CHAPTER 1

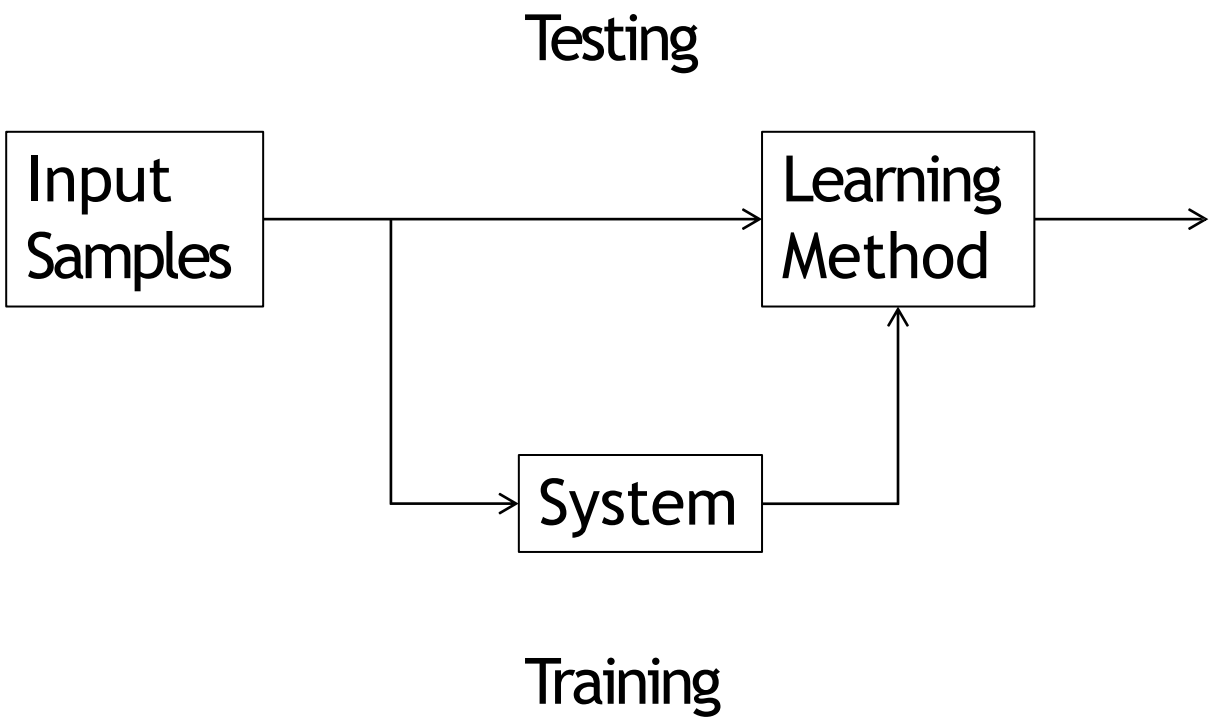
- INTRODUCTION

What is machine learning?

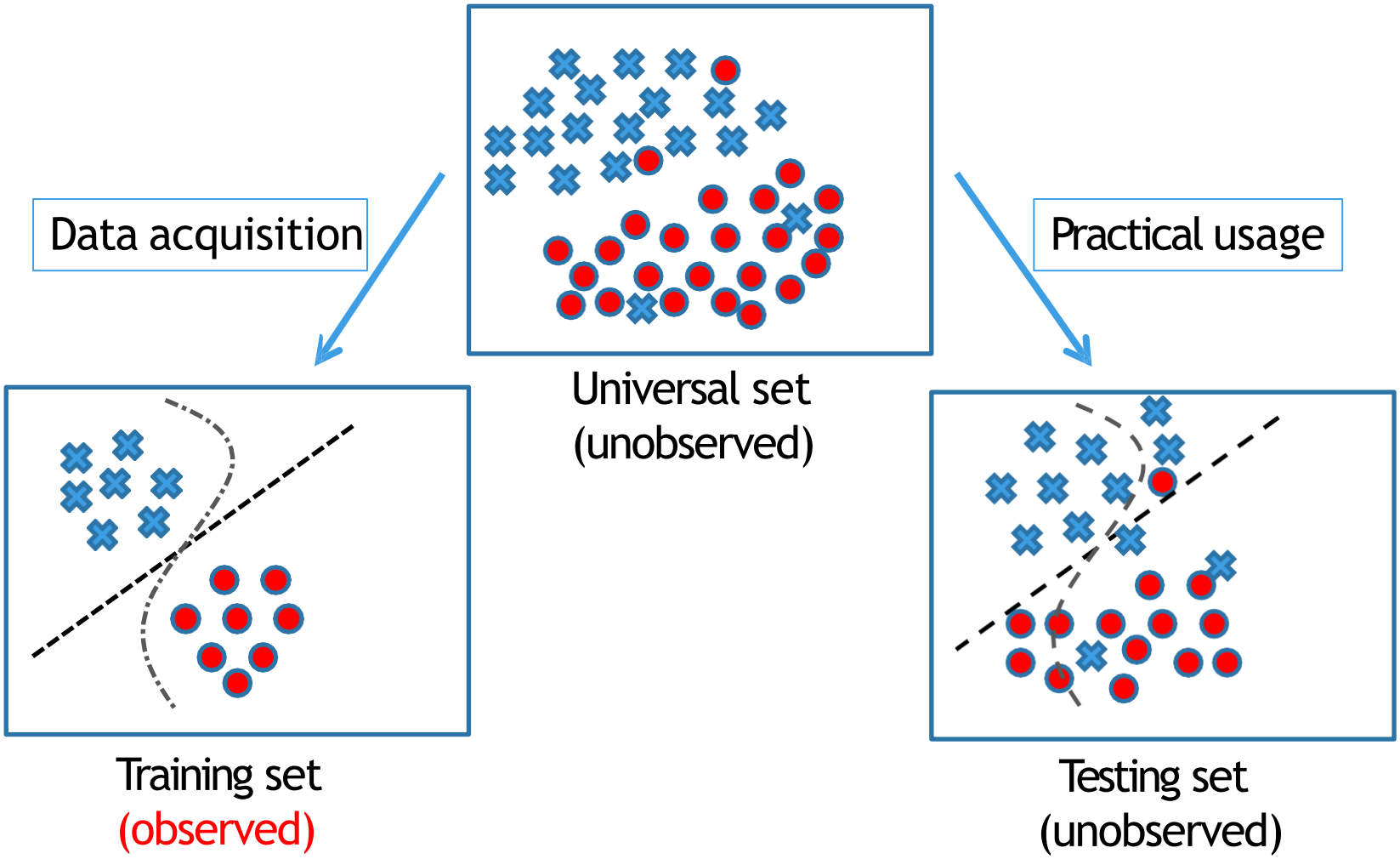
- A branch of **artificial intelligence**, concerned with the design and development of algorithms that allow computers to evolve behaviors based on empirical data.

- As intelligence requires knowledge, it is necessary for the computers to acquire knowledge.

Learning system model

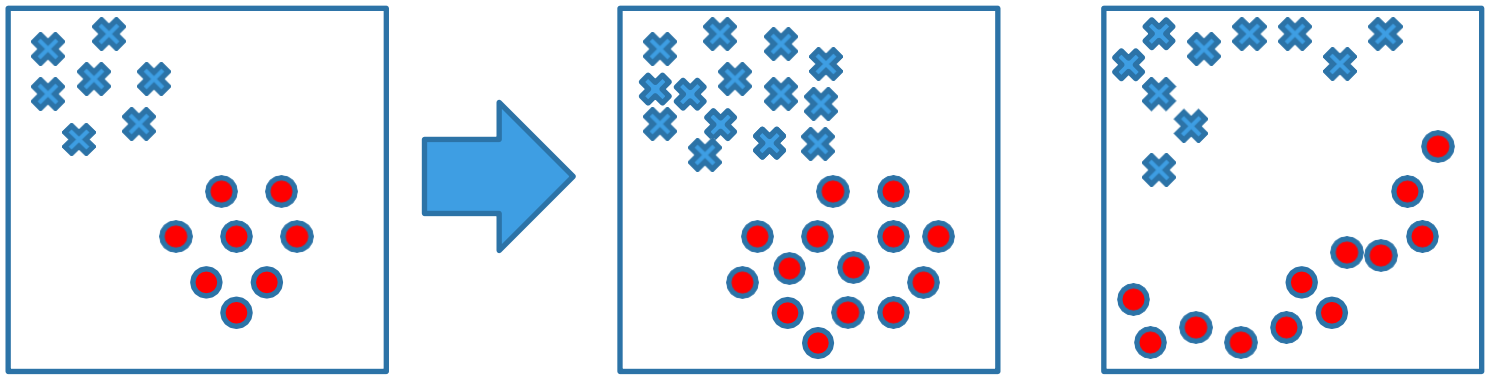


Training and testing

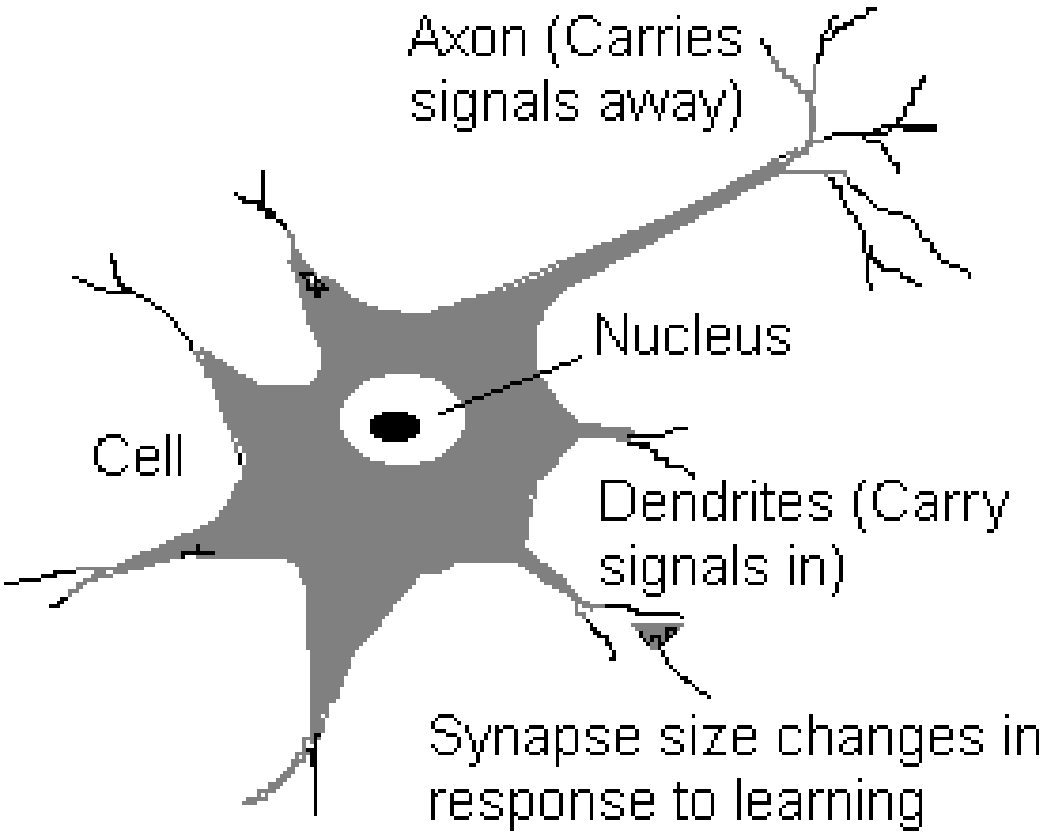


Training and testing

- Training is the process of making the system able to learn.
- No rule:
  - Training set and testing set come from the same distribution
  - Need to make some assumptions or bias

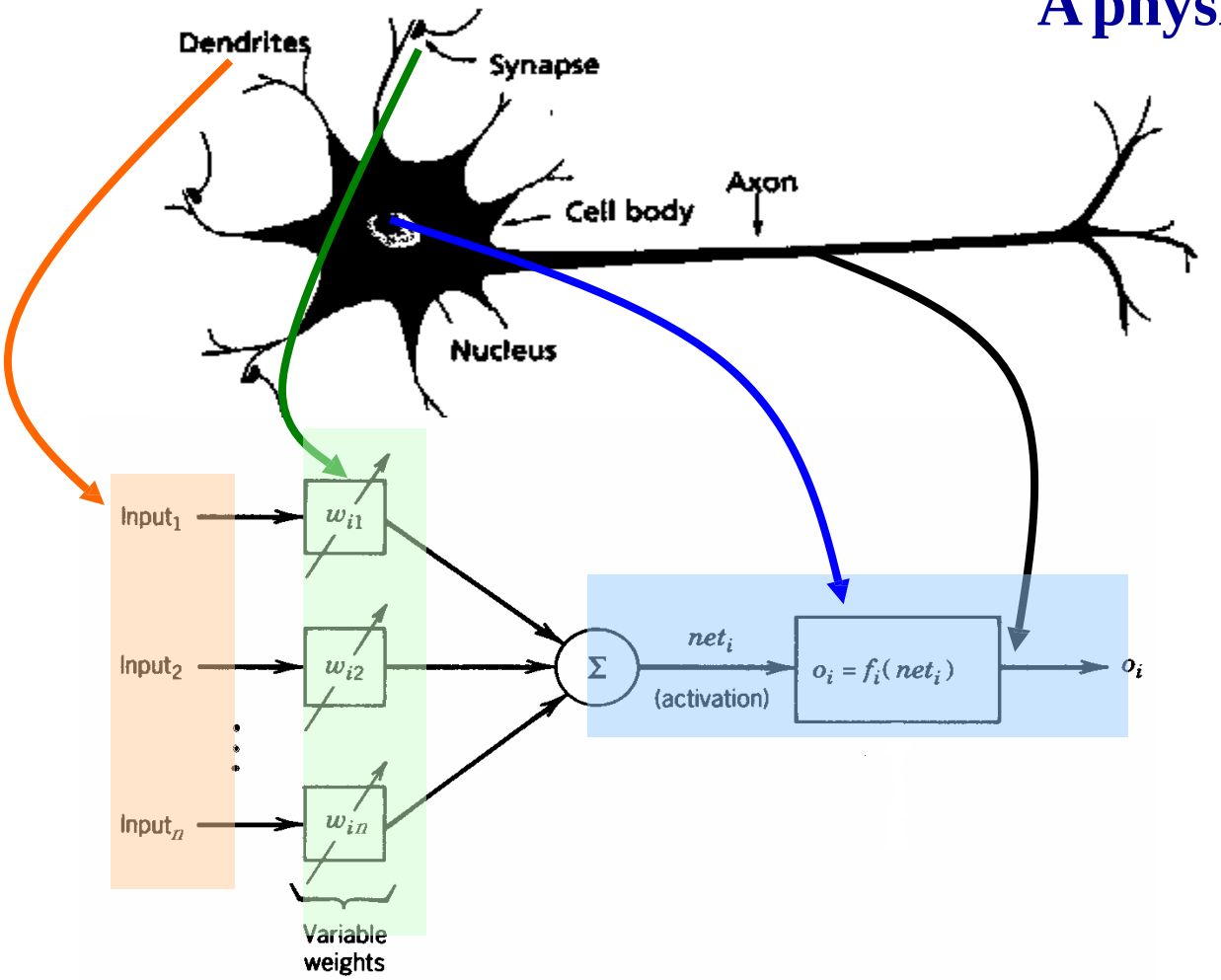


Biological Neurons

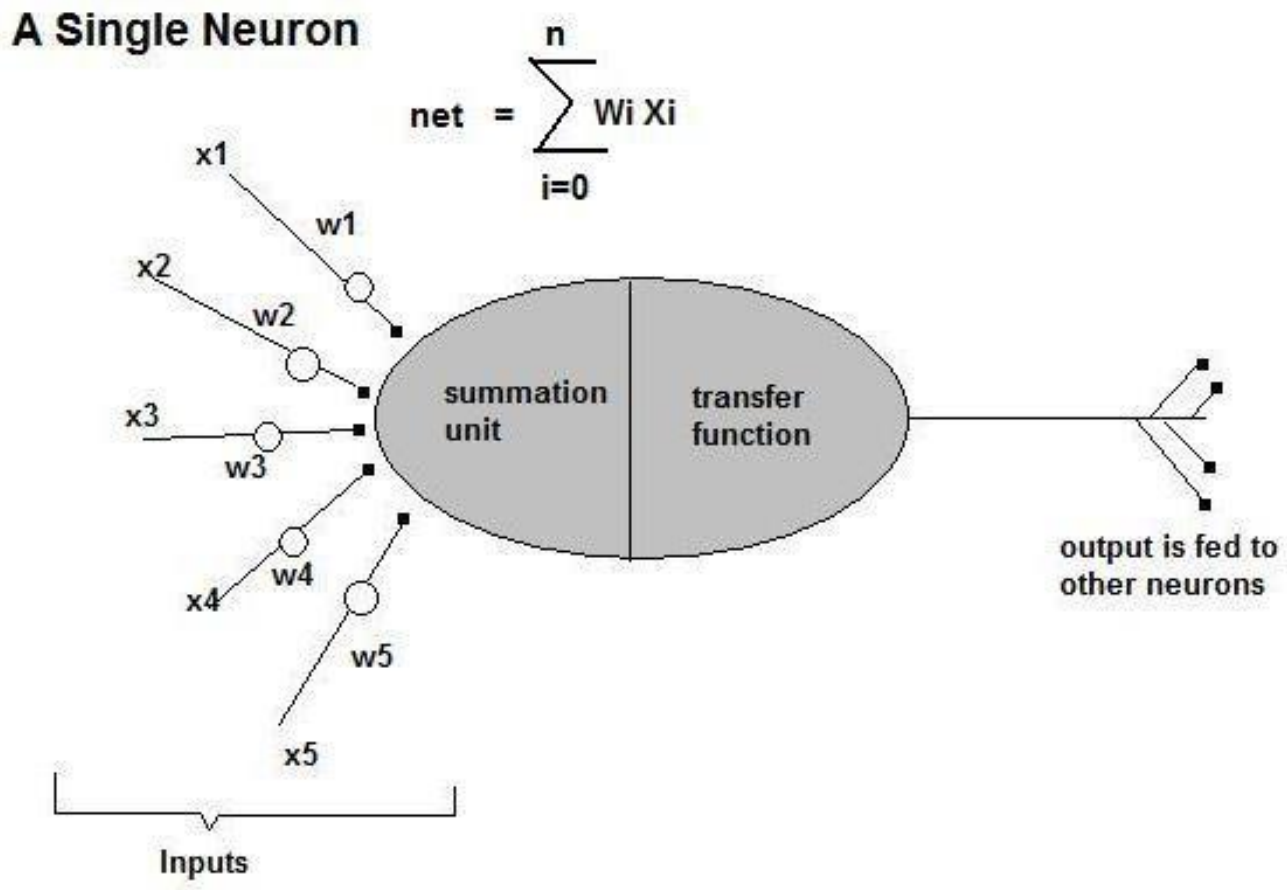


Artificial Neurons

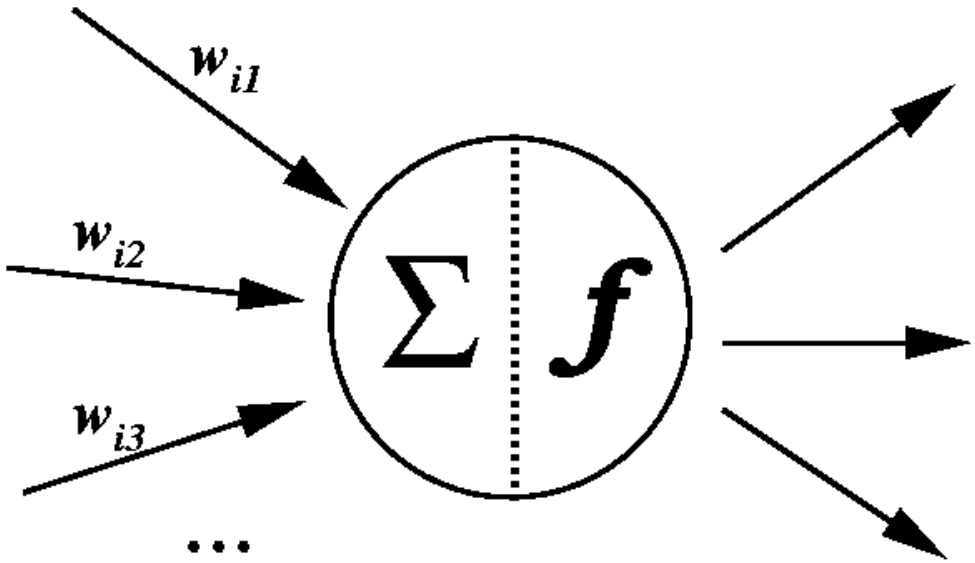
A physical neuron



ARTIFICIAL NEURON MODEL



ARTIFICIAL NEURON MODEL



$$y_i = f(net_i)$$

Basic elements of neural networks are:

- Input nodes
- Weights
- Activation function
- Total signal reaching at output are given by:

$$\text{Output (y)} = \sum_{i=1}^{n} Wi\, Xi$$

- Output may be more than one it depends on number of neuron i.e. multiple neuron will cause multiple output.

Types of Learning

- **Supervised (inductive) learning**
- Training data includes desired outputs
- **Unsupervised learning**
  - Training data does not include desired outputs
- **Semi-supervised learning**
  - Training data includes a few desired outputs
- **Reinforcement learning**
  - Rewards from sequence of actions

Performance

- Several factors affecting the performance:
  - Types of training provided
    - The form and extent of any initial background knowledge
  - The type of feedback provided
  - The learning algorithms used

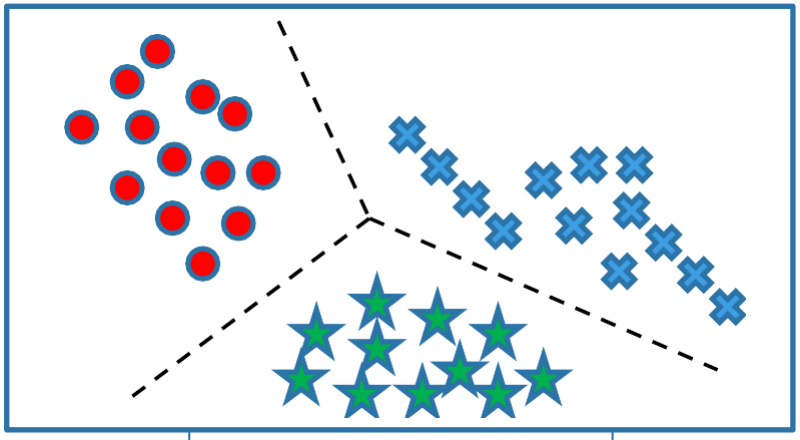
Algorithms

- The success of machine learning system also depends on the algorithms.
- The algorithms control the search to find and build the knowledge structures.
- The learning algorithms should extract useful information from training examples.

