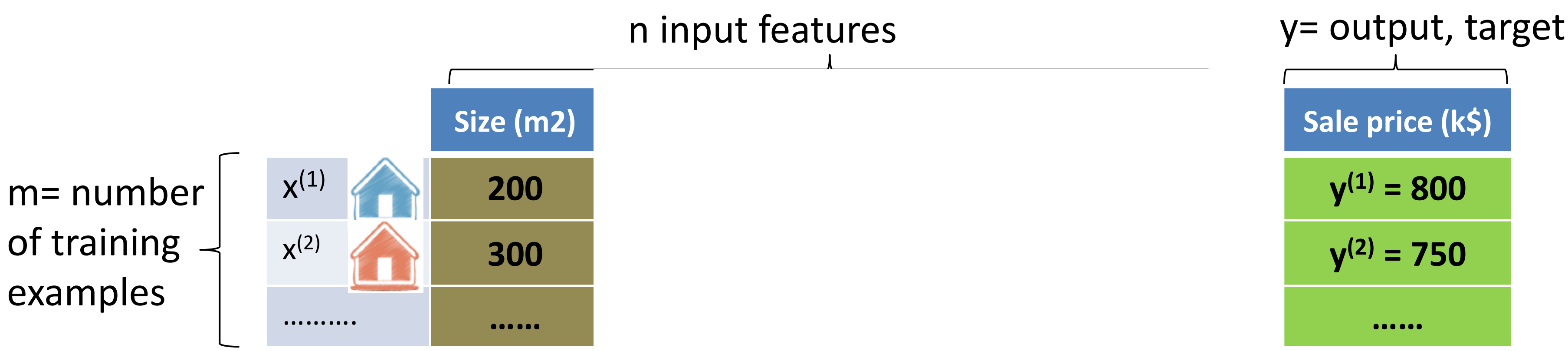
- An R^2 statistic that is close to 1 indicates that a large proportion of the variability in the response has been explained by the regression.

- A number near 0 indicates that the regression did not explain much of the variability in the response

1.2
Multivariate Linear Regression

Multiple Linear Regression

- In simple linear regression, we use one feature x to predict (y)
- In multiple linear regression, we have multiple features $X=(x_1,x_2, \dots, x_n)$



- $X^{(i)}$ is an n-dimensional feature vector
- $X^{(1)} = (200, 2010, 2, \dots.)^T$ the feature vector of the first training example.
- $x_j^{(i)}$ is the value of feature *j* in the i^{th} training example. $x_2^{(1)} = 2010$

Multiple Linear Regression

- In simple linear regression, $h_\theta(x) = \theta_0 + \theta_1 x$
- In multiple linear regression, $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$
- For convenience of notation, define $x_0 = 1$ $(x_0^{(i)} = 1)$

$$h_\theta(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

- Rewrite in matrix notation

$$\begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \cdots\cdot \\ \theta_n \end{bmatrix} \qquad \theta, x \in R^{n+1} \qquad \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \cdots\cdot \\ x_n \end{bmatrix}$$

$$h_\theta(x) = \sum_{i=1}^{n} \theta_i x_i = \theta^T x = \theta x T$$

Multiple Linear Regression

- Cost function:

$$J(\theta_0, \theta_1, \ldots, \theta_n) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

Simple Linear Regression, n=1

Repeat {

$$\theta_0 := \theta_0 - \alpha \underbrace{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})}_{\frac{\partial}{\partial \theta_0} J(\theta)}$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)}) x^{(i)}$$

(simultaneously update θ_0, θ_1) }

Multiple Linear Regression, n>1

Repeat {

$$\theta_j := \theta_j - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

(simultaneously update θ_j for $j = 0, \ldots, n$)

}

$$\theta_0 := \theta_0 - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)}) x_1^{(i)}$$

$$\theta_2 := \theta_2 - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)}) x_2^{(i)}$$

$\ldots$

OLS for multiple features

- Cost function with matrix notations:

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 = \frac{1}{2m}(X\theta - y)^T(X\theta - y)$$

- Where

$$X = \begin{bmatrix} — (x^{(1)})^T — \\ — (x^{(2)})^T — \\ \vdots \\ — (x^{(m)})^T — \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

- Derivatives with respect to θ $\quad \nabla_\theta J(\theta) = X^T X\theta - X^T y$

- By setting them to zero $\quad \theta = (X^T X)^{-1} X^T y$

When to use OLS or GD ?

