



# CS60010: Deep Learning

## Spring 2023

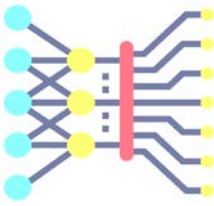
Sudeshna Sarkar

**Module 2 Part B**

**Linear Models for Classification**  
**Gradient Descent**

19 Jan 2023

# Linear Regression: Analytic Solution



$$L = \sum_{i=1}^m (\hat{y}^{(i)} - y^{(i)})^2 = \sum_{i=1}^m (\theta_0 + \theta_1 x^{(i)} - y^{(i)})^2$$

Since the loss is differentiable, we set

$$\frac{dL}{d\theta_0} = 0 \quad \text{and} \quad \frac{dL}{d\theta_1} = 0$$

We want the loss-minimizing values of  $\theta$ , so we set

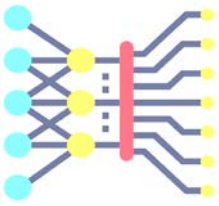
$$\frac{dL}{d\theta_1} = 0 = 2\theta_1 \sum_{i=1}^N (x^{(i)})^2 + 2\theta_0 \sum_{i=1}^N x^{(i)} - 2 \sum_{i=1}^N x^{(i)} y^{(i)}$$

$$\frac{dL}{d\theta_0} = 0 = 2\theta_1 \sum_{i=1}^N x^{(i)} + 2\theta_0 N - 2 \sum_{i=1}^N y^{(i)}$$

These being linear equations of  $\theta$ , have a unique closed form solution

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

# Multivariate Linear Regression



$$x \in \mathcal{R}^d$$

$$\hat{y} = f(x; \theta) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_d x_d$$

$$\begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix} = \begin{bmatrix} x_0^{(1)} & x_1^{(1)} & x_2^{(1)} & \dots & x_d^{(1)} \\ x_0^{(2)} & x_1^{(2)} & x_2^{(2)} & \dots & x_d^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_0^{(m)} & x_1^{(m)} & x_2^{(m)} & \dots & x_d^{(m)} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_d \end{bmatrix}$$
$$\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}$$

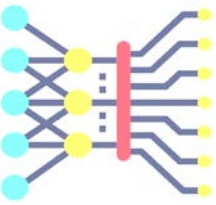
Define  $x_0 = 1$

$$f(x; \theta) = \theta^T \mathbf{x}$$

Cost Function:

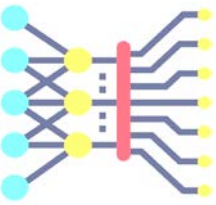
$$J(\boldsymbol{\theta}) = J(\theta_0, \theta_1, \dots, \theta_d) = \frac{1}{m} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2$$

# Multivariate Linear Regression



$$\begin{aligned} J(\boldsymbol{\theta}) &= \frac{1}{m} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2 = \frac{1}{m} (\hat{y}^{(i)} - y^{(i)})^2 \\ &= \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 = \frac{1}{m} (\hat{\mathbf{y}} - \mathbf{y})^T (\hat{\mathbf{y}} - \mathbf{y}) \\ &= \frac{1}{m} (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^T (\mathbf{X}\boldsymbol{\theta} - \mathbf{y}) \\ &= \frac{1}{m} \{\boldsymbol{\theta}^T (X^T X) \boldsymbol{\theta} - \boldsymbol{\theta}^T \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \boldsymbol{\theta} + \mathbf{y}^T \mathbf{Y}\} \\ &= \frac{1}{m} \{\boldsymbol{\theta}^T (X^T X) \boldsymbol{\theta} - (\mathbf{X}^T \mathbf{y})^T \boldsymbol{\theta} - (\mathbf{X}^T \mathbf{y})^T \boldsymbol{\theta} + \mathbf{y}^T \mathbf{Y}\} \\ &= \frac{1}{m} \{\boldsymbol{\theta}^T (X^T X) \boldsymbol{\theta} - 2(\mathbf{X}^T \mathbf{y})^T \boldsymbol{\theta} + \mathbf{y}^T \mathbf{Y}\} \end{aligned}$$

# Multivariate Linear Regression

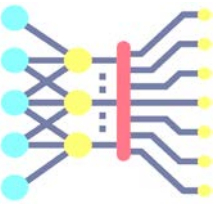


- Equating the gradient of the cost function to 0,

$$\begin{aligned}\nabla_{\theta} J(\boldsymbol{\theta}) &= \frac{1}{m} \{2\mathbf{X}^T \mathbf{X} \boldsymbol{\theta} - 2\mathbf{X}^T \mathbf{y} + 0\} = 0 \\ \mathbf{X}^T \mathbf{X} \boldsymbol{\theta} - \mathbf{X}^T \mathbf{y} &= 0 \\ \boldsymbol{\theta} &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}\end{aligned}$$

**This gives a closed form solution, but another option is to use iterative solution**

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



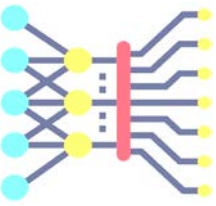
# Partial derivatives

- Let  $y = f(\mathbf{x}) = f(x_1, x_2, \dots, x_n)$  be a multivariate function with  $n$  variables
  - The mapping is  $f: \mathbb{R}^n \rightarrow \mathbb{R}$
- The **partial derivative** of  $y$  with respect to its  $i^{\text{th}}$  parameter  $x_i$  is

$$\frac{\partial y}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x_1, x_2, \dots, x_i + h, \dots, x_n) - f(x_1, x_2, \dots, x_i, \dots, x_n)}{h}$$

- To calculate  $\frac{\partial y}{\partial x_i}$ , we can treat  $x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_n$  as constants and calculate the derivative of  $y$  only with respect to  $x_i$
- For notation of partial derivatives, the following are equivalent:

$$\frac{\partial y}{\partial x_i} = \frac{\partial f}{\partial x_i} = \frac{\partial}{\partial x_i} f(\mathbf{x}) = f_{x_i} = f_i = D_i f = D_{x_i} f$$

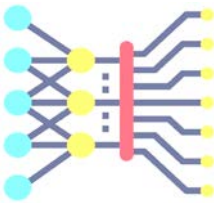


# Multidimensional derivative: Gradient

**Gradient** vector: The gradient of the multivariate function  $f(\mathbf{x})$  with respect to the  $n$ -dimensional input vector  $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$ , is a vector of  $n$  partial derivatives

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[ \frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \dots, \frac{\partial f(\mathbf{x})}{\partial x_n} \right]^T$$

- In ML, the gradient descent algorithm relies on the opposite direction of the gradient of the loss function  $\mathcal{L}$  with respect to the model parameters  $\theta$  ( $\nabla_{\theta} \mathcal{L}$ ) for minimizing the loss function



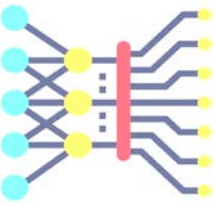
$$f(x, y, z) = x^3zy^2 - xz + yz.$$

Which of the following is the gradient vector  $\begin{pmatrix} \partial f / \partial x \\ \partial f / \partial y \\ \partial f / \partial z \end{pmatrix}$  ?