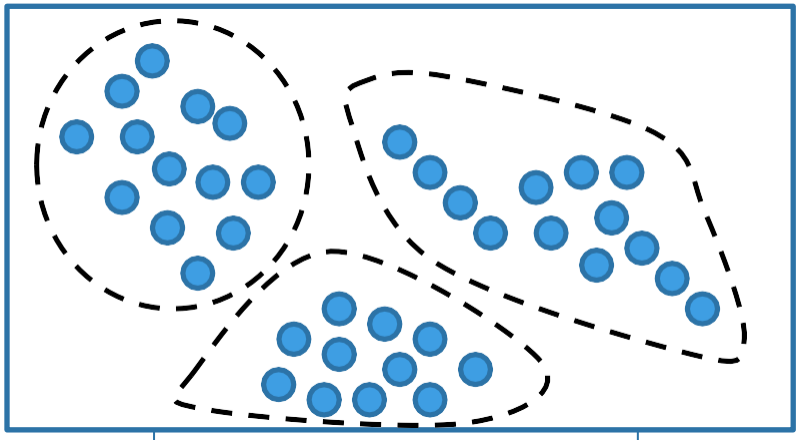
Algorithms

- **Supervised learning**
  - Prediction
  - Classification (discrete labels), Regression (real values)
- **Unsupervised learning**
  - Clustering
  - Probability distribution estimation
  - Finding association (in features)
  - Dimension reduction
- **Semi-supervised learning**
- **Reinforcement learning**
  - Decision making (robot, chess machine)

Algorithms

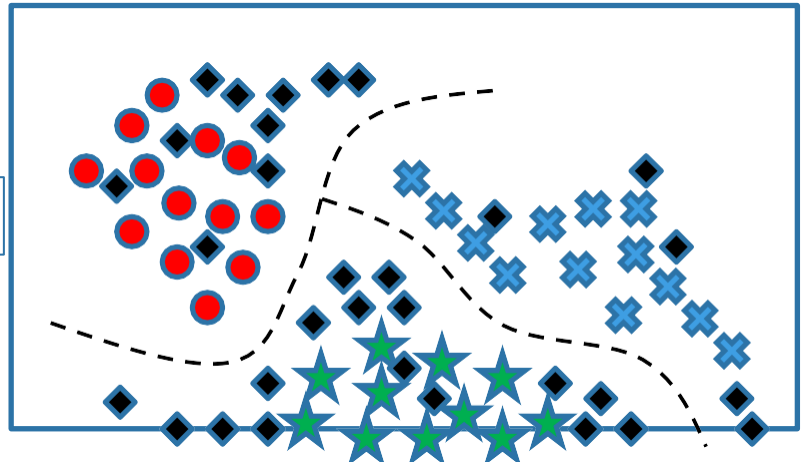


Supervised learning



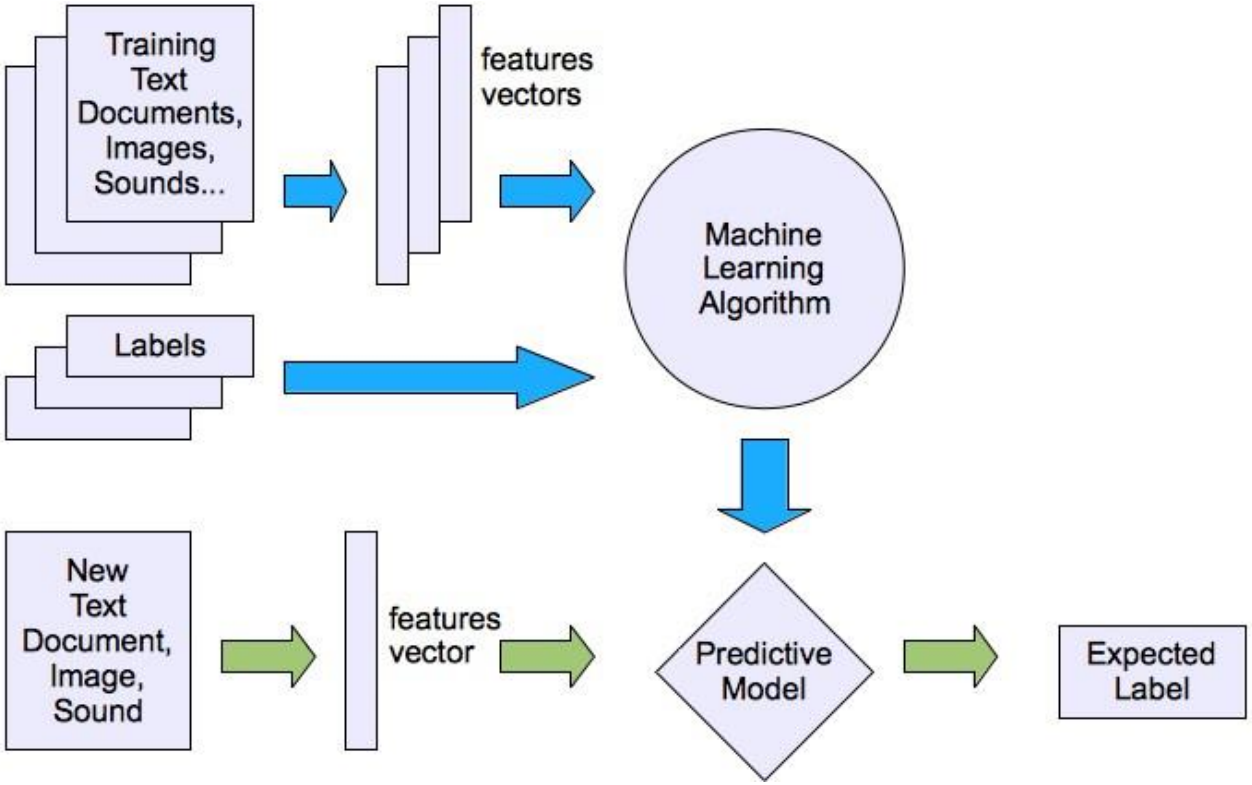
Unsupervised learning

Semi-supervised learning



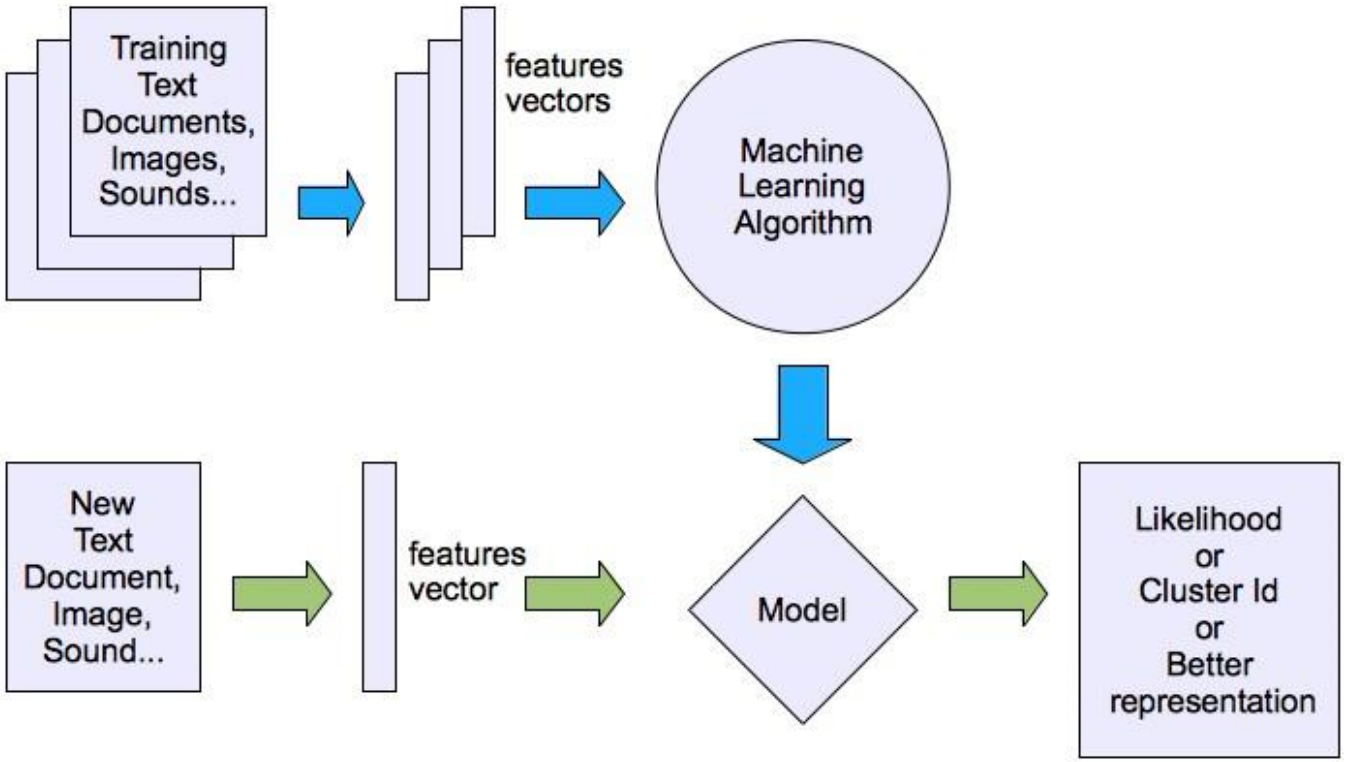
Machine learning structure

- Supervised learni



Machine learning structure

- Unsupervised learning



DEFINITIONS OF NEURAL NETWORKS

According to Nigrin (1993), p. 11:

A neural network is a circuit composed of a very large number of simple processing elements that are neurally based. Each element operates only on local information.

Furthermore each element operates asynchronously; thus there is no overall system clock.

According to Zurada (1992):

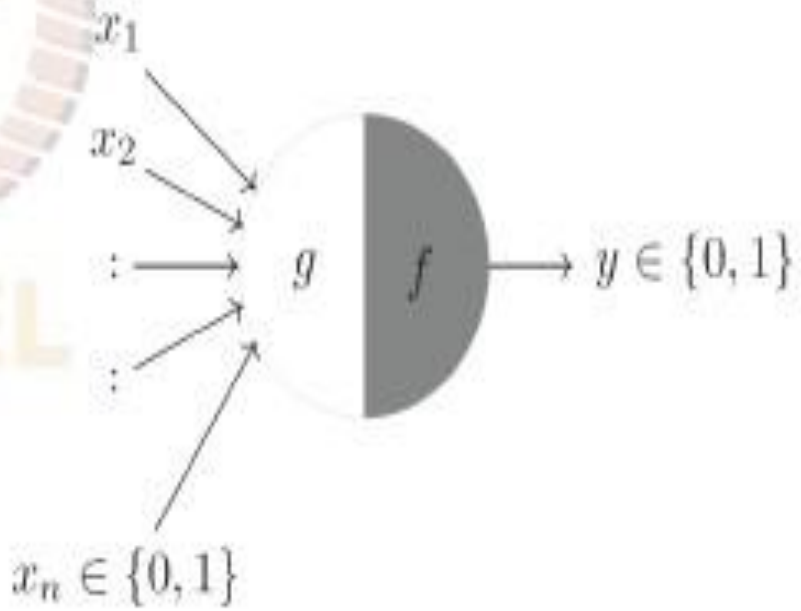
Artificial neural systems, or neural networks, are physical cellular systems which can acquire, store and utilize experiential knowledge.

McCulloch-Pitts Neuron

- McCulloch (neuroscientist) and Pitts (logician) proposed a highly simplified computational model of the neuron (1943)
- g aggregates the inputs and the function f takes a decision based on this aggregation
- The inputs can be excitatory or inhibitory
- $y = 0$ if any x_i is inhibitory, else

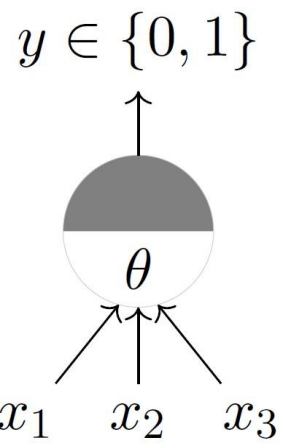
$$g(x_1, x_2, \ldots, x_n) = g(\mathbf{x}) = \sum_{i=1}^{n} x_i$$

$$y = f(g(\mathbf{x})) = 1 \text{ if } g(\mathbf{x}) \geq \theta$$
$$= 0 \text{ if } g(\mathbf{x}) < \theta$$

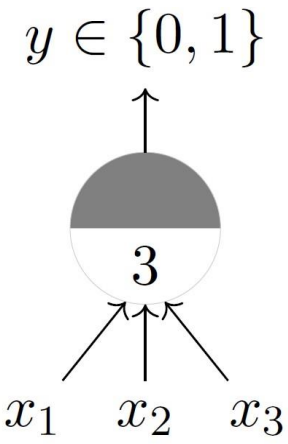


- θ is a thresholding parameter

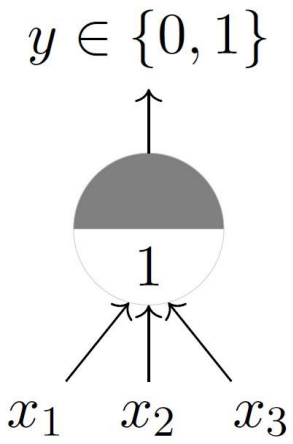
McCulloch-Pitts Neuron



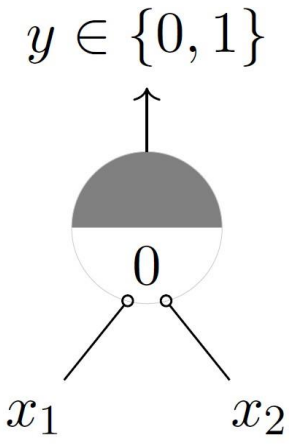
A McCulloch-Pitts Unit



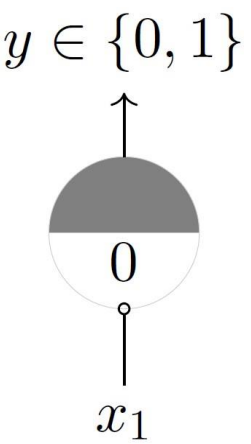
AND function



OR function



NOR function



NOT function

- Feedforward MP networks can compute any Boolean function $f : \{0, 1\}^n \to \{0, 1\}$
- Recursive MP networks can simulate any Deterministic Finite Automaton (DFA) (S

Perceptrons

- Frank Rosenblatt, an American psychologist, proposed the perceptron model (1958)
- Later refined and carefully analyzed by Minsky and Papert (1969)
- A more general computational model than McCulloch-Pitts neurons
- Inputs are no longer limited to boolean values

$$g(x_1, x_2, \ldots, x_n) = g(\mathbf{x}) = \sum_{i=1}^{n} w_i * x_i$$

$$y = f(g(\mathbf{x})) = 1 \text{ if } g(\mathbf{x}) \geq \theta$$
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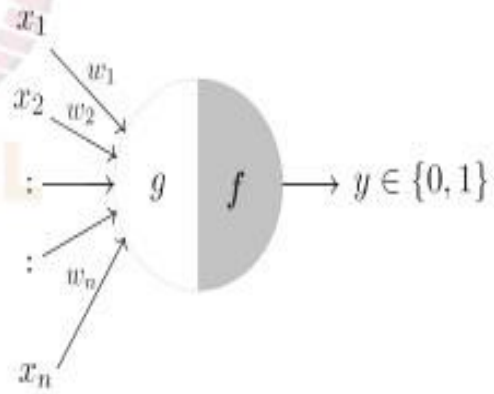

Perceptrons

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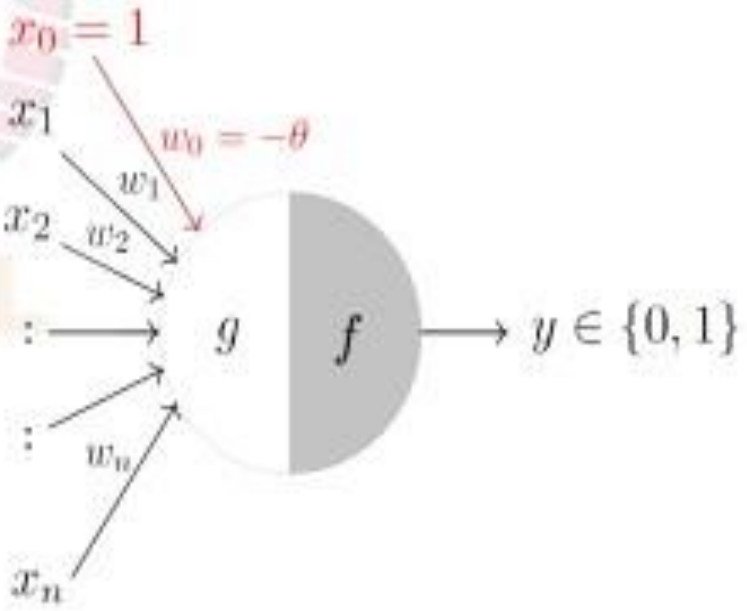
- Inputs are no longer limited to boolean values

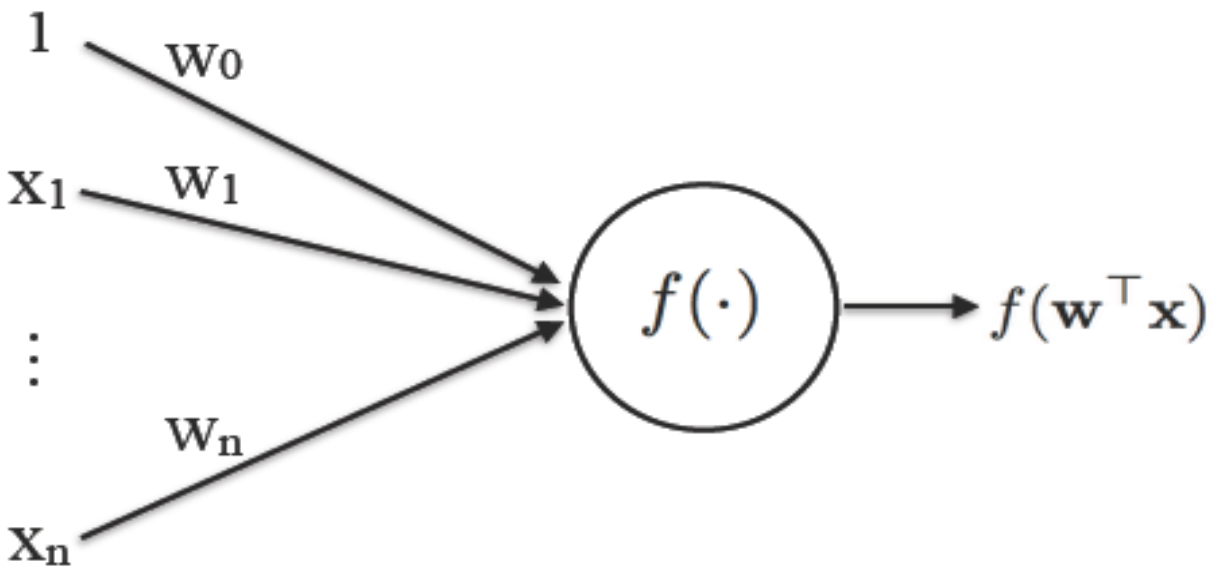
- A more accepted convention

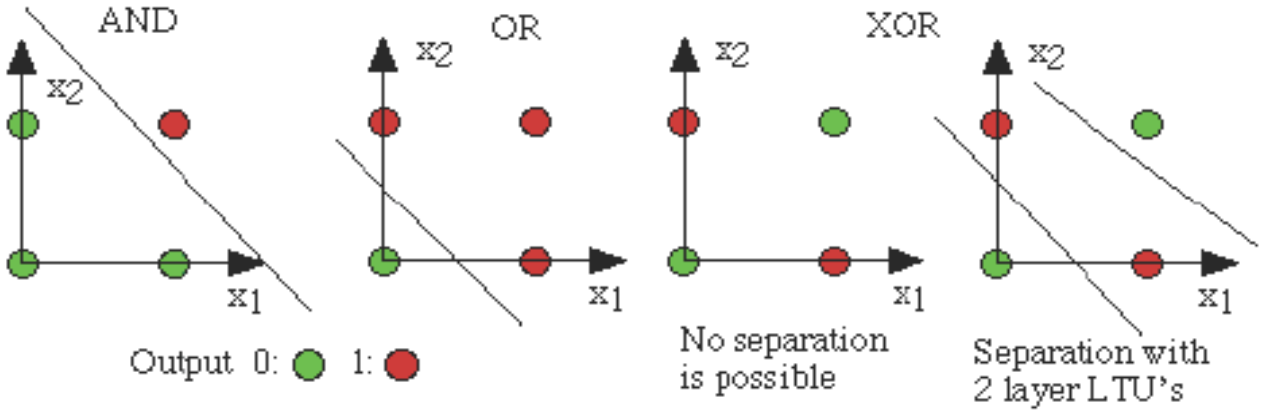
$$g(x_1, x_2, \ldots, x_n) = g(\mathbf{x}) = \sum_{i=0}^{n} w_i * x_i$$

$$y = f(g(\mathbf{x})) = 1 \text{ if } g(\mathbf{x}) \geq 0$$
$$= 0 \text{ if } g(\mathbf{x}) < 0$$
$$\text{where } x_0 = 1 \text{ and } w_0 = -\theta$$



F


1
W0
X1
W1
f(·)
f(w⊤x)
Wn
Xn

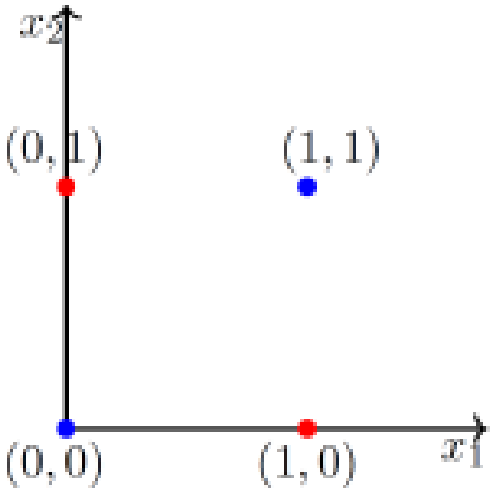

AND
x2
x1
OR
x2
x1
XOR
x2
x1
x2
x1
Output 0:
1:
No separation
is possible
Separation with
2 layer LTU's

The X O R Problem

x_1	x_2	XOR	
0	0	0	$w_0 + \sum_{i=1}^{2} w_i x_i < 0$
1	0	1	$w_0 + \sum_{i=1}^{2} w_i x_i \geq 0$
0	1	1	$w_0 + \sum_{i=1}^{2} w_i x_i \geq 0$
1	1	0	$w_0 + \sum_{i=1}^{2} w_i x_i < 0$

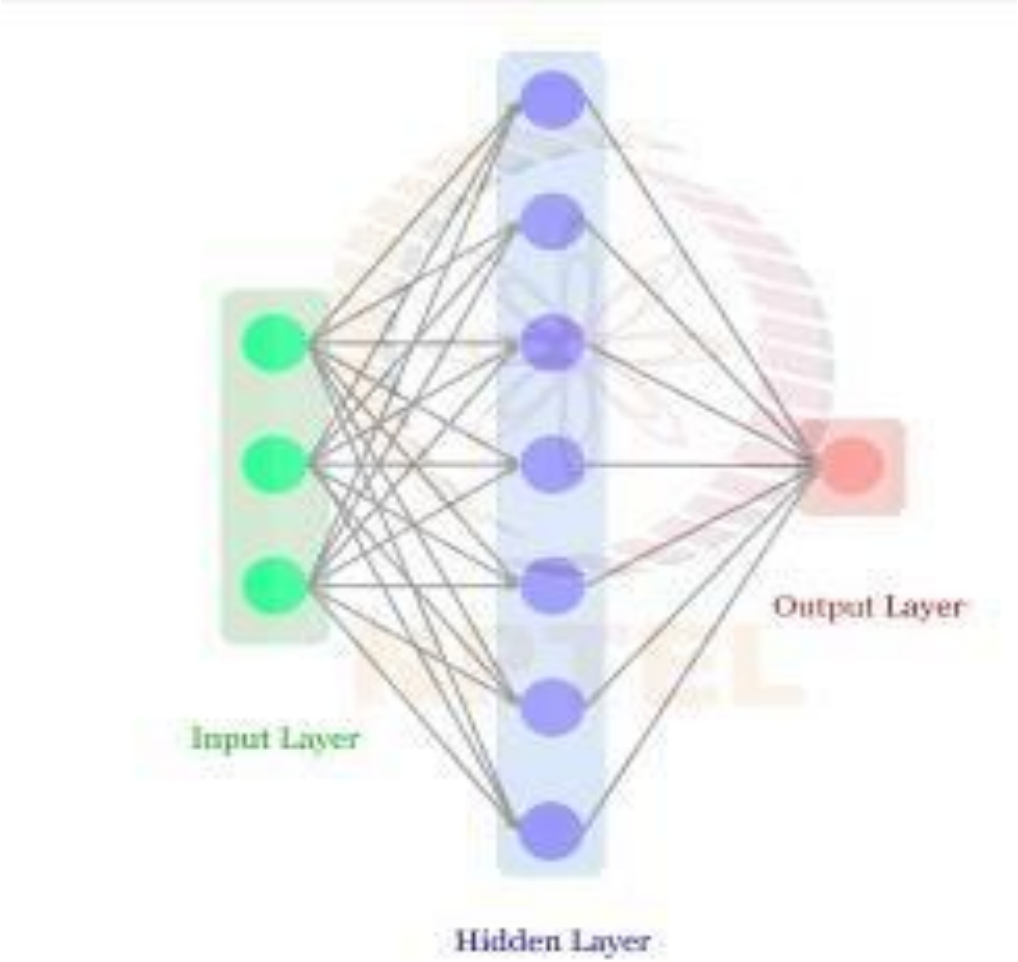
$$w_0 + w_1 \cdot 0 + w_2 \cdot 0 < 0 \implies w_0 < 0$$
$$w_0 + w_1 \cdot 1 + w_2 \cdot 0 \geq 0 \implies w_1 > -w_0$$
$$w_0 + w_1 \cdot 0 + w_2 \cdot 1 \geq 0 \implies w_2 > -w_0$$
$$w_0 + w_1 \cdot 1 + w_2 \cdot 1 < 0 \implies w_1 + w_2 < -w_0$$