- The following is a comparison of GD and the OLS (normal equation):

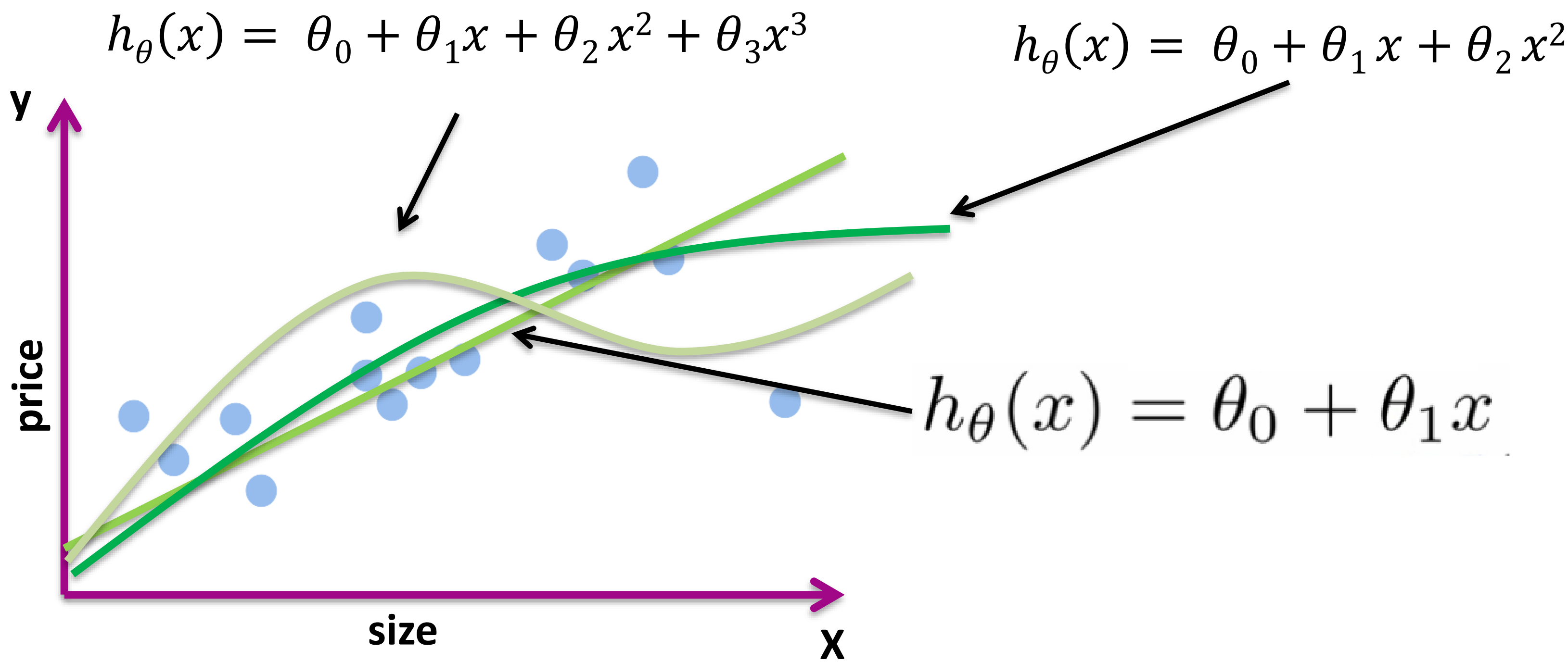
Gradient Descent	OLS (Normal Equation)
Need to choose alpha	No need to choose alpha
Needs feature scaling	No need for feature scaling
Needs many iterations	No need to iterate
$O(kn^2)$	$O(n^3)$, need to calculate inverse of X^TX
Works well when n is large	Slow if n is very large

- $n=10^4$-10^5 is usually the threshold of choosing GD over OLS
- Feature scaling helps converting the features to the same scale.
- For example, if x_i represents housing prices with a range of 100 to 2000 and a mean value of 1000, then,

$$x_i = \frac{price - 1000}{2000 - 100}$$

Polynomial Regression

- Polynomial regression is a particular case of multiple regression where the features are powers of one single feature x



