

# Machine Learning with Python

### Multivariate Linear Models For Regression And Classification

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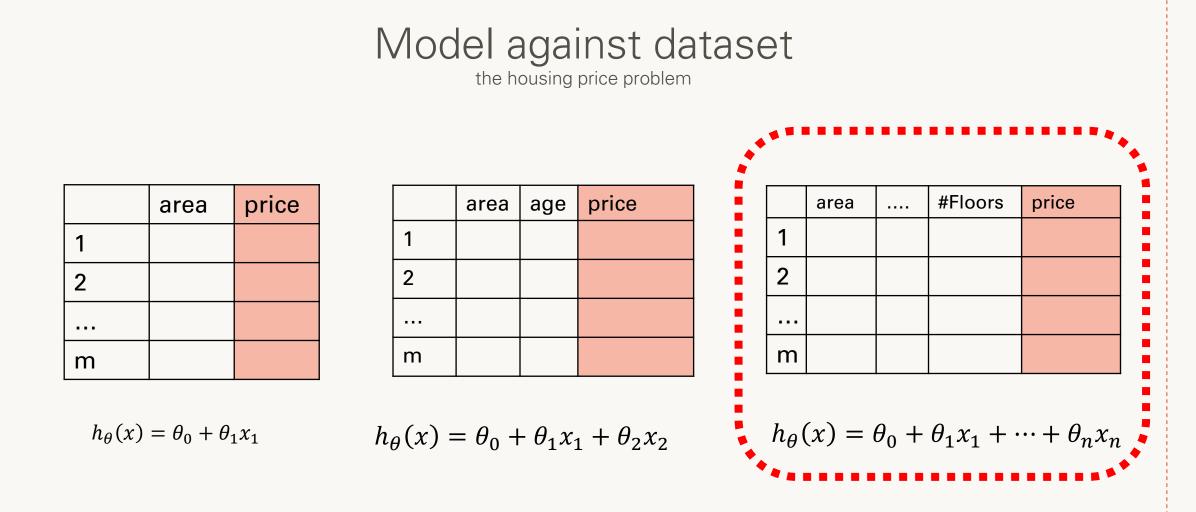
Taibah University

2021-2022

# Agenda

- Multivariant linear regression
  - Feature scaling
  - Polynomial Regression
- Logistic Regression: Binary-class classification
  - Sigmoid function
  - Decision boundary
  - Cost function
- Logistic Regression: Multi-class classification
  - SoftMax function

### Motivation



### Predict the house's price using many features

- In original version we had
  - X = house size, use this to predict
  - $\circ$  y = house price

If in a new scheme we have more variables (such as number of bedrooms, number floors, age of the home)
 x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub> are the four features

- x<sub>1</sub> size (feet squared)
- $x_2$  Number of bedrooms
- x<sub>3</sub> Number of floors
- x<sub>4</sub> Age of home (years)
- y is the output variable (price)



Multi-variante Multi-features Multi-variables

- *Multivariate linear regression* is the generalization of the univariate linear regression (seen earlier).
- As the name suggests, there are more than one independent variables,  $x1, x2, \dots, xn$  and a dependent variable y.

### Notation

- $x_1, x_2 \cdots, x_n$  denote the n features
- y denotes the output variable to be predicted
- n is number of features
- *m* is the number of training examples
- $x^{(i)}$  is the  $i^{th}$  training example
- $x_{j}^{(i)}$  is the  $j^{th}$  feature of the  $i^{th}$  training example

### Multivariate Hypothesis

The hypothesis in case of univariate linear regression was,

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

Extending the above function to multiple features, hypothesis of multivariate linear regression is given by,

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$
  
=  $\theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$ , where  $x_0 = 1$  (1)  
=  $\theta^T x$ , vectorizing above equation

Where,

$$\circ \ heta = egin{bmatrix} heta_0 \ heta_1 \ dots \ heta_n \end{bmatrix} \in \mathbb{R}^{n+1} ext{ and } x = egin{bmatrix} x_0 \ x_1 \ dots \ x_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

### Multivariate Cost Function

• 1

The cost function for univariate linear regression was,

$$J( heta_0, heta_1) = rac{1}{2m}\sum_{i=1}^m \left(h_ heta(x^{(i)}) - y^{(i)}
ight)^2$$

Extending the above function to multiple features, the cost function for multiple features is given by,

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

$$= \frac{1}{2m} \sum_{i=1}^{m} \left( \theta^{T} x^{(i)} - y^{(i)} \right)^{2}$$

$$= \frac{1}{2m} \sum_{i=1}^{m} \left( \left( \sum_{j=0}^{n} \theta_{j} x_{j}^{(i)} \right) - y^{(i)} \right)^{2}$$
Where  $\theta$  is a vector give by  $\theta = \begin{bmatrix} \theta_{0} \\ \theta_{1} \\ \vdots \\ \theta_{n} \end{bmatrix}$ 

$$(2)$$

### Multivariate Gradient Descent

Hypothesis:  $h_{\theta}(x) = \theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$ Parameters:  $\theta_0, \theta_1, \dots, \theta_n$ Cost function:  $J(\theta_0, \theta_1, \dots, \theta_n) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$ 

 $\begin{array}{l} \text{Gradient descent:} \\ \text{Repeat } \{ \\ \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \dots, \theta_n) \\ \} \\ \begin{array}{l} \text{(simultaneously update for every } j = 0, \dots, n) \end{array} \end{array}$ 

### Multivariate Gradient descent

$$h_{\theta}(x) = \theta_{0}x_{0} + \theta_{1}x_{1} + \theta_{2}x_{2} + \dots + \theta_{n}x_{n}, \quad x_{0} =$$

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

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} ((\theta_{0}x_{0} + \theta_{1}x_{1} + \theta_{2}x_{2} + \dots + \theta_{n}x_{n}) - y^{(i)})^{2}$$

 $ext{repeat until convergence} \left\{ heta_j := heta_j - lpha rac{\partial}{\partial heta_j} J( heta) 
ight.$ 

(3)

1

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

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

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

Evaluating the partial derivative  $\frac{\partial}{\partial \theta_i} J(\theta)$  gives,

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m \left( h_\theta(x^{(i)}) - y^{(i)} \right) x_j^{(i)} \tag{4}$$

Multivariate Gradient descent

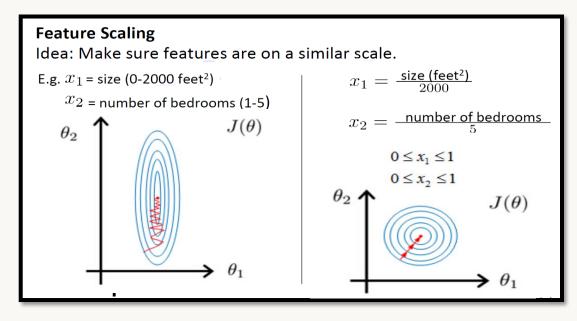
Univariate Gradient decent **Gradient Descent** Previously (n=1): Repeat {  $\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})$  $\frac{\partial}{\partial \theta_0} J(\theta)$  $heta_1 := heta_1 - lpha rac{1}{m} \sum_{i=1}^m (h_ heta(x^{(i)}) - y^{(i)}) x^{(i)}$ (simultaneously update  $heta_0, heta_1$ )

# $$\label{eq:main_state_state} \begin{split} & \text{New algorithm } (n \geq 1); \\ & \text{Repeat } \Big\{ \\ & \theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} \\ & \quad (\text{simultaneously update } \theta_j \text{ for } \\ & \quad j = 0, \dots, n) \Big\} \end{split}$$

# **Feature Scaling**

### Feature Scaling (Normalization)

• *Normalization* refers to normalizing the data dimensions so that they are of approximately the same scale.