- The fourth condition contradicts conditions 2 and 3
- No solution possible satisfying this set of inequalities

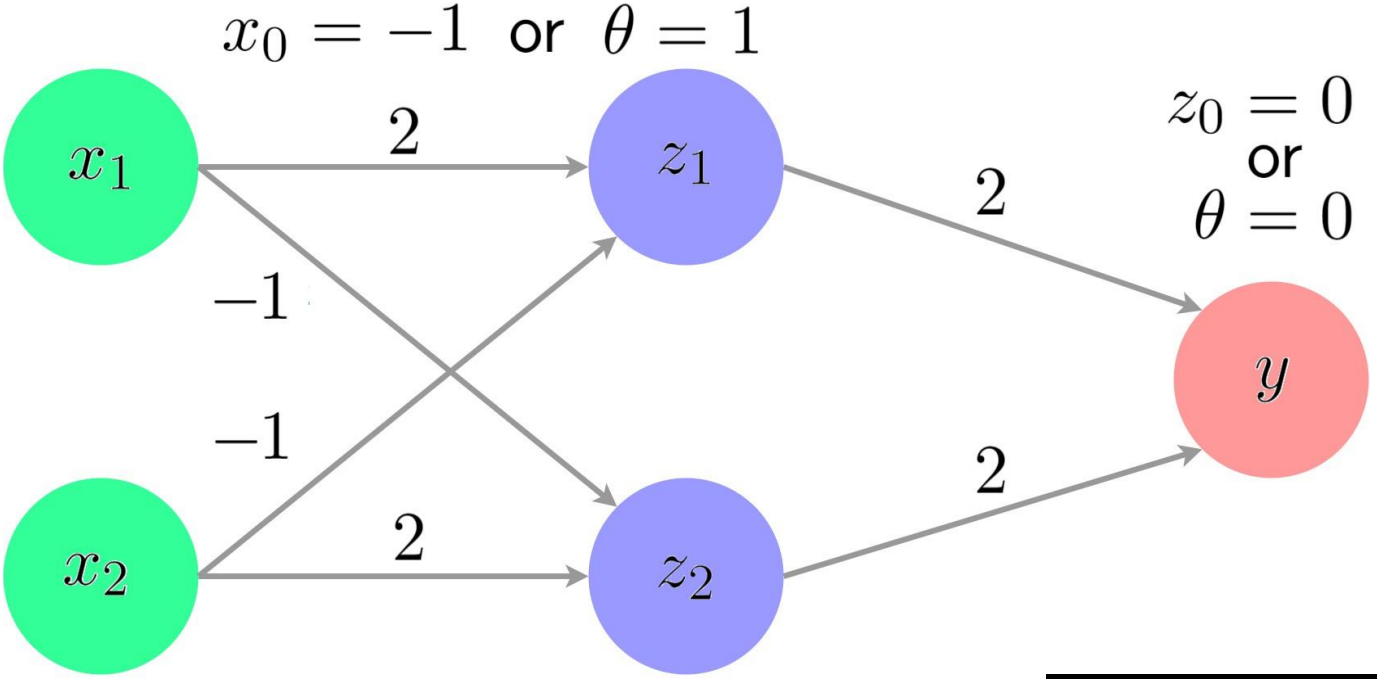


- Indeed you can see that it is impossible to draw a line which separates the red points from the blue points

Multi-Layer Perceptrons



Solving XOR with Multi-Layer Perceptrons



(x_1, x_2)	(z_1, z_2)	y
(0,0)	(0,0)	0
(0,1)	(0,0)	1
(1,0)	(1,0)	1
(1,1)	(0,0)	0

Going Beyond Binary Inputs and Outputs

Question

- What about arbitrary functions of the form $y = f(x)$ where $x \in \mathbf{R}^n$ (instead of $\{0,1\}^n$) and $y \in \mathbf{R}$ (instead of $\{0,1\}$)?
- Can we use the same perceptron model to represent such functions?

Need of activation function

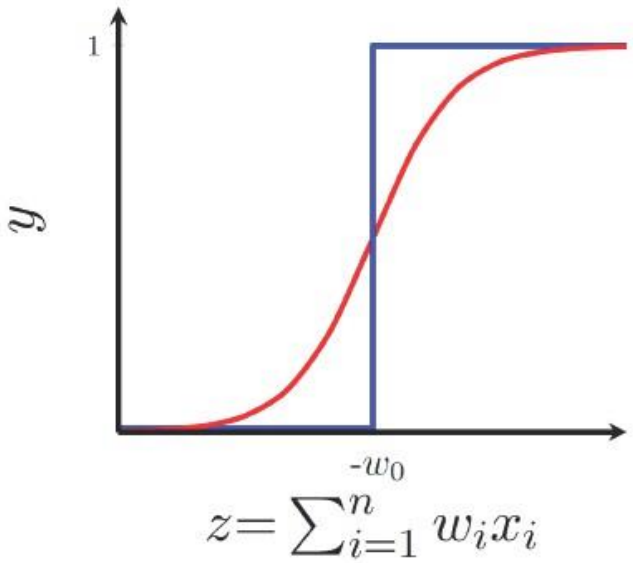
1. Introducing Non-Linearity:
•Without activation functions, a neural network would simply be a linear combination of inputs and weights, limited to modeling only linear relationships.
2. Learning Complex Representations:
•Activation functions enable neurons to learn more intricate representations of data.
3. Decision-Making Capabilities:
•Activation functions introduce decision-making power to neurons.
•Based on the activation function's output, a neuron can decide whether to "fire" or not, influencing the flow of information through the network and ultimately shaping the model's output.
4. Controlling Output Range:
•Activation functions can regulate the output range of neurons.
•Some activation functions, like sigmoid and tanh, constrain outputs between 0 and 1 or -1 and 1, making them suitable for probability-related tasks.
•Others, like ReLU, allow for unbounded positive outputs, useful for representing real-valued quantities.

Need for activation function
Sigmoid function

- We could use any logistic function to obtain a smoother output function than a step function
- One form is the sigmoid function:

$$y = \frac{1}{1 + e^{-(w_0 + \sum_{i=0}^{n} w_i x_i)}}$$

- No longer a sharp transition at the threshold $-w_0$
- Also, output is no longer binary but a real value between 0 and 1 which can be interpreted as a probability
- Unlike the step function, this one is smooth, continuous at $-w_0$ and most importantly **differentiable**

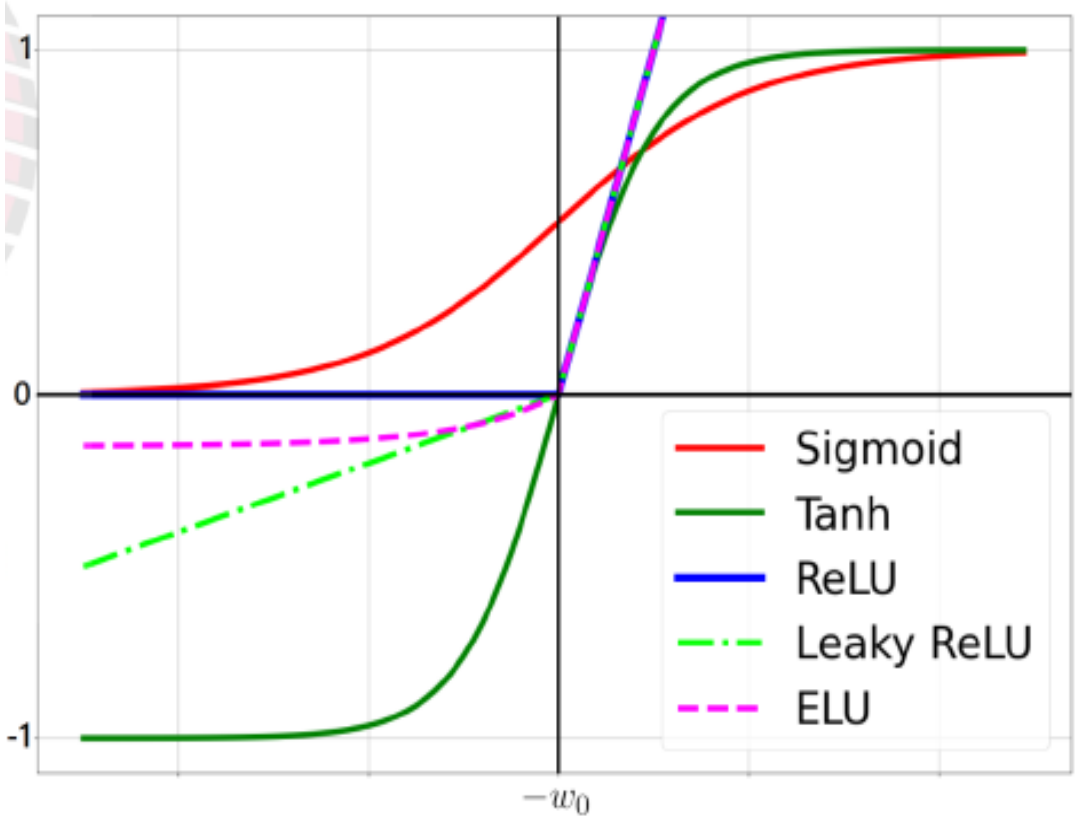


Activation Function

Identity		$f(x) = x$
Binary step		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
Logistic (a.k.a. Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$
TanH		$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$
ArcTan		$f(x) = \tan^{-1}(x)$
Softsign [7][8]		$f(x) = \frac{x}{1 + \lvert x \rvert}$
Rectified linear unit (ReLU)[9]		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$

Activation Function

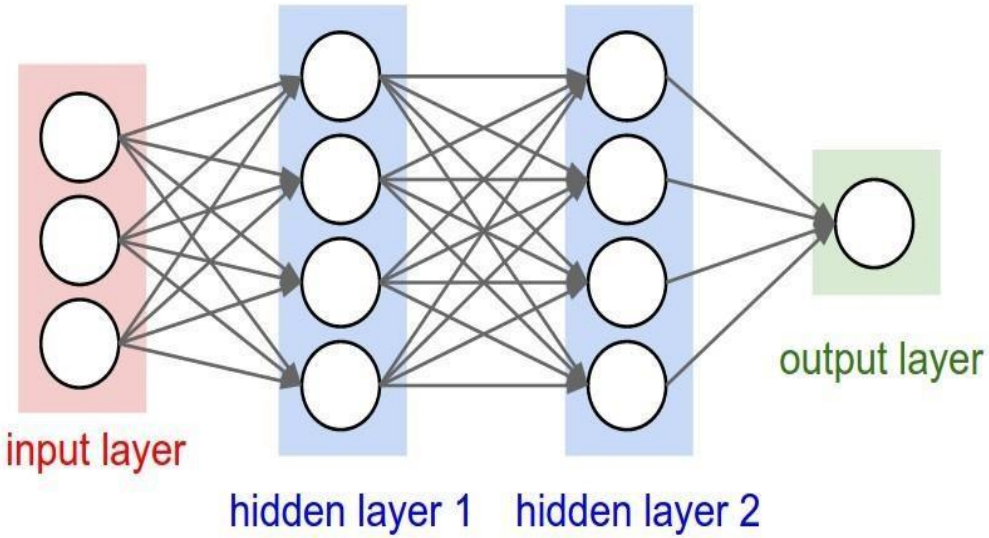
- **Leaky ReLU:** $y = \max(\alpha z, z), \alpha \in (0, 1)$
- **Exponential Linear Unit (ELU):**
  $y = \max(\alpha(e^z - 1), z)$, where $\alpha > 0$



Feedforward Neural Networks and Backpropagation

Feedforward Networks

A feedforward neural network, also called a multi-layer perceptron, is a collection of neurons, organized in *layers*.



It is used to approximate some function f^*. For instance, f^* could be a classifier that maps an input vector $\boldsymbol{x}$ to a category $\boldsymbol{y}$.

The neurons are arranged in the form of a directed acyclic graph i.e., the information only flows in one direction - input $\boldsymbol{x}$ to output $\boldsymbol{y}$. Hence the term **feedforward**.

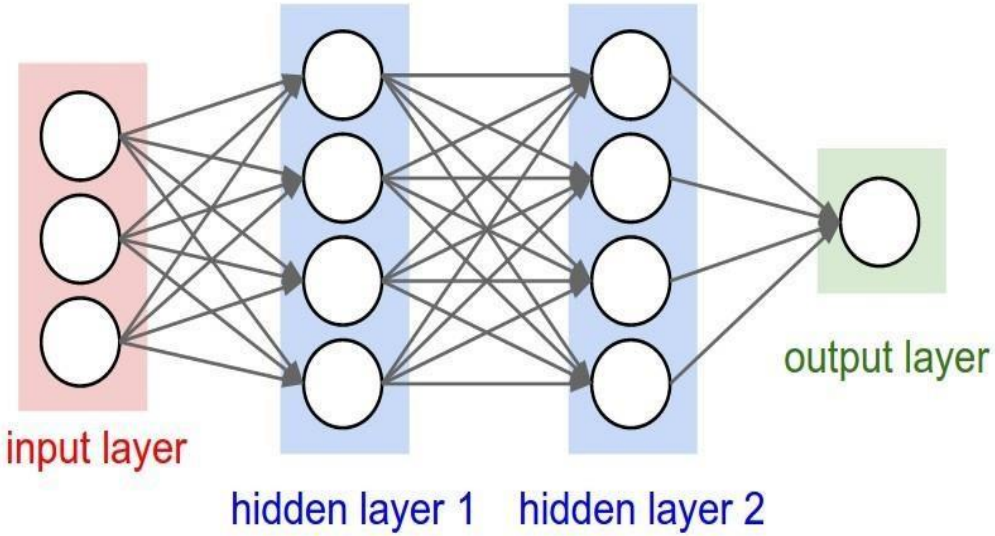
- How Do FNNs Work?
- Imagine a network of interconnected artificial neurons, each capable of processing information and making simple decisions. In an FNN, these neurons are organized in layers:

- Input layer: Receives the raw data.

- Hidden layers: Perform computations and extract features from the data. There can be one or several hidden layers depending on the complexity of the problem.

- Output layer: Produces the final prediction or result.

Feedforward Networks



The number of layers in the network (excluding the input layer) is known as depth

Each neuron can be seen as a **vector**-to-**scalar** function which takes a vector of inputs

from the previous layer and computes a scalar value.

Above network can be seen as a composition of functions $y = f^{(3)}(f^{(2)}(f^{(1)}(x)))$, $f^{(1)}$ being the first hidden layer, $f^{(2)}$ being the second and $f^{(3)}$ being the final output layer.

- How information travels through the Forward Network:

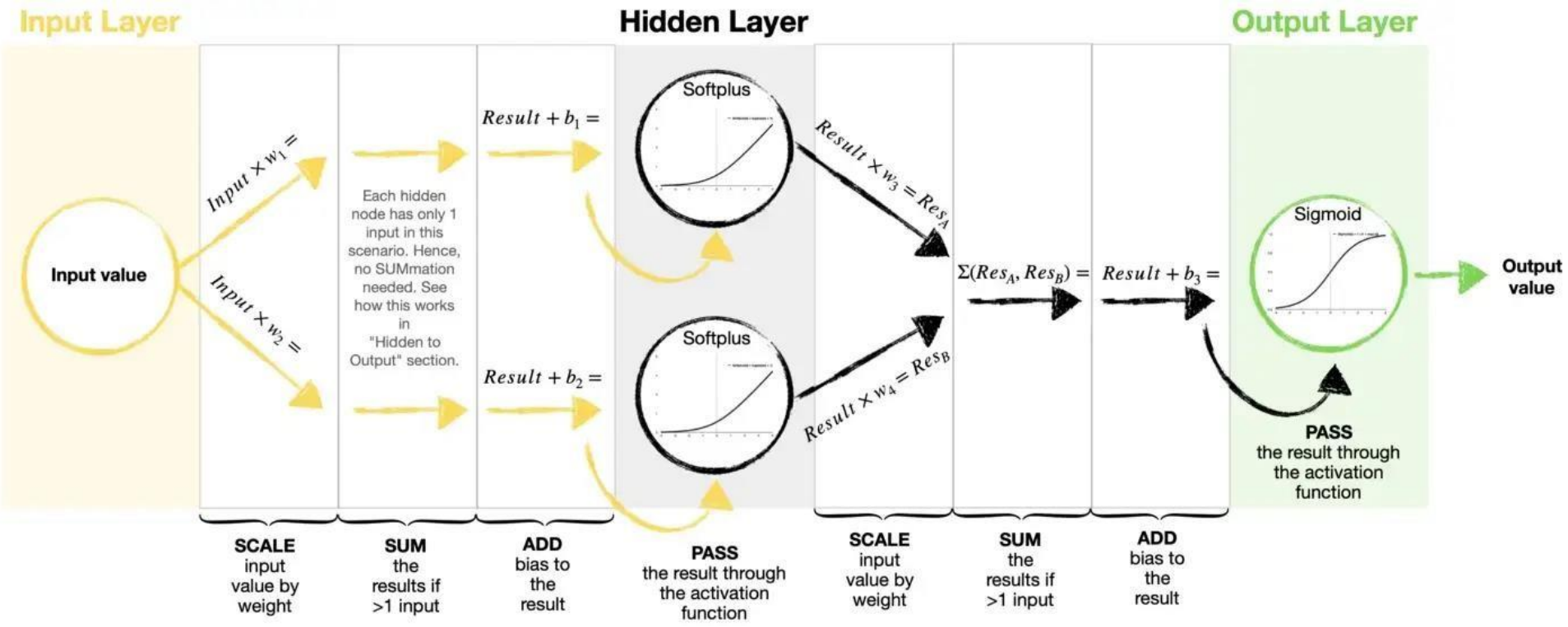
1.Inputs:

- Each neuron in the input layer receives a specific element from the data point.
- 2. Weighted Sum:
- Each hidden neuron sums the products of its inputs with their corresponding weights (coefficients).
- 3. Activation:
- The neuron applies an activation function (e.g., sigmoid, ReLU) to the weighted sum to introduce non-linearity.
- 4. Output:
- The output neuron combines the activated signals from the hidden layer and performs its own activation, producing the final prediction.

Feedforward Networks

- To approximate some function f^*, we are generally given noisy estimates of $f^*(\boldsymbol{x})$ at different points, in the form of a dataset $\{\boldsymbol{x}_i, y_i\}_{i=1}^{M}$.
- Our neural network defines a function $y = f(\boldsymbol{x}; \theta)$. Our goal is to learn the parameters (weights and biases) θ such that f best approximates f^*.
- How to find the values of the parameters i.e., train the network?
- **Gradient Descent**, the go-to method to train neural networks

Feedforward Networks



Gradient Descent

- Gradient descent is an optimization algorithm used to adjust the weights and biases of the network, ultimately leading it to learn and improve its performance on a specific task.
- How it works:
- 1. Objective Function and Error:
- We start with an objective function, which quantifies the network's performance on the training data. Examples include mean squared error for regression or cross-entropy for classification.
- During training, the network predicts outputs for each data point, and these predictions are compared to the actual targets. The difference between the prediction and the target is called the error.

Gradient Descent

- 2. Gradient Calculation:
- Gradient descent relies on the concept of a gradient, which essentially tells us how quickly the error changes with respect to each weight and bias in the network.
- By calculating the gradients for each parameter, we understand how changing that parameter would affect the overall error.

- 3. Weight and Bias Update:
- The core idea of gradient descent is to take small steps in the direction that reduces the error.
- We use the calculated gradients to update the weights and biases of the network. The update typically follows a rule like weight = weight - learning_rate * gradient, where learning_rate determines the step size.

Gradient Descent

- 4. Iteration and Optimization:
- This process of calculating gradients, updating weights, and computing predictions is repeated iteratively over the entire training data multiple times (epochs).
- With each iteration, the network gradually adjusts its parameters, learning the underlying patterns in the data and improving its ability to make accurate predictions.

Gradient Descent:A 1D Example

- Neural networks are usually trained by minimizing a loss function, such as mean square error:

$$Loss_{MSE} = \frac{1}{M}\sum_{i=1}^{M}(f^*(x) - f(x;\theta))^2$$

- Let us consider a simple 1D example, where we try to minimize the function $f(x) = \frac{1}{2}x^2$.
  Specifically, we find out the value x^* gives the smallest value for $f(x)$ i.e., $f(x^*)$.

$$x^* = \arg\min_x f(x)$$

Gradient Descent: A 1D Example

- We can obtain the slope of the function $f(x)$ at x by taking its derivative i.e., $f'(x)$.

Gradient Descent: A 1D Example

- We can obtain the slope of the function $f(x)$ at x by taking its derivative i.e., $f'(x)$.
- This means, if we give a very small *push* to x in the direction (sign) of the slope, we're sure that the function will increase.

$$f(x + p \cdot \text{sign}(f'(x))) > f(x) \quad \text{for an infinitesimally small } p$$

Gradient Descent: A 1D Example

- We can obtain the slope of the function $f(x)$ at x by taking its derivative i.e., $f'(x)$.
- This means, if we give a very small *push* to x in the direction (sign) of the slope, we're sure that the function will increase.

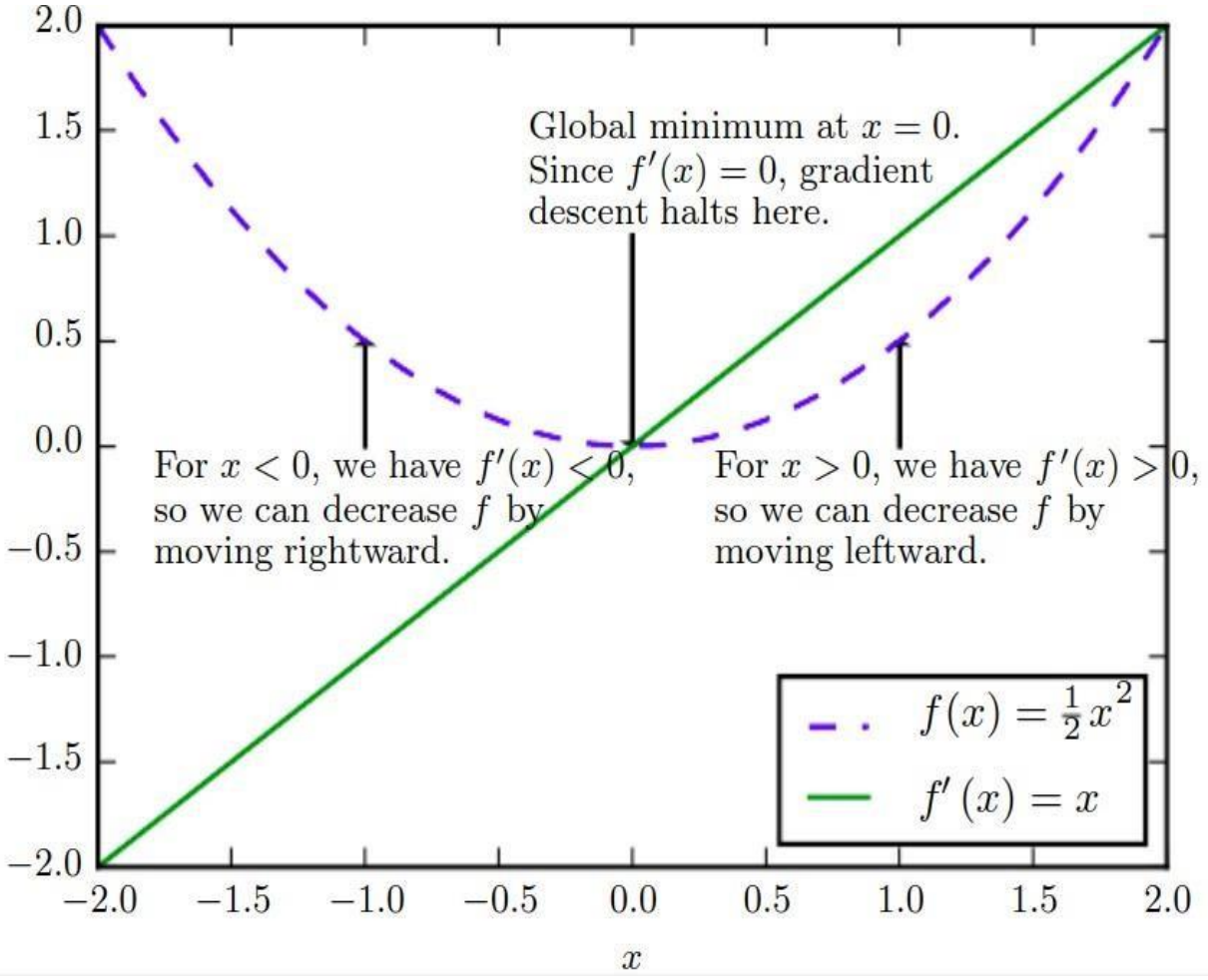
$$f(x + p \cdot \text{sign}(f'(x))) > f(x) \quad \text{for an infinitesimally small } p$$

- The reverse is also true i.e.,

$$f(x - p \cdot \text{sign}(f'(x))) < f(x) \quad \text{for an infinitesimally small } p$$

- This forms the basis for gradient descent - we start off at a random x, and take small steps in the direction of the **negative** gradient.