- General model:

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 \theta_1 x + \cdots + \theta_p x^p + \varepsilon$$

1.3
Assessing Performance

Assessing Performance

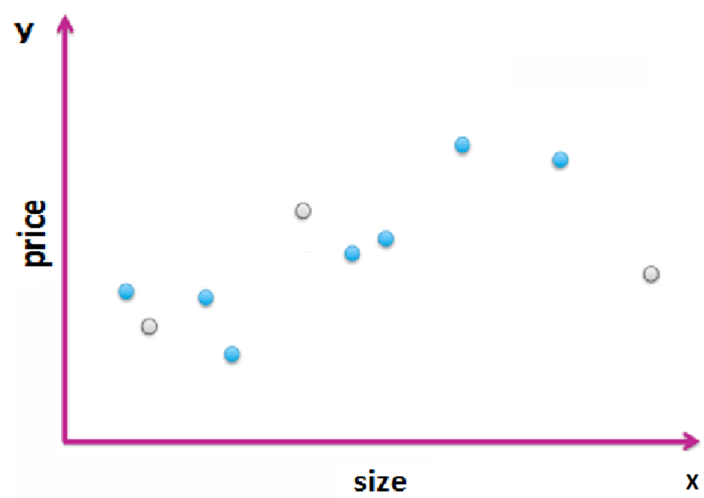
- This is about knowing how well the model will **generalize** to unseen data.
- One of the most used methods is splitting the data into train/test sets.

