COMP 554 / CSDS 553 Advanced NLP

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Basics of Neural Networks

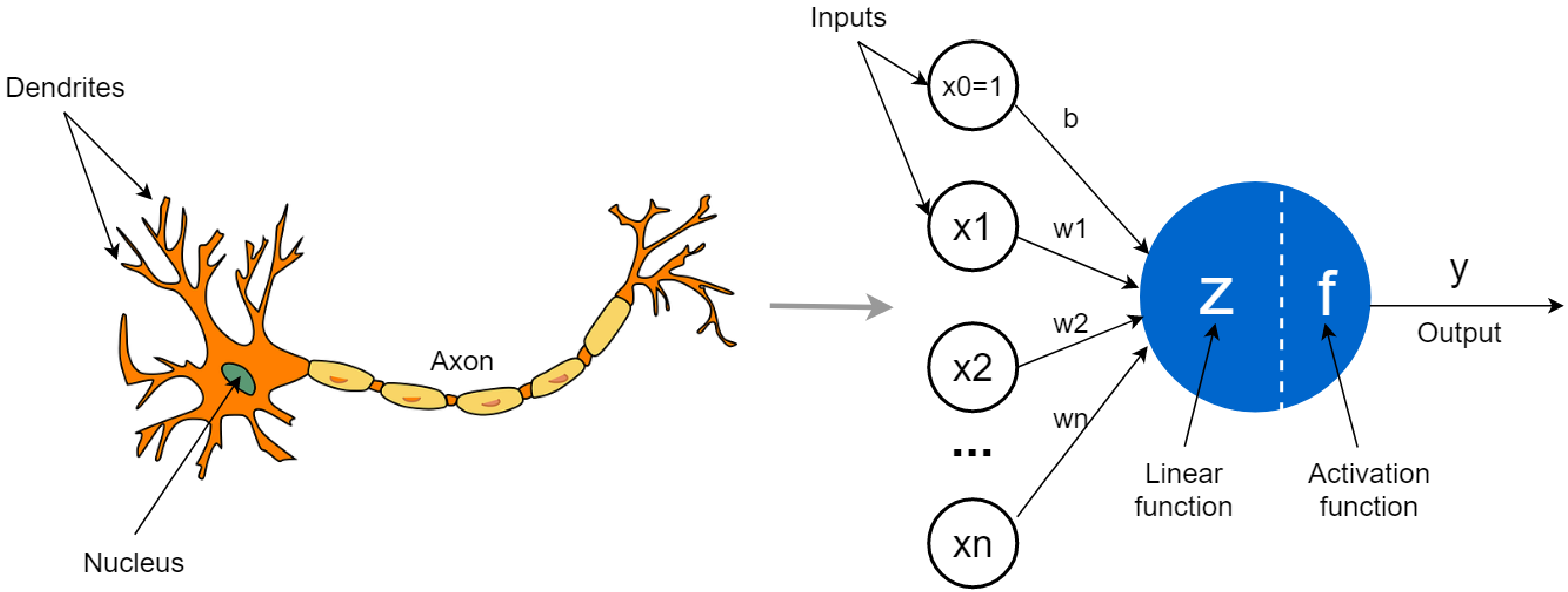
Four Components for ML Systems

- A feature representation of the input, i.e., $[x_1, x_2, ..., x_n]$
- A classification function that computes `\hat{y}`, the estimated class, via `p(y|x)`. Sigmoid, softmax, etc.
- An objective function that we want to optimize for learning, usually involving minimizing a loss function corresponding to error on training examples. Cross-entropy loss function, MAE, MSE, etc.
- An algorithm for optimizing the objective function. The gradient descent

Four Components for ML Systems

- Training: We train the system (specifically the weights w and b) using stochastic gradient descent and the cross-entropy loss.

- Testing: Given a test example x we compute $p(y|x)$ and return the higher probability label $y = 1$ or $y = 0$.

