### Recall from last time ...

## Logistic Regression

#### Classification

Email: Spam / Not Spam?

Content Video: Sensitive / Non-sensitive?

Skin Lesion: Malignant / Benign?

 $y \in \{0,1\}$  0: "Negative Class" (e.g., Benign skin lesion) 1: "Positive Class" (e.g., Malignant skin lesion)

## Hypothesis Representation

#### Logistic Regression Model

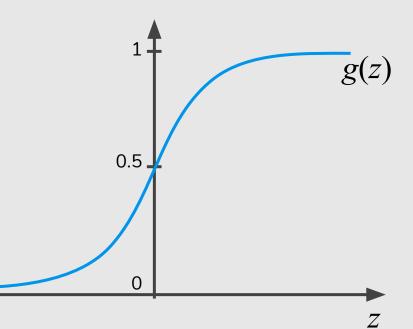
Want  $0 \le h_{\theta}(x) \le 1$ 

$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^{T} x}}$$

$$h_{\theta}(x) = g(\theta^{T}x)$$

$$g(z) = \frac{1}{1+e^{-2}}$$

Sigmoid Function Logistic Function

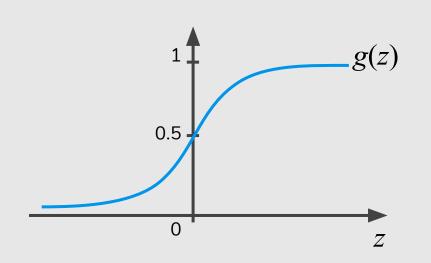


## Decision Boundary

#### **Logistic Regression**

$$h_{\theta}(x) = g(\theta^{\mathrm{T}} x)$$

$$g(z) = \frac{1}{1 + e^{-z}}$$



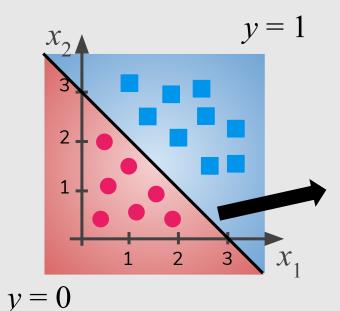
Suppose predict "
$$y = 1$$
" if  $h_{\theta}(x) \ge 0.5$ 

predict "
$$y = 0$$
" if  $h_{a}(x) < 0.5$ 

$$g(z) \ge 0.5$$
 when  $z \ge 0$ 

$$g(z) < 0.5 \text{ when } z < 0$$

#### **Decision Boundary**



$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

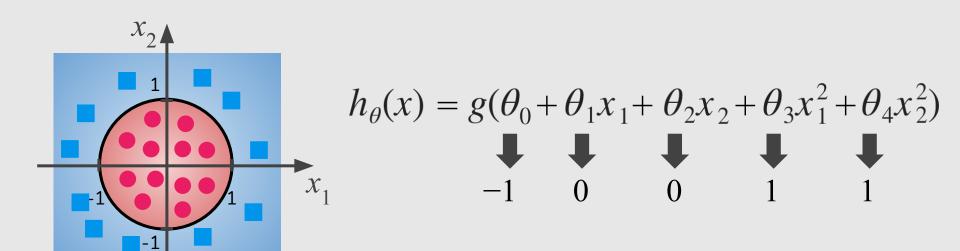
#### **Decision Boundary**

$$x_1 + x_2 = 3$$
$$h_{\theta}(x) = 0.5$$

 $y = 0, x_1 + x_2 < 3$ 

Predict "
$$y = 1$$
" if  $-3 + x_1 + x_2 \ge 0$   
 $x_1 + x_2 \ge 3$ 

#### Non-linear Decision Boundaries



Predict "
$$y = 1$$
" if  $-1 + x_1^2 + x_2^2 \ge 0$   
 $x_1^2 + x_2^2 \ge 1$ 

## **Cost Function**

Training set:  $\{(x^{(1)},y^{(1)}), (x^{(2)},y^{(2)}), ..., (x^{(m)},y^{(m)})\}$ 

$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^{T}x}} \qquad x \in \begin{bmatrix} x_{0} \\ x_{1} \\ \vdots \\ x_{n} \end{bmatrix} \quad x_{0} = 1, y \in \{0,1\}$$

How to choose parameters  $\theta$  ?

Linear regression: 
$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$
Logistic

$$Cost(h_{\theta}(x), y) = \frac{1}{2} (h_{\theta}(x) - y)^2$$
  $h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$ 



#### **Derivative of Logistic Function**

$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = \frac{d}{dz} \frac{1}{1 + e^{-z}}$$

$$= \frac{0 \cdot (1 + e^{-z}) - 1 \cdot (-e^{-z})}{(1 + e^{-z})^2} \quad \text{(quotient rule)}$$

$$= \frac{e^{-z}}{(1 + e^{-z})^2}$$

$$= \left(\frac{1}{1 + e^{-z}}\right) \left(1 - \frac{1}{1 + e^{-z}}\right)$$

$$= g(z)(1 - g(z))$$

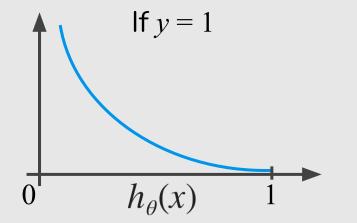
$$Cost(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1\\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$