Gradient Descent: A 1D Example



Gradient Descent 1D Example

Imagine a hiker descending a hilly terrain to reach the lowest point (valley). Gradient descent mimics this process to find the minimum of a function.

Key concepts:

•Function: The hill you're navigating, represented by a mathematical equation (e.g., f(x) = x^2).

•Gradient: The slope of the hill at any point, indicating the direction of steepest ascent or descent.

•Learning rate: The hiker's step size, controlling how far they move in each iteration.

Steps:

1.Start: Choose an initial position (x-value) on the hill.

2.Calculate gradient: Determine the slope (derivative) of the function at this position.

3.Take a step: Move in the direction opposite to the gradient (downhill), with a step size determined by the learning rate.

4.Repeat: Calculate the gradient at the new position and take another step, continuing until you reach the valley (or a close approximation).g

Example

Function:

•We're working with the function f(x) = x^2, which represents a parabolic curve (like a hill) with its minimum at x = 0.

Initial Position:

•We start at x = 3, meaning the hiker is standing on the hill at a point where the value of f(x) is 9.

Learning Rate:

•The learning rate is set to 0.1, which controls how large each step the hiker takes will be.

Iteration 1:

1.Calculate gradient:

- •The gradient of f(x) = x^2 is 2x.
- •At x = 3, the gradient is 6 (the slope of the hill is positive and steep).

2.Take a step:

- •Since we want to move downhill, we take a step in the opposite direction of the gradient.
- •The step size is -0.1 * 6 (learning rate multiplied by gradient), which equals -0.6.

3.New position:

- •The hiker's new position becomes x = 3 - 0.6 = 2.4.

Example…

Iteration 2:

1.Calculate gradient:

- At x = 2.4, the gradient of f(x) = x^2 is 4.8.

2.Take a step:

- The step size is -0.1 * 4.8 = -0.48.

3.New position:

- The hiker moves to x = 2.4 - 0.48 = 1.92.

Repeat iterations:

- This process continues, with the hiker taking steps based on the gradient, gradually moving closer to the minimum of the function.
- The iterations stop when the hiker reaches a point where the gradient is very close to zero, indicating they're at (or very near) the bottom of the valley.

Why Negative Gradient?

•The gradient of the loss function points in the direction of the steepest increase in loss.
•We want to minimize the loss, so we take a step in the opposite direction, which is achieved by multiplying the gradient by -1.

Imagine a landscape:
•The loss function forms a landscape with valleys (minima) and hills (maxima).
•The negative gradient points us down the steepest slope of the hill towards the valley.
•By iteratively taking steps in this direction, we eventually reach the bottom of the valley (minimum loss), improving the network's accuracy.

Why Negative Gradient?

Benefits of using the negative gradient:

- Helps find the optimal parameters that minimize the loss function.
- Enables efficient learning by guiding the network towards better predictions.
- Forms the basis for various optimization algorithms used in neural network training.
- the negative gradient in neural networks plays a critical role in guiding the learning process and adjusting parameters to minimize the loss function, ultimately leading to improved network performance and accurate predictions.

Why Negative Gradient?

- Consider the multivariate case, since while training neural networks, the loss function we minimize is parametrized by multiple weights, ϑ
- For simplicity, we denote our loss function as $L(\vartheta)$. Our aim is to find the weight vector ϑ which minimizes $L(\vartheta)$
- Let **u**, a unit vector, be the direction that takes us to the minimum, i.e.:

$$\min_{\mathbf{u}, \mathbf{u}^T\mathbf{u}=1} \mathbf{u}^T \nabla_\theta L(\theta)$$

$$= \min_{\mathbf{u}, \mathbf{u}^T\mathbf{u}=1} \|\mathbf{u}\|_2 \|\nabla_\theta L(\theta)\|_2 \cos\beta$$

- Since $\|\boldsymbol{u}\|_2 = 1$, we can minimize the above function when $\beta = 180^0$, i.e. when **u** is the direction of **negative** gradient

How to use Gradient Descent

We can use Gradient Descent to train neural networks as follows:

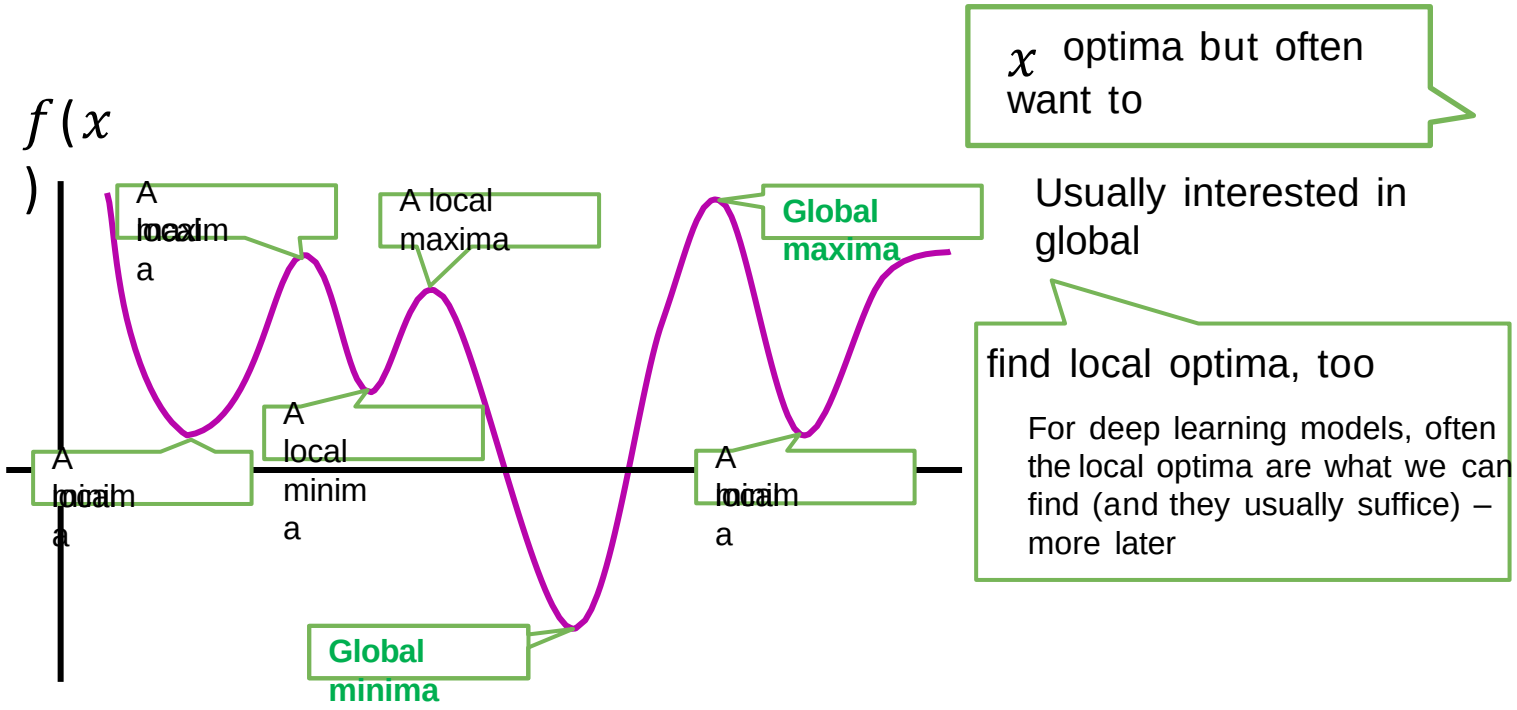
- Start with a random weight vector θ.
- Compute the loss function over the dataset, i.e., $L(\theta)$ with the current network, using a suitable loss function such as mean-squared error
- Compute the gradients of the loss function with respect to each weight value $\frac{\delta L}{\delta \theta_i}$.
- Update the weights as follows, where η is the learning rate i.e., the amount by which the weight is changed in each step:

$$\theta_i^{next} = \theta_i^{curr} - \eta \frac{\delta L}{\delta \theta_i^{curr}}$$

We can repeat the above steps until the gradient is zero.

Functions and their optima

- Many ML problems require us to optimize a function f of some variable(s) x
- For simplicity, assume f is a scalar-valued function of a scalar $x (f: \mathbb{R} \rightarrow \mathbb{R})$



- Any function has one/more optima (maxima, minima), and maybe saddle points
- Finding the optima or saddles requires derivatives/gradients of the function

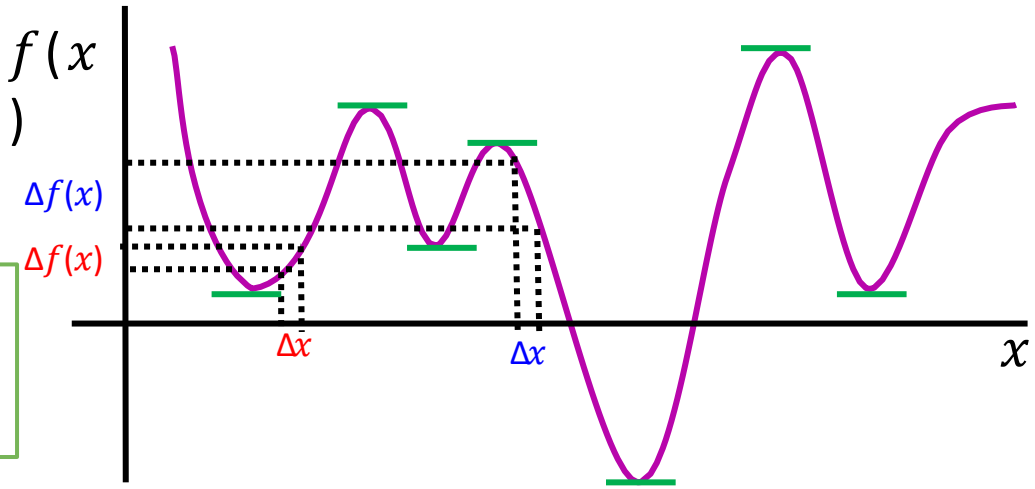
Derivatives

- Magnitude of derivative at a point is the rate of change of the func at that point

$$\frac{df(x)}{dx} = \lim_{\Delta x \to 0} \frac{\Delta f(x)}{\Delta x}$$

Sign is also important: Positive derivative means f is increasing at x if we increase the value of x by a very small amount; negative derivative means it is decreasing

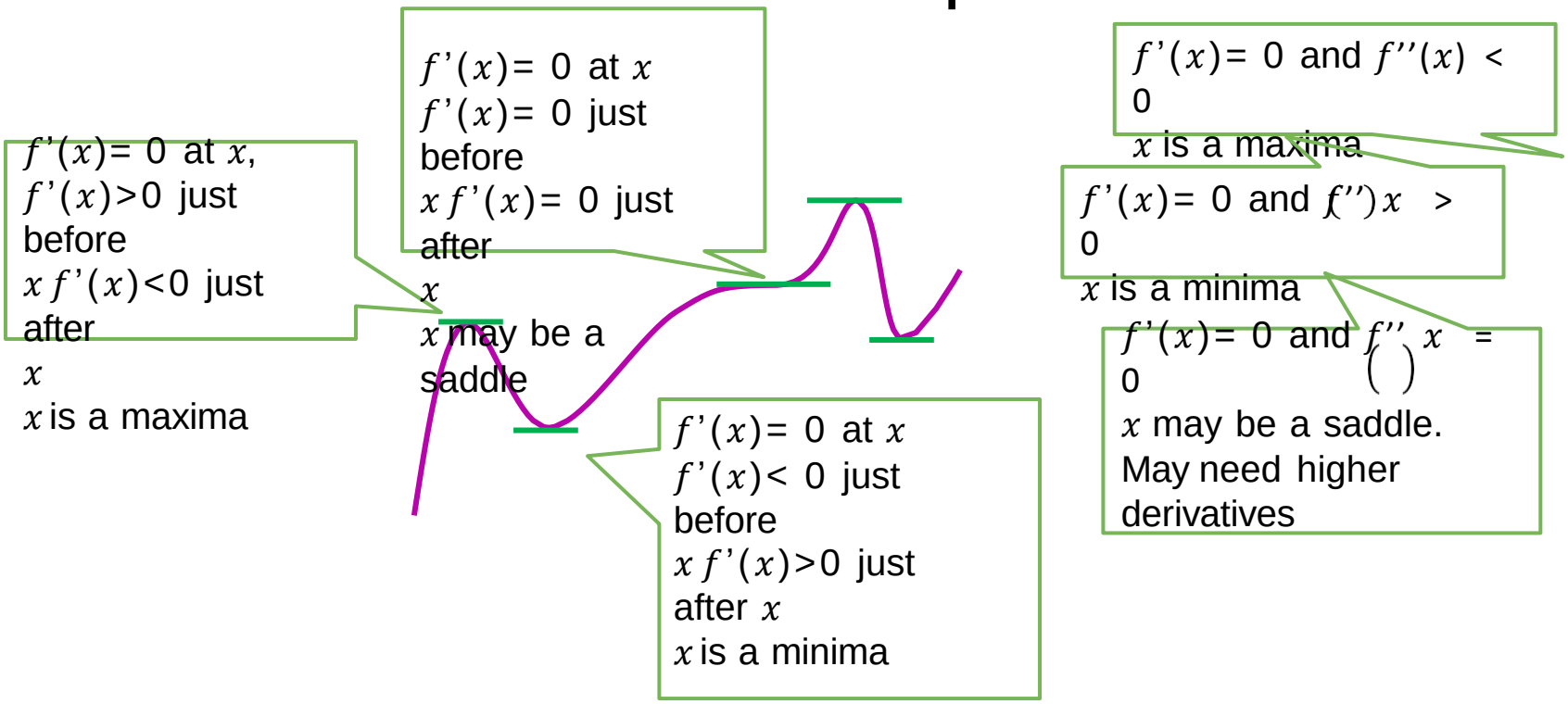
Understanding how f changes its value as we change x is helpful to understand optimization (minimization/maximization) algorithms



- Derivative becomes zero at stationary points (optima or saddle points)
  - The function becomes "flat"((Δf x = 0 if we change x by a very little at such points)
  - These are the points where the function has its maxima/minima (unless they are saddles)

Derivatives

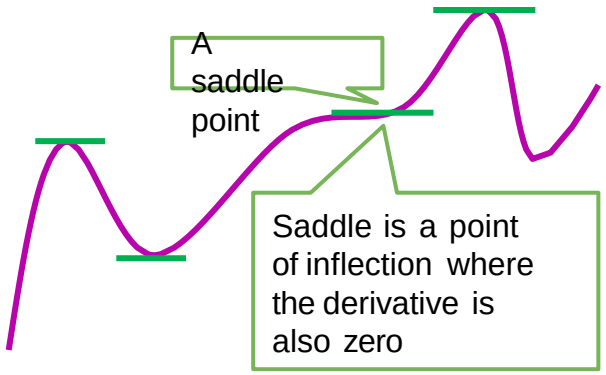
- How the derivative itself changes tells us about the function's optima

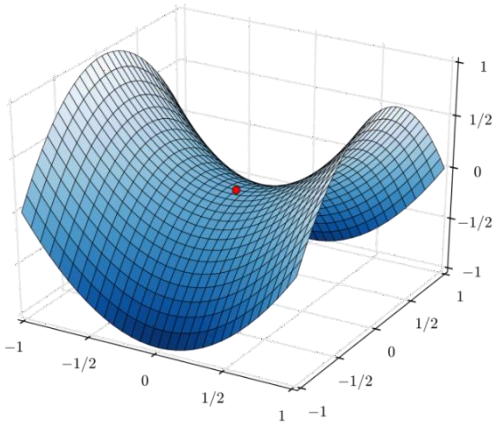


- The second derivative $f''(x)$ can provide this information

Saddle Points

- Points where derivative is zero but are neither minima nor maxima [49]



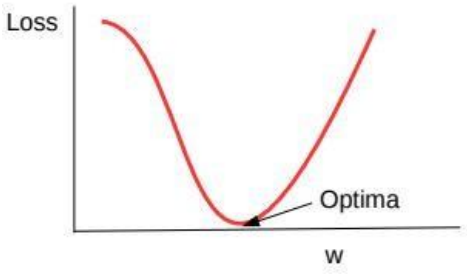


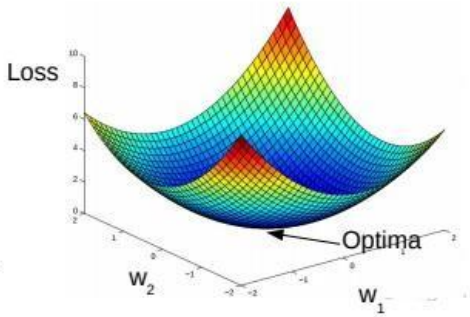
- Saddle points are very common for loss functions of deep learning models
  - Need to be handled carefully during optimization

- Second or higher derivative may help identify if a stationary point is a saddle

Convex and Non-Convex Functions

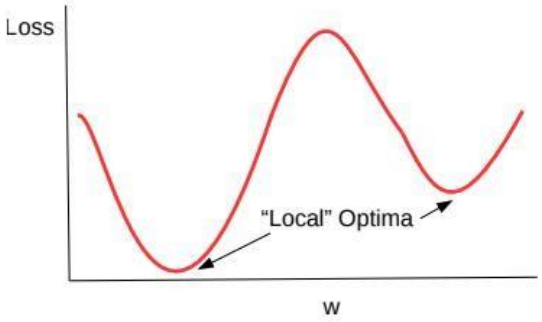
- A function being optimized can be either convex or non- convex

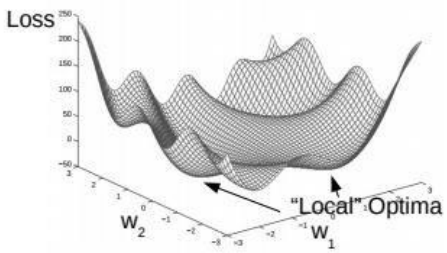




Convex functions are bowl-shaped. They have a unique optima (minima)

Negative of a convex function is called a concave function, which also has a unique optima (maxima)



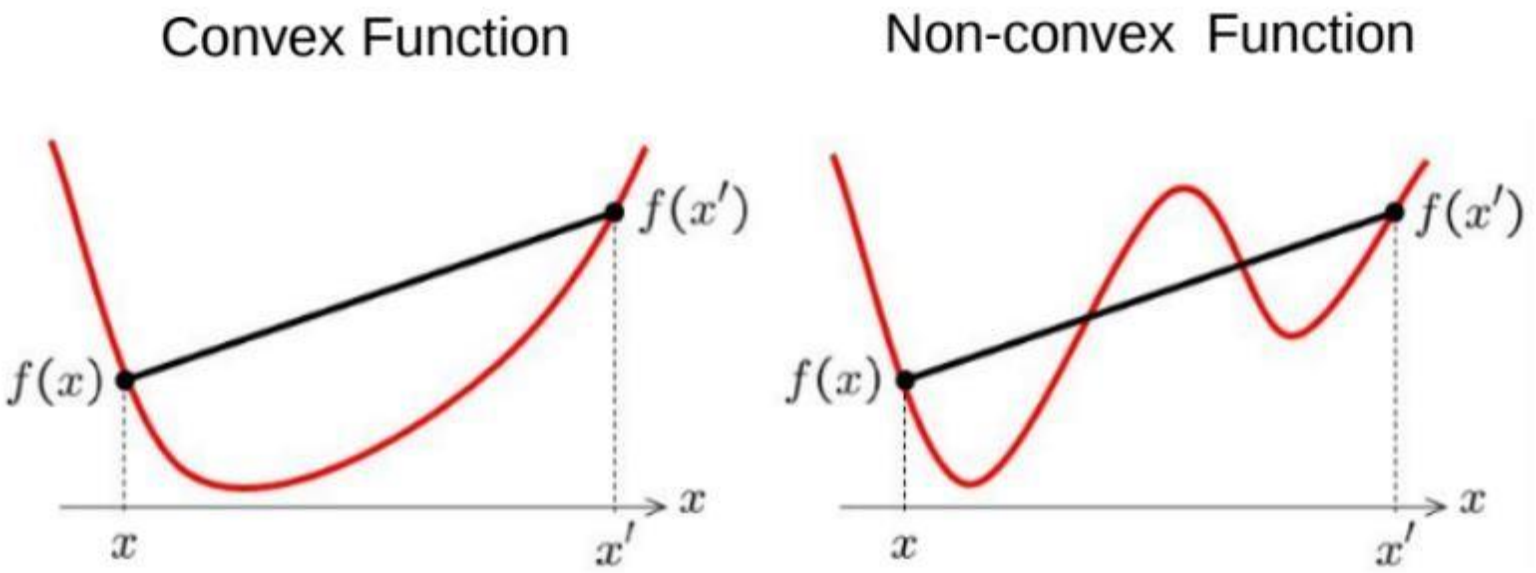


Non-convex functions have multiple minima. Usually harder to optimize as compared to convex functions

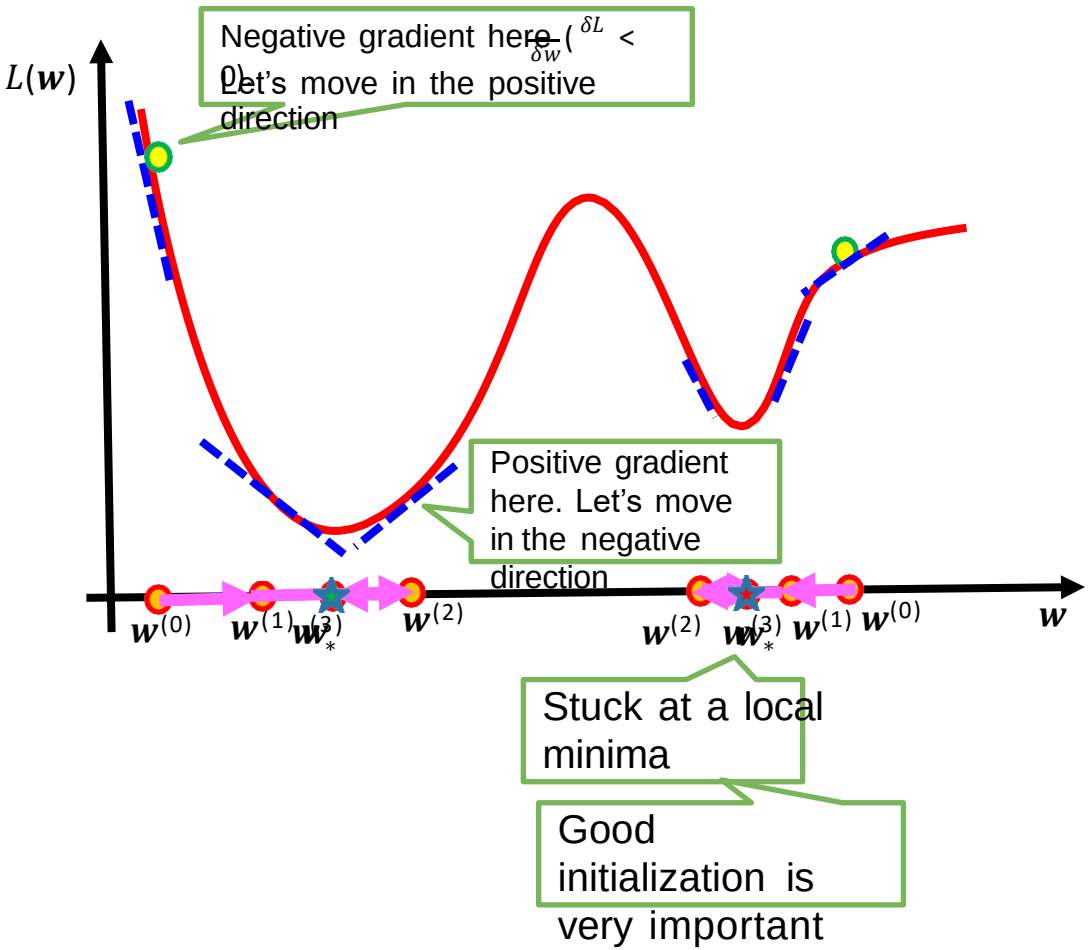
Loss functions of most deep learning models are non-convex