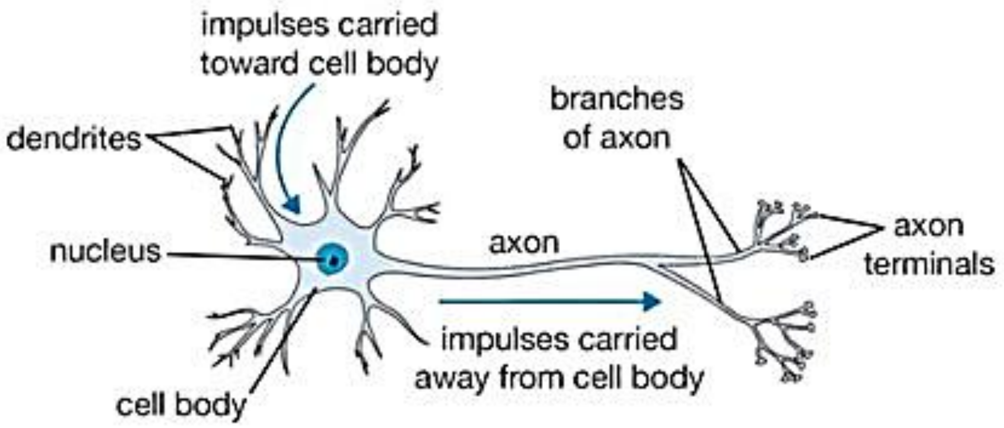


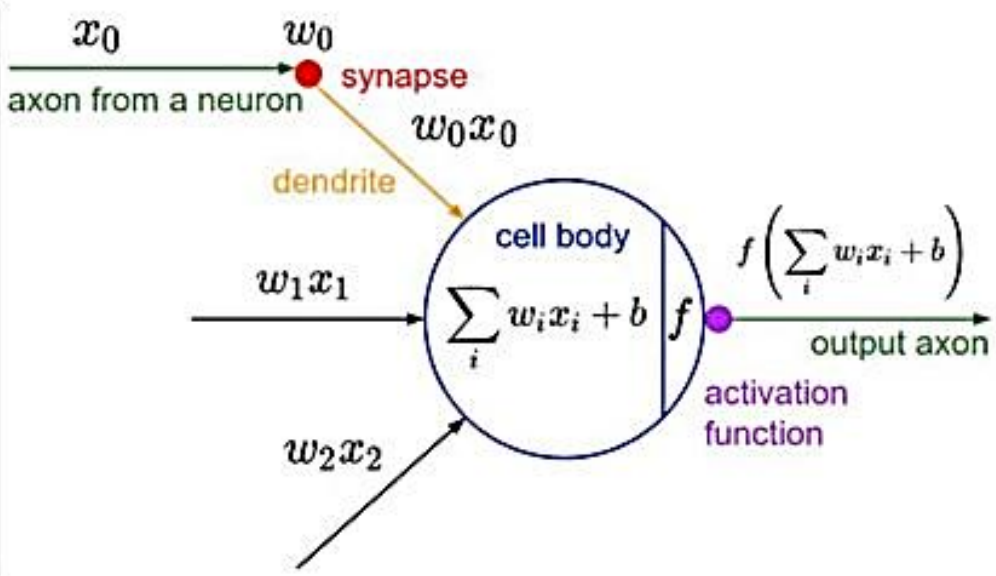
Dendrites receive signals from other neurons