- (a)  $\begin{pmatrix} 3x^2y^2 \\ y \\ 3x^2y^2 - x \end{pmatrix}$
- (b)  $\begin{pmatrix} 3x^2zy^2 - z \\ 2x^3zy + z \\ x^3y^2 - x + y \end{pmatrix}$
- (c)  $\begin{pmatrix} 2x^3zy + z \\ x^3y^2 + y \\ 3x^2zy^2 - z + y \end{pmatrix}$



# Gradient as directional derivative

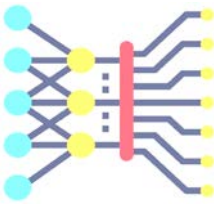


$$\begin{aligned} f(x + h, y + h) &\approx f(x, y) + h_1 \left. \frac{\partial f}{\partial x} \right|_{(x,y)} + h_2 \left. \frac{\partial f}{\partial y} \right|_{(x,y)} \\ &= f(x, y) + (h_1, h_2) \cdot \left( \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right) = f(x, y) + \vec{h} \cdot \nabla f \end{aligned}$$

Gradient Descent:  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla f$

↑  
learning rate

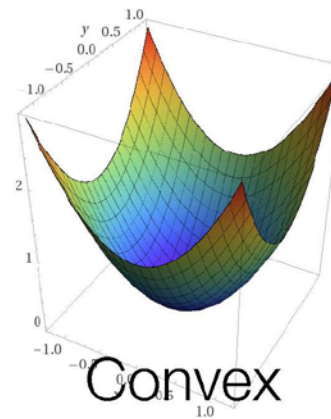
# Gradient Descent Algorithm



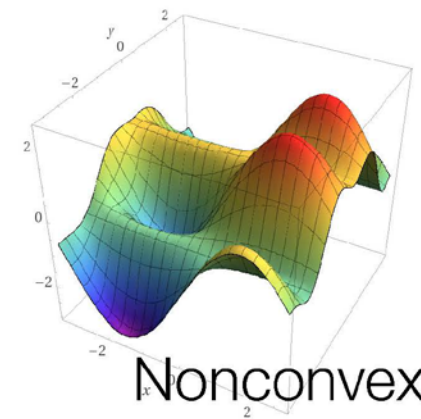
Starting at some suitable  $w^{(0)} \in \mathfrak{R}^d$  do for  $t = 0, 1, \dots, T - 1$   
 $\{ w^{(t+1)} \leftarrow w^{(t)} - \eta \cdot \nabla f|_{w^{(t)}} \}$

- “Like water flowing down a slope.”
- Stops making progress when  $\nabla f = 0$  (“Stationary point”)
- Will reach minimizer of  $f(x)$  if  $f$  is a convex function
- No guarantees for non convex  $f$ . At best find “local minima.” (Finding global minimum is NP-hard in worst case).

convex vs nonconvex losses was a big argument in AI/ML 15+ years ago. (Nonconvex side won)

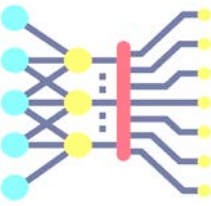


Convex

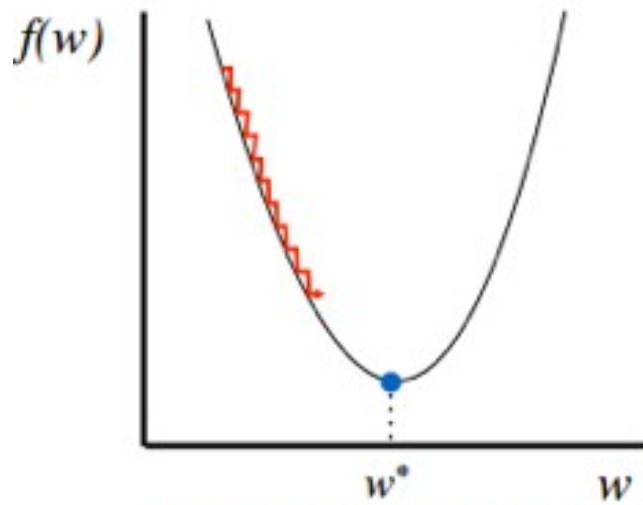


Nonconvex

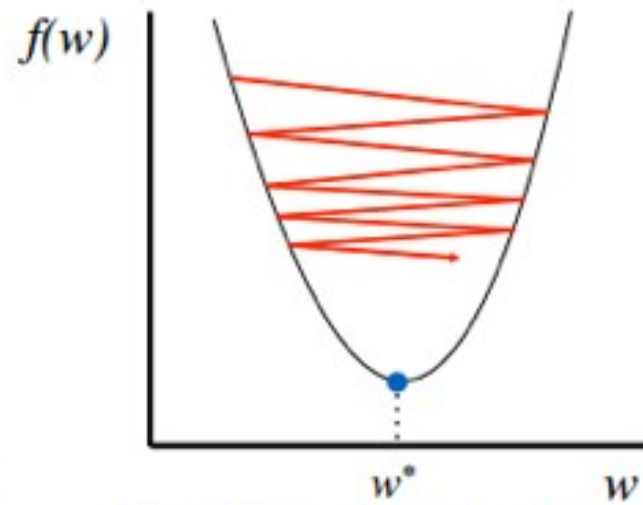
# Step Size



- Determines how quickly training loss goes down; hence “learning rate”

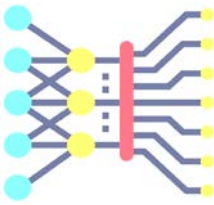


Too small: converge  
very slowly

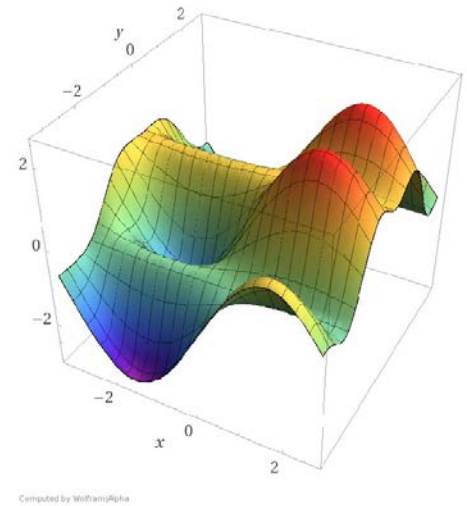
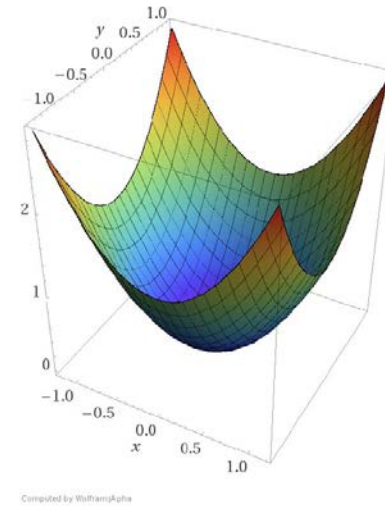


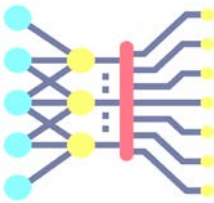
Too big: overshoot and  
even diverge

# Importance of Initialization



- Simple convex functions have unique optimum.
- But in practice loss functions are non convex and have multiple optima (test accuracies all over the map). Initialization (and even choice of LR) affects where you end up!
- With non convex loss (e.g., in deep learning) good initialization is a must. No good theory for it. In deep learning, Gaussian initialization is common...