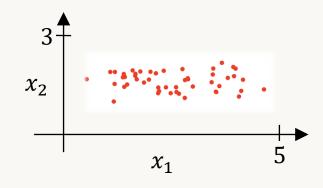
 $h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$ 

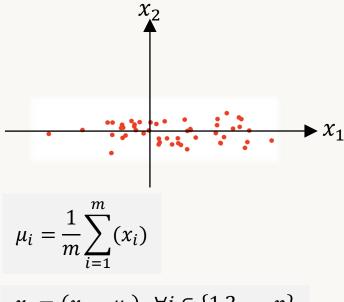
After **normalization** Contours become more like circles (as scaled between 0 and 1)

- As seen above, if the contours are *skewed* then learning steps would take longer to converge as the steps would be more prone to *oscillatory behavior* as shown in <u>the left plot</u>.
- Whereas <u>if the features are properly scaled</u>, then the plot is *evenly distributed*, and the steps of gradient descent have better profile of convergence.

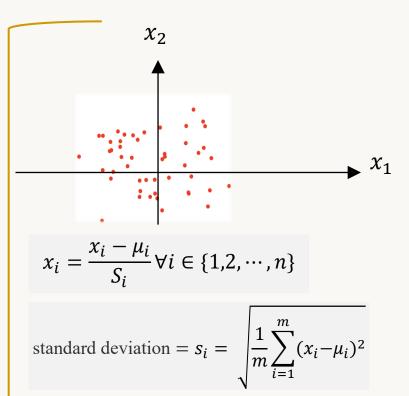
### Feature Scaling (Normalization)

• Normalizing training sets



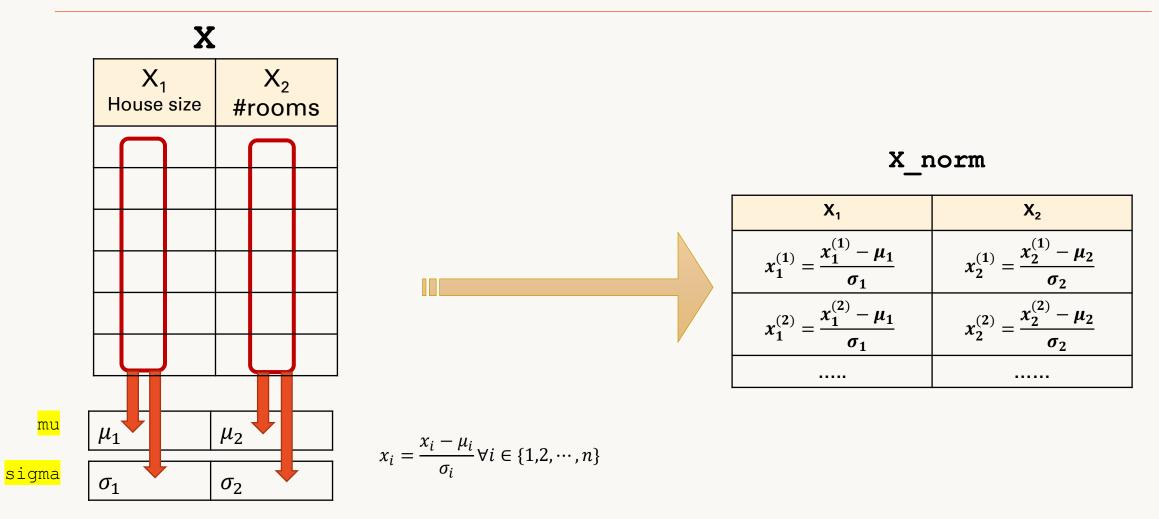


- $x_i = (x_i \mu_i) \quad \forall i \in \{1, 2, \cdots, n\}$
- Mean Normalization is the most common form of preprocessing. It involves subtracting the mean across every individual *feature* in the data and has the geometric interpretation of *centering the cloud of data around the origin* along every dimension.
  - Not applied to the feature  $X_0$  as it always =1



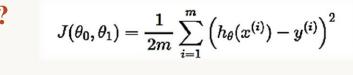
- $x_i$  is the feature value
- $\mu_i$  is the mean
- *S<sub>i</sub>* is the standard deviation or the range i.e., max-min

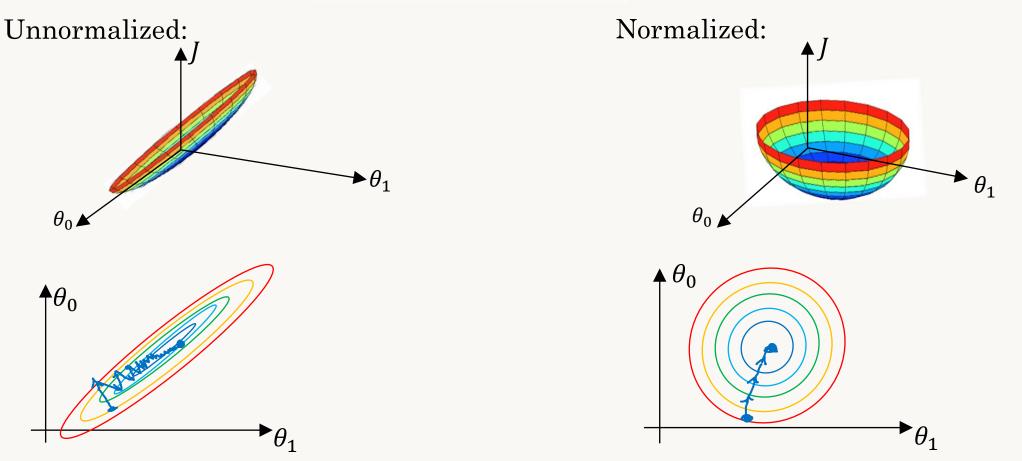
### Feature Normalization



### Feature Normalization

• Why normalize inputs?

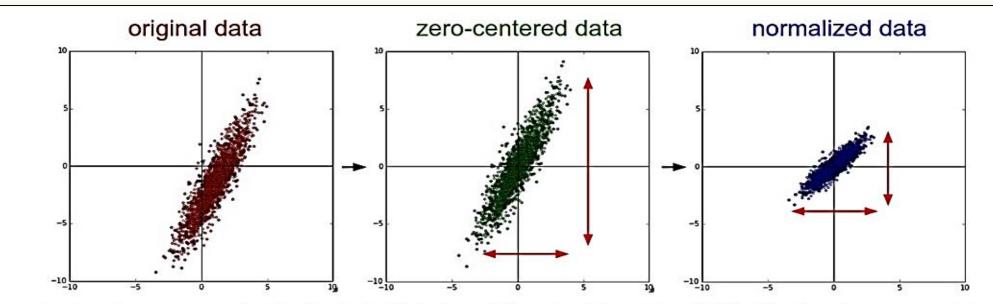




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## Feature Normalization

• More illustrations



Common data preprocessing pipeline. Left: Original toy, 2-dimensional input data. Middle: The data is zero-centered by subtracting the mean in each dimension. The data cloud is now centered around the origin. Right: Each dimension is additionally scaled by its standard deviation. The red lines indicate the extent of the data - they are of unequal length in the middle, but of equal length on the right.

Note: The *feature normalization* must be applied to both instances from the **training** and **testing** sets



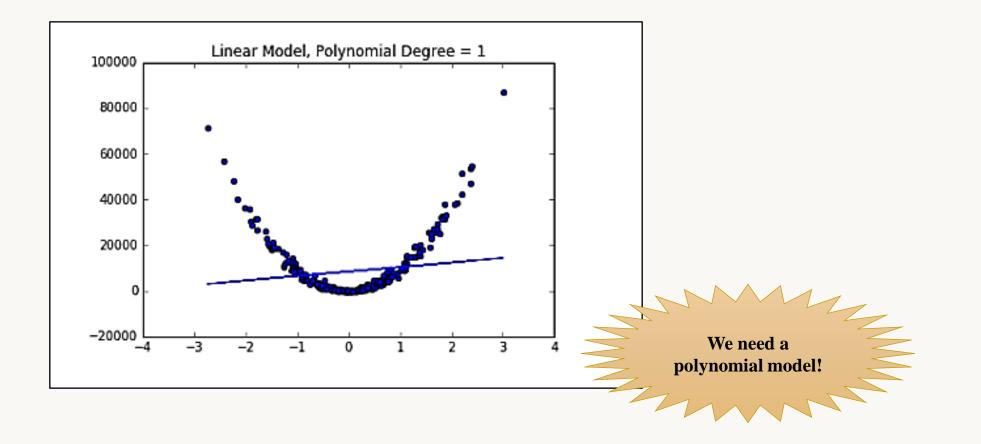


### • In Feature Engineering

- ✓ Sometimes it might be fruitful to *generate new features* by combining the existing ones.
  - For example, given *width* and *length* of a property to predict *price*
- ✓ It might be helpful to use *area* of the property, i.e., *width* \* *length* as an additional feature.