Soma processes the information

Axons transmit the output

Synapses are the connections to other neurons





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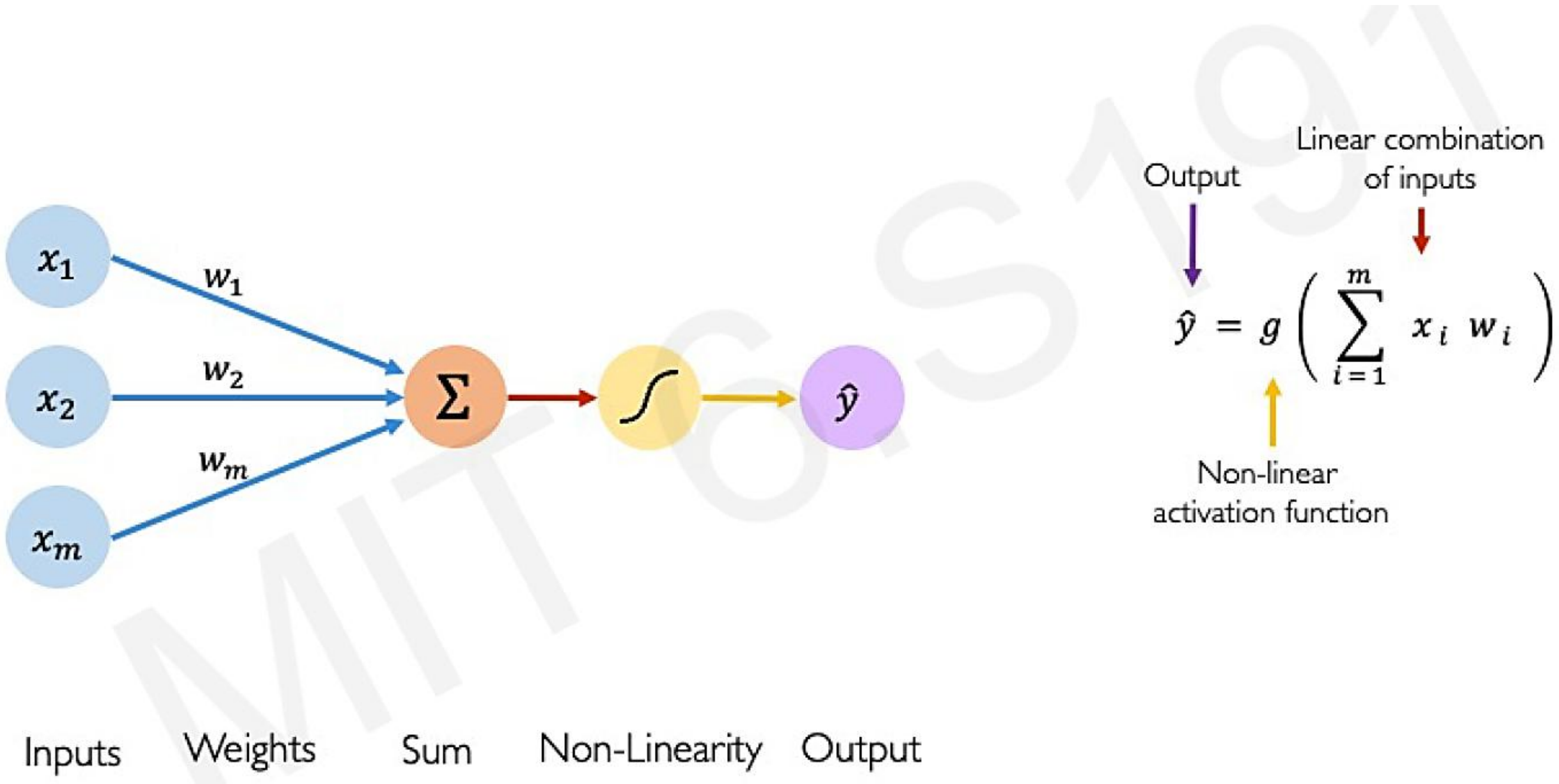
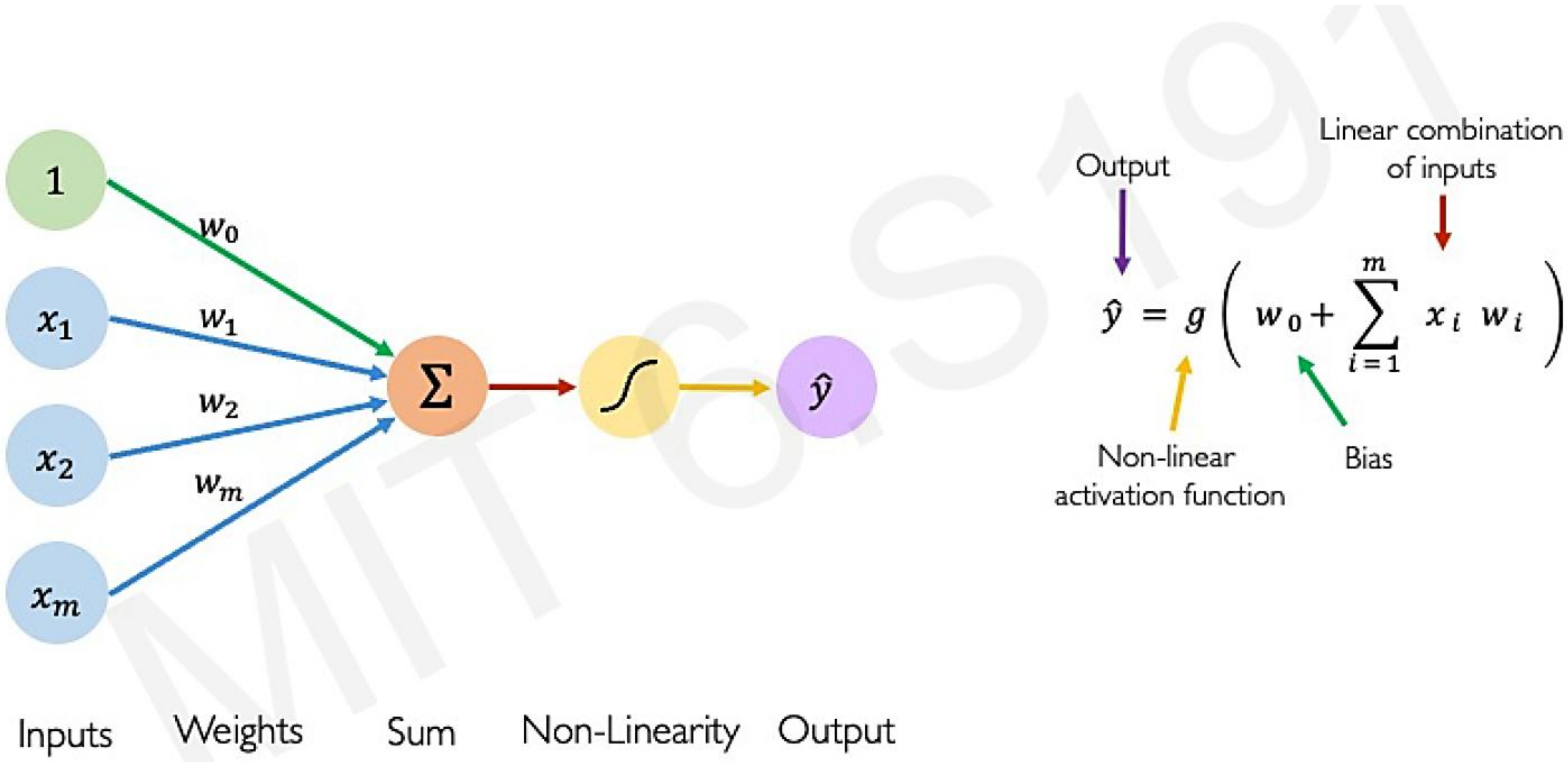
Perceptron