Training set – 70%

Size	Price
2104	400
1600	330
2400	369
1416	232
3000	540
1985	300
1534	315

Test set 30%

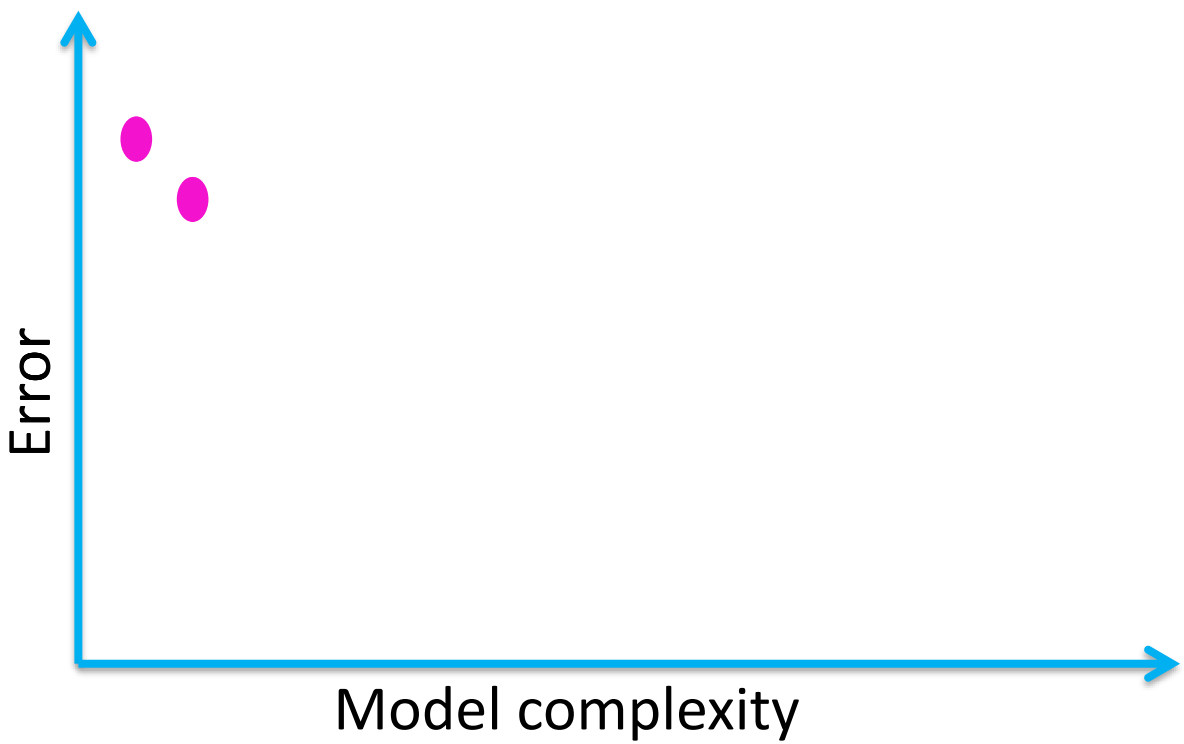
Size	Price
1427	199
1380	212
1494	243

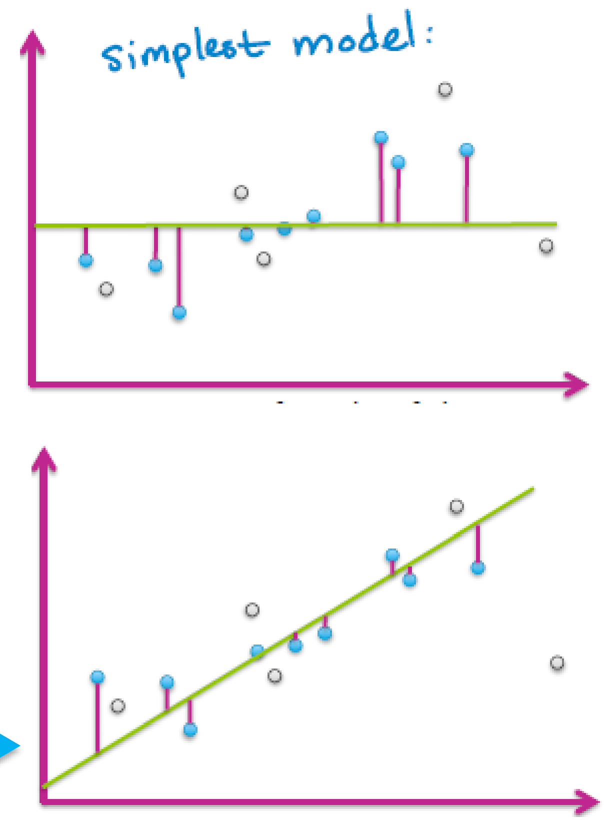


- Learn θ from training data (minimizing training error $J_{train}(\theta)$)
- Compute test error $J_{test}(\theta) = \frac{1}{2mtest} \sum_{i}^{m_{test}} (h_\theta(x^{(i)}) - y^{(i)})^2$

Training error vs. model complexity

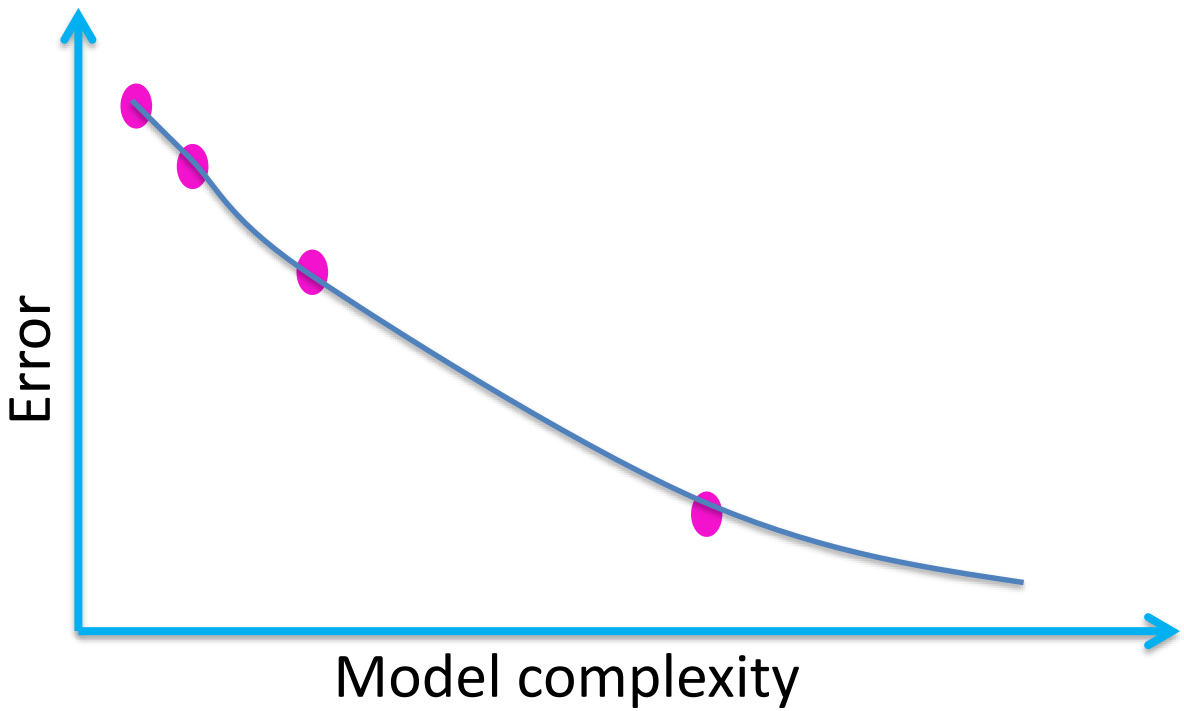
- Let’s take polynomial regression as an example