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*Polynomial regression* is useful as it allows us to fit a model to nonlinear data.

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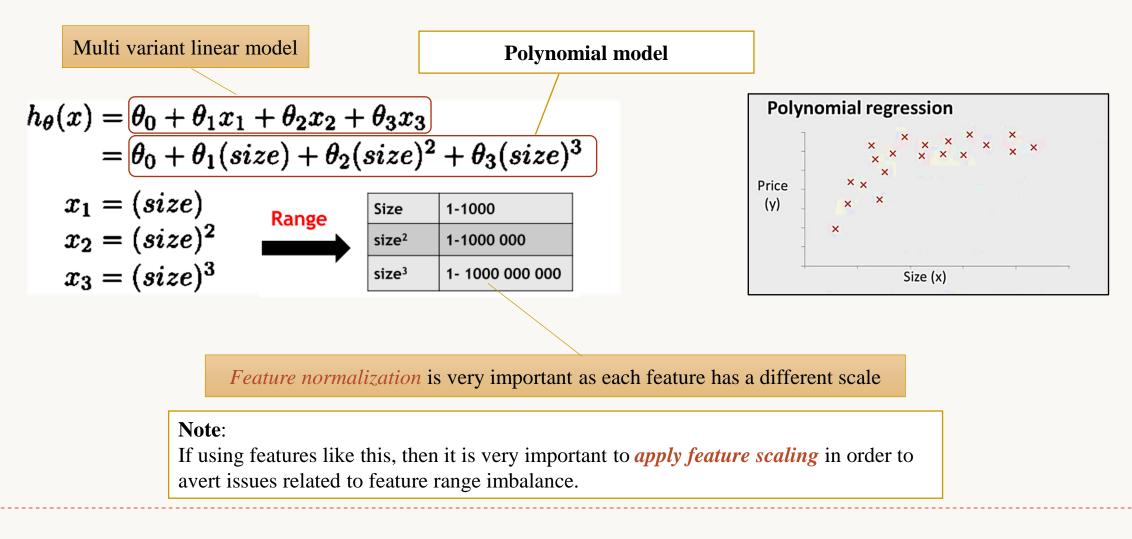
The concept of feature engineering can be used to achieve **polynomial regression**. Say the polynomial hypothesis chosen is,

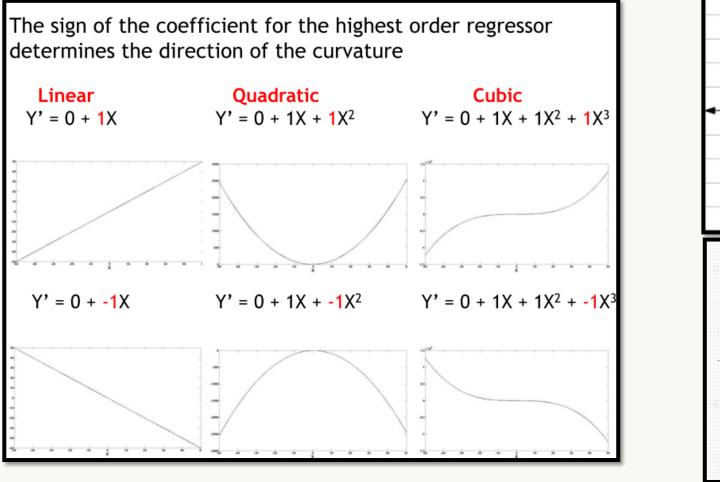
 $h_ heta(x) = heta_0 + heta_1 \, x + heta_2 \, x^2 + \dots + heta^n \, x^n$ 

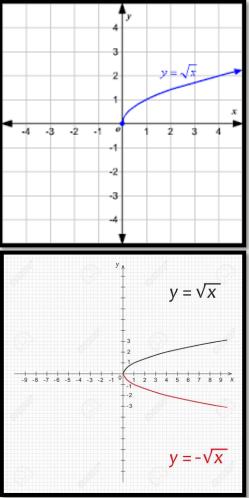
This function can be addressed as multivariate linear regression by substitution and is given by,

$$h_ heta(x) = heta_0 + heta_1 \, x_1 + heta_2 \, x_2 + \dots + heta_n \, x_n$$

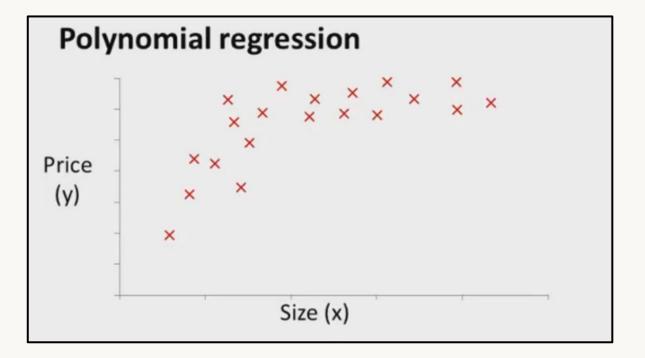
• Where  $x_n = x^n$ 



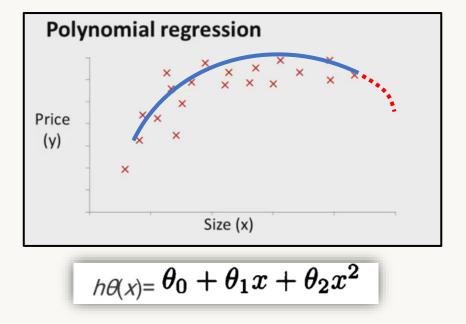




• Which model is the best ?



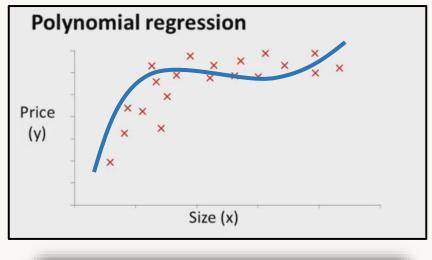
• Which model is the best ?



Not accurate: the price should be increased when size increases

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• Which model is the best ?

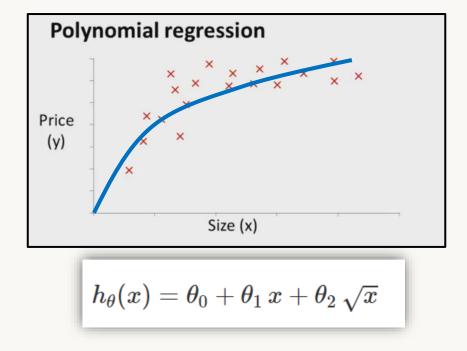


$$h\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$

**Overfitting**: lack of generalization

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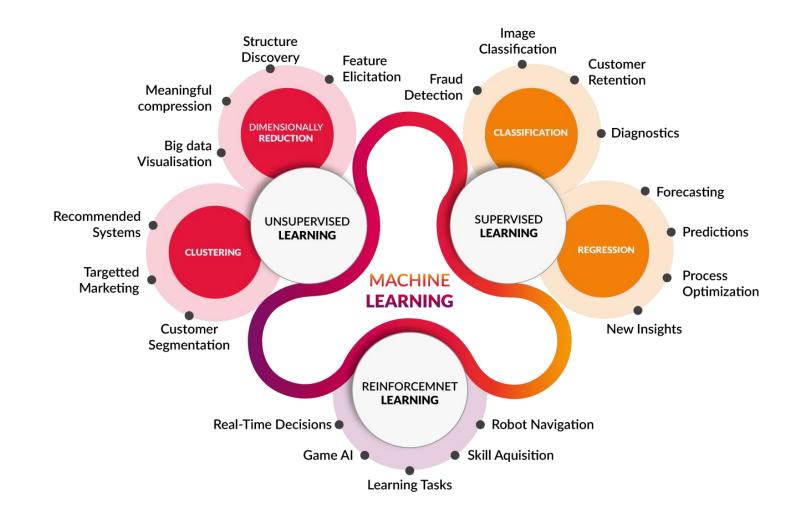
• Which model is the best ?