#### Why use log function?

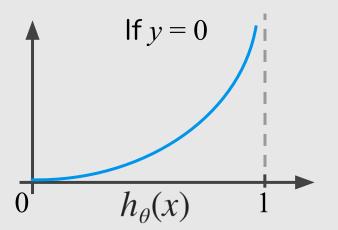
https://math.stackexchange.com/questions/886555/deriving-cost-function-using-mle-why-use-log-function

$$Cost(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1\\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$



$$\begin{aligned} \operatorname{Cost} &= 0 \text{ if } y = 1, \, h_{\theta}(x) = 1 \\ \operatorname{But as} & h_{\theta}(x) \longrightarrow 0 \\ \operatorname{Cost} & \longrightarrow \infty \end{aligned}$$

$$Cost(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1\\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$



## Simplified Cost Function and Gradient Descent

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \text{Cost}(h_{\theta}(x^{(i)}), y^{(i)})$$

$$= -\frac{1}{m} \left[ \sum_{i=1}^{m} y^{(i)} \log(h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)})) \right]$$

To fit parameters  $\theta$ :  $\min_{\alpha} J(\theta)$ 

To make a new prediction given new x: Output  $h_{\theta}(x) = \frac{1}{1 + e^{-\theta^{T}x}}$ 

#### **Gradient Descent**

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

$$\begin{aligned} & \text{Want } \min_{\theta} J(\theta) \colon \\ & \text{repeat } \{ & & \underbrace{\frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}}_{i} \\ & \theta_j := \theta_j - \alpha \underbrace{\frac{\partial}{\partial \theta_j} J(\theta)}_{j} \\ & \text{ } \{ \text{simultaneously update } \theta_i \text{ for } j = 0, 1, ..., n \} \end{aligned}$$

#### **Gradient Descent**

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

Want 
$$\min_{\theta} J(\theta)$$
:

$$h_{\theta}(x) = \theta^{T}x \implies h_{\theta}(x) = \frac{1}{1 + e^{-\theta^{T}x}}$$

repeat {

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

} (simultaneously update  $\theta_i$  for j = 0, 1, ..., n)

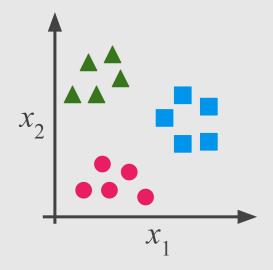
Algorithm looks identical to linear regression!

## Multiclass Classification: One-vs-all

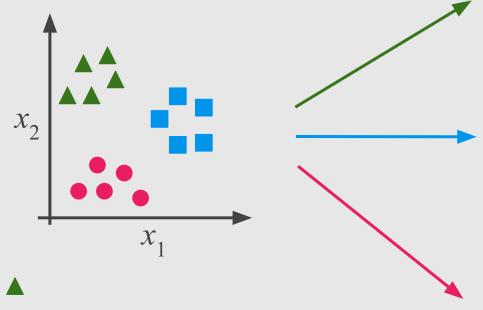
#### **Binary Classification**

# $x_2$

#### Multi-class Classification



#### One-us-All (One-us-Rest)



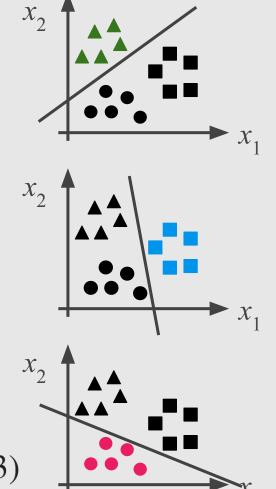
Class 1: ▲

Class 2:

Class 3: •

$$h_{\theta}^{(i)}(x) = P(y = i \mid x; \theta)$$

$$(i=1,2,3)$$



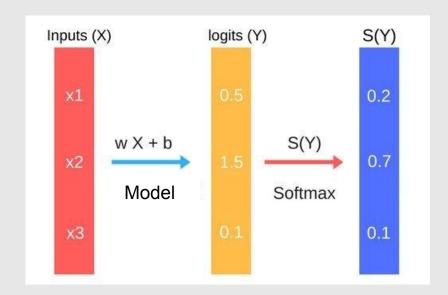
#### One-us-All (One-us-Rest)

Train a logistic regression classifier  $h_{\theta}^{(i)}(x)$  for each class i to predict the probability that y = i.

One a new input x, to make a prediction, pick the class i that maximizes

$$\max_{i} h_{\theta}^{(i)}(x)$$

#### Multinomial Logistic Regression



http://dataaspirant.com/2017/03/14/multinomial-logistic-regression-model-works-machine-learning/

#### References

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#### **Machine Learning Books**

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 4
- Pattern Recognition and Machine Learning, Chap. 4

#### **Machine Learning Courses**

- https://www.coursera.org/learn/machine-learning, Week 3
- Logistic Regression The Math of Intelligence (Week 2): https://youtu.be/D8alok2P468
- http://cs229.stanford.edu/notes/cs229-notes1.pdf



## Regularization Machine Learning and Pattern Recognition

(Largely based on slides from Andrew Ng)

#### Prof. Sandra Avila

Institute of Computing (IC/Unicamp)