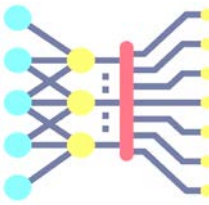
- Gradient is a linear operator.

$$\nabla \left( f_1(\vec{\theta}) + f_2(\vec{\theta}) \right) = \nabla \left( f_1(\vec{\theta}) \right) + \nabla \left( f_2(\vec{\theta}) \right)$$

- Training Loss = Sum of Losses on individual datapoints.
- Gradient of training loss = sum of gradients of loss on individual datapoints.
- For large datasets evaluating exact derivative gets expensive
- **Stochastic GD:** Estimate the sum via a small random sample of datapoints, and use it instead of exact gradient. (Like an opinion poll over datapoints.)

$$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} + \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} + \dots + \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

# Batch, Stochastic and Mini-batch Stochastic Gradient Descent



## Algorithm 1 Batch Gradient Descent at Iteration $k$

**Require:** Learning rate  $\epsilon_k$

**Require:** Initial Parameter  $\theta$

- 1: **while** stopping criteria not met **do**
- 2:     Compute gradient estimate over  $N$  examples:
- 3:      $\hat{\mathbf{g}} \leftarrow +\frac{1}{N} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$
- 4:     Apply Update:  $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$
- 5: **end while**

## Algorithm 2 Stochastic Gradient Descent at Iteration $k$

**Require:** Learning rate  $\epsilon_k$

**Require:** Initial Parameter  $\theta$

- 1: **while** stopping criteria not met **do**
- 2:     Sample example  $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$  from training set
- 3:     Compute gradient estimate:
- 4:      $\hat{\mathbf{g}} \leftarrow +\nabla_{\theta} L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$
- 5:     Apply Update:  $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$
- 6: **end while**

## Mini-batch

### Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration $k$

**Require:** Learning rate  $\epsilon_k$ .

**Require:** Initial parameter  $\theta$

**while** stopping criterion not met **do**

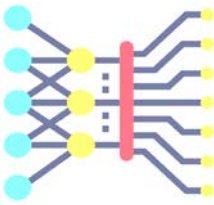
    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient estimate:  $\hat{\mathbf{g}} \leftarrow +\frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Apply update:  $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$

**end while**

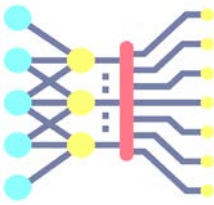
# Iterative Gradient Descent for Regression



- Iterative Gradient Descent needs to perform many iterations and need to choose a stepsize parameter judiciously. But it works equally well even if the number of features ( $d$ ) is large.
- For the least square solution, there is no need to choose the step size parameter or no need to iterate. But, evaluating  $(\mathbf{X}^T \mathbf{X})^{-1}$  can be slow if  $d$  is large.



# The loss “landscape”

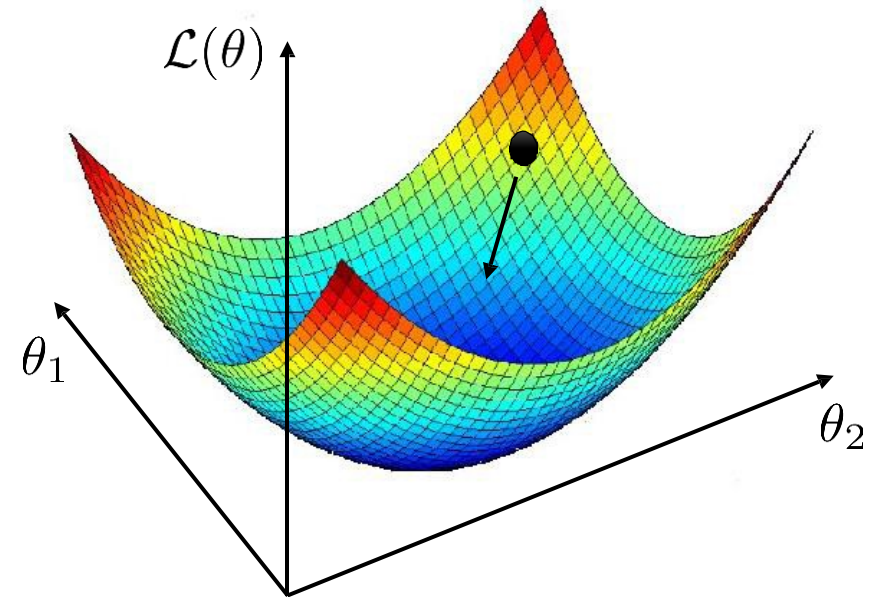


$$\theta^* \leftarrow \arg \min_{\theta} - \underbrace{\sum_i \log p_{\theta}(y_i | x_i)}_{\mathcal{L}(\theta)}$$

let's say  $\theta$  is 2D

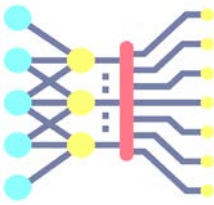
An algorithm:

1. Find a *direction*  $v$  where  $\mathcal{L}(\theta)$  decreases
  2.  $\theta \leftarrow \theta + \alpha v$
- some small constant  
called “learning rate” or  
“step size”





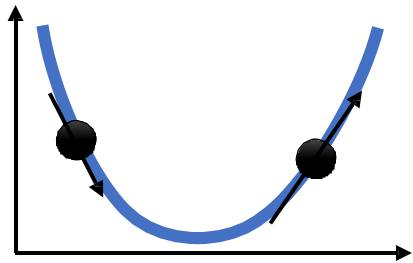
# Gradient descent



An algorithm:

1. Find a *direction*  $v$  where  $\mathcal{L}(\theta)$  decreases
2.  $\theta \leftarrow \theta + \alpha v$

Which way does  $\mathcal{L}(\theta)$  decrease?