### Seems to be good:

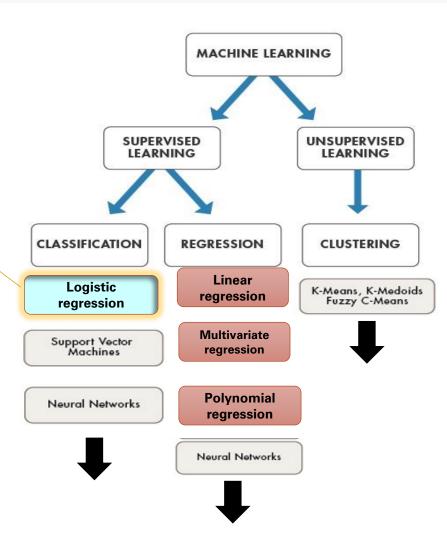
a non-decreasing function as opposed to quadratic function which comes back down

# **Logistic Regression Model**

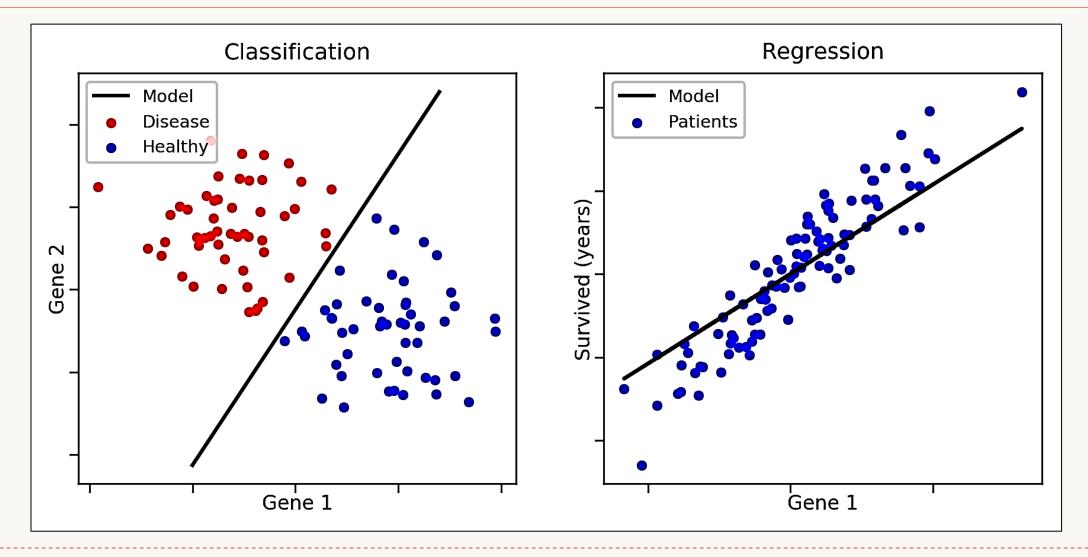


### Note:

*Logistic regression* is used for classification not for regression (prediction) like linear/polynomial regression.



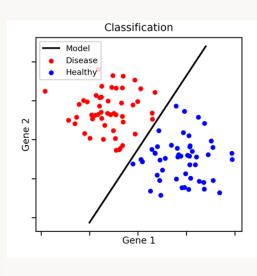
### Classification vs. Prediction (regression)

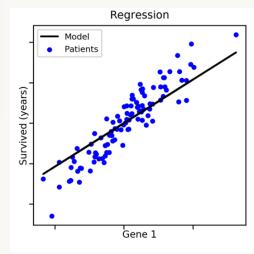


# Classification vs. Prediction (regression)

### Classification:

- predicts categorical class labels
- classifies data (constructs a model) based on the training set and the values (class labels) in a classifying attribute and uses it in classifying new data
- Prediction:
  - models <u>continuous-valued functions</u>, i.e., predicts unknown or missing values





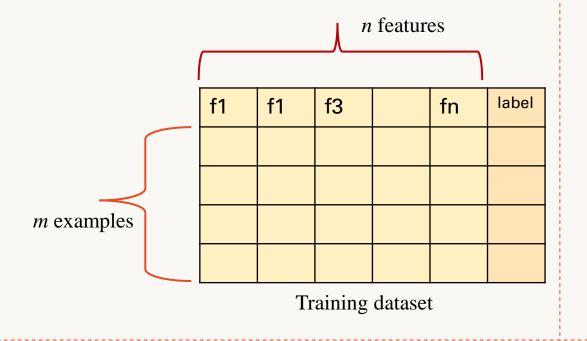
# Classification applications

- Typical Applications of Classification
  - credit approval
  - target marketing
  - medical diagnosis
  - treatment effectiveness analysis

- **Email**: Spam / Not Spam?
- **Online Transactions**: Fraudulent (Yes / No)?
- **Tumor**: Malignant / Benign ?

 $label \in \{0,1\}$ 

0: "Negative Class" (e.g., benign tumor) 1: "Positive Class" (e.g., malignant tumor)

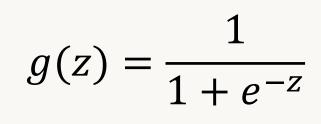


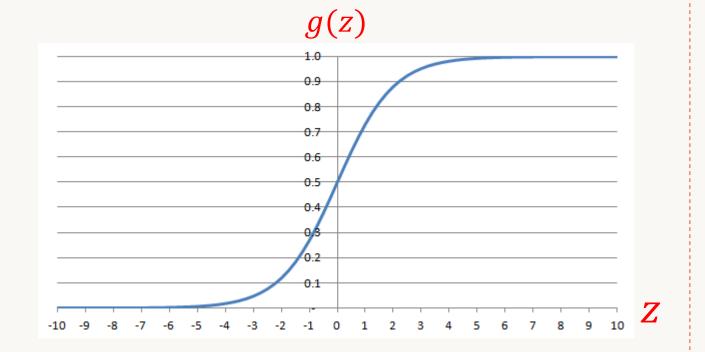
- The output is the class label  $\rightarrow 0$  or 1
- Our hypothesis should produce zero or one
- ML job is to find the weights for the features for a function where its output is zero or one
- And we need a model where:  $0 \le h_{\theta}(x) \le 1$

## Suggestion is to use the sigmoid function

### Sigmoid Function or Logistic Function.

• *Plot of the sigmoid function* is given below which shows no matter what the value of *z*, the function returns a value between 0 and 1





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#### Logistic Regression

- for 0 ≤ h<sub>θ</sub>(x) ≤ 1 is to be true, there is a need of squashing function, i.e., a function which limits the output of hypothesis between given range.
- For logistic regression sigmoid function is used as the squashing function.
- The hypothesis for logistic regression is give by:  $h_{\theta}(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$

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

## Logistic Regression (Cont.)

• The value of hypothesis  $h_{\theta}(x)$  is interpreted as the probability that the input x belongs to class y=1, i.e., probability that y=1, given x, parametrized by  $\theta$ .