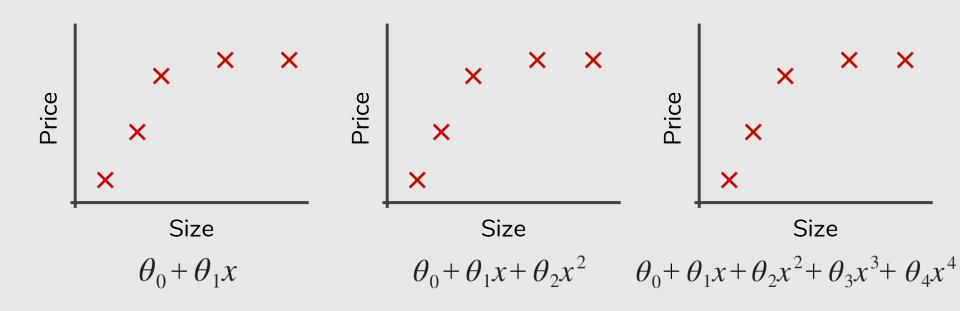
#### Today's Agenda

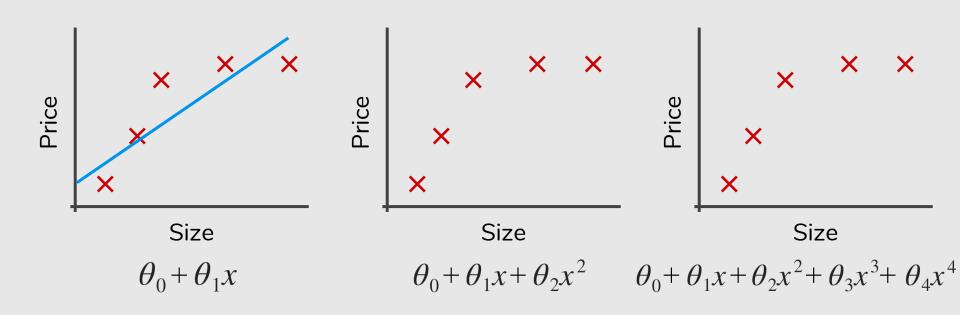
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- Regularization
  - The Problem of Overfitting
  - Diagnosing Bias vs. Variance
  - Cost Function
  - Regularized Linear Regression
  - Regularized Logistic Regression