Convex Functions

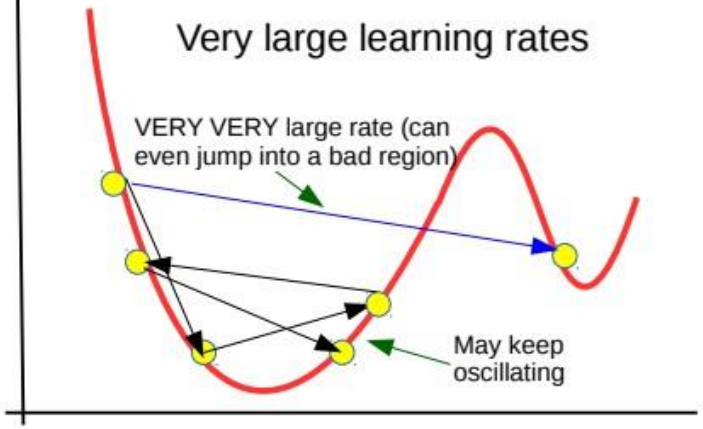
- Informally, $f(x)$ is convex if all of its chords lie above the function everywhere

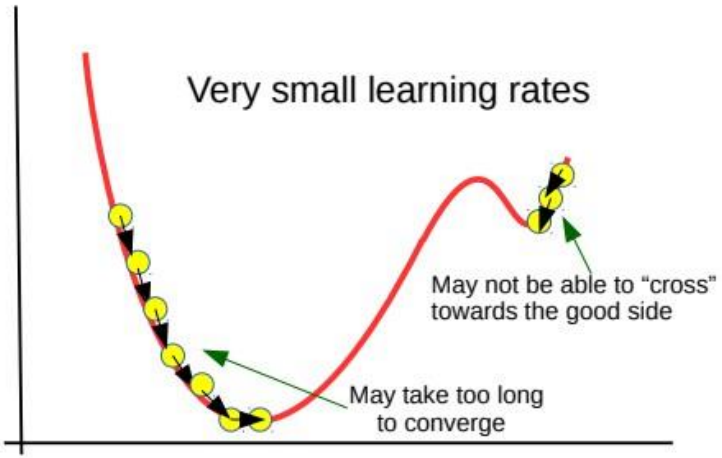


Gradient Descent:An Illustration



Learning rate is very important



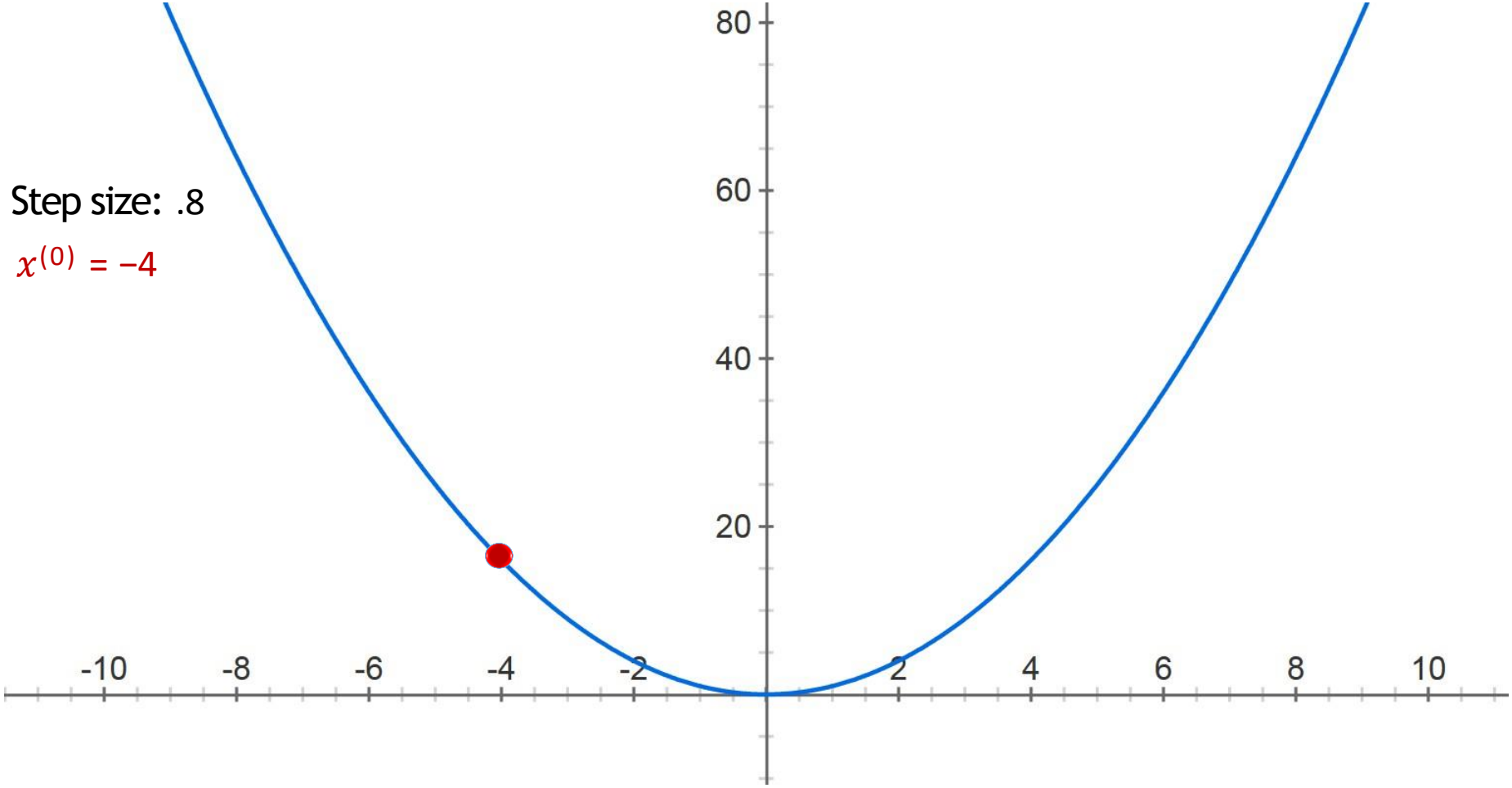


Gradient Descent

$f(x) = x^2$

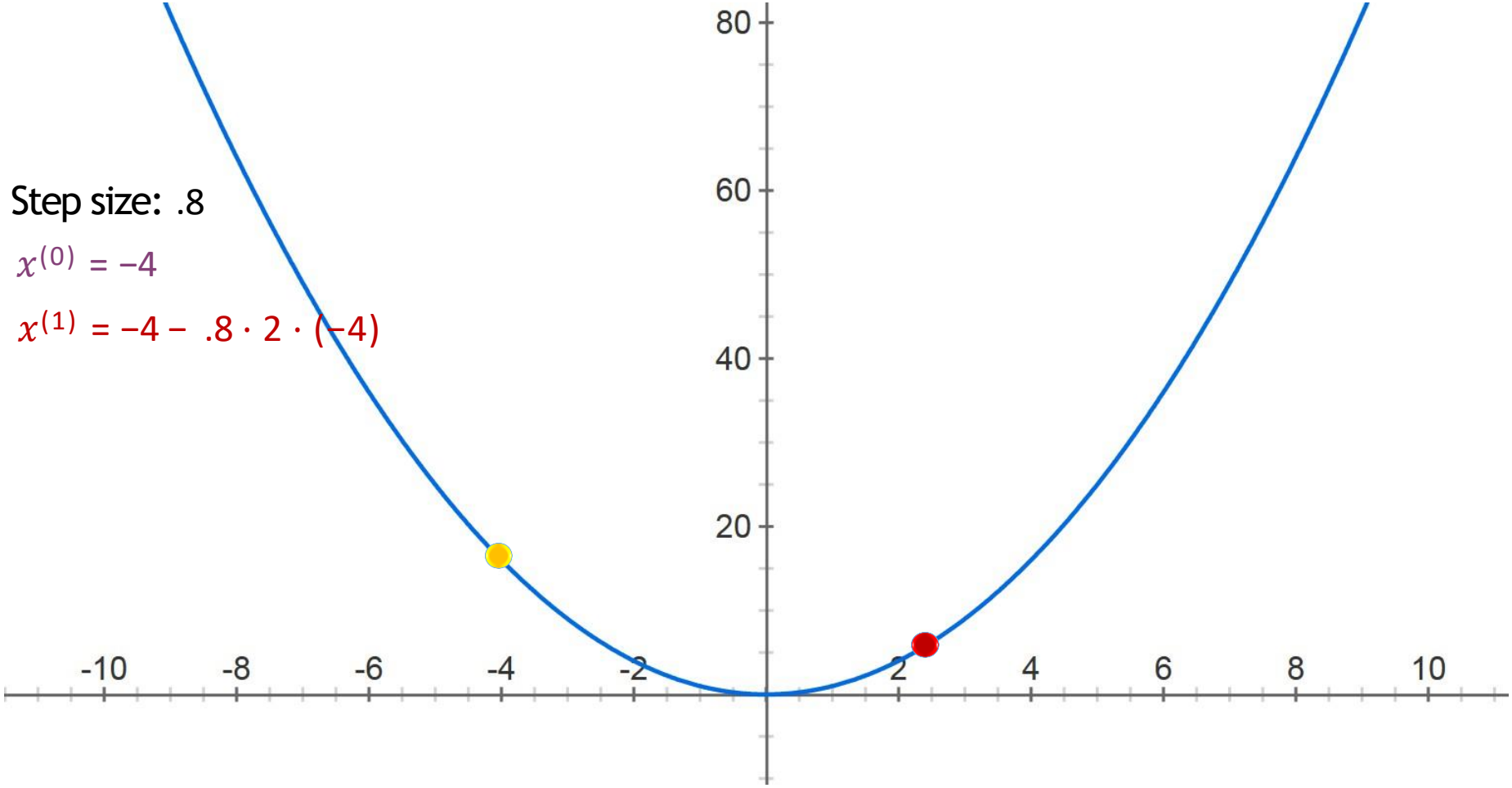
Step size: .8

$x^{(0)} = -4$



Gradient Descent

$f(x) = x^2$



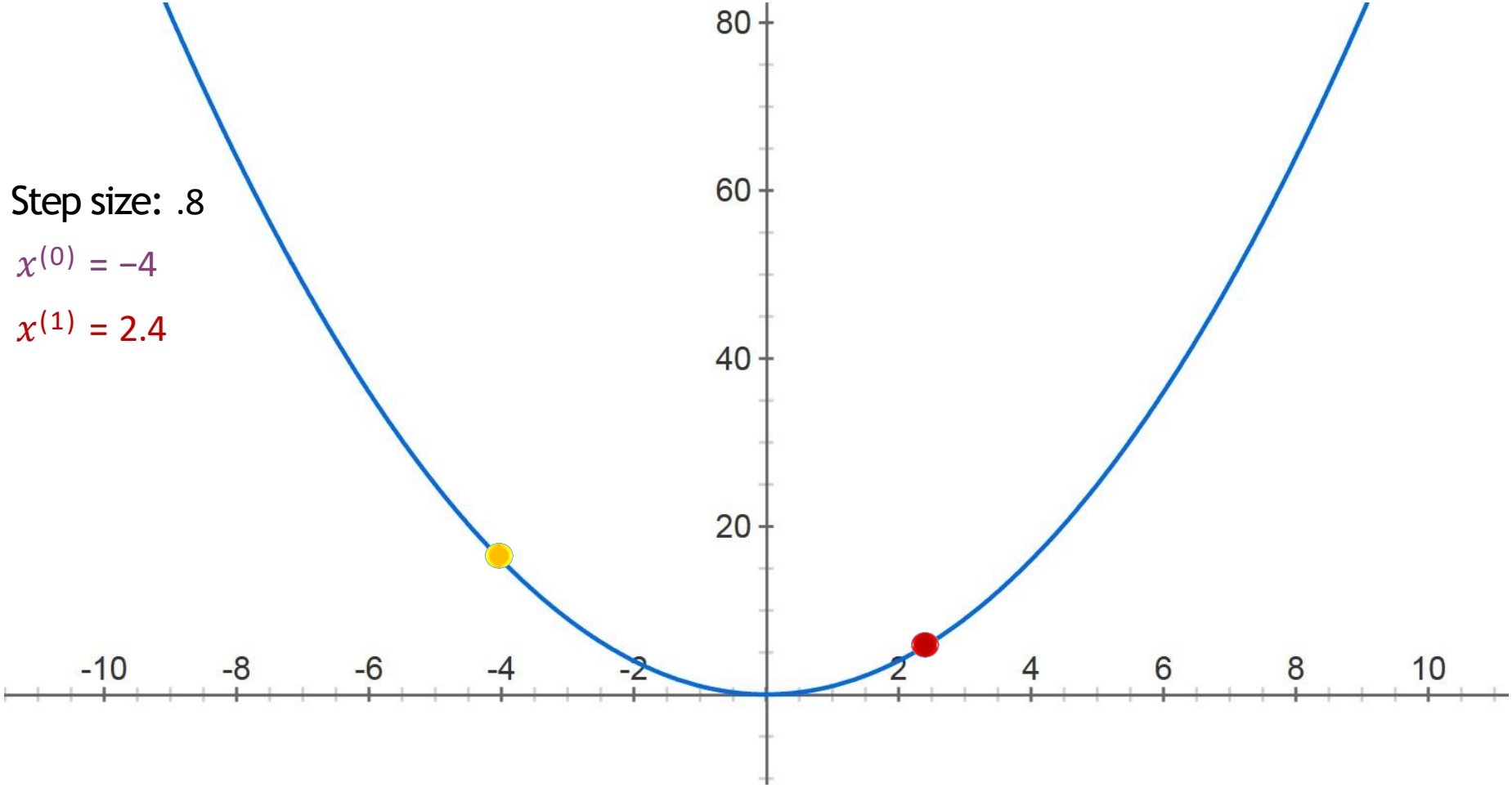
Step size: .8

$x^{(0)} = -4$

$x^{(1)} = -4 - .8 \cdot 2 \cdot (-4)$

Gradient Descent

$f(x) = x^2$



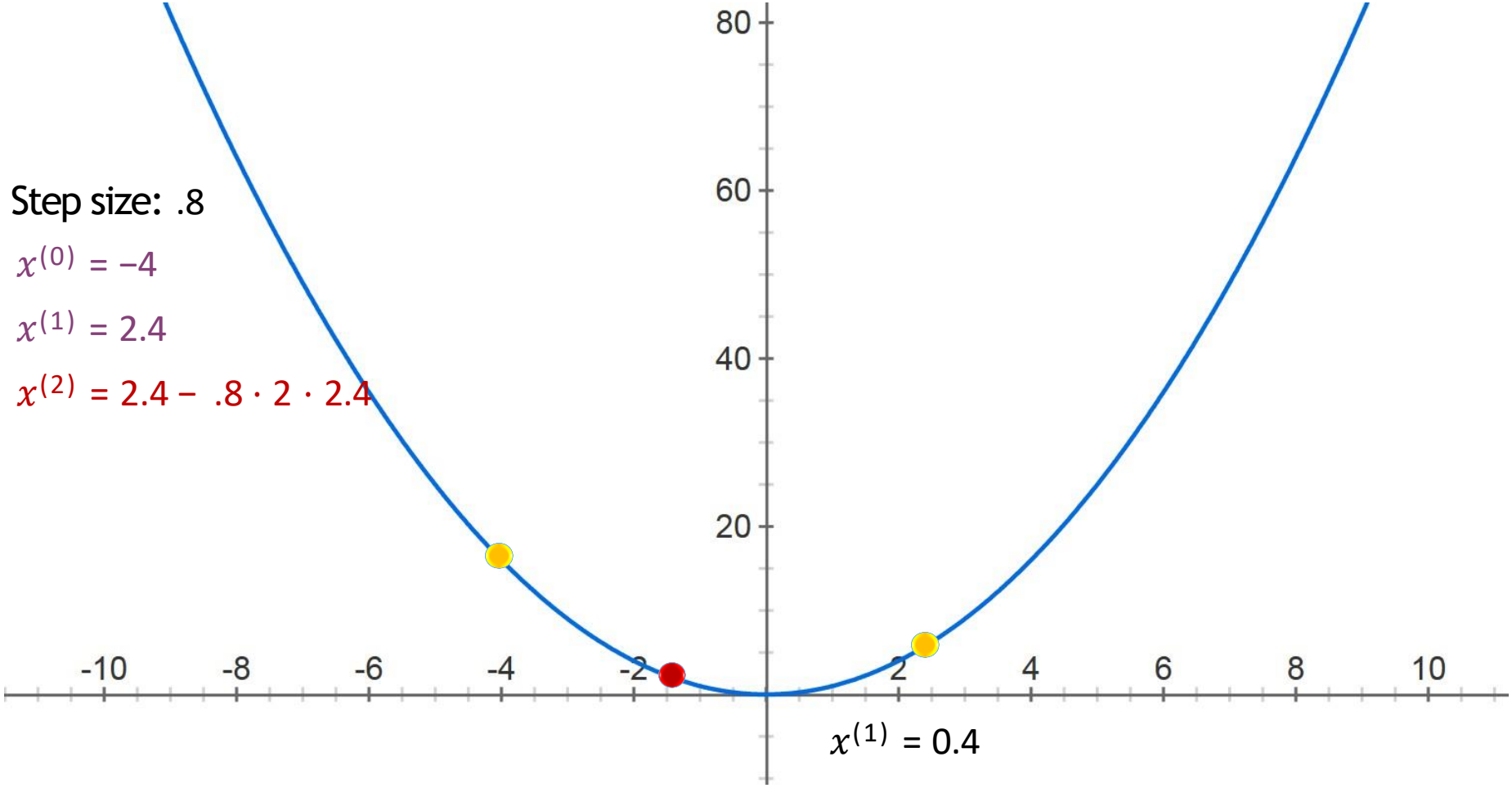
Step size: .8

$x^{(0)} = -4$

$x^{(1)} = 2.4$

Gradient Descent

$f(x) = x^2$



Step size: .8

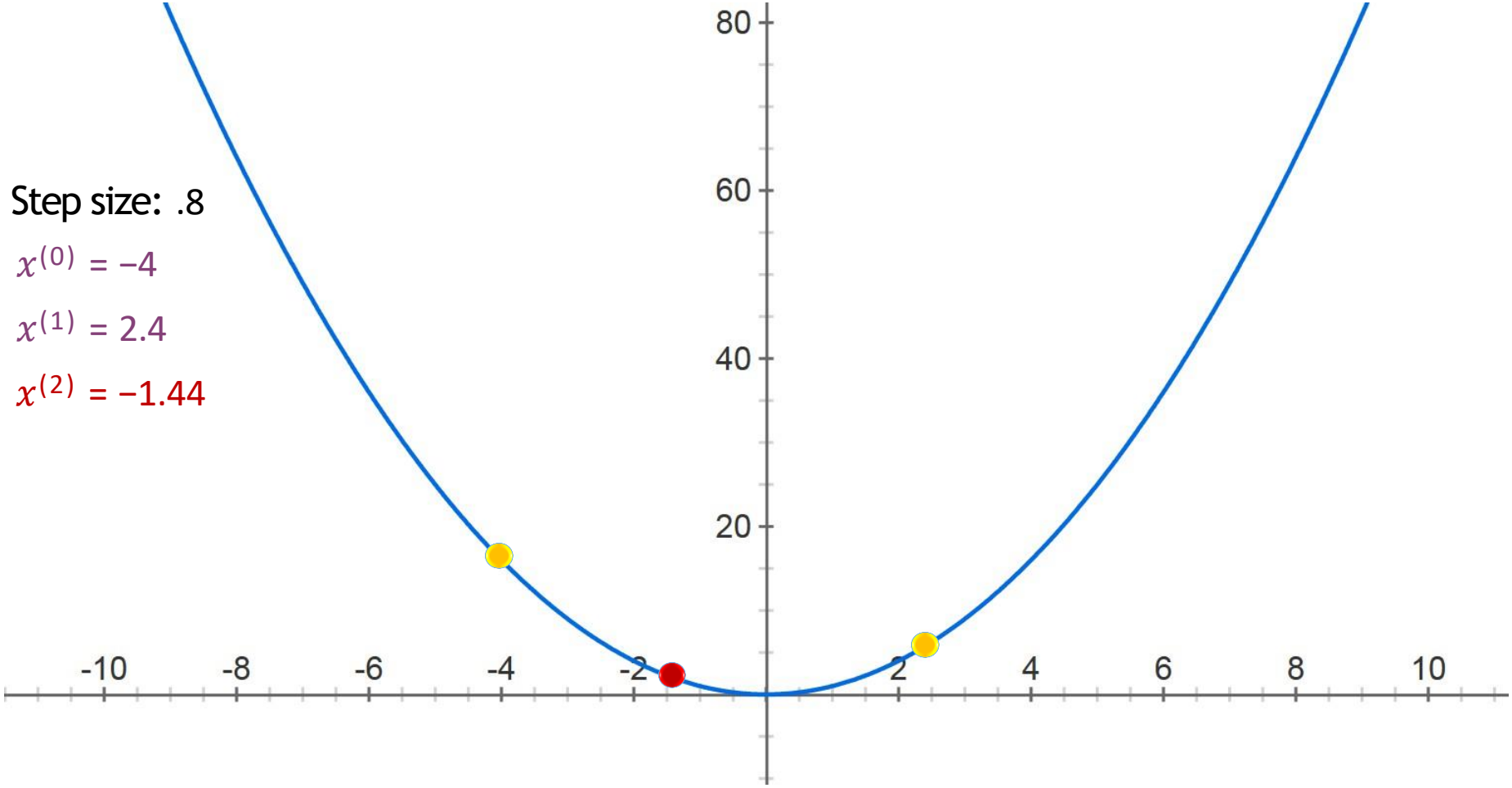
$x^{(0)} = -4$

$x^{(1)} = 2.4$

$x^{(2)} = 2.4 - .8 \cdot 2 \cdot 2.4$

Gradient Descent

$f(x) = x^2$



Step size: .8

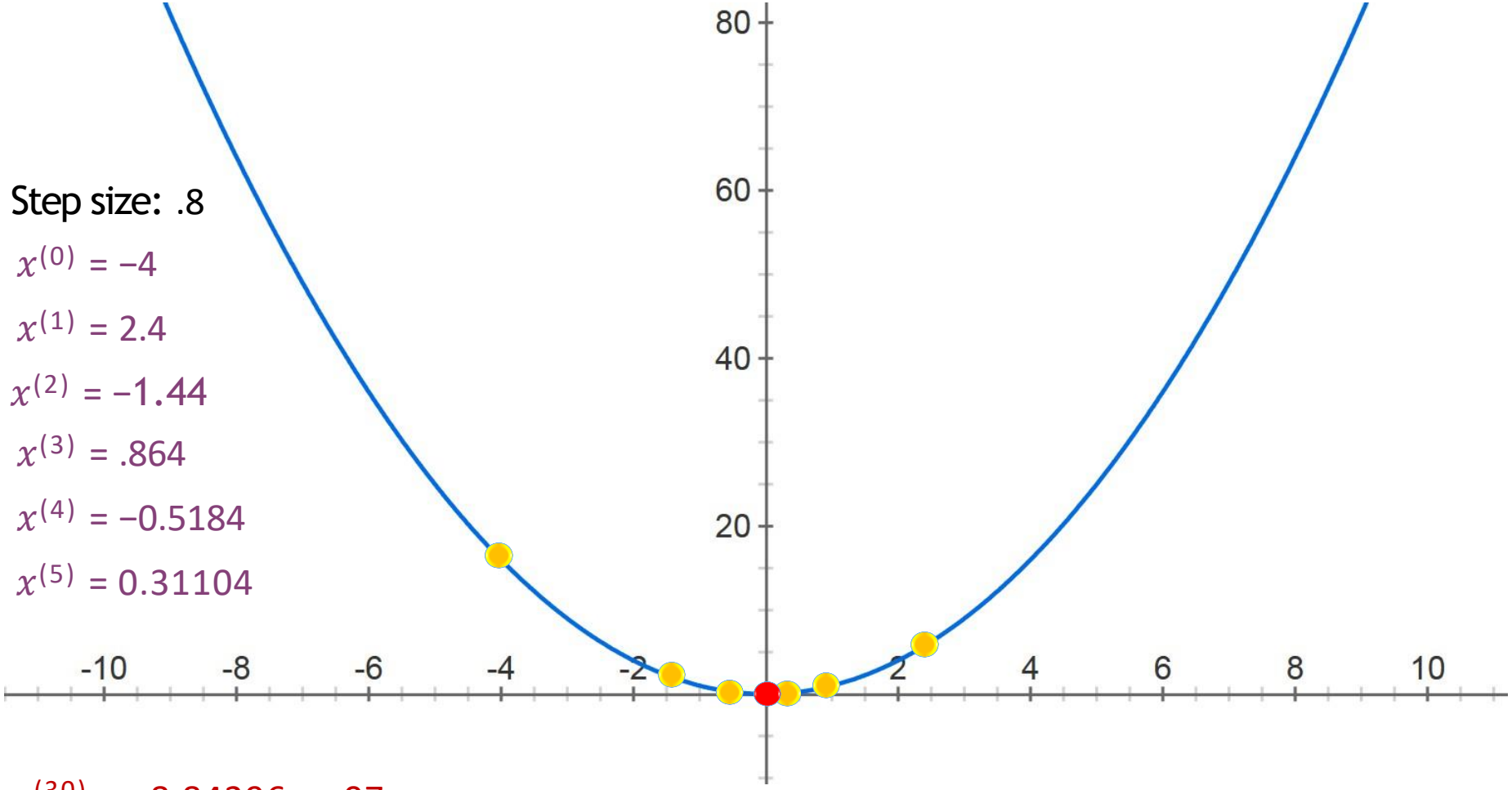
$x^{(0)} = -4$

$x^{(1)} = 2.4$

$x^{(2)} = -1.44$

Gradient Descent

$f(x) = x^2$



Step size: .8

$x^{(0)} = -4$

$x^{(1)} = 2.4$

$x^{(2)} = -1.44$

$x^{(3)} = .864$

$x^{(4)} = -0.5184$

$x^{(5)} = 0.31104$

$x^{(30)} = -8.84296e-07$

Gradient Descent: Convex Functions

For convex functions, local optima are always global optima (this follows from the definition of convexity)