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

It can be mathematically represented as,

$$h_{ heta}(x) = P(y = 1 | x; heta)$$

The fundamental properties of probability holds here, i.e.,

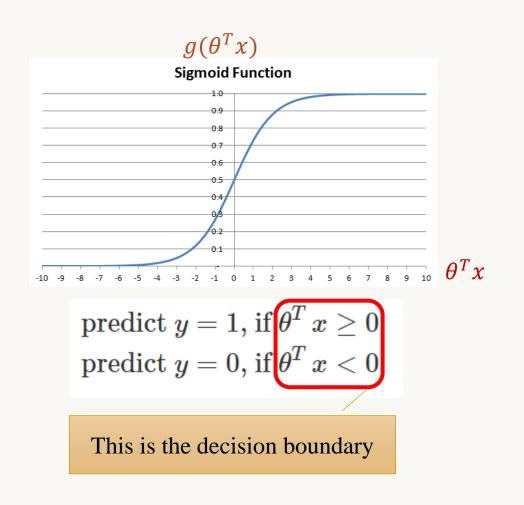
$$P(y=0|x; heta)+P(y=1|x; heta)=1$$

# **Decision Boundary**

#### **Decision Boundary**

• For the given hypothesis of logistic regression, say  $\delta = 0.5$  is chosen as the **threshold for the binary classification.** 

$$label \in \{0,1\} \quad \stackrel{\text{O: "Negative Class"}}{_{1: \text{"Positive Class"}}}$$
$$h_{\theta}(x) = g(\theta^{T}x) = \frac{1}{1 + e^{-\theta^{T}x}}$$



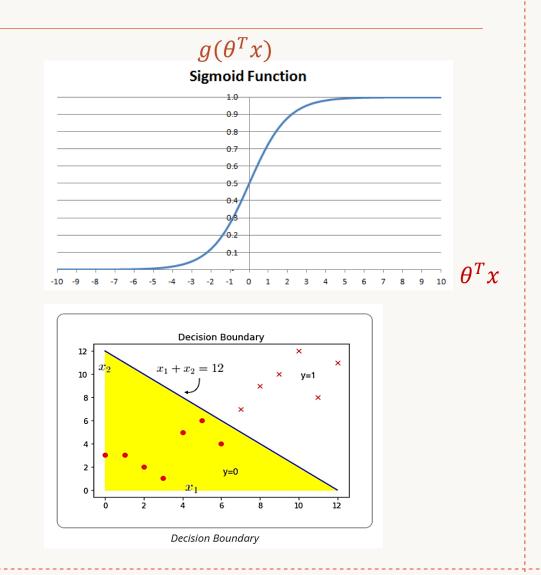
#### Linear Decision Boundary

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

In this example  $\theta^T x = -12 + x_1 + x_2$ 

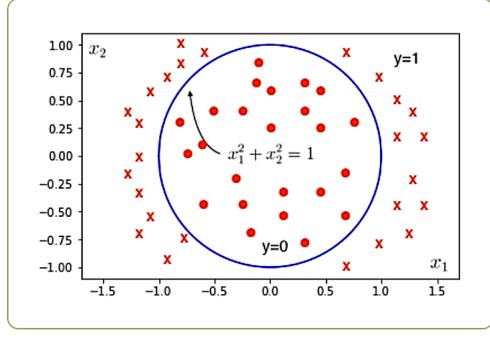
$$ext{predict } y = 1, ext{if} heta^T x \geq 0 \ ext{predict } y = 0, ext{if} heta^T x < 0 \ ext{}$$

$$ext{predict } y = 1, ext{if } -12 + x_1 + x_2 \geq 0 ext{ or } x_1 + x_2 \geq 12 ext{predict } y = 0, ext{if } -12 + x_1 + x_2 < 0 ext{ or } x_1 + x_2 < 12 ext{}$$

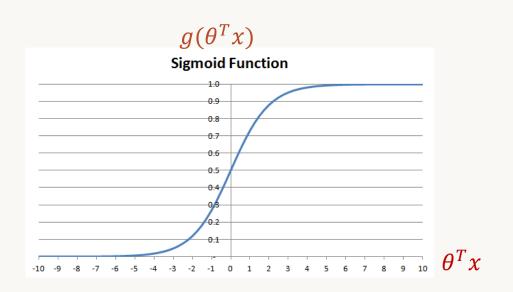


### Nonlinear Decision Boundary

• It is possible to achieve *non-linear decision boundaries* by using the higher order polynomial terms and can be incorporated in a way similar to how multivariate linear regression handles polynomial regression.



Non-Linear Decision Boundary



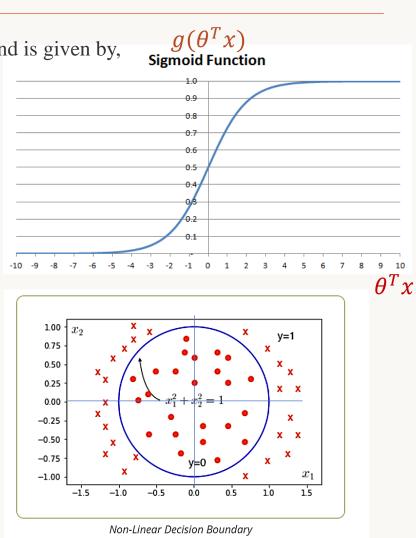
## Nonlinear Decision Boundary (Cont.)

Say, the hypothesis of the logistic regression has higher order polynomial terms, and is given by,  $\theta^T x = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2$ 

$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

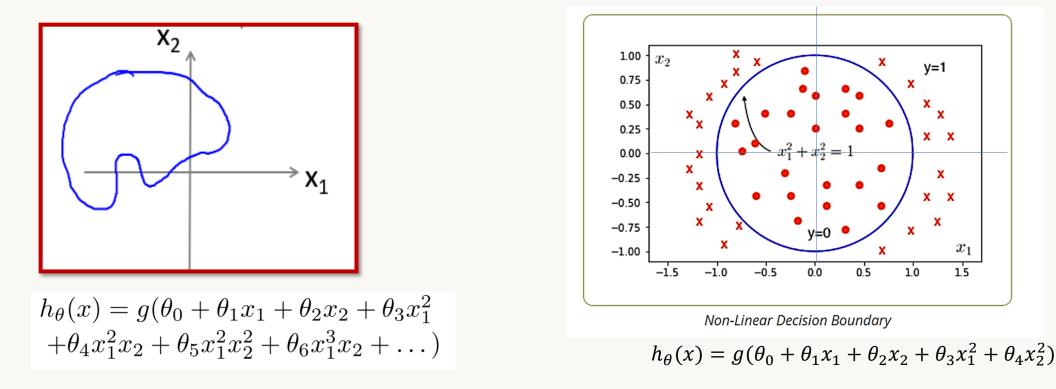
let optimal  $\theta$  given below would form an optimal decision boundary  $\theta^T = [-1 \ 0 \ 0 \ 1 \ 1]$ 

Substituting 
$$\theta^T x = -1 + x_1^2 + x_2^2$$
  
Decision boundary is  $x_1^2 + x_2^2 = 1$   
predict  $y = 1$ , if  $-1 + x_1^2 + x_2^2 \ge 0$  or  $x_1^2 + x_2^2 \ge 1$   
predict  $y = 0$ , if  $-1 + x_1^2 + x_2^2 < 0$  or  $x_1^2 + x_2^2 < 1$ 



## Nonlinear Decision Boundary (Cont.)

• As the order of features is increased more and more **complex decision** boundaries can be achieved by logistic regression. *Be aware of overfitting !!* 



Gradient Descent is used to search for the best parameter values of  $\theta$  that make the decision boundary