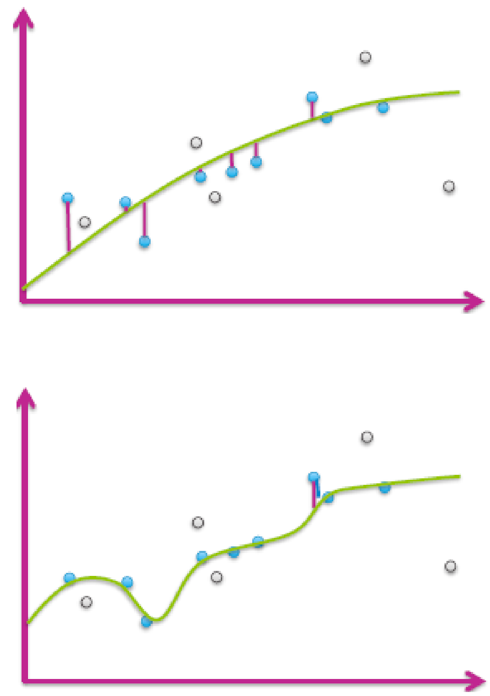




Training error vs. model complexity

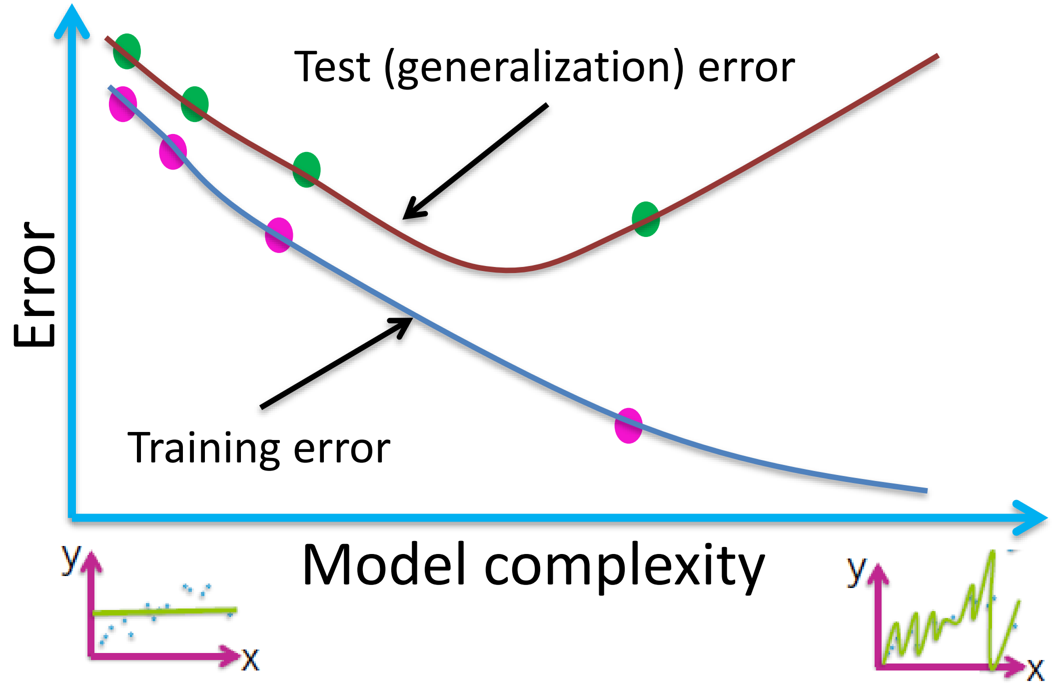
- Training error decreases with increasing model complexity