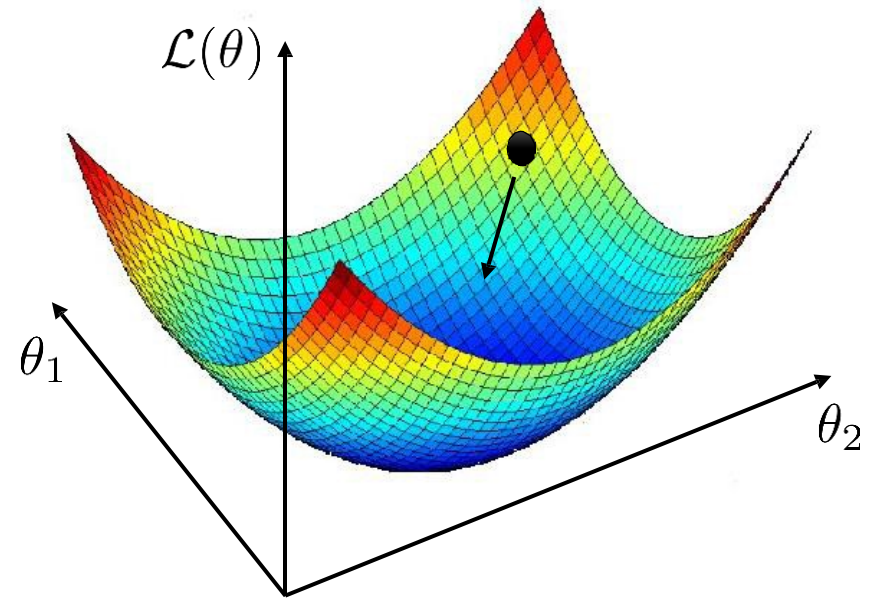
negative slope = go to the right

positive slope = go to the left

in general:

for each dimension, go in the direction  
opposite the slope **along that dimension**

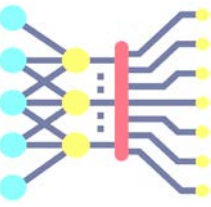
$$v_1 = -\frac{d\mathcal{L}(\theta)}{d\theta_1} \quad v_2 = -\frac{d\mathcal{L}(\theta)}{d\theta_2} \quad \text{etc.}$$



gradient:

$$\nabla_{\theta} \mathcal{L}(\theta) = \begin{bmatrix} \frac{d\mathcal{L}(\theta)}{d\theta_1} \\ \frac{d\mathcal{L}(\theta)}{d\theta_2} \\ \vdots \\ \frac{d\mathcal{L}(\theta)}{d\theta_n} \end{bmatrix}$$

# Gradient descent

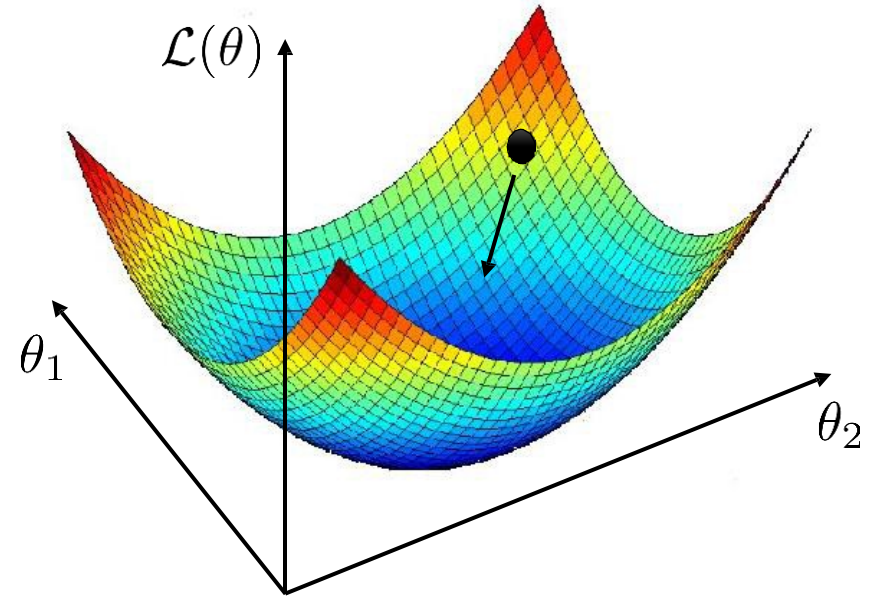


An algorithm:

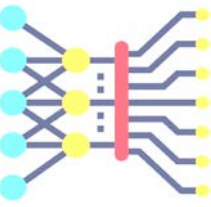
- 1. Find a *direction*  $v$  where  $\mathcal{L}(\theta)$  decreases
- 2.  $\theta \leftarrow \theta + \alpha v$

Gradient descent:

- 1. Compute  $\nabla_{\theta} \mathcal{L}(\theta)$
- 2.  $\theta \leftarrow \theta - \alpha \nabla_{\theta} \mathcal{L}(\theta)$



$$\nabla_{\theta} \mathcal{L}(\theta) = \begin{bmatrix} \frac{d\mathcal{L}(\theta)}{d\theta_1} \\ \frac{d\mathcal{L}(\theta)}{d\theta_2} \\ \vdots \\ \frac{d\mathcal{L}(\theta)}{d\theta_n} \end{bmatrix}$$