x_1
x_2
x_m
w_1
w_2
w_m
Σ
$\hat{y}$
Inputs
Weights
Sum
Non-Linearity
Output
Output
Linear combination of inputs
$\hat{y} = g\left(\sum_{i=1}^{m} x_i \, w_i\right)$
Non-linear activation function

Perceptron



1
w_0
x_1
w_1
x_2
w_2
x_m
w_m
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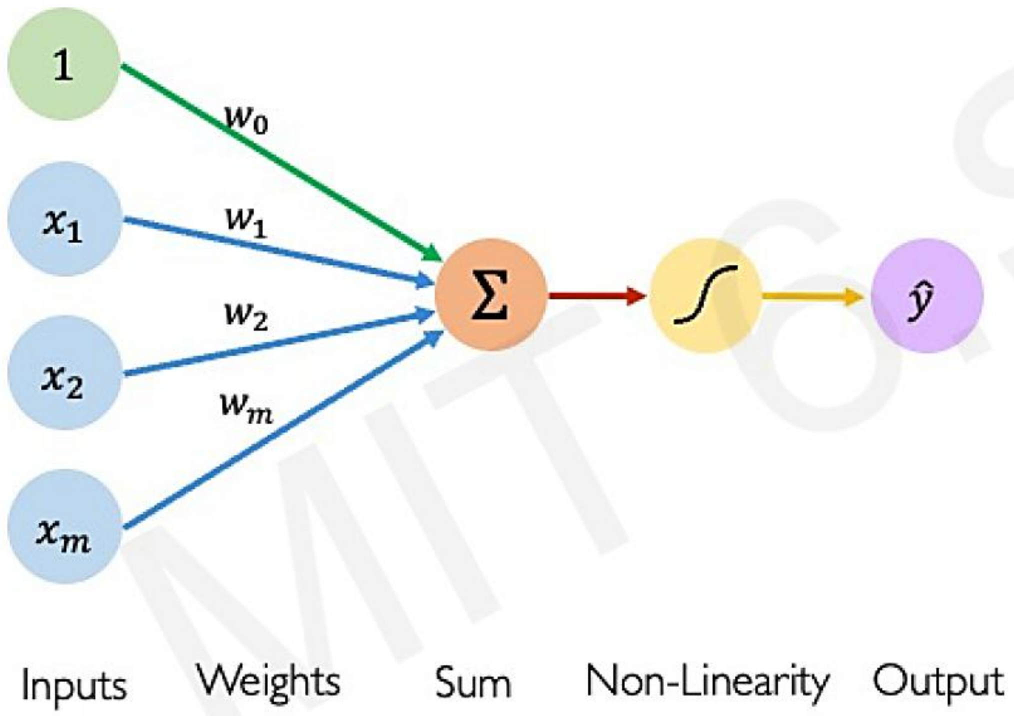
Non-linear activation function
Bias
MIT 6.S191