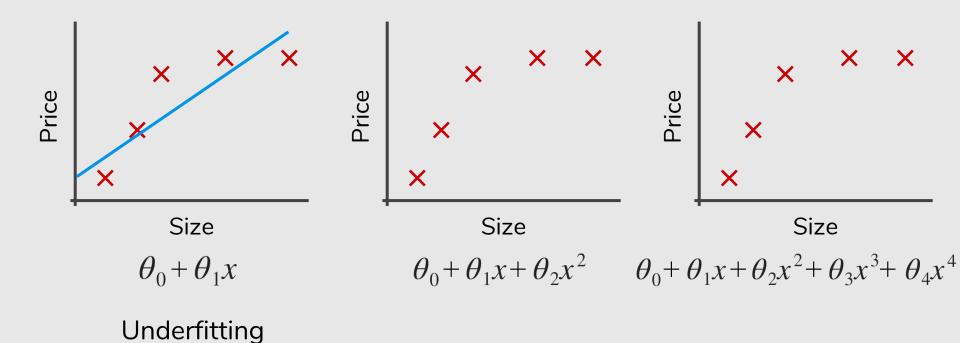
## The Problem of Overfitting

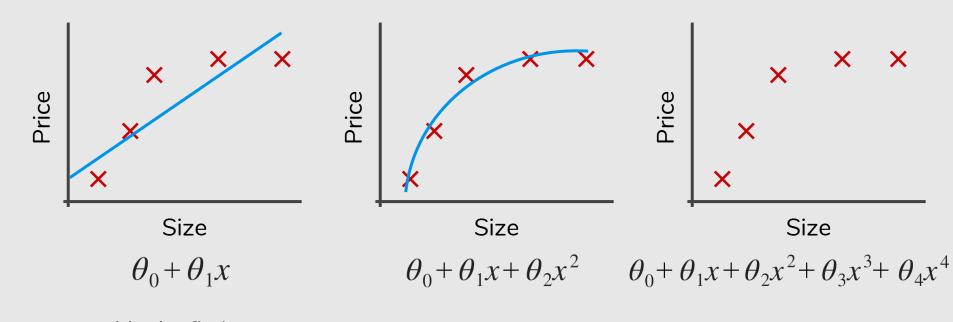




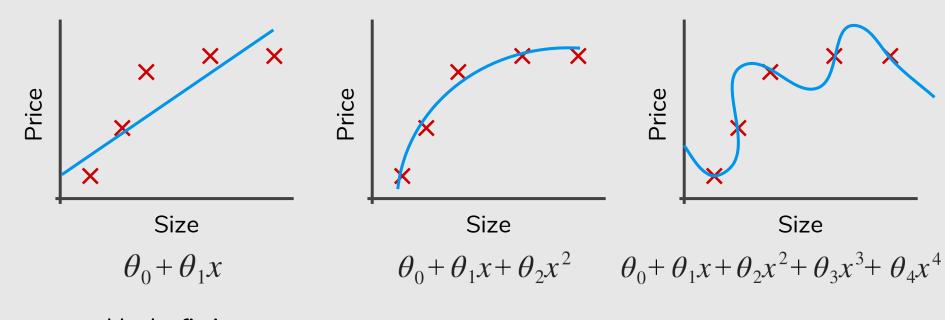


High bias



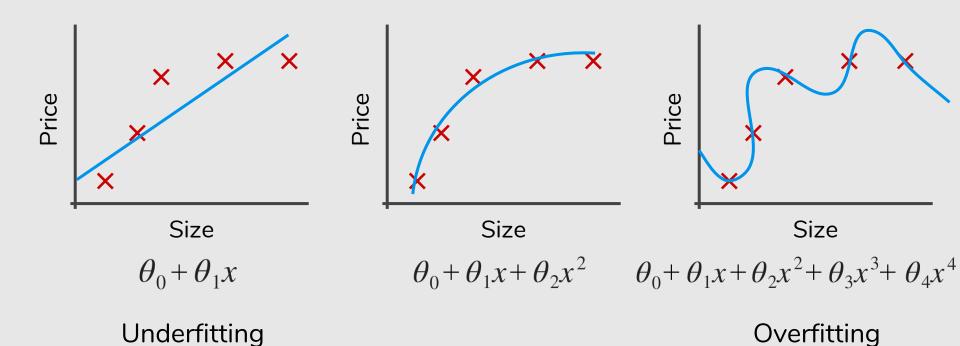


Underfitting High bias

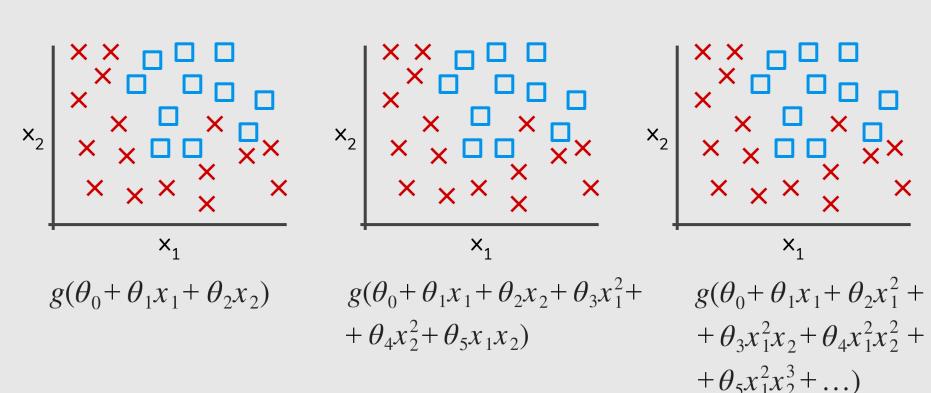


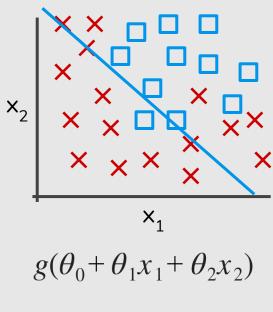
Underfitting High bias

High bias

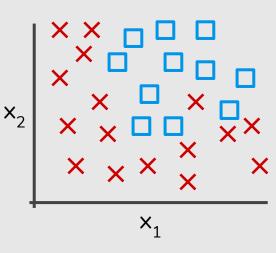


High variance

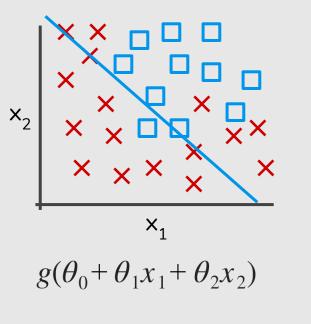




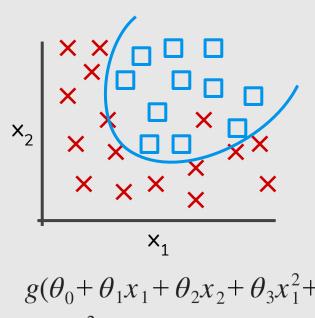
Underfitting High bias



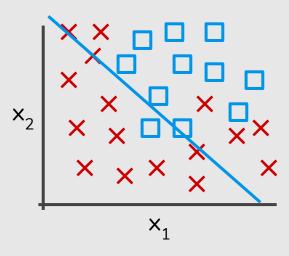
$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2)$$



Underfitting High bias

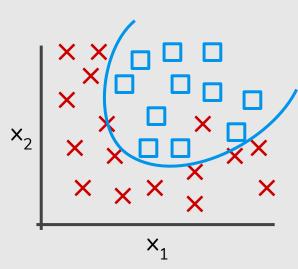


$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2)$$



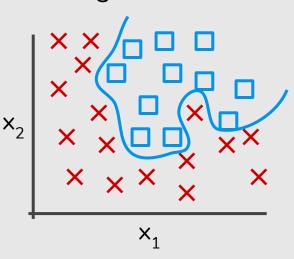
$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

Underfitting High bias



$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2)$$

Overfitting
High variance



$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

A model's generalization error can be expressed as the sum of **three** very different errors:

- Bias
- Variance
- Irreducible error

A model's generalization error can be expressed as the sum of **three** very different errors:

#### Bias

- Due to wrong assumptions, such as assuming that the data is linear when it is actually quadratic.
- A high-bias model is most likely to underfit the training data.
- Variance
- Irreducible error

A model's generalization error can be expressed as the sum of **three** very different errors:

- Bias
- Variance
  - Due to the model's excessive sensitivity to small variations in the training data.
  - A model with many degrees of freedom is likely to have high variance, and thus to overfit the training data.
- Irreducible error

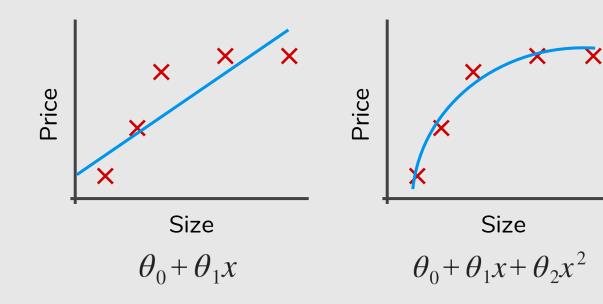
A model's generalization error can be expressed as the sum of **three** very different errors:

- Bias
- Variance
- Irreducible error
  - Due to the noisiness of the data itself.
  - The only way to reduce this part of the error is to clean up the data.