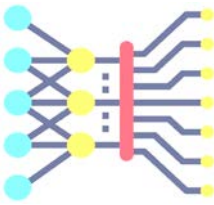


# Classification problems

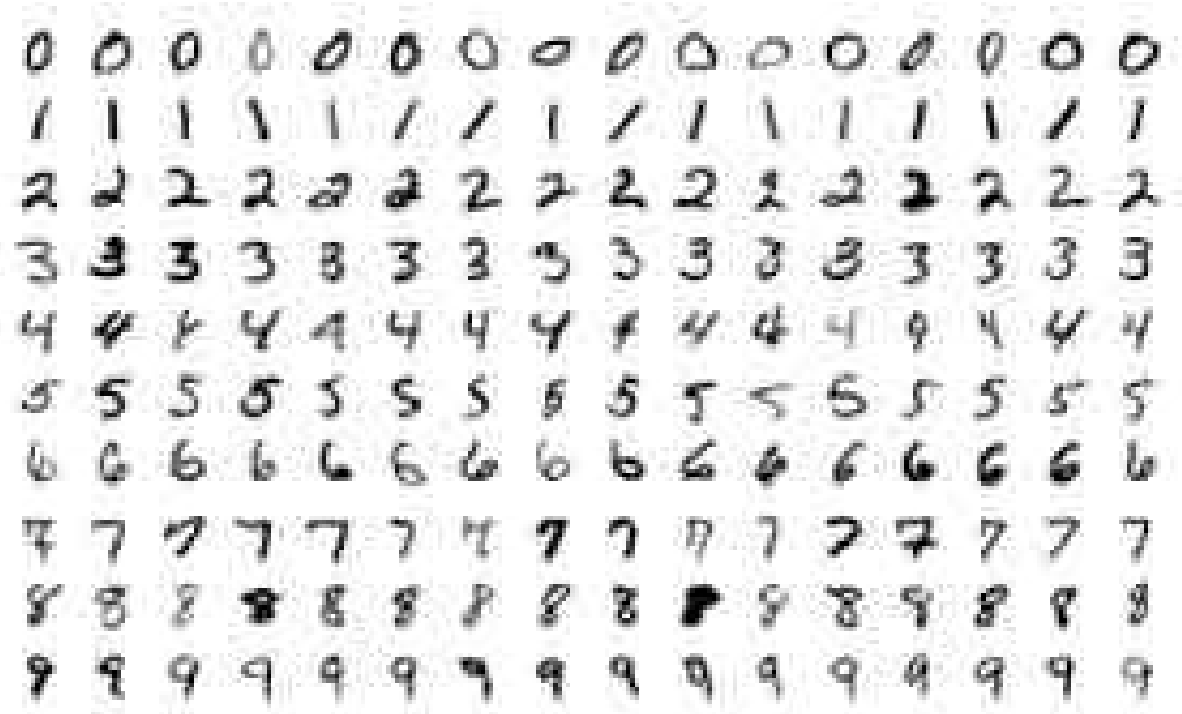
Linear Models for Classification

Logistic Regression

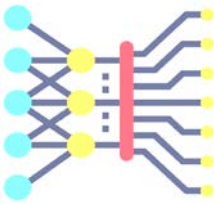
# Binary classification



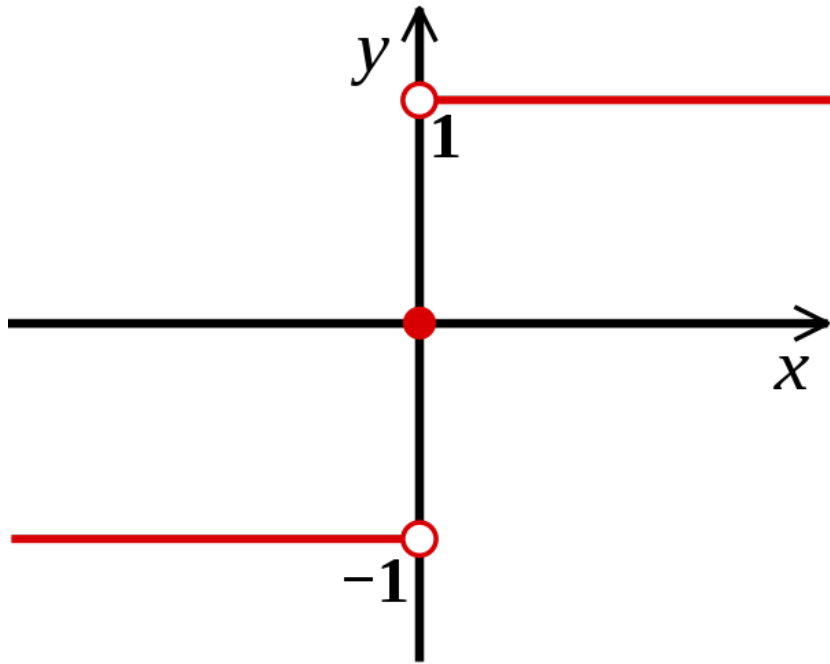
- Binary classification:
  - Training datapoints have one of two labels (0/1) or (-1/+1).
- Multiclass classification
  - Training datapoints have one of  $k$  labels (0, 1, 2,...,  $k-1$ )



# Binary Classification

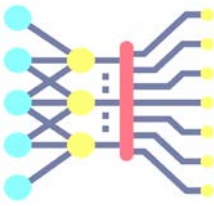


We want the possible outputs of  $\mathbf{h}_{\theta}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}$  to have values 0 or 1.

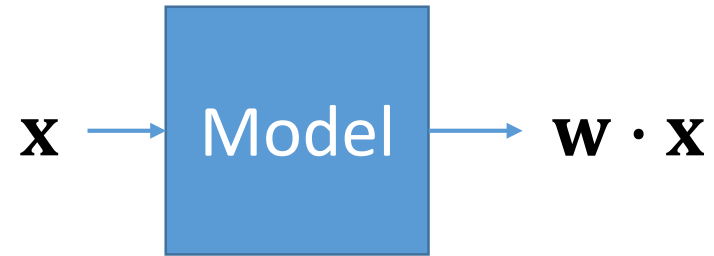


What is derivative of  $f(x) = \text{sign}(x)$  in the interval  $(0, \infty]$ ?

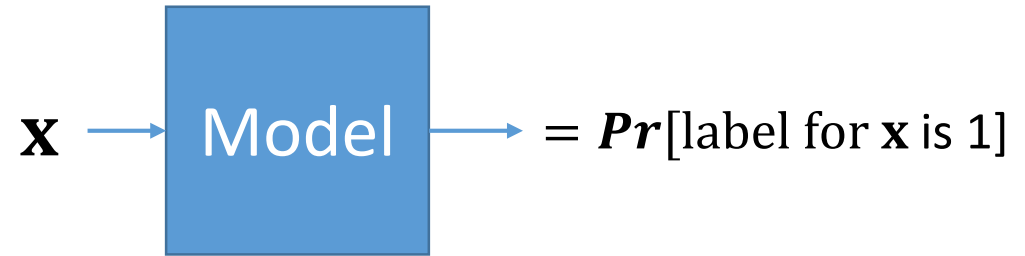
# Logistic regression: output is a probability



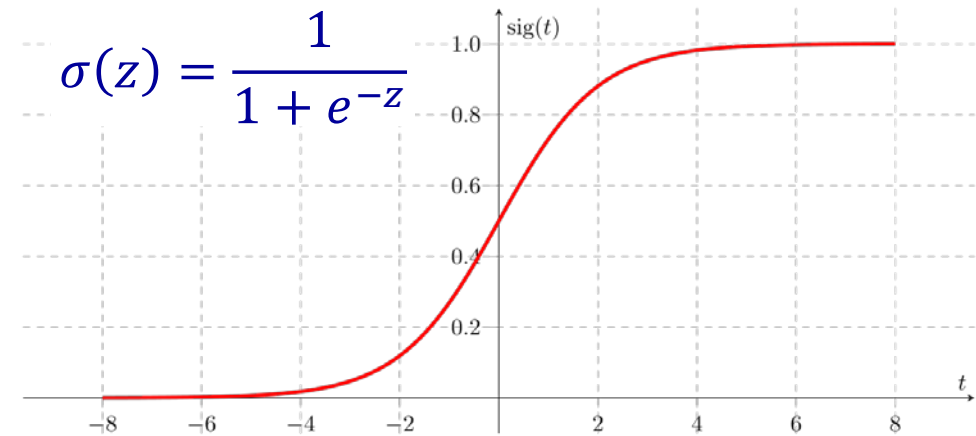
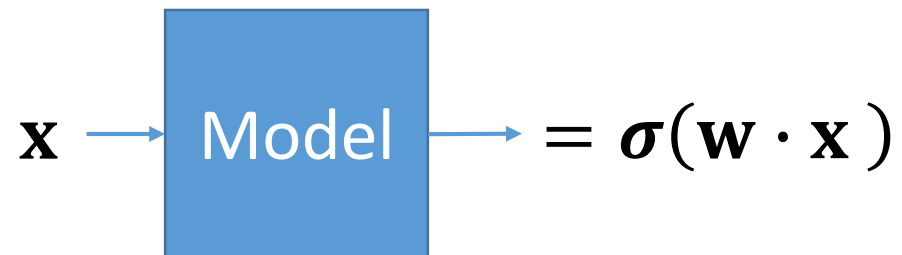
Linear Regression