## **Logistic Regression Cost Function**

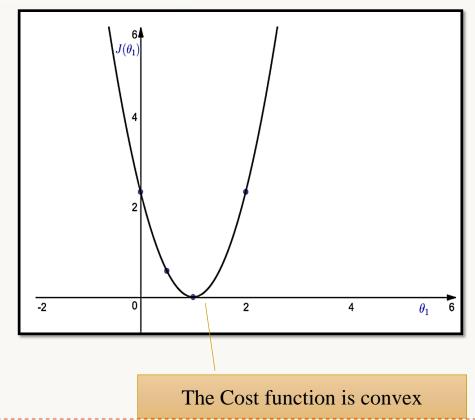
#### Logistic Regression (Cost Function)

#### **Recall that previously in linear regression:**

It can be seen in <u>Mulivariate Linear Regression</u> that the cost function for the linear regression is given by,

$$egin{split} J( heta) &= rac{1}{m} \sum_{i=1}^m rac{1}{2} \Big( h_ heta(x^{(i)}) - y^{(i)} \Big)^2 \ &= rac{1}{m} \sum_{i=1}^m Cost(h_ heta(x^{(i)}), y^{(i)}) \end{split}$$

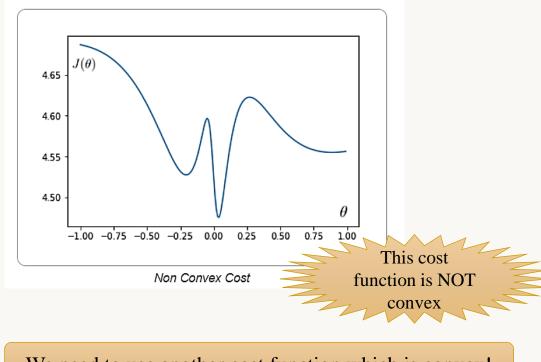
 $h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$ 



- The same cost function of multivariate regression would not work well for the logistic regression because the hypothesis for logistic regression is the complex sigmoid function
- Below, gives **non-convex** curve with many **local minima** as shown in the plot below.
- So, gradient descent will not work properly for such a case and therefore it would be very difficult to minimize this function.

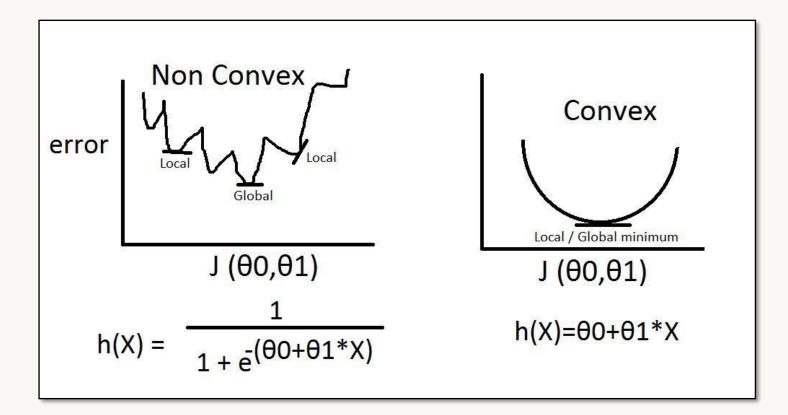
$$egin{aligned} h_{ heta}(x) &= g( heta^T x) = rac{1}{1+e^{- heta^T x}} \ J( heta) &= rac{1}{m} \sum_{i=1}^m rac{1}{2} \Big(h_{ heta}(x^{(i)}) - y^{(i)}\Big)^2 \end{aligned}$$

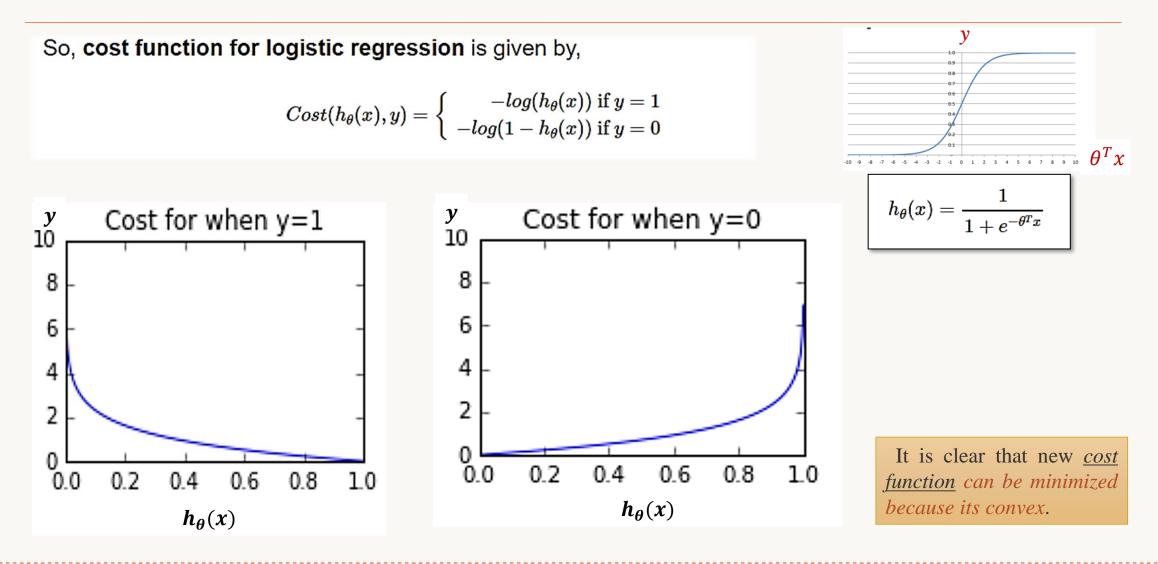
$$=rac{1}{m}\sum_{i=1}^{m}Cost(h_{ heta}(x^{(i)}),y^{(i)})$$

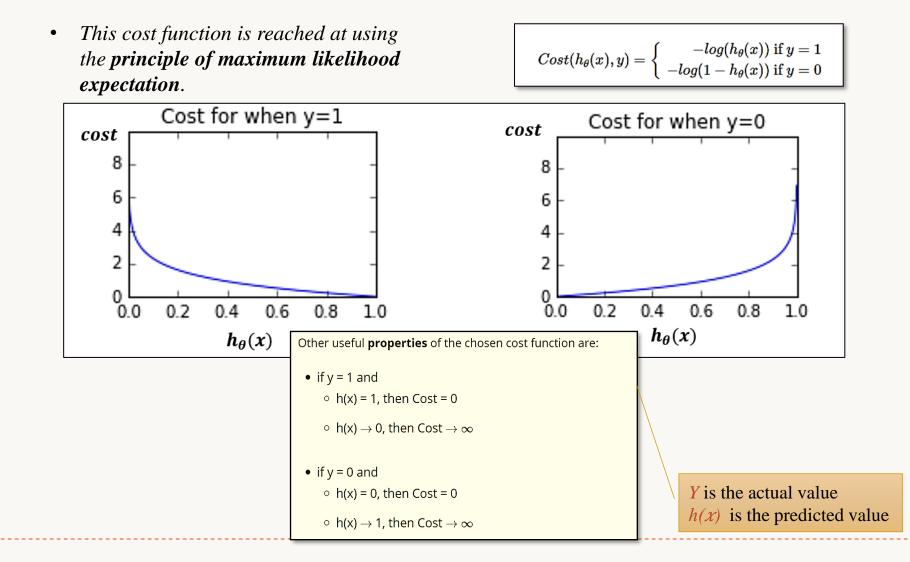


We need to use another cost function which is convex!