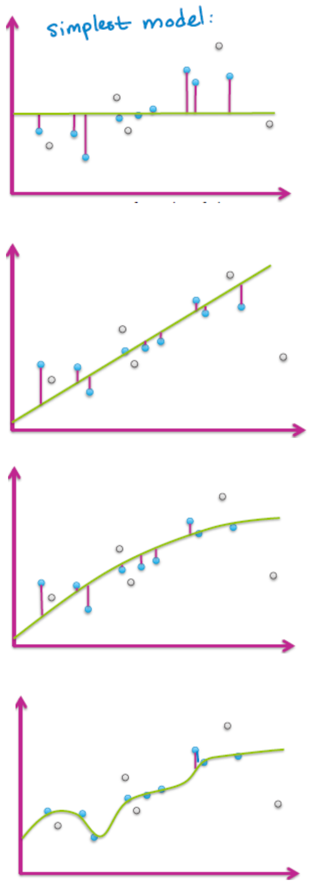




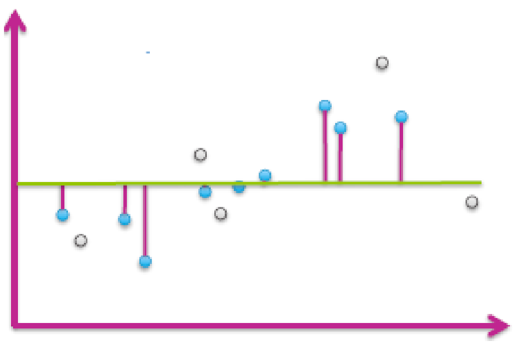
Testing error vs. model complexity

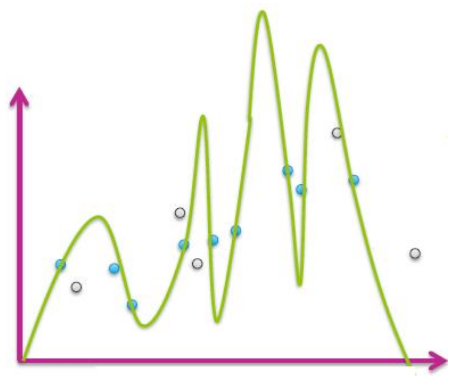
- Test error can be used as an approximation of the generalization error