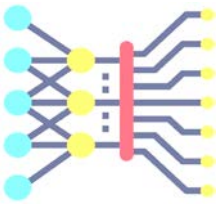
Logistic Model: Output is a probability



Logistic Model: Output is a probability



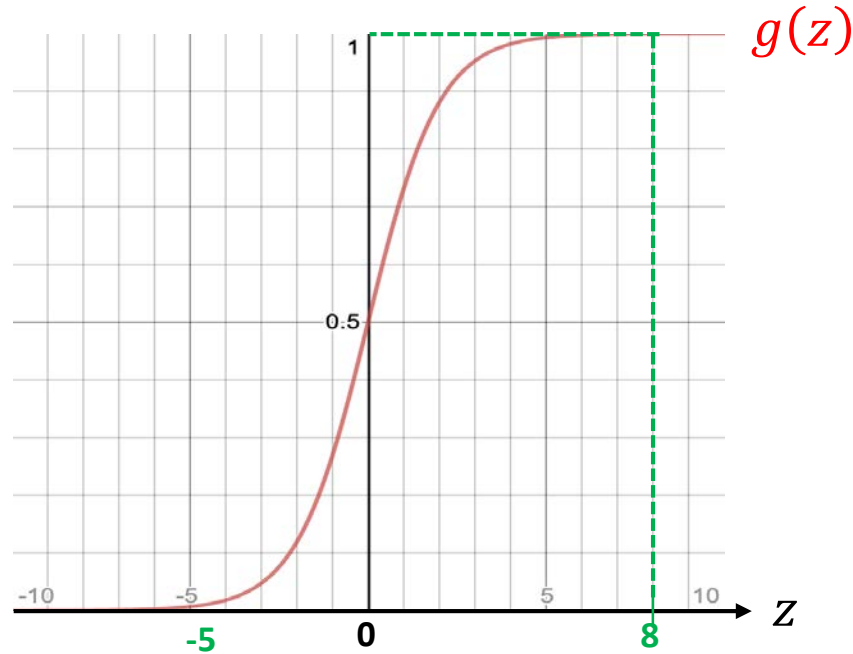
# Logistic Loss



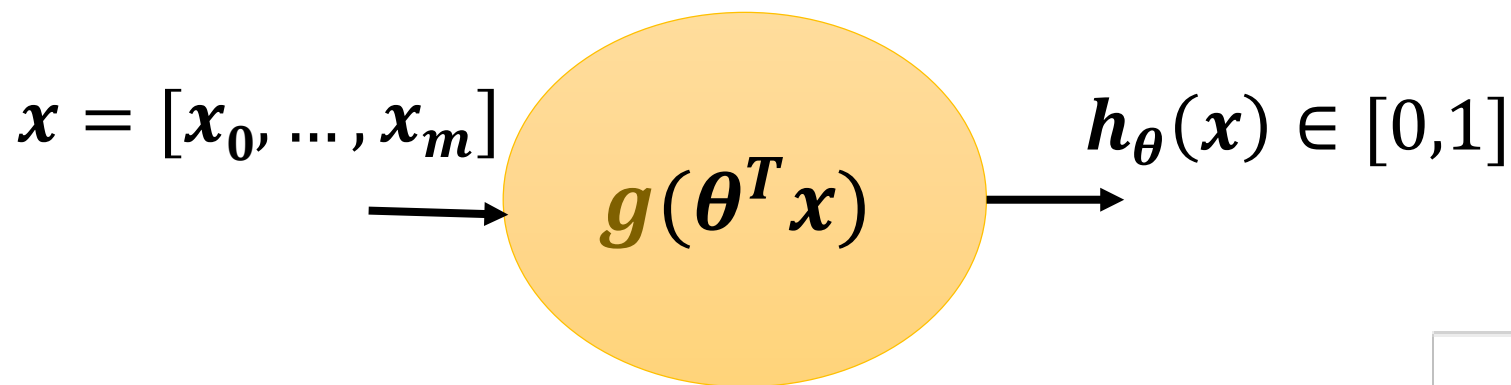
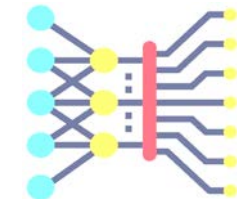
Use an **activation function** (e.g., **sigmoid or logistic function**)

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

$z \in \mathbb{R}$ , but  
 $g(z) \in [0,1]$



# Classification



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

Thresholding:

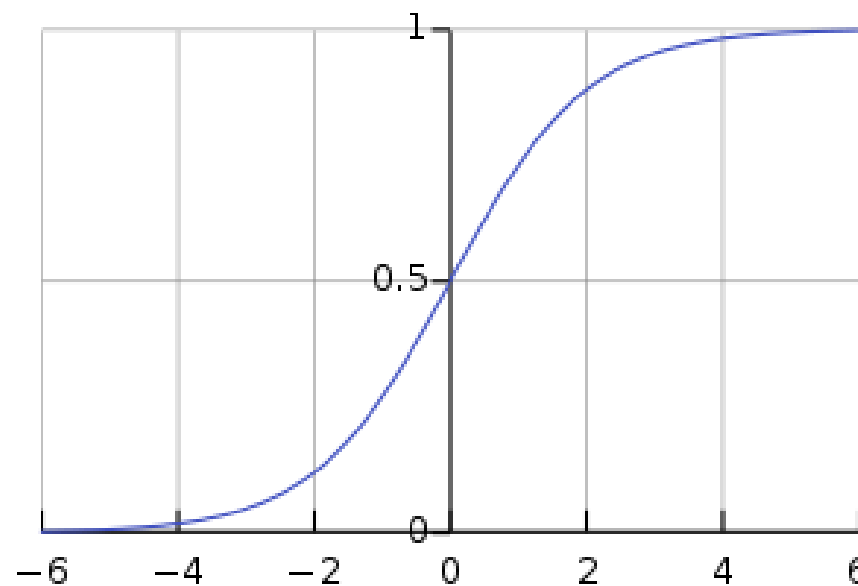
predict “y = 1” if  $h_\theta(x) \geq 0.5$

$$z = \theta^T x \geq 0$$

predict “y = 0” if  $h_\theta(x) < 0.5$

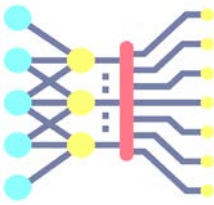
$$z = \theta^T x < 0$$

**Alternative Interpretation:  $h_\theta(x)$  = estimated probability that  $y = 1$  on input  $x$**



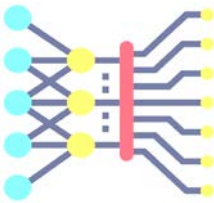


# Example: Probabilistic Weather Predictions



	Mon	Tue	Wed	Thu	Fri
Rained?	Y	N	Y	N	N
M1 Pr[rain]	60%	20%	90%	50%	40%
M2 Pr[rain]	70%	50%	80%	20%	60%

Which model seems to be a better predictor to you?