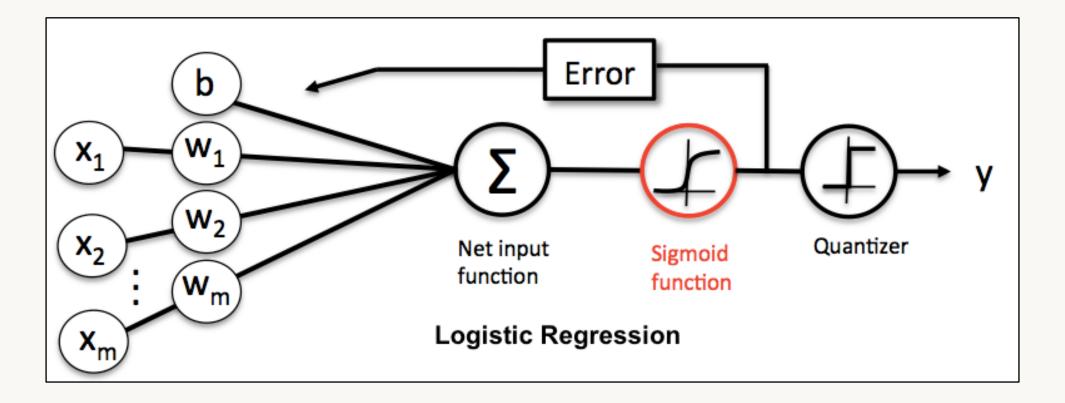
• More illustration:







#### **Summary:**



#### **Gradient Descent for Logistic Regression**

## Gradient Descent for Logistic Regression

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

$$Cost(h_{\theta}(x, y) = \left\{ -\frac{1}{\log(1 - h_{\theta}(x))} \text{ if } y = 0 \right\}$$
Want  $\min_{\theta} J(\theta)$ :
Repeat  $\left\{ \theta_{j} := \theta_{j} - \alpha \frac{\partial}{\partial \theta_{j}} J(\theta) \right\}$  (simultaneously update all  $\theta_{j}$ )
Repeat  $\left\{ \theta_{j} := \theta_{j} - \alpha \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) x_{j}^{(i)} \right\}$  (simultaneously update all  $\theta_{j}$ )
$$\theta = \begin{bmatrix} \theta_{0} \\ \theta_{1} \\ \vdots \\ \theta_{n} \end{bmatrix} \in \mathbb{R}^{n+1} \text{ and } x = \begin{bmatrix} x_{0} \\ x_{1} \\ \vdots \\ x_{n} \end{bmatrix} \in \mathbb{R}^{n+1}$$

Note: Feature Scaling is as important for logistic regression as it is for linear regression as it helps the process of gradient descent.

# Gradient Descent for Logistic Regression (Cont.)

#### **Advanced Optimization**

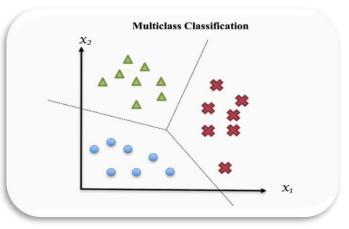
Given the functions for calculation of  $J(\theta)$  and  $\frac{\partial}{\partial \theta}J(\theta)$  one can apply one of the many **optimization techniques other than gradient descent**:

- Conjugate Descent
- BFGS
- L-BFGS

Advantage	Disadvantages
No need to manually pick $lpha$	More complex
Often faster than gradient descent	Harder to debug

*These algorithms automatically find out the best* α *value.* 

# **Multiclass Logistic Regression**



### Multiclass Logistic Regression

• Multiclass logistic regression is an extension of the binary classification making use of the **one-vs-all** or **one-vs-rest** classification strategy.

#### Intuition

Given a classification problem with n distinct classes, train n classifiers, where each classifier draws a decision boundary for one class vs all the other classes. Mathematically,

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

For Example:

• Email foddering/tagging:

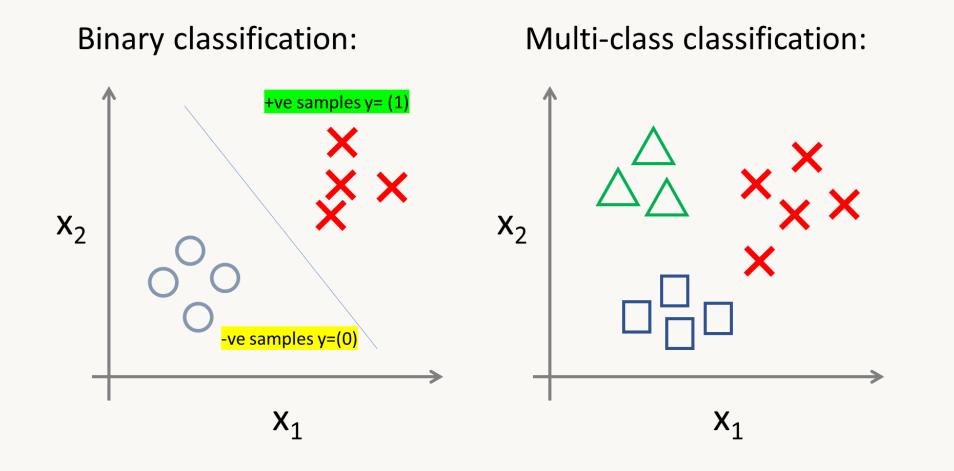
Work, Friends, Family, Hobby y=1 y=2 y=3 y=4

• Medical diagrams:

Not ill, Cold, Flu y=1 y=2 y=3

• Weather:

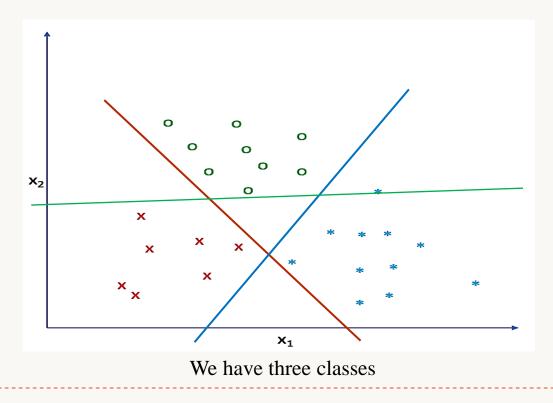
Sunny, Cloudy, Rain, Snow y=1 y=2 y=3 y=4



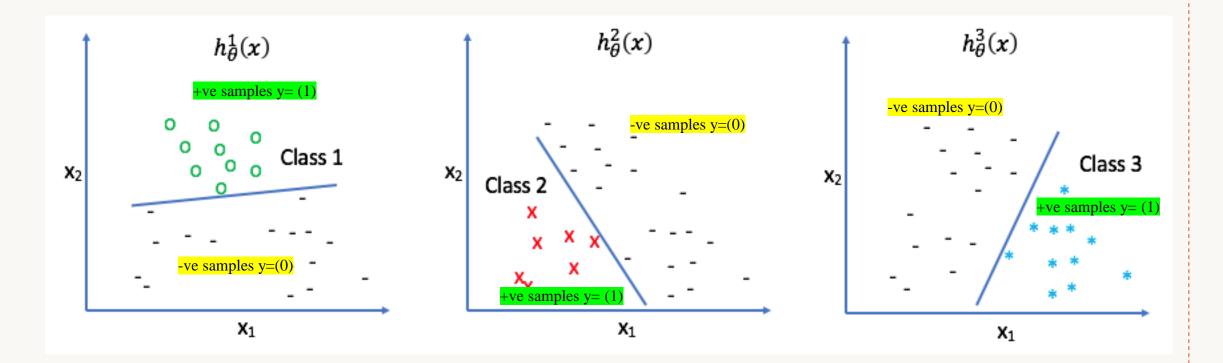
$$x \in egin{bmatrix} 1 \ x_1 \ dots \ x_n \end{bmatrix}, \hspace{0.1cm} y \in \{1,2,\ldots,k\}$$

For a dataset with k classes, you'd train a collection of k classifiers.