Bias – Variance tradeoff





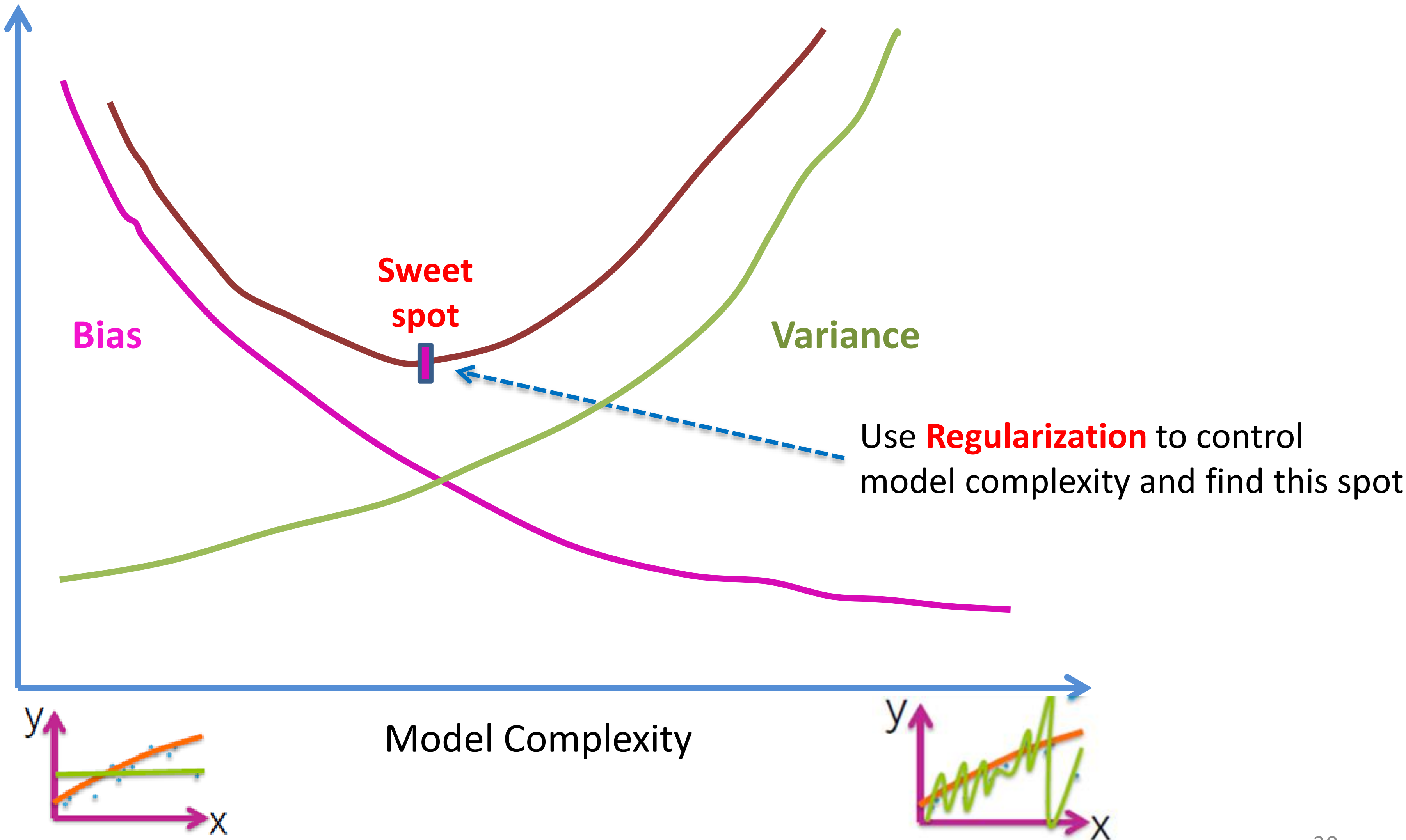
- **<u>High bias model</u>**

The model does not capture enough
The structure of the training set
Parameters tend to be small

- **<u>High variance model</u>**

The model is too specific to the structure
Of the training set
Parameters tend to be very large

Bias – Variance tradeoff



1.4
Regularization

Regularization

- It's about finding balance between:
  - How well the model fits the data
  - The magnitude of coefficients

- This is achieved by incorporating a penalty on weights θ in the cost function

- Ridge Regression (L_2 regularization)

$$J(\theta) = \frac{1}{2m} \left[\sum_{i=0}^{m} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2 + \lambda \sum_{j=1}^{n} (\theta_j)^2 \right]$$

- Lasso Regression (L_1 regularization)

$$J(\theta) = \frac{1}{2m} \left[\sum_{i=0}^{m} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2 + \lambda \sum_{j=1}^{n} | \theta_j | \right]$$

- λ is the regularization parameter:
  - Ridge: Encourages small weights θ but not exactly 0
  - Lasso: "Shrink" some weights θ exactly to 0

GD with Regularization

- Reminder of the L2 regularization cost function:

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

- Previously:

$$\theta_0 := \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \quad \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

- With regularization: $\theta_j := \theta_j(1 - \alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$

- α, λ are learning parameters to choose manually

- In practice: $(1 - \alpha\lambda/m)$ is between 0.99 and 0.95

Other Linear Regression Models

- Number of visiting customers to a website
- Product demand, inventory, failure, …
- Stock pricing
- Insurance claims severity

"Remember that all models are wrong;
the practical question is how wrong do they
have to be **to not be useful**."

George Box, 1987