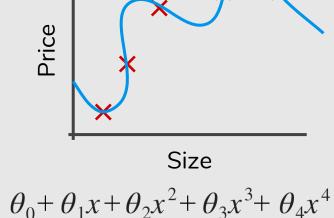
**Increasing a model's complexity** will typically increase its variance and reduce its bias.

Reducing a model's complexity increases its bias and reduces its variance.

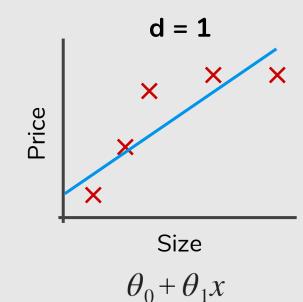
This is why it is called a **tradeoff**.



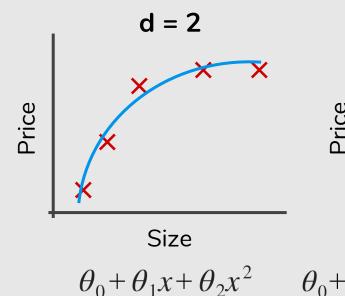
Underfitting High bias

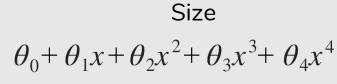


Overfitting High variance



Underfitting High bias



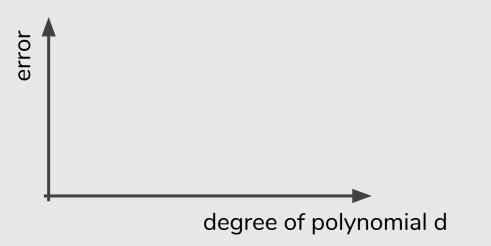


d = 4

Overfitting High variance

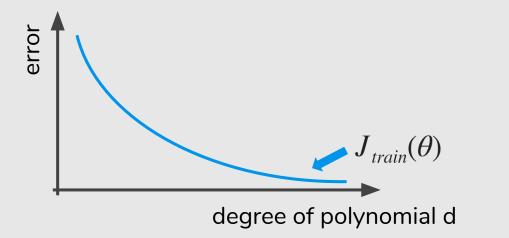
Training error: 
$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^{n} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

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$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$
  
Cross-validation error:  $J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_{\theta}(x^{(i)}_{cv}) - y^{(i)}_{cv})^2$ 



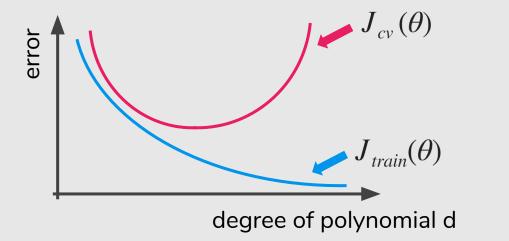
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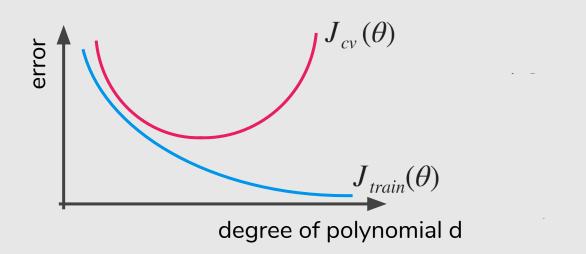


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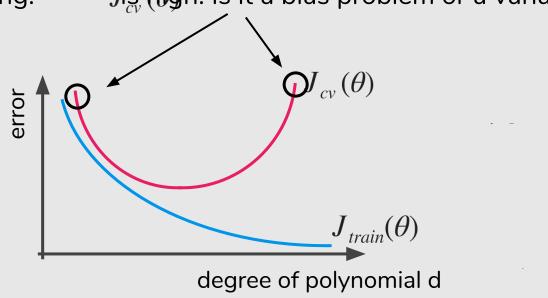
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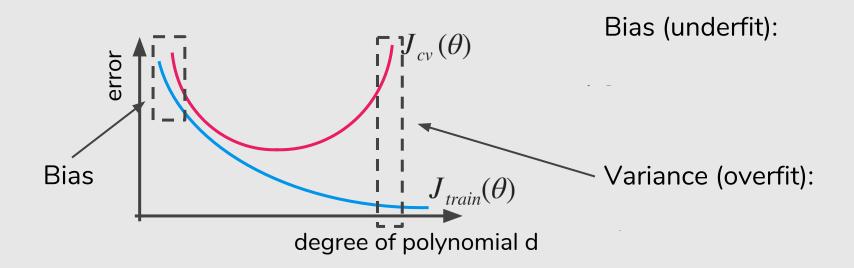
Suppose your learning algorithm is performing less well than you were hoping: Jis high. Is it a bias problem or a variance problem?