	Mon	Tue	Wed	Thu	Fri
Rained?	Y	N	Y	N	N
M1 Pr[rain]	60%	20%	90%	50%	40%
M2 Pr[rain]	70%	50%	80%	20%	60%

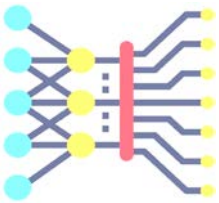
Max Likelihood Principle: The **better** model is one that assigned **more probability** to the events that actually happened (i.e., YNYNN)

$\text{Pr}[YNYNN] = \text{Pr}[Y \text{ on M}] \cdot \text{Pr}[N \text{ on Tu}] \cdot \text{Pr}[Y \text{ on W}] \cdot \text{Pr}[N \text{ on Th}] \cdot \text{Pr}[N \text{ on F}]$

$\text{Pr}[YNYNN] \text{ according to Model 1} = (0.6)(1 - 0.2)(0.9)(1 - 0.5)(1 - 0.4)$

$\text{Pr}[YNYNN] \text{ according to Model 2} =$

# Formulating loss function for logistic regression



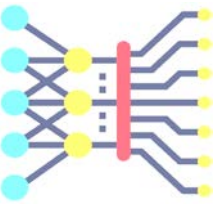
- $\Pr[x = 1] = \sigma(z) = \frac{1}{1+e^{-\mathbf{w} \cdot \mathbf{x}}}$
- $\Pr[x = 0] = 1 - \sigma(z) = 1 - \frac{1}{1+e^{-\mathbf{w} \cdot \mathbf{x}}} = \frac{e^{-\mathbf{w} \cdot \mathbf{x}}}{1+e^{-\mathbf{w} \cdot \mathbf{x}}}$

$$= \frac{\frac{1}{e^{\mathbf{w} \cdot \mathbf{x}}}}{1 + \frac{1}{e^{\mathbf{w} \cdot \mathbf{x}}}} = \frac{1}{e^{\mathbf{w} \cdot \mathbf{x}}} \cdot \frac{e^{\mathbf{w} \cdot \mathbf{x}}}{1 + e^{\mathbf{w} \cdot \mathbf{x}}} = \frac{1}{1 + e^{\mathbf{w} \cdot \mathbf{x}}}$$

- Max Likelihood Fit: Find  $\mathbf{w}$  that maximizes probability assigned to data.
- Probability assigned by model to the dataset

$$= \prod_i \frac{1}{1 + \exp(-y_i \mathbf{w} \cdot \mathbf{x}_i)}$$

# Optimization for logistic loss



Max Likelihood Fit: Find  $\mathbf{w}$  that maximizes probability assigned to data.

Training Dataset:  $\{(x_i, y_i)\}$

Probability assigned by model to the dataset

$$= \prod_i \frac{1}{1 + \exp(-y_i \mathbf{w} \cdot x_i)}$$

- Maximizing this is equivalent to Minimizing the reciprocal
- Training Objective:

$$\min_{\mathbf{w}} \prod_i (1 + \exp(-y_i \mathbf{w} \cdot x_i))$$

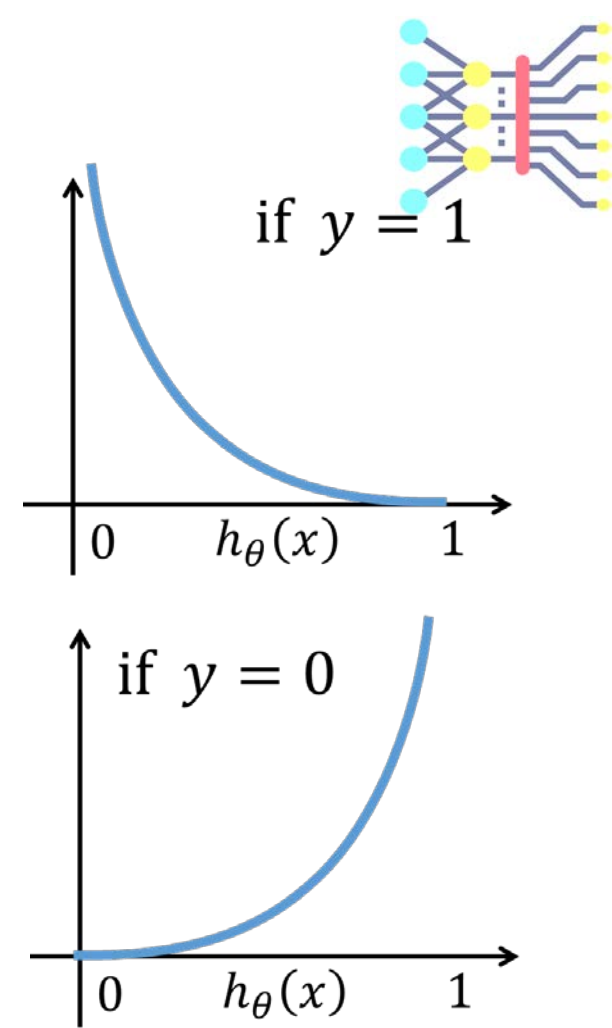
$$\min_{\mathbf{w}} \sum_i \log(1 + \exp(-y_i \mathbf{w} \cdot x_i))$$

# Cost function for Logistic Regression

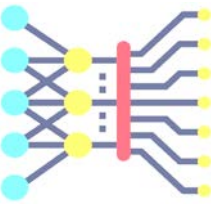
## Logistic Regression

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

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



# Gradient descent



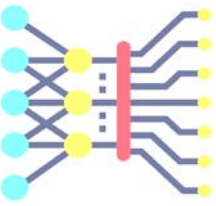
$$J(\theta) = -\frac{1}{m} \left[ \sum_{i=1}^m y^{(i)} \log(h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)})) \right]$$

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

**Good news:** Convex function!

**Bad news:** No analytical solution

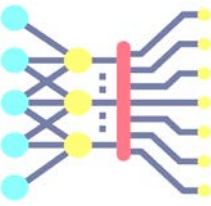
# Gradient descent



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

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

# Gradient descent



(Simultaneously update all  $\theta_j$ )

Repeat {

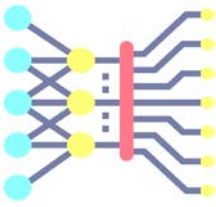
$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

}

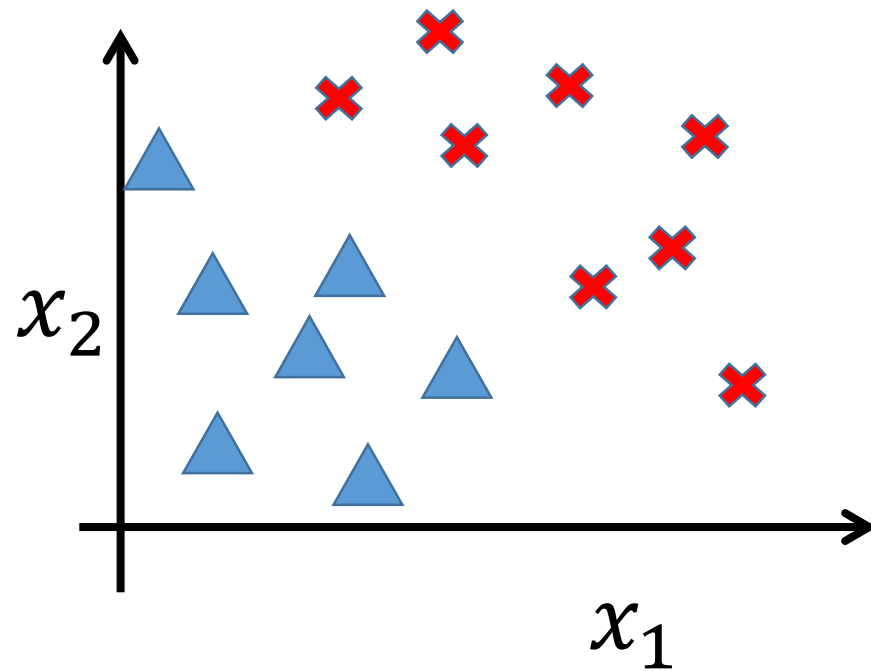
$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}$$