If gradient descent converges to a critical point, then the result is a global minimizer

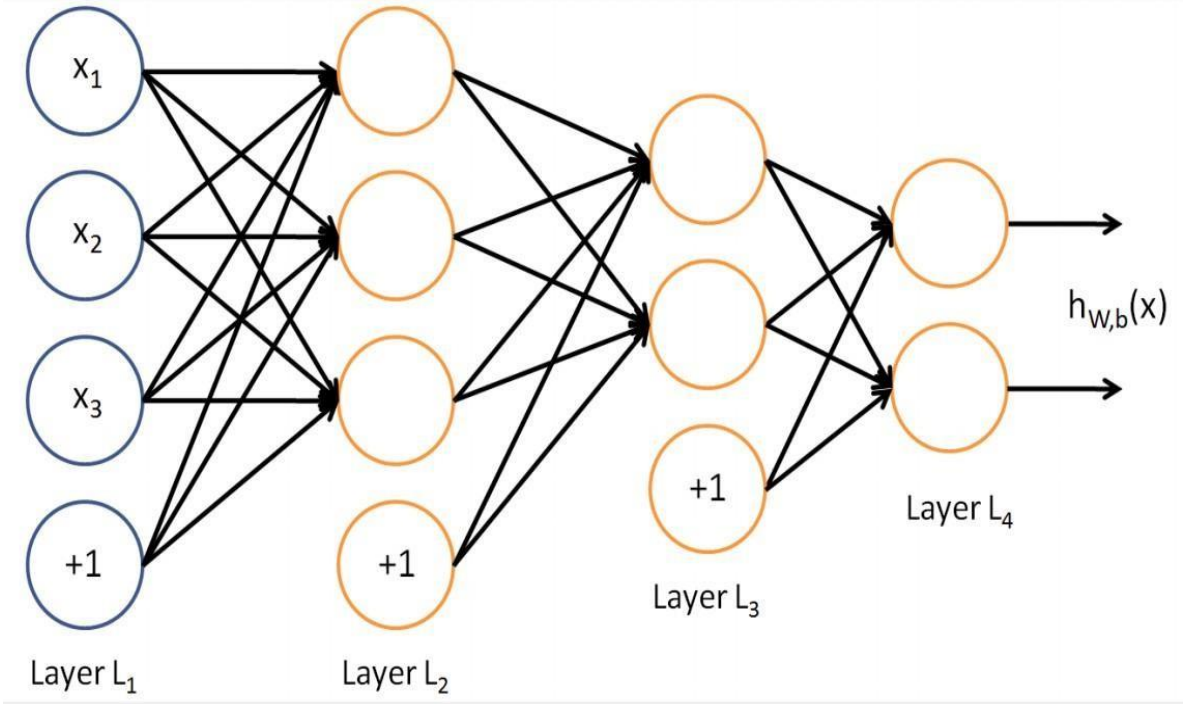
Not all convex functions are differentiable, can we still apply gradient descent?

Diminishing Step Size Rules

- A fixed step size may not result in convergence for non-differentiable functions
- Instead, can use a diminishing step size:
  - Required property: step size must decrease as number of iterations increase but not too quickly that the algorithm fails to make progress
- Common diminishing step size rules:
  - $\gamma_t = \frac{a}{b+t}$ for some $a > 0, b \geq 0$
  - $\gamma_t = \frac{a}{\sqrt{t}}$ for some $a > 0$

Gradient Descent

A feedforward neural network is a composition of multiple functions, organized as layers



What do we need to implement gradient descent? Compute gradient of loss function w.r.t. each weight in the network. How to do this?

Gradient Descent

Back-propagation, a procedure which combines gradient computation using chain rule and parameter updation using Gradient Descent, thus fully describing the neural network training algorithm.

Backpropagation

- Backpropagation is an algorithm that trains neural networks by effectively adjusting their weights and biases to minimize the error between their predictions and the desired outputs.
- It works by propagating the error back through the network, layer by layer, using the chain rule of calculus to calculate how much each weight and bias contributed to the error.

Steps of Backpropagation

1.Forward Pass:

1. Input data is fed into the input layer of the network.
2. Each neuron in the network performs calculations based on its inputs and activation function, passing its output to the neurons in the next layer.
3. This process continues until the output layer produces a prediction.

2.Error Calculation:

1. The predicted output is compared to the actual target value, and the difference (error) is calculated using a loss function.

3.Backward Pass:

1. The error signal is propagated backward through the network, layer by layer, using the chain rule of differentiation.
2. At each layer, the algorithm calculates the partial derivative of the error with respect to each weight and bias.

Steps of Backpropagation

4. Parameter Update:
    1. The calculated partial derivatives are used to update the weights and biases of the network, moving them in a direction that reduces the error.
    2. The amount of change is determined by the learning rate, which controls how quickly the network learns.
5. Iteration:
    1. Steps 1-4 are repeated for a large number of training examples, adjusting the weights and biases after each example.
    2. Over time, the network learns to make better predictions by minimizing the error on the training data.

Backpropagation

Consider a simple feed forward neural network (or multilayer perceptron)

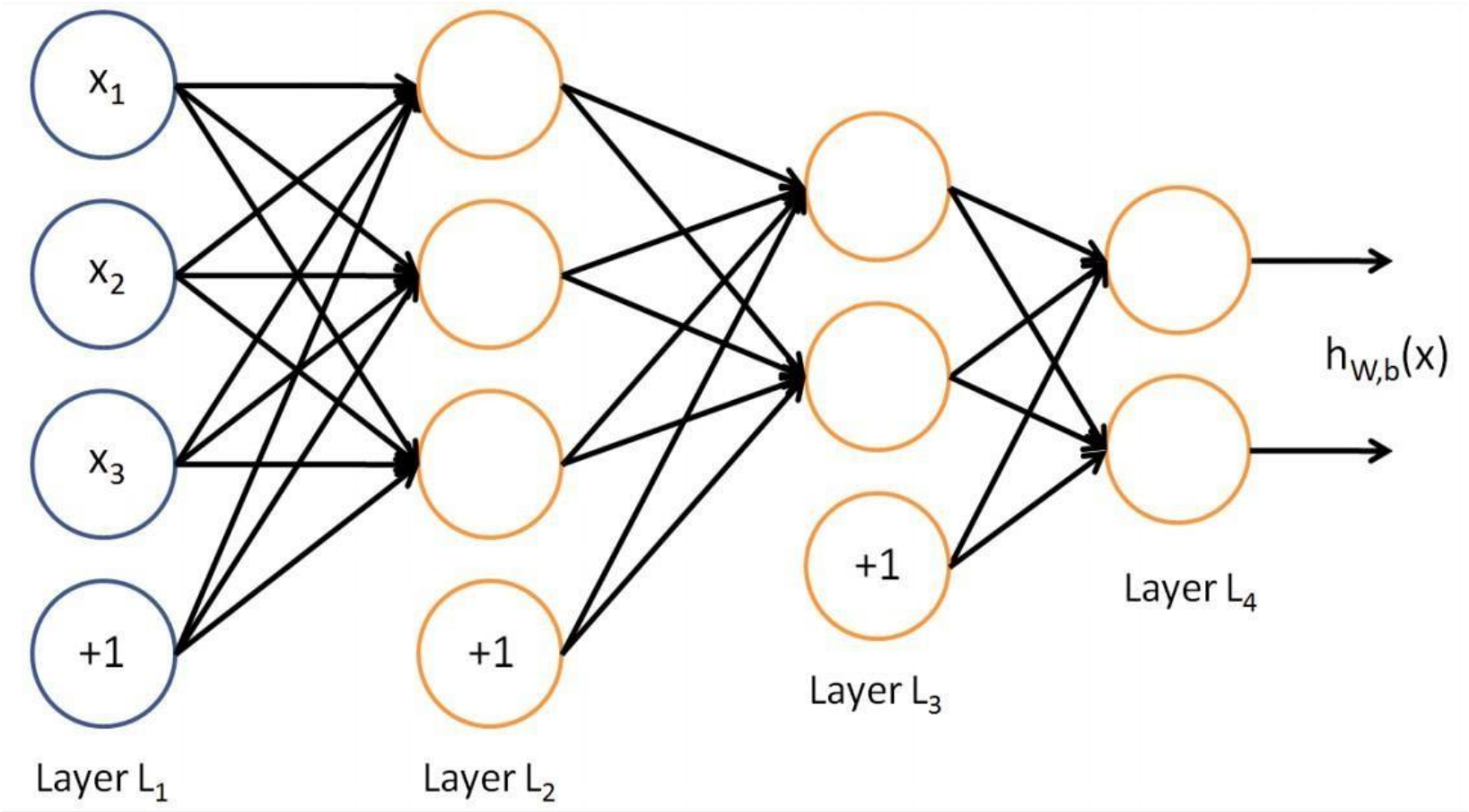


Figure Credit: Stanford UFLDL Tutorial

Backpropagation

- A fixed training set $\{x^{(i)}, y^{(i)}\}_{i=1}^{M}$ of M training samples
- Parameters = θ $\{W, b\}$, weights and biases

Backpropagation

- A fixed training set $\{x^{(i)}, y^{(i)}\}_{i=1}^{M}$ of M training samples
- Parameters $\theta = \{W, b\}$, weights and biases
- Mean square cost function for a single example:

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

- Overall cost function is given by:

$$L(\theta) = \frac{1}{M}\sum_{i=1}^{M} L(\theta; x^{(i)}, y^{(i)})$$

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

Backpropagation: Notations

- We have n_l layers in the network, $l = 1, 2, .., n_l$

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Backpropagation: Notations

We have n_l layers in the network, $l = 1, 2, .., n_l$

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- For a 3-layer network shown earlier, compact vectorized form of a **forward pass** to compute neural network's output is shown below:

$$z^{(2)} = W^{(1)}x + b^{(1)}$$

$$a^{(2)} = f(z^{(2)})$$

$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$

Backpropagation: Notations

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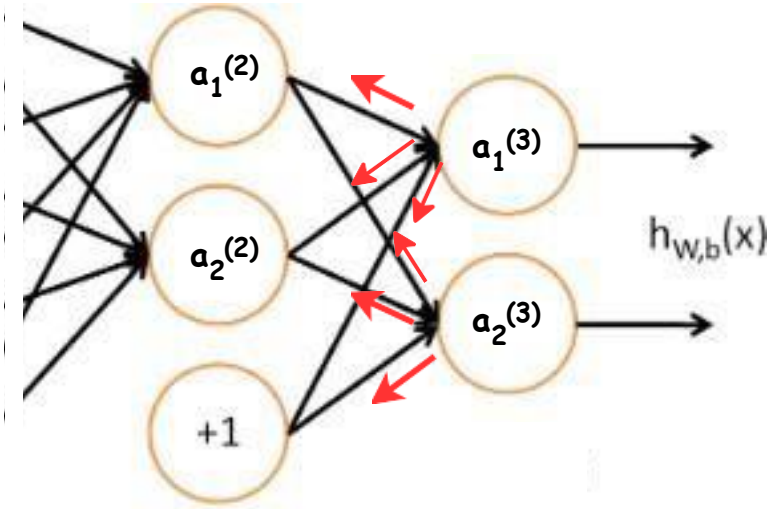
$$a^{(2)} = f(z^{(2)})$$
$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$
$$h(x) = a^{(3)} = f(z^{(3)})$$

- Function f can denote any activation function such as sigmoid, ReLU, identity, etc.

Backpropagation: Backward Pass

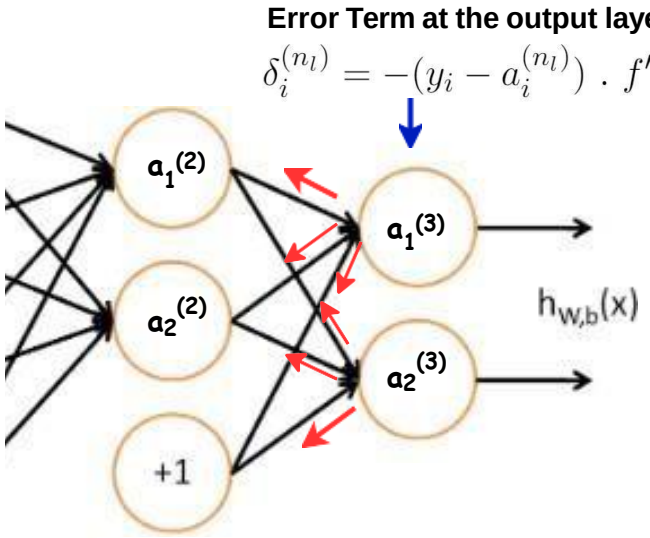
- During the forward pass, we successively compute each layer's outputs from left to right.
- During backward pass, we aim to compute derivatives of each parameter starting from the right most layer to the left most one i.e., layer $n_l, n_l - 1, \ldots, 1$.
- Once the derivatives are computed, we use Gradient Descent to update the parameters.



Backpropagation: Backward Pass

- For each node, we define an **error term** $\delta_i^{(l)}$ to denote how much the node was responsible for the loss computed
- If $l = n_l$ i.e., **last layer**, error term computation is straightforward, since we directly take derivative of loss function (MSE, in this case, between output and target values)

$$\delta_i^{(n_l)} = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$



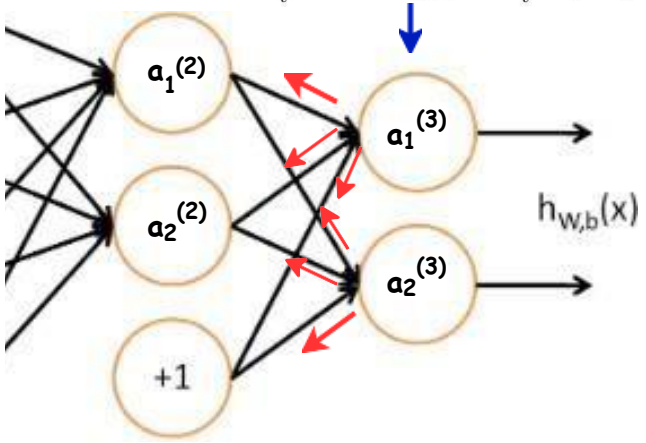
Backpropagation: Backward Pass

- To compute error term for **hidden layers**, $l = n_l - 1, n_l - 2, \ldots$, we rely on error terms from subsequent layers
- In particular, we compute error term as sum of error terms in next layer, weighted by weights along connections to next layer:

$$\delta_i^{(l)} = \left(\sum_{j=1}^{s_{l+1}} W_{ij}^{(l)} \delta_j^{(l+1)} \right) f'(z_i^{(l)})$$

Error Term at the output layer

$$\delta_i^{(n_l)} = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$



Error Term at the hidden layer

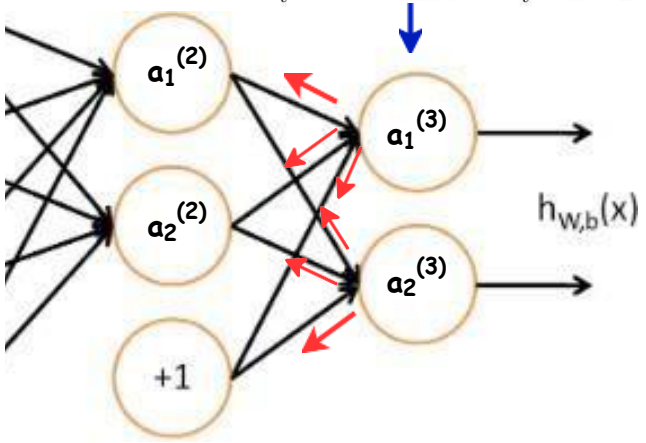
$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)} \right) \circ f'(z^{(l)})$$

Backpropagation: Backward Pass

- Note that f' denotes derivative of activation function
- For a linear neuron $f(x) = x$, derivative is 1
- For a sigmoid neuron $f(x) = \sigma(x) = \frac{1}{1+e^{-x}}$, derivative turns out to be $\sigma(x)(1-\sigma(x))$

Error Term at the output layer

$$\delta_i^{(n_l)} = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$



Error Term at the hidden layer

$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)}\right) \circ f'(z^{(l)})$$

Backpropagation:Algorithm

- Perform a feedforward pass, computing the activations for layers 1, 2, ...n_l.
- For each output unit i in layer n_l set,

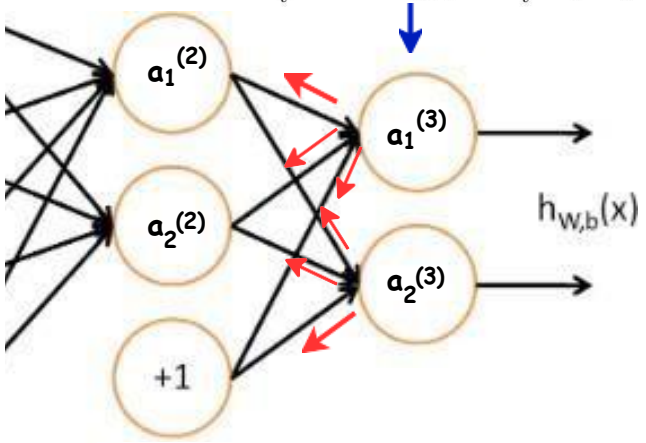
$$\delta^{(n_l)} = -(y - a^{(n_l)}) \circ f'(z^{(n_l)})$$

- For $l = n_l - 1, n_l - 2, n_l - 3, .., 2$
  For each node in layer l set,

$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)}\right) \circ f'(z^{(l)})$$

Error Term at the output layer

$$\delta_i^{(n_l)} = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$



Error Term at the hidden layer

$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)}\right) \circ f'(z^{(l)})$$

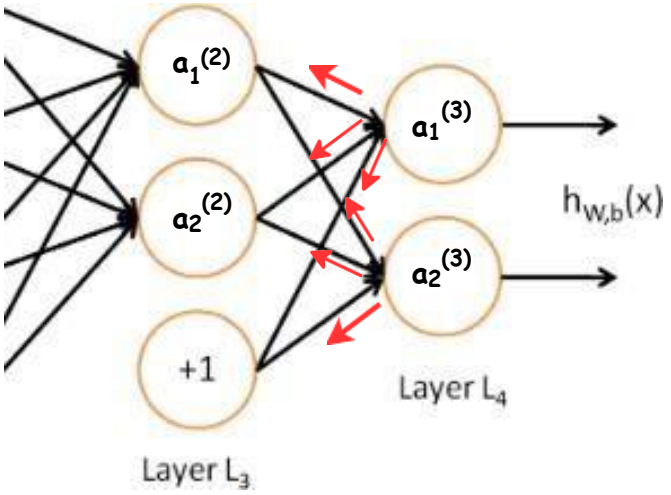
Backpropagation:Algorithm

- Compute the desired partial derivatives, as:

$$\nabla_{W^{(l)}} L(W, b; x, y) = \delta^{l+1} (a^{(l)})^T$$
$$\nabla_{b^{(l)}} L(W, b; x, y) = \delta^{l+1}$$

Error Term at the output layer

$$\delta_i^{(n_l)} = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$



Error Term at the hidden layer

$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)}\right) \circ f'(z^{(l)})$$

Gradient Descent using Backpropagation

1. Set $\Delta W^{(l)} := 0, \Delta b^{(l)} = 0$ (matrix/vector of zeros) for all l.
2. For $i = 1$ to M
   1. Use backpropagation to compute $\nabla_{\theta^{(i)}} L(\theta; x, y)$.
   2. Set $\Delta\theta^{(l)} := \Delta\theta^{(l)} + \nabla_{\theta^{(i)}} L(\theta; x, y)$
3. Update the parameters:

$$W^{(l)} = W^{(l)} - \eta \left[\frac{1}{M} \Delta W^{(l)} \right]$$

$$b^{(l)} = b^{(l)} - \eta \left[\frac{1}{M} \Delta b^{(l)} \right]$$

4. Repeat for all points until convergence.

Math behind Machine Learning

Probability

- Probability-
- Probability Vs Odds-
- Conditional Probabilities-the probability of a given event based on the existing presence of another event occurring
  - P(E |F
) where:
  - E is the event for which we're interested in a probability.
  - F is the event that has already occurred.

Probability

- Conditional Probabilities-
  - BAYES'S THEOREM

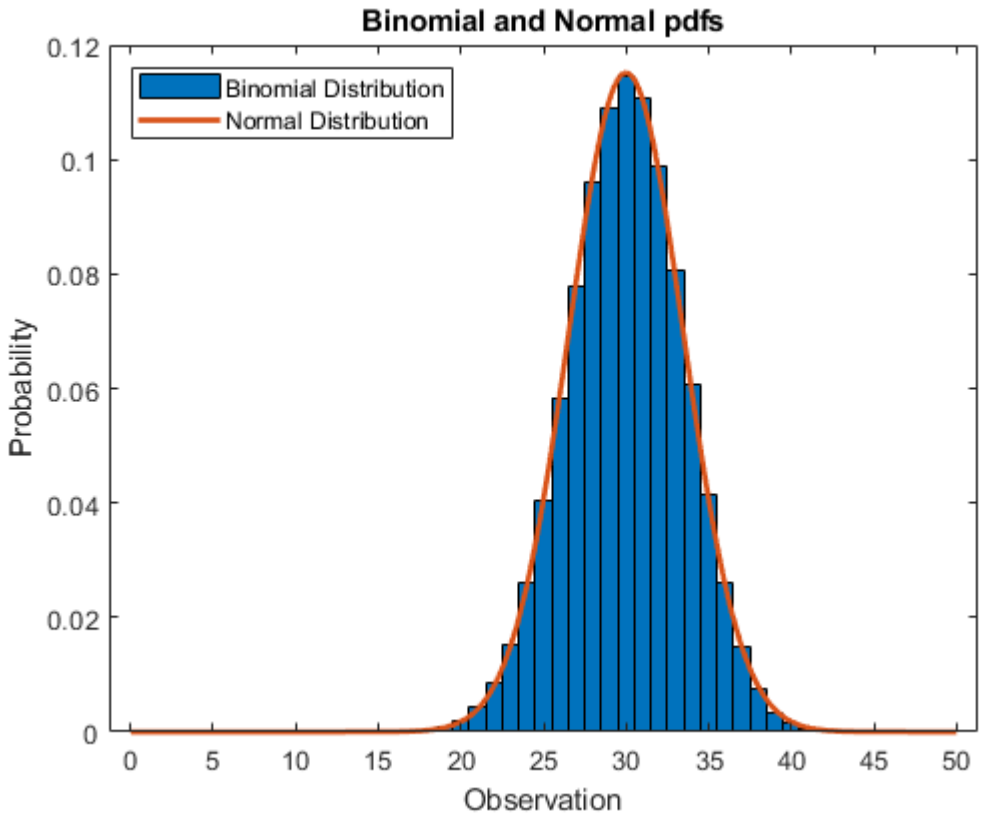
$$P(A \mid B) = \frac{P(B \mid A)\,P(A)}{P(B)}$$

Probability

- Posterior Probability-
  - conditional probability we assign after the evidence is considered.
  - Posterior probability distribution is defined as the probability distribution of an unknown quantity conditional on the evidence collected from an experiment treated as a random variable

Distributions

- Continuous –
  - Defined by mean and std deviation
  - normal distributio
- Discrete- binomial distribution



SamplesVersus Population

- Population - All of the units we'd like to study
  or model in our experiment.
- Sample- Subset of the population of data that hopefully represents the accurate distribution of the data without introducing sampling bias

Resampling Methods

- **Bootstrapping-**
  - Random samples drawn from another sample to generate a new sample that has a balance between the number of samples per class.
  - Used to develop a model against a dataset with highly unbalanced classes.