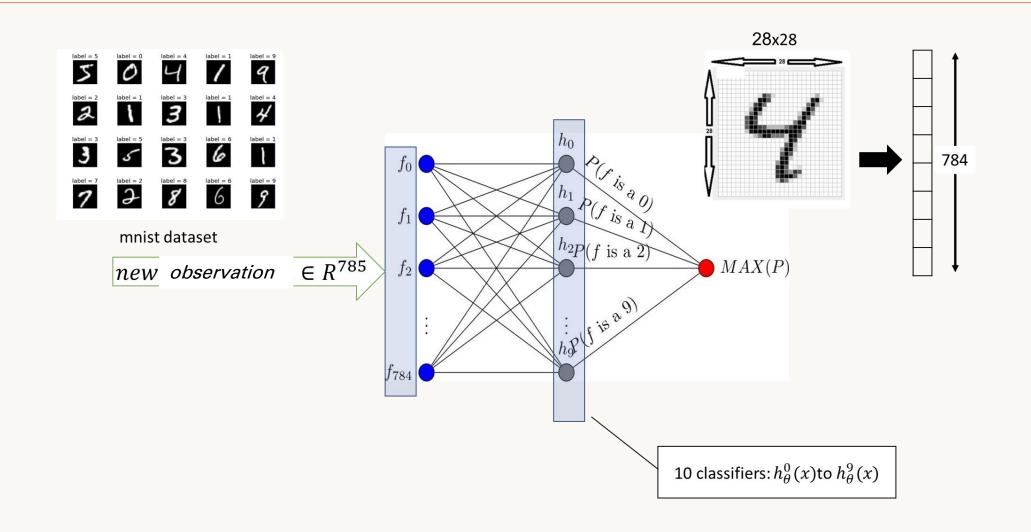
 $h_{ heta}^{1}\left(x
ight),h_{ heta}^{2}\left(x
ight),\ldots h_{ heta}^{k}\left(x
ight)$ 



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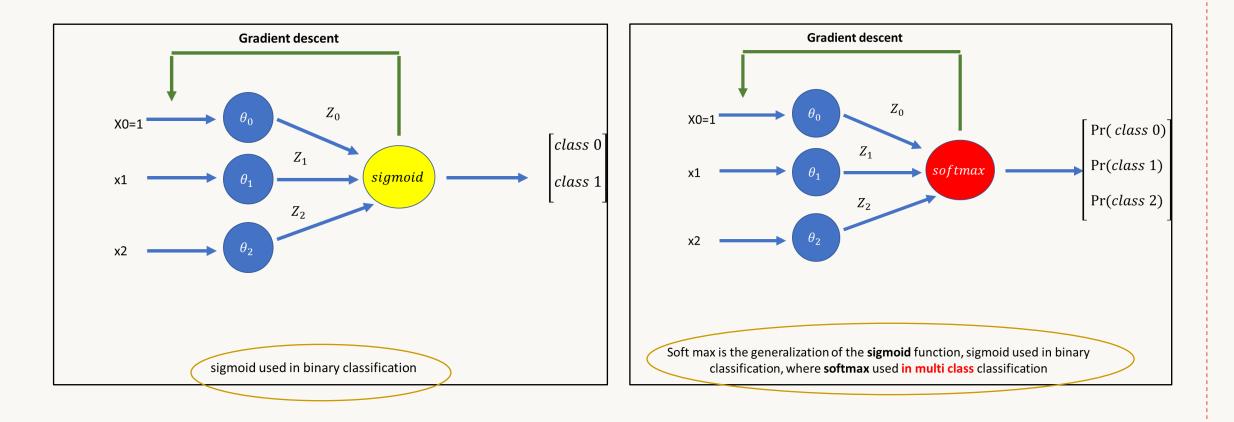


- Each classifier  $h_{\theta}^{i}(x)$  returns the probability that an observation belongs to **class i.**
- All we have to do in order to predict the class of an *observation* is to select the class of whichever classifier returns the **highest probability**.

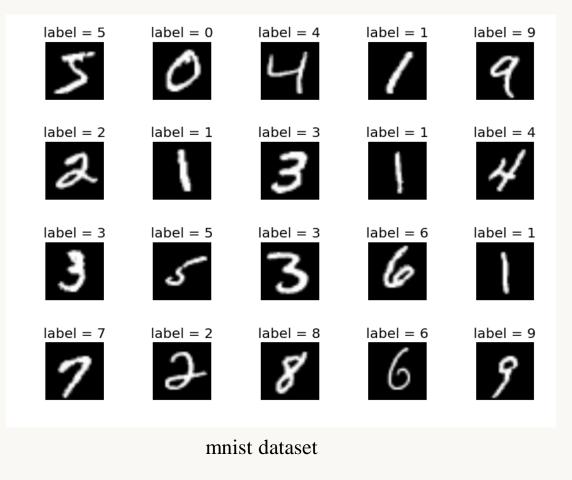


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#### Multiclass Logistic Regression (Squashing Function)

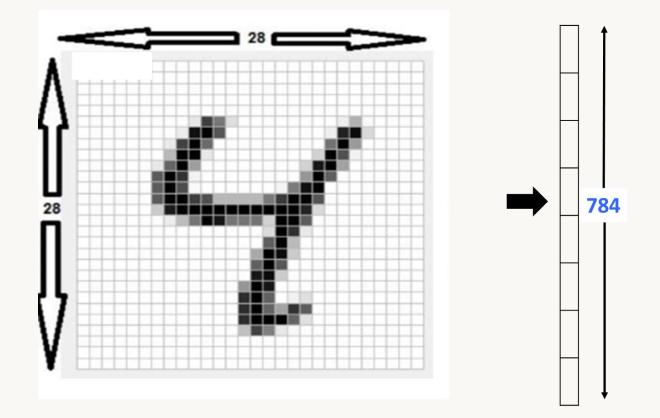


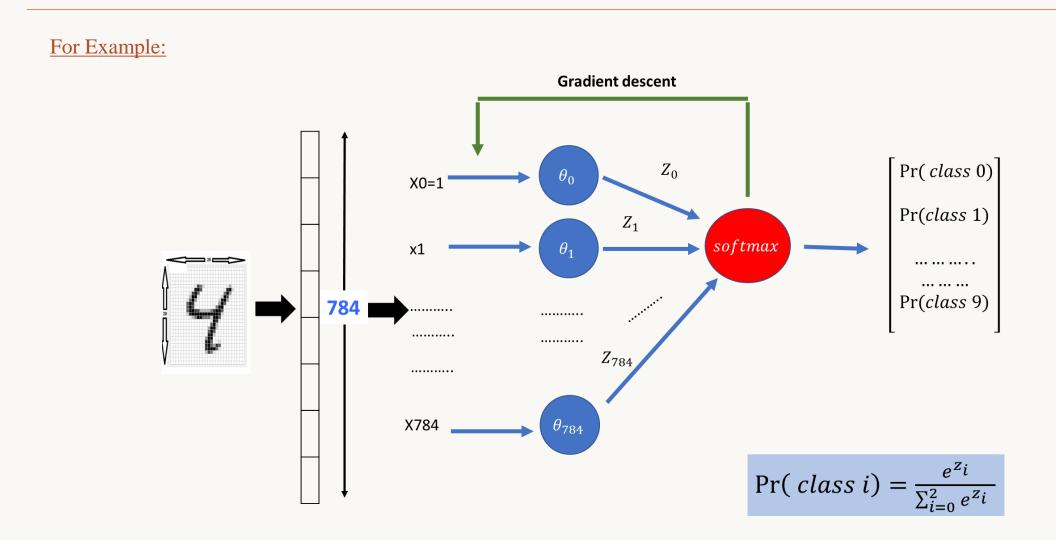
For Example:



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#### For Example:





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# Summary

**Implementation Note:** In the multivariate case, the cost function can also be written in the following vectorized form:

$$J(\theta) = \frac{1}{2m} \left( X\theta - \vec{y} \right)^T \left( X\theta - \vec{y} \right)$$

where

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

The vectorized version is efficient when you're working with numerical computing tools like Octave/MATLAB. If you are an expert with matrix operations, you can prove to yourself that the two forms are equivalent.

- Multi-class Classification (Useful videos):
  - ✓ <u>https://www.youtube.com/watch?v=LLux1SW--oM</u>
  - ✓ <u>https://www.youtube.com/watch?v=ueO\_Ph0Pyqk</u>