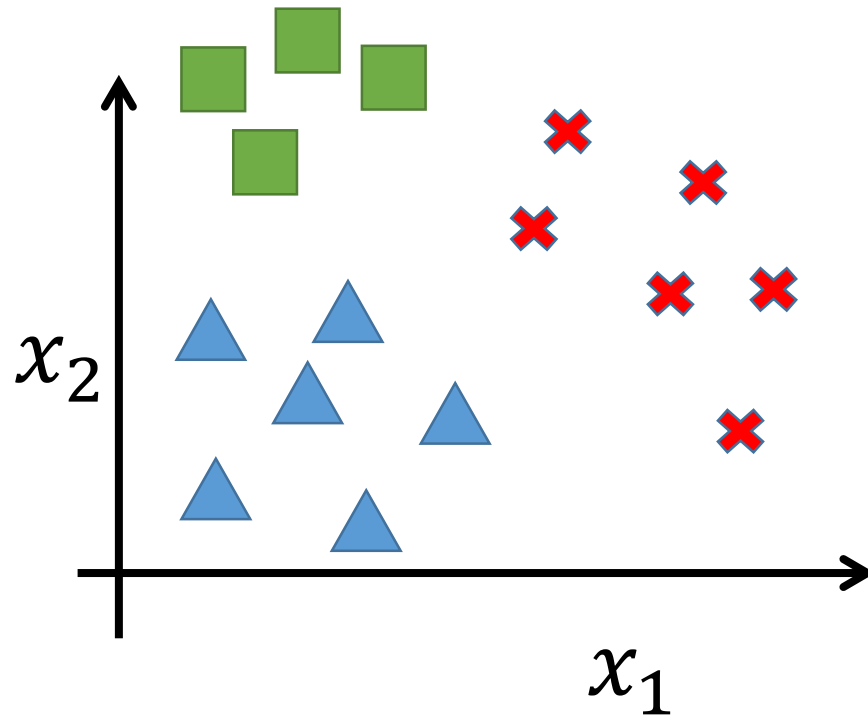
# Multiclass classification

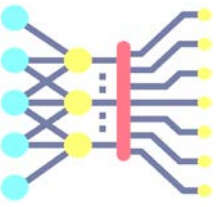


## Binary classification



## Multiclass classification





# Multi-class Classification

- Multi-class Classification:  $y$  can take on  $K$  different values  $\{1, 2, \dots, k\}$
- $h_{\theta}(x)$  estimates the probability of belonging to each class

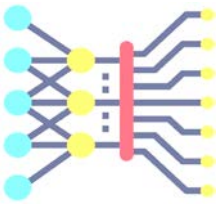
$$P(y = k|x, \theta) \propto \exp(\theta_k^T x)$$

$$\theta = \begin{bmatrix} \vdots & \vdots & \vdots \\ \theta_1 & \theta_2 & \theta_k \\ \vdots & \vdots & \vdots \end{bmatrix}$$

$$P(y = k|x, \theta) = \frac{\exp(\theta_k^T x)}{\sum_{j=1}^K \exp(\theta_j^T x)}$$

$$J(\theta) = - \left[ \sum_{i=1}^m \sum_{j=1}^K 1\{y^{(i)} = k\} \log \frac{\exp(\theta_k^T x^{(i)})}{\sum_{j=1}^K \exp(\theta_j^T x^{(i)})} \right]$$

# Empirical risk minimization



$$\text{Empirical risk} = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(x_i, y_i, \theta) \approx E_{x \sim p(x), y \sim p(y|x)} [\mathcal{L}(x, y, \theta)]$$

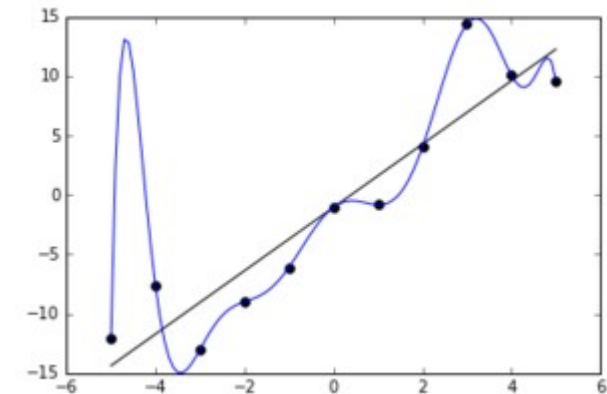
Supervised learning is (usually) *empirical* risk minimization

Is this the same as *true* risk minimization?

**Overfitting:** when the empirical risk is low, but the true risk is high

can happen if the dataset is too small

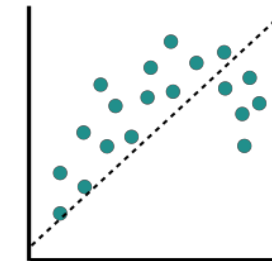
can happen if the model is too powerful (has too many parameters/capacity)



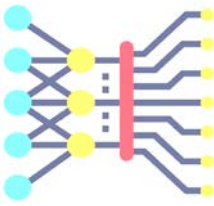
**Underfitting:** when the empirical risk is high, and the true risk is high

can happen if the model is too weak (has too few parameters/capacity)

can happen if your optimizer is not configured well (e.g., wrong learning rate)



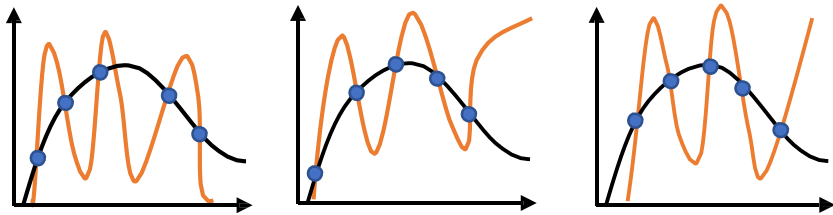
# Overfitting and Underfitting



$$\mathcal{L}(\theta, x, y) = -\frac{1}{2} ||f_{\theta}(x) - y||^2$$

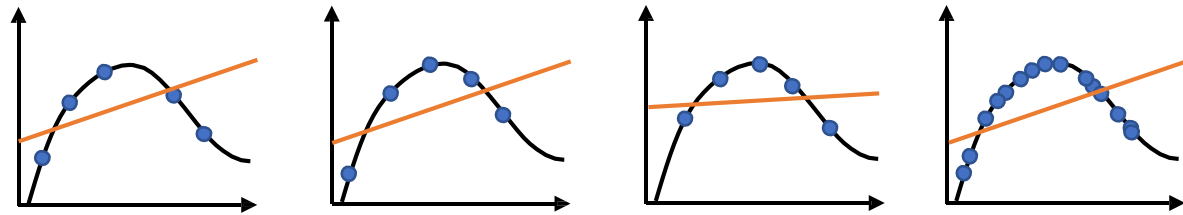
**Question:** how does the error change for different **training sets**?

overfitting



- The training data is fitted well
- The true function is fitted poorly
- **The learned function looks different each time!**

underfitting



- The training data is fitted poorly
- The true function is fitted poorly
- **The learned function looks similar, even if we pool together all the datasets!**