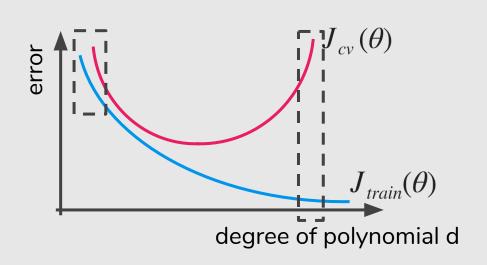
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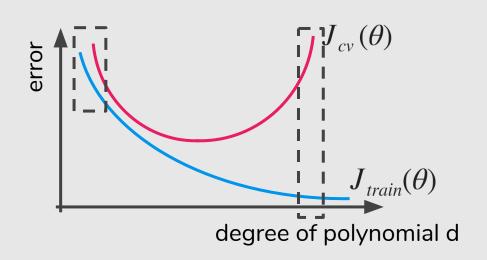
Bias (underfit):

 $J_{\textit{train}}(\theta)$  will be high

$$J_{cv}(\theta) \approx J_{train}(\theta)$$

Variance (overfit):

Suppose your learning algorithm is performing less well than you were hoping: Jis high. Is it a bias problem or a variance problem?



Bias (underfit):

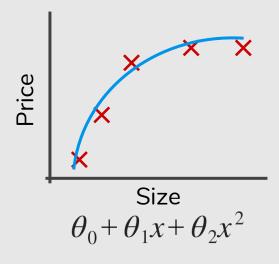
 $J_{\textit{train}}(\theta)$  will be high

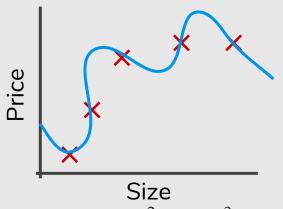
$$J_{cv}(\theta) \approx J_{train}(\theta)$$

Variance (overfit):

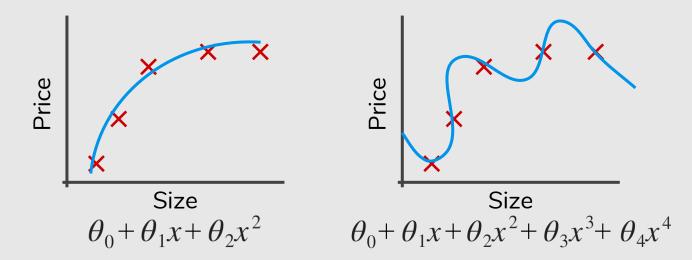
$$egin{aligned} J_{ extit{train}}( heta) & ext{will be low} \ J_{ extit{cv}}( heta) \gg J_{ extit{train}}( heta) \end{aligned}$$

# **Cost Function**



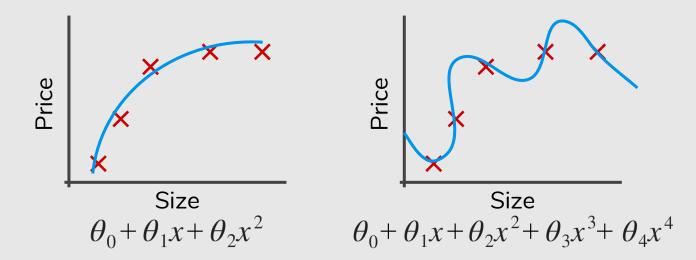


Size 
$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$



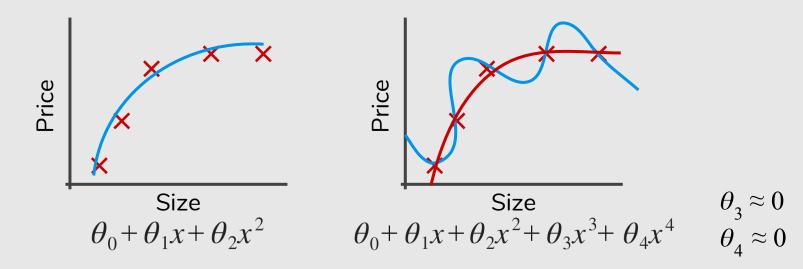
Suppose we penalize and make  $\theta_{\rm 3},\,\theta_{\rm 4}$  really small.

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



Suppose we penalize and make  $\theta_3$ ,  $\theta_4$  really small.

$$\min_{\theta} \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^{2} + 1000 \theta_{3}^{2} + 1000 \theta_{4}^{2}$$



Suppose we penalize and make  $\theta_3$ ,  $\theta_4$  really small.

$$\min_{\theta} \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^{2} + 1000 \theta_{3}^{2} + 1000 \theta_{4}^{2}$$

Small values for parameters  $\theta_0, \theta_1, ..., \theta_n$ 

- "Simpler" hypothesis
- Less prone to overfitting

Small values for parameters  $\theta_0, \theta_1, ..., \theta_n$ 

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- Less prone to overfitting

#### Housing

- Features:  $x_0, x_1, ..., x_{100}$
- Parameters:  $\theta_0, \theta_1, \theta_2, ..., \theta_{100}$

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

Small values for parameters  $\theta_0, \theta_1, ..., \theta_n$ 

- "Simpler" hypothesis
- Less prone to overfitting

#### Housing

- Features:  $x_0, x_1, ..., x_{100}$
- Parameters:  $\theta_0, \theta_1, \theta_2, ..., \theta_{100}$

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

 $J(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^{2} + \lambda \sum_{j=1}^{n} \theta_{j}^{2} \right]$ to fit the training to keep the data well parameters small

Regularization parameter

In regularized linear regression, we choose  $\theta$  to minimize

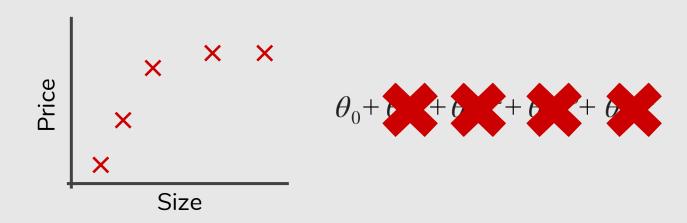
$$J(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{i=1}^{n} \theta_i^2 \right]$$

What if  $\lambda$  is set to an extremely large value (perhaps for too large for our problem, say  $\lambda = 10^{10}$ )?