Perceptron

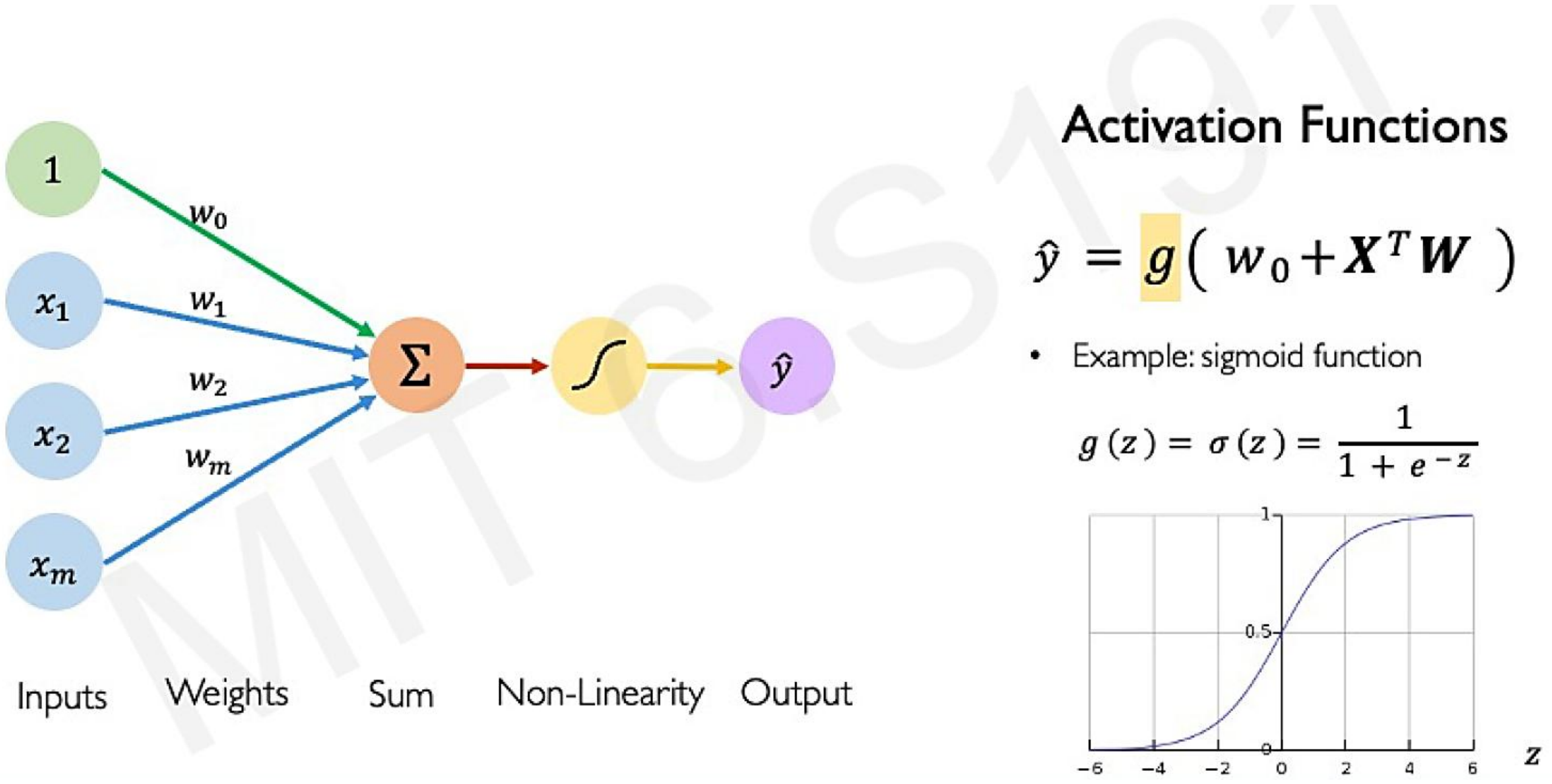


$$\hat{y} = g\left(w_0 + \sum_{i=1}^{m} x_i \, w_i \right)$$

$$\hat{y} = g\left(w_0 + \boldsymbol{X}^T \boldsymbol{W} \right)$$

where: $\boldsymbol{X} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$ and $\boldsymbol{W} = \begin{bmatrix} w_1 \\ \vdots \\ w_m \end{bmatrix}$

Perceptron



1
x_1
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$\hat{y}$
Inputs
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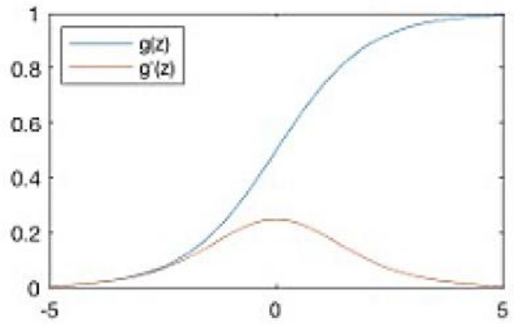
Output
Activation Functions
$\hat{y} = g(\, w_0 + \boldsymbol{X}^T \boldsymbol{W} \,)$
• Example: sigmoid function
$g(z) = \sigma(z) = \dfrac{1}{1 + e^{-z}}$
z
MIT 6.S191

Activation Functions

Sigmoid Function



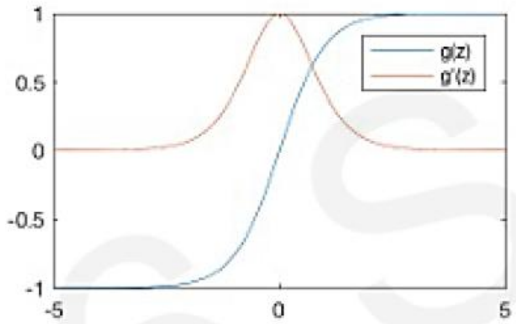
$$g(z) = \frac{1}{1 + e^{-z}}$$

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

```
tf.math.sigmoid(z)
```

```
torch.sigmoid(z)
```