Resampling Methods

- Cross-validation-
  - Method used to estimate how well a model generalizes on a training dataset
  - Split the training dataset into N number of splits and then separate the splits into training and test groups.
  - Train on the training group of splits and then test the model on the test group of splits.
  - Rotate the splits between the two groups many times until
    we've exhausted all the variations.
  - No hard number for the number of splits to use but researchers have found 10 splits to work well in practice.
  - Common approach – Use a separate portion of the held- out data used as a validation dataset during training.

Resampling Methods

Method	Definition	Limitations
Holdout	The original data is divided into two sets, training and test set. The model is induced using the training set and then its performance is evaluated using the test set. The accuracy of the induced model on the test set is used to estimate the accuracy of the classifier	1. Because the data was divided into two sets fewer label examples are available for training. As a result, the induced model may not be as good 2. It may be highly dependent on the composition of the training and test sets. 3. The two sets are no longer independent because they are subsets of a larger set.
Random Subsampling	Repeats the holdout method several times to improve estimation of a classifier's performance. Overall accuracy, acc_{sub} is based on the accuracy for each run, acc_i. $acc_{sub} = \sum_{i=1}^{k} {acc_i}/{k}$	1. Still encounters some of the holdout problems. 2. Some records might be used for training more often than others.
Cross-Validation	Partitions the data into k disjoint subset. It then uses k-1 subsets for the training model and one set for the test set. It does this k number of times switching the test set each time thereby each record is used the same number of times for training and exactly one time for testing. The total error is found by summing the errors of all k runs. Leave-one-out k=n:-basically all the data except for one is used for the training set and the one is used for the test set. This is good because it uses as much data as possible for training	1. Training algorithm has to be rerun from scratch k times. 2. When the data set size is small splitting it compromises it integrity. 1. Computationally expensive 2. The variance of the estimated performance metric is high
Bootstrap	The training records are sampled with replacement. "A common variation used is the .632 bootstrap which computes the overall accuracy by combining the accuracies of each bootstrap sample with the accuracy computed from a training set that contains all the labeled examples in the original data[1]"	1. Bootstrap can yield poor results in certain situations 2. Though the bootstrap easily accommodates some violations of traditional statistical assumptions (e.g., non-normality), it is susceptible to others (e.g., non-independence)[2].

Selection Bias

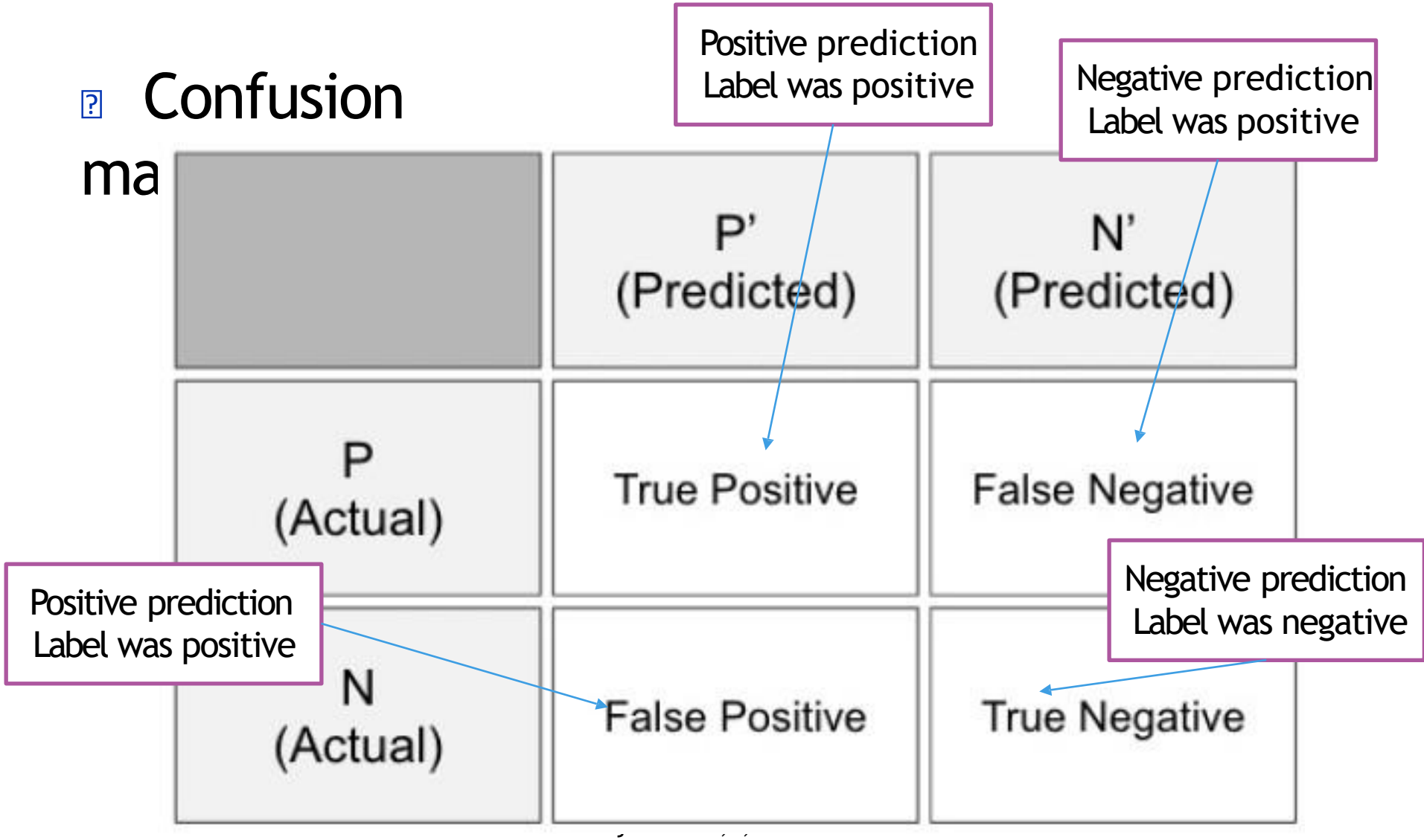
- Sampling method that does not have proper randomization and skews the sample in a way such that the sample is not representative of the population we'd like to model.
- Possibility of introducing bias into our models that will lower our model's accuracy on data from the larger population

Likelihood

- Likeliness that an event will occur yet do not specifically reference its numeric probability.
- About an event that has a reasonable probability of happening but still might not.
- Informally, likelihood is also used as a synonym for probability.

Evaluating Models

- Confusion ma



Evaluating Models

- False positive - “type I error”
- False negative - “type II error”

Evaluating Models

- Sensitivity versus specificity-
  - two different measures of a binary classification model. -
  - Sensitivity-
  - The true positive rate measures how often we classify an input record as the positive class and its correct classification.
  - This also is called sensitivity ,or recall;.
  - Sensitivity quantifies how well the model avoids false negatives.
  - Sensitivity = TP / (TP + FN)

Evaluating Models

- Sensitivity versus specificity-
  - Specificity-Specificity quantifies how well the model avoids false positives.
  - Specificity = TN / (TN + FP)

Evaluating Models

- Accuracy-
  - Accuracy is the degree of closeness of measurements of a quantity to that quantity's true value.
  - Accuracy = (TP + TN) / (TP + FP + FN + TN)
  - Accuracy can be misleading in the quality of the model when the class imbalance is high.

Evaluating Models

- Precision
  - The degree to which repeated measurements under the same conditions give us the same results in the context of science and statistics.
  - Positive prediction value.
  - Precision = TP / (TP + FP)
  - A measurement can be accurate yet not precise, not accurate but still precise, neither accurate nor precise, or both accurate and precise.
  - We consider a measurement to be valid if it is both accurate and precise.

Evaluating Models

- Recall-
  - Same as sensitivity and is also known as the true positive rate or the hit rate.
- F1 score-
  - In binary classification we consider the F1 score (or F- score, F-measure) to be a measure of a model's accuracy.
  - Harmonic mean of both the precision and recall measures (described previously) into a single score:
  - $F1 = 2TP / (2TP + FP + FN)$

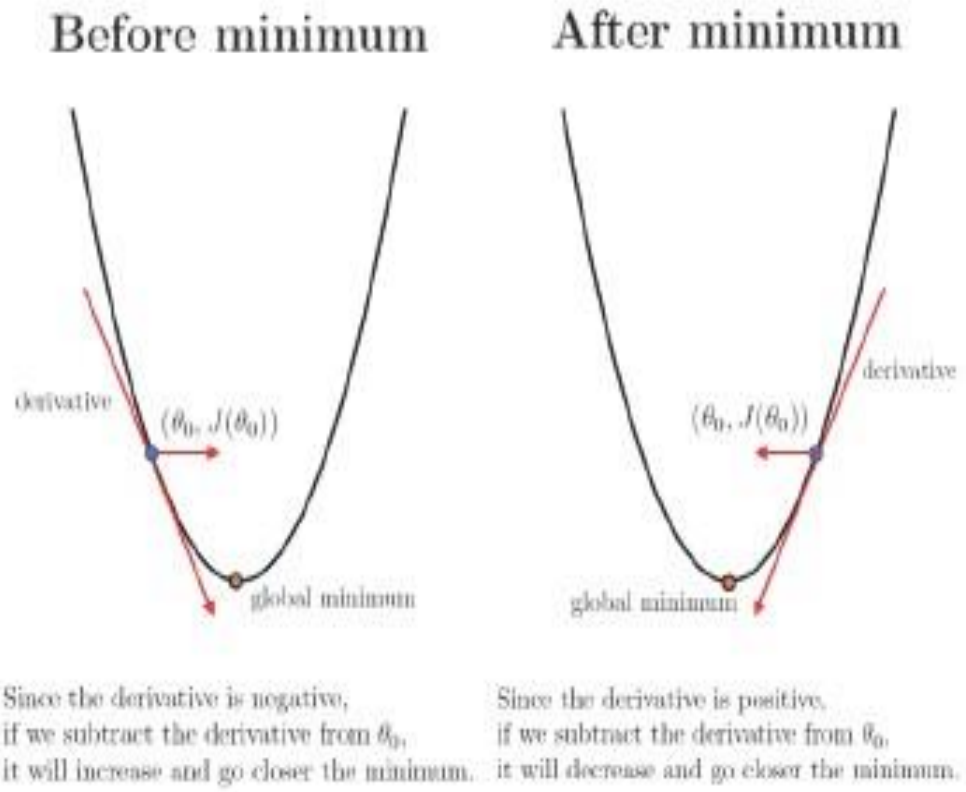
Gradient Descent and Variants

Review:Gradient Descent (GD)

- Optimization algorithm used to find minima of a given differentiable function
- At each step, parameters (θ) are pushed in negative direction of gradient of a cost function ($J(\theta\, x, y)$, in figure alongside) w.r.t parameters

$$\theta_{new} = \theta_{old} - \alpha \Delta \theta_{old}$$

where α is learning rate



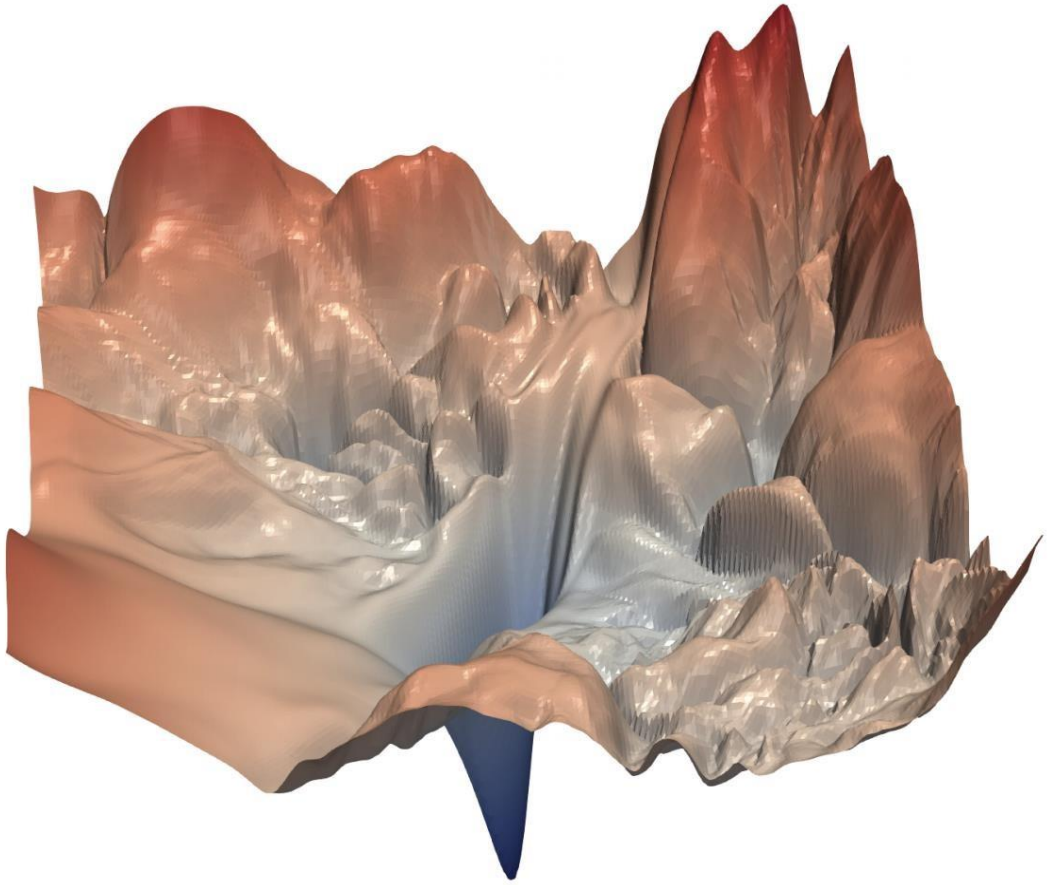
Gradient Descent Algorithm

Require: Learning rate α, initial parameters θ_t, training dataset $\mathcal{D}_{tr}$

1: **while** stopping criterion not met **do**
2: Initialize parameter updates $\Delta\theta_t = 0$
3: **for each** $(x^{(i)}, y^{(i)})$ in $\mathcal{D}_{tr}$ **do**
4: Compute gradient using backpropagation $\nabla_{\theta_t}\mathcal{L}(\theta_t; x^{(i)}, y^{(i)})$
5: Aggregate gradient $\Delta\theta_t = \Delta\theta_t + \nabla_{\theta_t}\mathcal{L}$
6: **end for**
7: Apply update $\theta_{t+1} = \theta_t - \alpha\frac{1}{|\mathcal{D}_{tr}|}\Delta\theta_t$
8: **end while**

Error Surface of Neural Networks

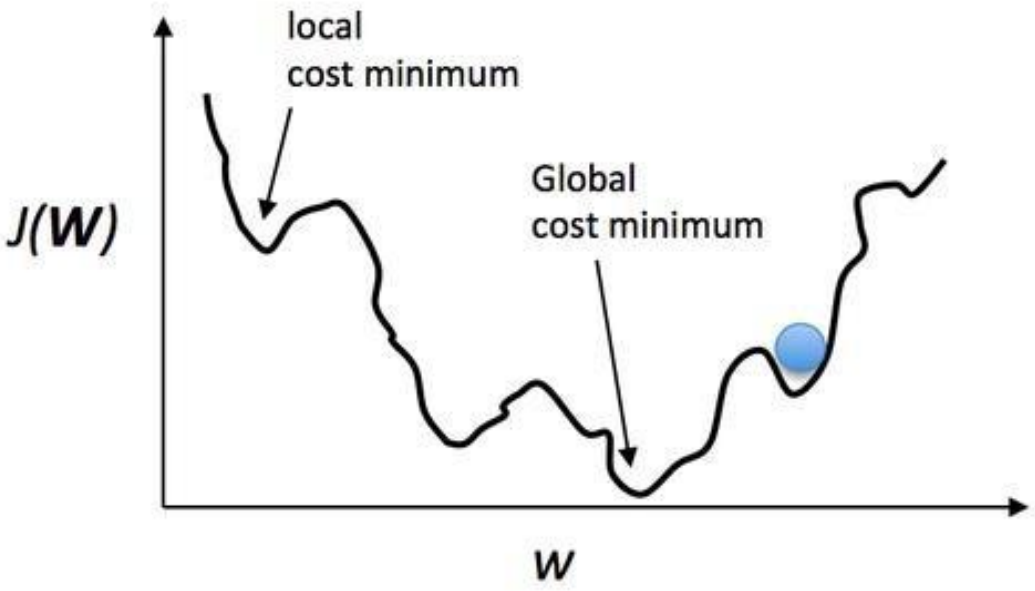
- Visualization of error surface of a neural network (ResNet-56)



Credit: Li et al,Visualizing the Loss Landscape of Neural Nets, NeurIPS 2018

Local Minima

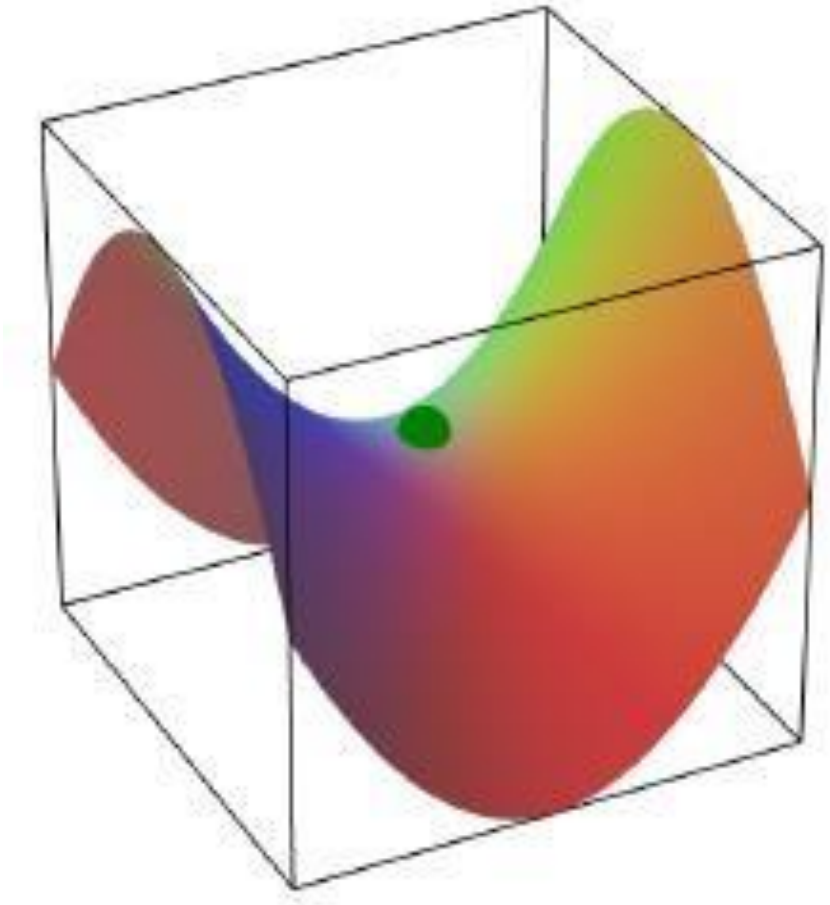
- Unlike convex objective functions that have a global minimum, non-convex functions as in deep neural networks have multiple local minima[1]



[1]Choromanska et al,The Loss Surface of Multilayer Nets,AISTATS 2015

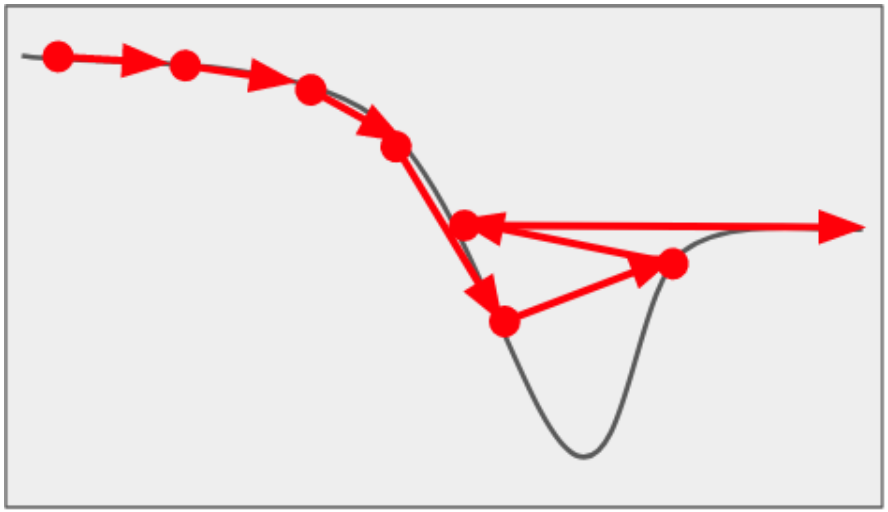
Saddle Points

- Local maximum along one cross-section of cost function and local minimum along another
- Though it isn't a local minimum, gradient is zero (or almost close to zero) =) gives impression of convergence
- Though local minima are prevalent in lower dimensional spaces, saddle points become more common in higher-dimensional spaces



Plateaus and Flat Regions

- They constitute portions of error surface where gradient is highly non-spherical
- Gradient descent spends a long time traversing in these regions as the updates are small
- How about increasing the learning rate?
- Though traversal becomes faster in plateaus, there is a risk of divergence



Momentum-based G D

- Intuition: With increasing confidence, increase step size; and with decreasing confidence, decrease step size
- Weight update given by:

Momentum Term

$$v_t = \gamma v_{t-1} + \alpha \nabla_{\theta_t} \mathcal{L}(\theta_t; x^{(i)}, y^{(i)})$$

$$\theta_{t+1} = \theta_t - v_t$$

Momentum-based GD: Algorithm

Require: Learning rate α, momentum parameter γ, initial parameters θ_t, training dataset $\mathcal{D}_{tr}$

Initialize $v_{t-1} = 0$
while stopping criterion not met **do**
    Initialize weight updates $\Delta\theta_t = 0$
    for each $(x^{(i)}, y^{(i)})$ in $\mathcal{D}_{tr}$ **do**
        Compute gradient using backpropagation $\nabla_{\theta_t}\mathcal{L}(\theta_t; x^{(i)}, y^{(i)})$
        Aggregate weight updates: $\Delta\theta_t = \Delta\theta_t + \nabla_{\theta_t}\mathcal{L}$
    end for
    Update velocity: $v_t = \gamma v_{t-1} + \alpha\Delta\theta_t$
    Apply update: $\theta_{t+1} = \theta_t - v_t$
end while

Nesterov Accelerated Momentum

- Based on Nesterov's Accelerated Gradient Descent published
  - in 19832; re-introduced by
- Sutskever in ICML'133
- Key idea: Look before you leap
- Assess how gradient changes after taking a step of momentum vt and use this to get better es