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

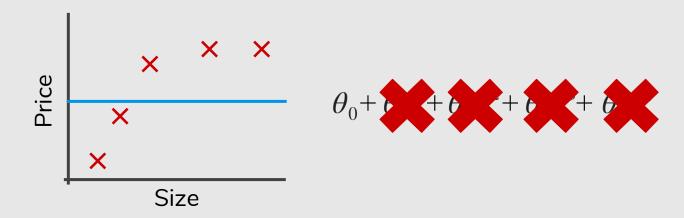
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$$J(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{i=1}^{n} \theta_i^2 \right]$$

What if  $\lambda$  is set to an extremely large value (perhaps for too large for our problem, say  $\lambda = 10^{10}$ )?



# Regularized Linear Function

#### **Gradient Descent**

```
repeat { \theta_j := \ \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} (simultaneously update \theta_j for j=0,\ 1,\ ...,\ n) }
```

#### **Gradient Descent**

repeat {  $\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)}$   $\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}$  { (simultaneously update  $\theta_i$  for j = 2 1, ..., n)

repeat {  $\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$   $\theta_j := \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$  (simultaneously update  $\theta_i$  for j = 1, ..., n)

repeat {  $\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)}$   $\theta_j := \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$ 

(simultaneously update  $\theta_j$  for j = 1, ..., n)

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

repeat {

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

$$\theta_{j} := \theta_{j} - \alpha \left[ \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) x_{j}^{(i)} + \frac{\lambda}{m} \theta_{j} \right]$$

} (simultaneously update  $\theta_j$  for j = 1, ..., n)

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

### **Normal Equation**

# **Normal Equation**

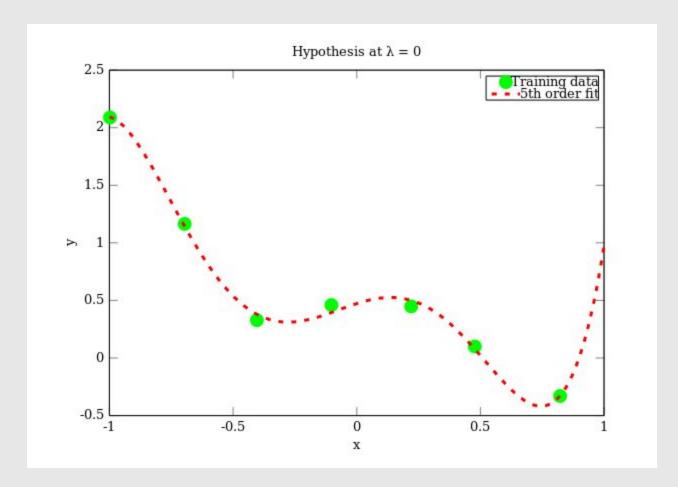
$$X = \begin{bmatrix} ---(x^{(1)})^{\mathrm{T}} - --- \\ ---(x^{(2)})^{\mathrm{T}} - --- \\ ---- \vdots ---- \\ ----(x^{(m)})^{\mathrm{T}} - --- \end{bmatrix} \quad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad \theta = (X^{T}X)^{-1}X^{T}y$$

$$\theta = \left( X^T X \right)^{-1} X^T y$$

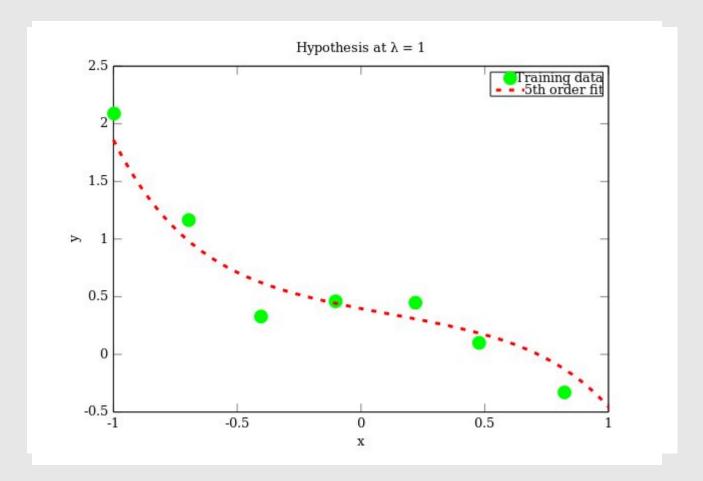
## **Normal Equation**

$$X = \begin{bmatrix} ---(x^{(1)})^{\mathrm{T}} - --- \\ ---(x^{(2)})^{\mathrm{T}} - --- \\ ---- \vdots ---- \\ ----(x^{(m)})^{\mathrm{T}} - --- \end{bmatrix} \quad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad \theta = (X^T X)^{-1} X^T y$$