Hyperbolic Tangent



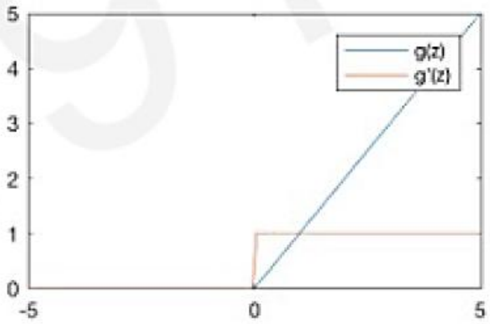
$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

```
tf.math.tanh(z)
```

```
torch.tanh(z)
```

Rectified Linear Unit (ReLU)



$$g(z) = \max(0, z)$$

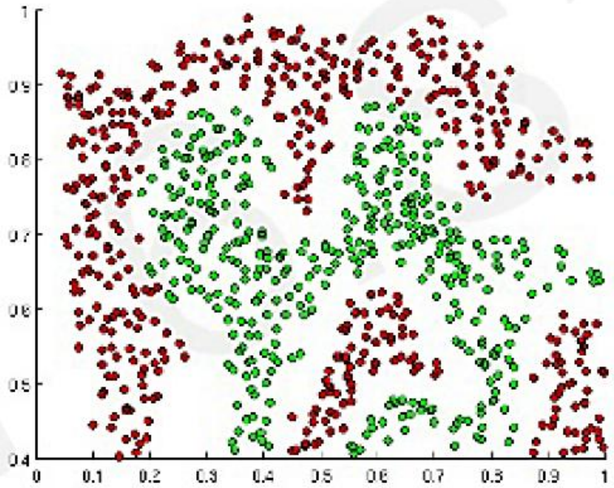
$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

```
tf.nn.relu(z)
```

```
torch.nn.ReLU(z)
```

Activation Functions and Non-Linearities

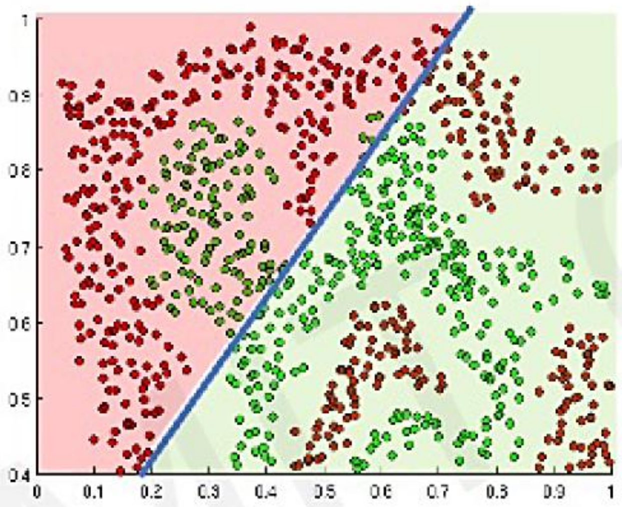
The purpose of activation functions is to ***introduce non-linearities*** *into the network*



What if we wanted to build a neural network to distinguish green vs red points?

Activation Functions and Non-Linearities

*The purpose of activation functions is to **introduce non-linearities** into the network*