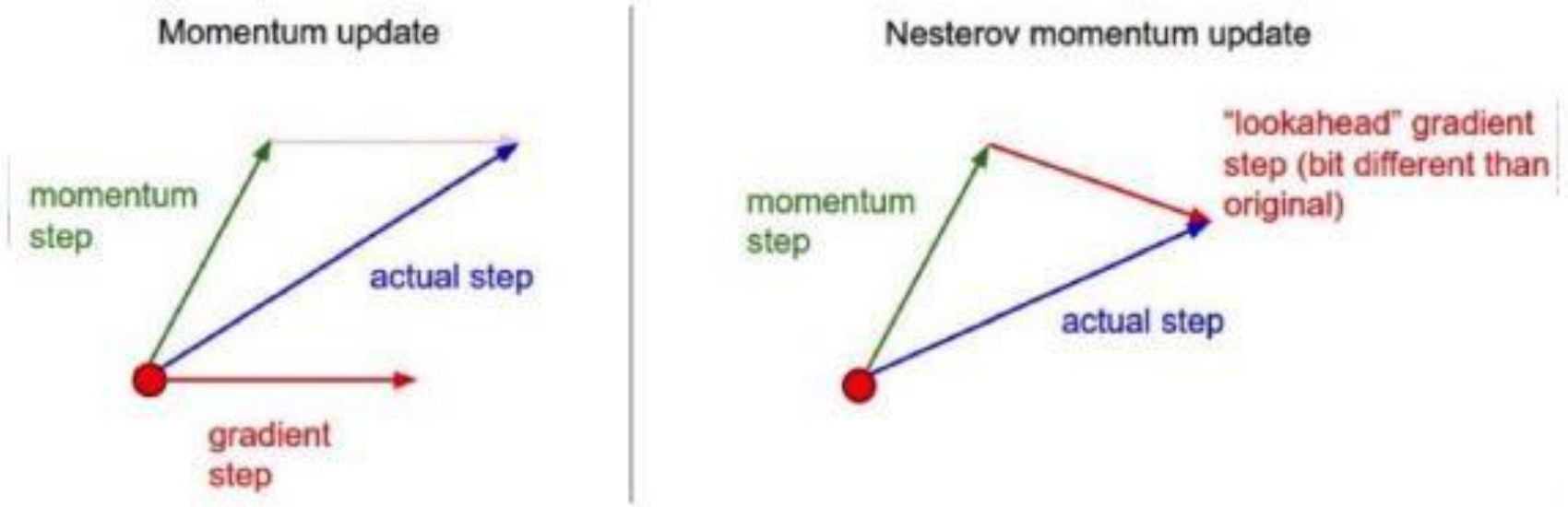
$$v_t = \gamma v_{t-1} + \alpha \nabla_{\tilde{\theta}_t} \mathcal{L}(\theta_t - \gamma v_{t-1}; x^{(i)}, y^{(i)})$$

-

$$\theta_{t+1} = \theta_t - v_t$$

- Empirically found to give good performance

Nesterov Accelerated Momentum: Visualization



Nesterov Accelerated Momentum: Algorithm

Require: Learning rate α, momentum parameter γ, initial parameters θ_t, training dataset $\mathcal{D}_{tr}$

Initialize $v_{t-1} = 0$
while stopping criterion not met **do**
    Initialize gradients $\Delta\theta_t = 0$
    Get look-ahead parameters $\tilde{\theta}_t = \theta_t - \gamma v_{t-1}$
    for each $(x^{(i)}, y^{(i)})$ in $\mathcal{D}_{tr}$ **do**
        Compute gradient using look-ahead parameters $\nabla_{\tilde{\theta}_t} \mathcal{L}(\tilde{\theta}_t; x^{(i)}, y^{(i)})$
        Aggregate gradient $\Delta\theta_t = \Delta\theta_t + \nabla_{\tilde{\theta}_t} \mathcal{L}$
    end for
    Update velocity $v_t = \gamma v_{t-1} + \alpha \Delta\theta_t$
    Apply update $\theta_{t+1} = \theta_t - v_t$
end while

GD: Pros and Cons

- For every parameter update, GD parses the entire dataset, hence called Batch GD
- Advantages of Batch GD
  - Conditions of convergence well-understood
  - Many acceleration techniques (e.g. conjugate gradient) operate in batch GD setting
- Disadvantages of Batch GD
  - Computationally slow
  - E.g. ImageNet (http://www.image-net.org), a commonly used dataset in vision, has ~14:2million samples; an iteration over it is going to be very slow

Stochastic Gradient Descent

Stochastic GD (SGD): Randomly shuffle the training set, and update parameters after gradients are computed for each training example

---

Require: Learning rate α, initial parameters θ_t, training dataset $\mathcal{D}_{tr}$

1: **while** stopping criterion not met **do**
2: **for each** $(x^{(i)}, y^{(i)})$ in $\mathcal{D}_{tr}$ **do**
3: Compute gradient using backpropagation $\nabla_{\theta_t}\mathcal{L}(\theta_t; x^{(i)}, y^{(i)})$
4: Gradient $\Delta\theta_t = \nabla_{\theta_t}\mathcal{L}$
5: Apply update $\theta_{t+1} = \theta_t - \alpha\Delta\theta_t$
6: **end for**
7: **end while**

Mini-batch Stochastic Gradient Descent

Mini-Batch Stochastic GD: Update parameters after gradients are computed for a randomly drawn mini-batch of training examples *(default option today, often simply called as SGD)*

Require: Learning rate α, initial parameters θ_t, mini-batch size m, training dataset $\mathcal{D}_{tr}$

---

while stopping criterion not met **do**
  Initialize gradients $\Delta\theta_t = 0$
  Sample m examples from $\mathcal{D}_{tr}$ (call it $\mathcal{D}_{mini}$)
  for each $(x^{(i)}, y^{(i)})$ in $\mathcal{D}_{mini}$ **do**
    Compute gradient using backpropagation $\nabla_{\theta_t}\mathcal{L}(\theta_t; x^{(i)}, y^{(i)})$
    Aggregate gradient $\Delta\theta_t = \Delta\theta_t + \nabla_{\theta_t}\mathcal{L}$
  end for
  Apply update $\theta_{t+1} = \theta_t - \alpha\Delta\theta_t$
end while

SGD: Pros and Cons

- Advantages of SGD
  - Usually much faster than batch learning; because there is lot of redundancy in batch learning
  - Often results in better solutions; SGD's noise can help in escaping local minima (provided neighborhood provides enough gradient information) and saddle points[1].
  - Can be used for tracking changes
- Disadvantages of SGD
  - Noise in SGD weight updates -can lead to no convergence!
  - Can be controlled using learning rate, but identifying proper learning rate is a problem of its own

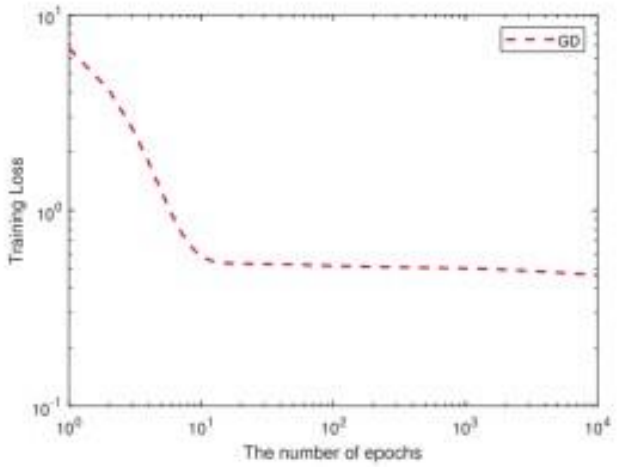
[1] http://mitliagkas.github.io/ift6085-2019/ift-6085-bonus-lecture-saddle-points-notes.pdf

Training NNs with SGD: Challenges

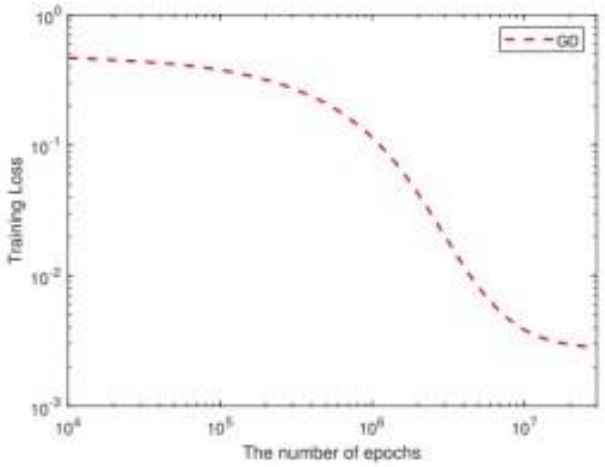
- Issues that we might encounter when traversing error surfaces using GD
  - Plateaus and flat regions
  - Local minima and saddle points
  - Vanishing and exploding gradients/cliffs
  - Other challenges
- Inexact gradients
  - Poor correspondence between local and global structure
  - Choosing learning rate and other hyperparameters

Training NNs with SGD: Challenges

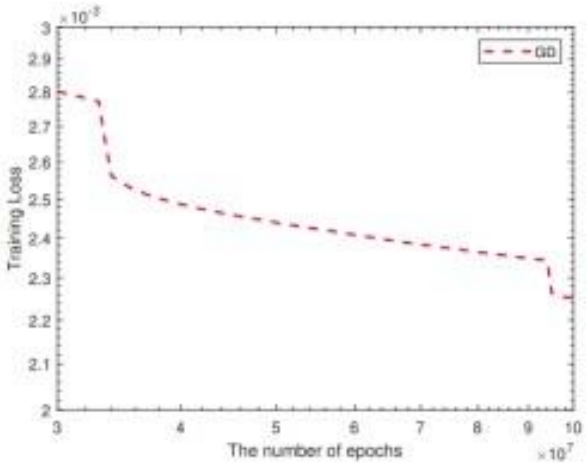
- Plateau
  - A plateau is a flat, elevated landform that rises sharply above the surrounding area on at least one



(a)

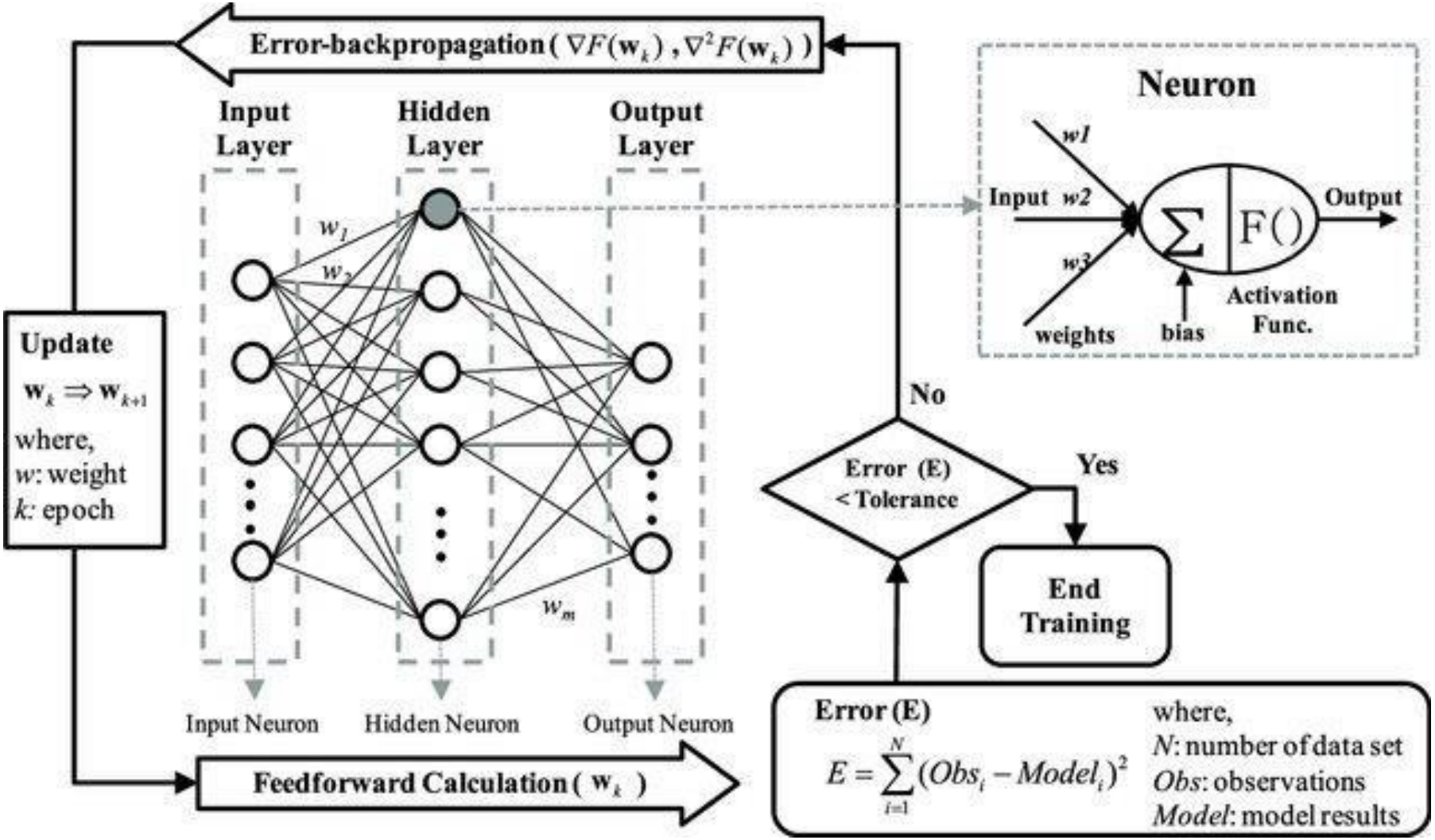


(b)



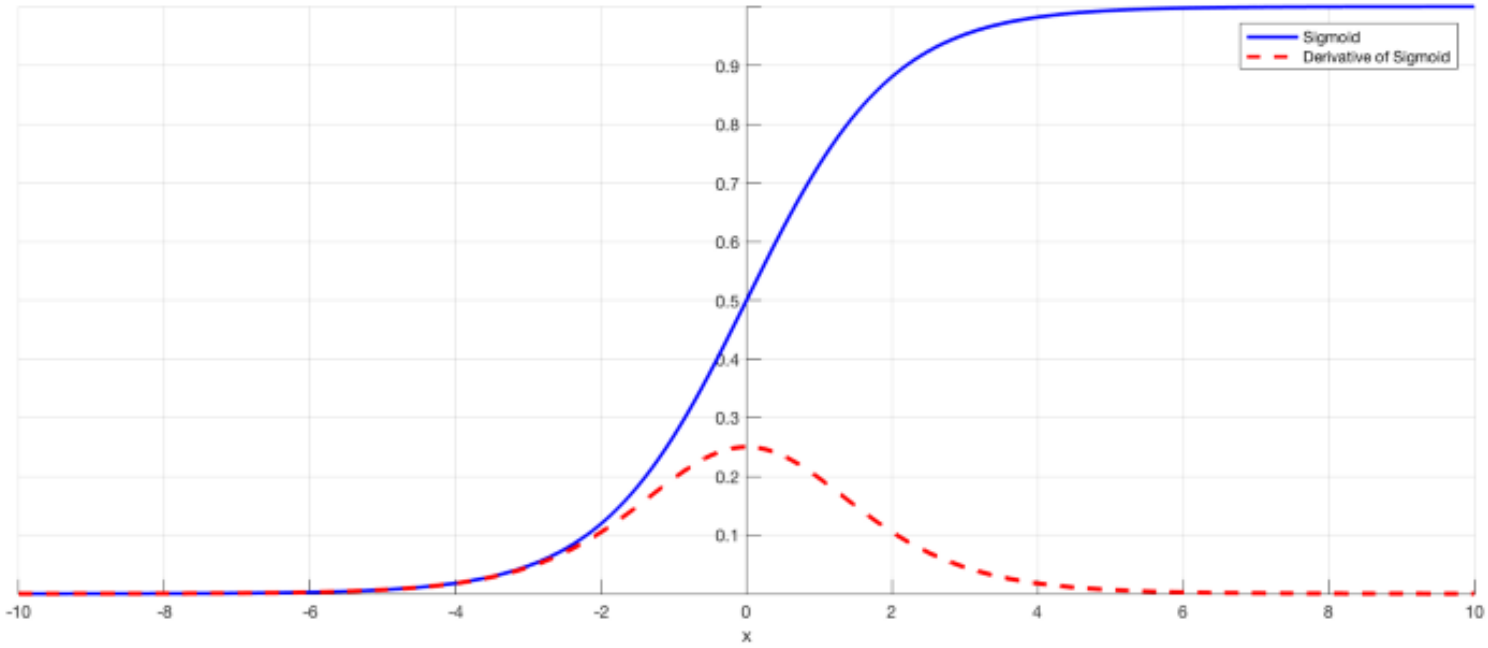
(c)

Back propagation

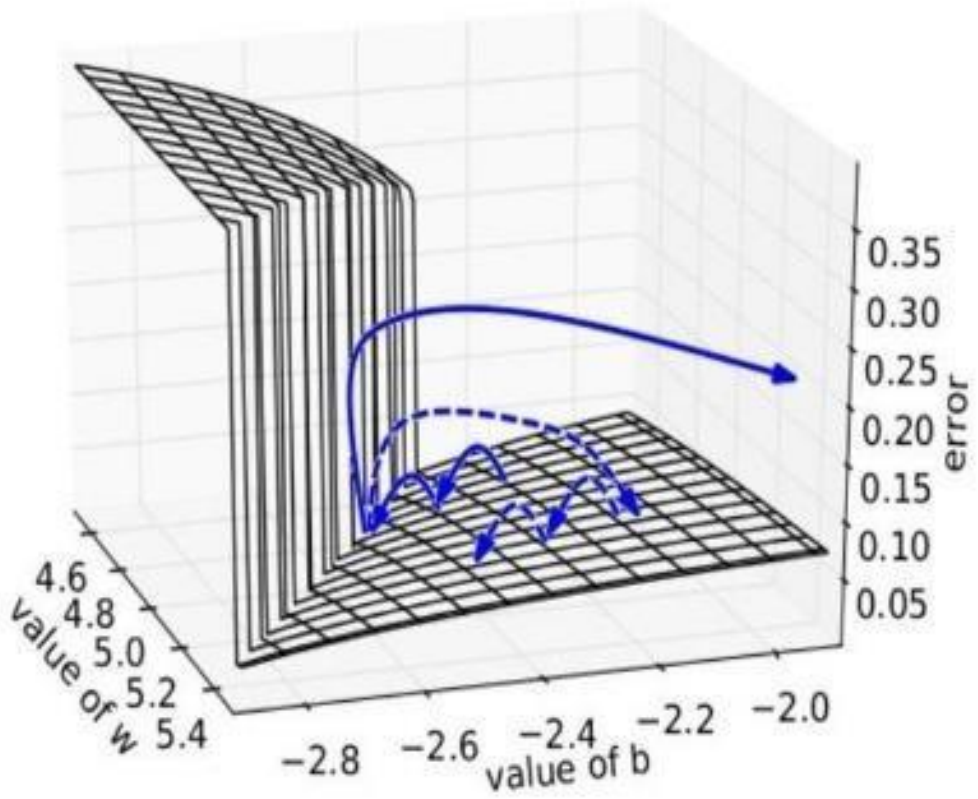


Source: Google Images

Vanishing Gradient



Exploding Gradient



How to know if our model is suffering from the Exploding/Vanishing gradient problem?

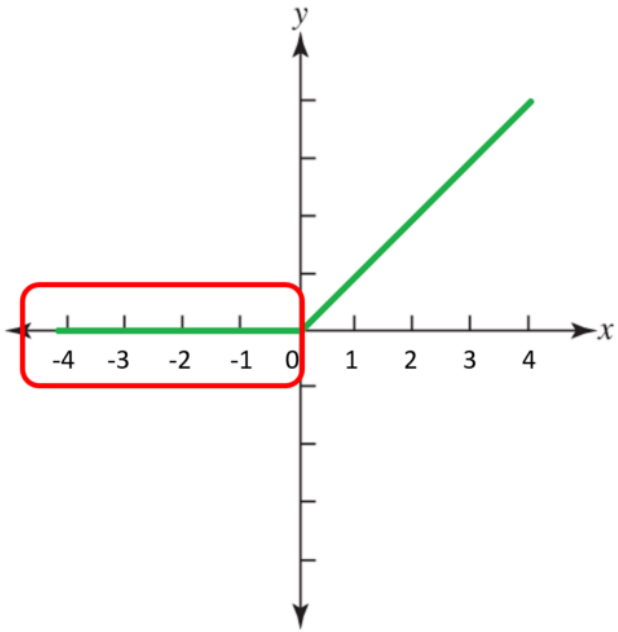
Exploding	**Vanishing**
There is an exponential growth in the model parameters.	The parameters of the higher layers change significantly whereas the parameters of lower layers would not change much (or not at all).
The model weights may become NaN during training.	The model weights may become 0 during training.
The model experiences avalanche learning.	The model learns very slowly and perhaps the training stagnates at a very early stage just after a few iterations.

- Solutions
  - **Proper Weight Initialization**
  - **Using Non-saturating Activation Functions**
  - **Gradient Clipping**

Dying ReLU

What's the Dying ReLU problem?

The dying ReLU problem refers to the scenario when many ReLU neurons only output values of 0. The red outline below shows that this happens when the inputs are in the **negative** range.



Dying ReLU- Causes

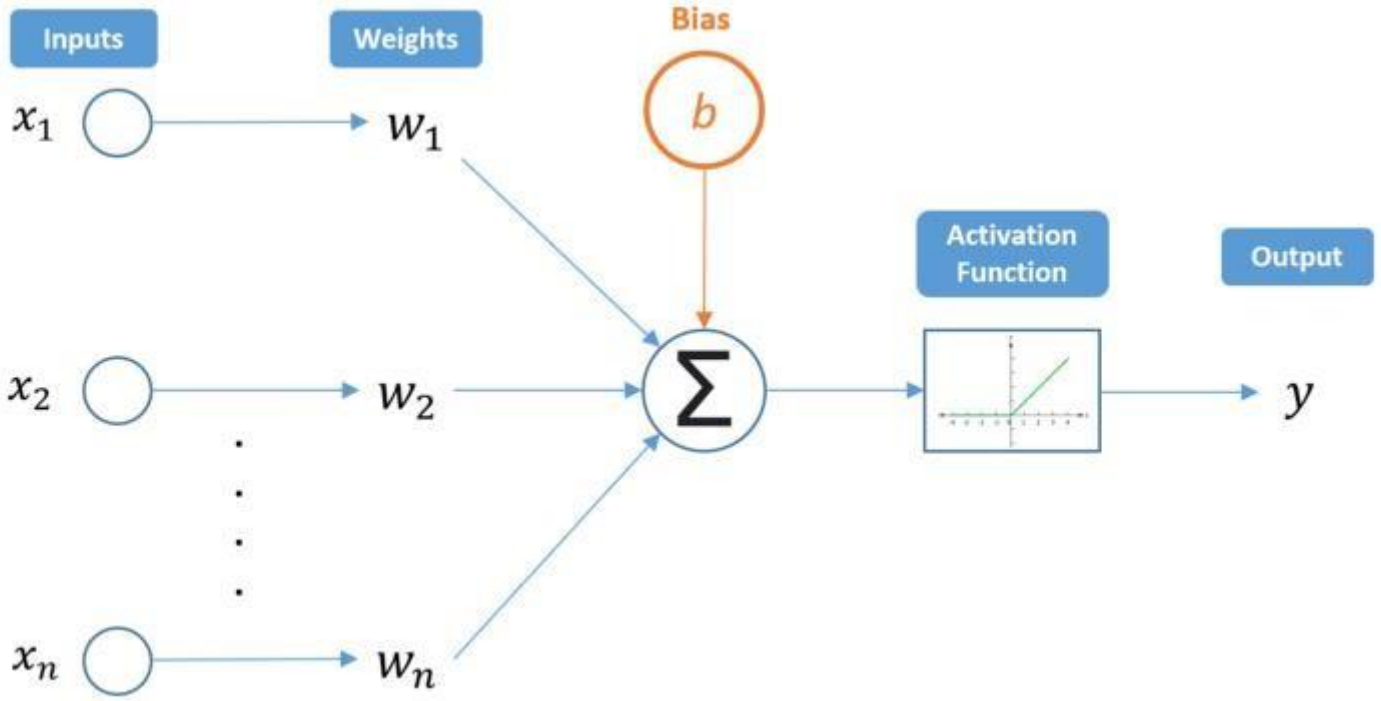
- High learning rate

$$W_{ij}^{*} = W_{ij} - a\left(\frac{\partial E}{\partial W_{ij}}\right)$$

New Weight — Old Weight — Learning Rate — Derivative of Error with respect to Weight

Dying ReLU- Causes

- Large negative bias



Solutions to the Dying ReLU problem?

- Use of a lower learning rate
- Variations of ReLU
- Modification of initialization procedure

References

- Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. MIT Press, 2016.
- https://cs231n.github.io/neural-networks-3/sgd