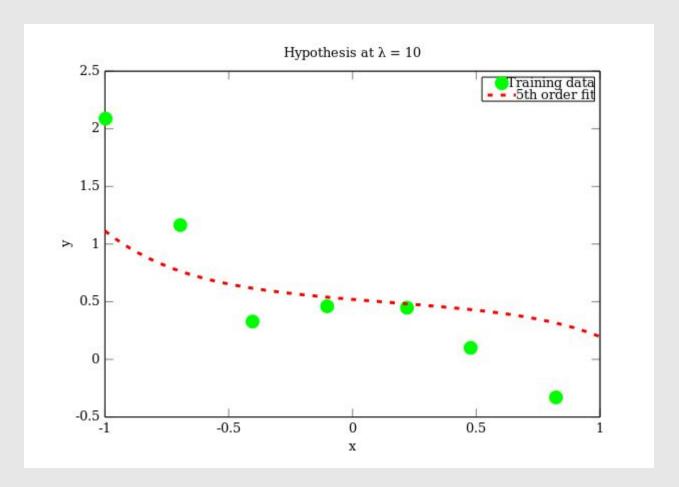
$$\theta = \left[ X^T X + \lambda \begin{bmatrix} 0 & & & \\ & 1 & & \\ & & 1 & \\ & & \ddots & \\ & & & 1 \end{bmatrix} \right]^{-1} X^T y$$



http://melvincabatuan.github.io/Machine-Learning-Activity-4/



http://melvincabatuan.github.io/Machine-Learning-Activity-4/



http://melvincabatuan.github.io/Machine-Learning-Activity-4/

# Regularized Logistic Function

repeat {  $\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)}$   $\theta_j := \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$ 

(simultaneously update  $\theta_j$  for j = 1, ..., n)

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

$$h_{\theta}(x) = \theta^T x \implies h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$

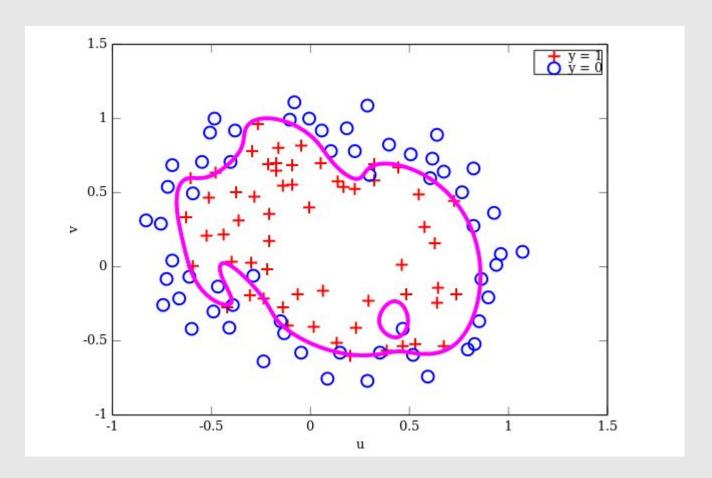
repeat {

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

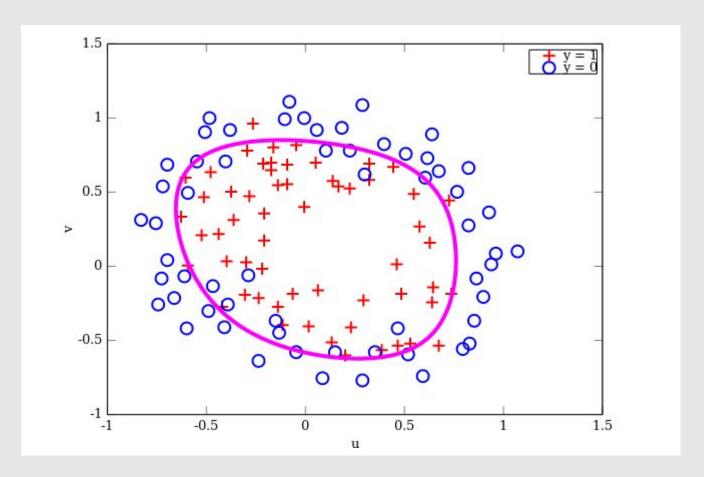
$$\theta_j := \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} + \frac{\lambda}{m} \theta_j \right]$$

} (simultaneously update  $\theta_j$  for j = 1, ..., n)

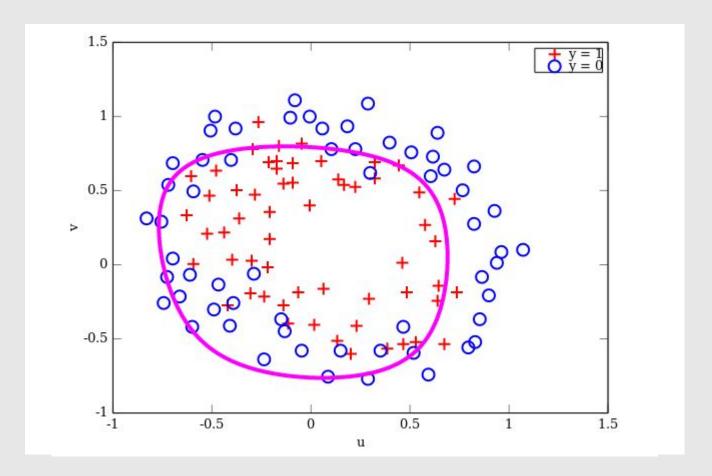
$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}$$



http://melvincabatuan.github.io/Machine-Learning-Activity-4/



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http://melvincabatuan.github.io/Machine-Learning-Activity-4/

# References

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### **Machine Learning Books**

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 4
- Pattern Recognition and Machine Learning, Chap. 3

#### **Machine Learning Courses**

https://www.coursera.org/learn/machine-learning, Week 3 & 6