Linear activation functions produce linear decisions no matter the network size

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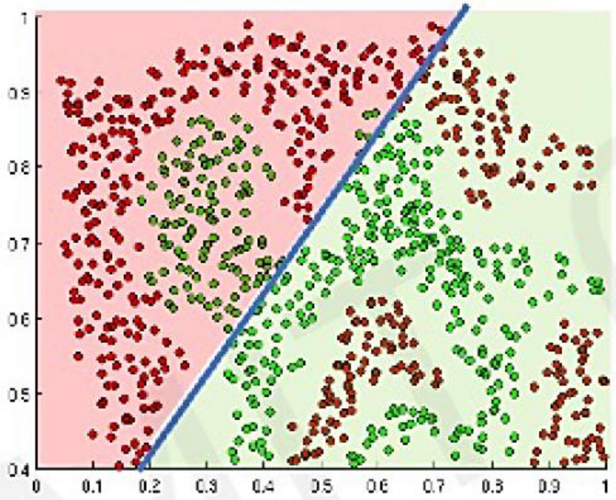
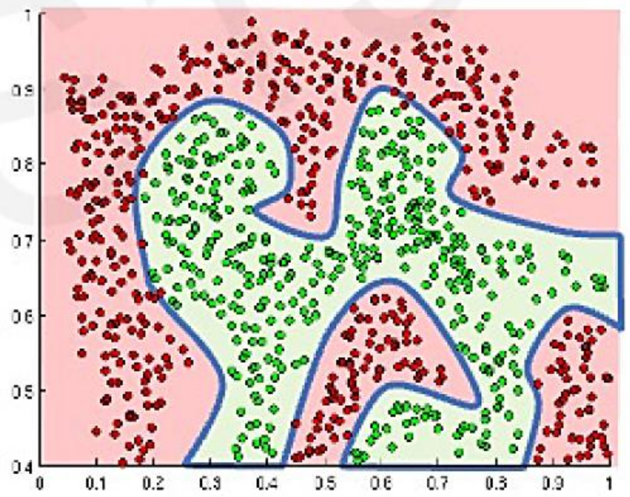
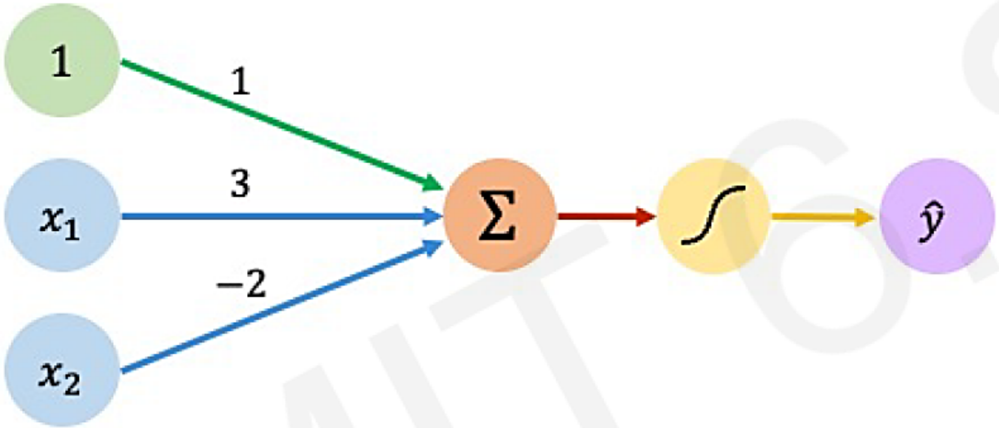


Linear activation functions produce linear decisions no matter the network size



Non-linearities allow us to approximate arbitrarily complex functions

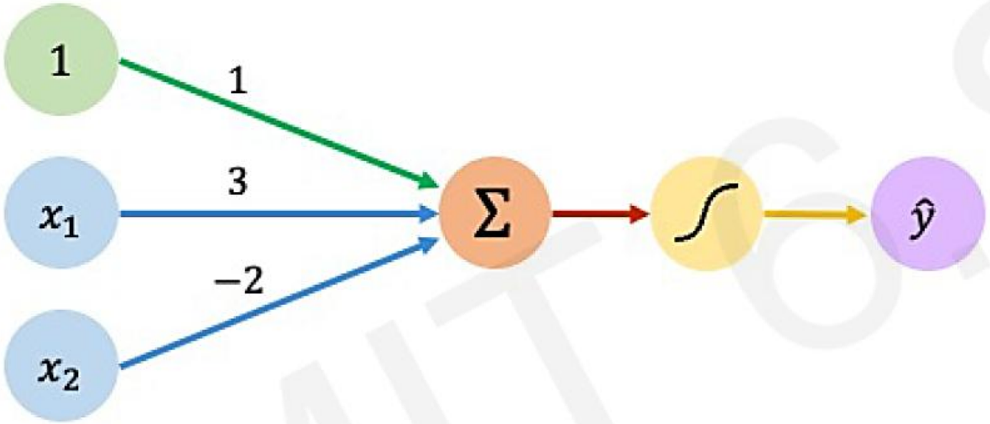
The Perceptron Example

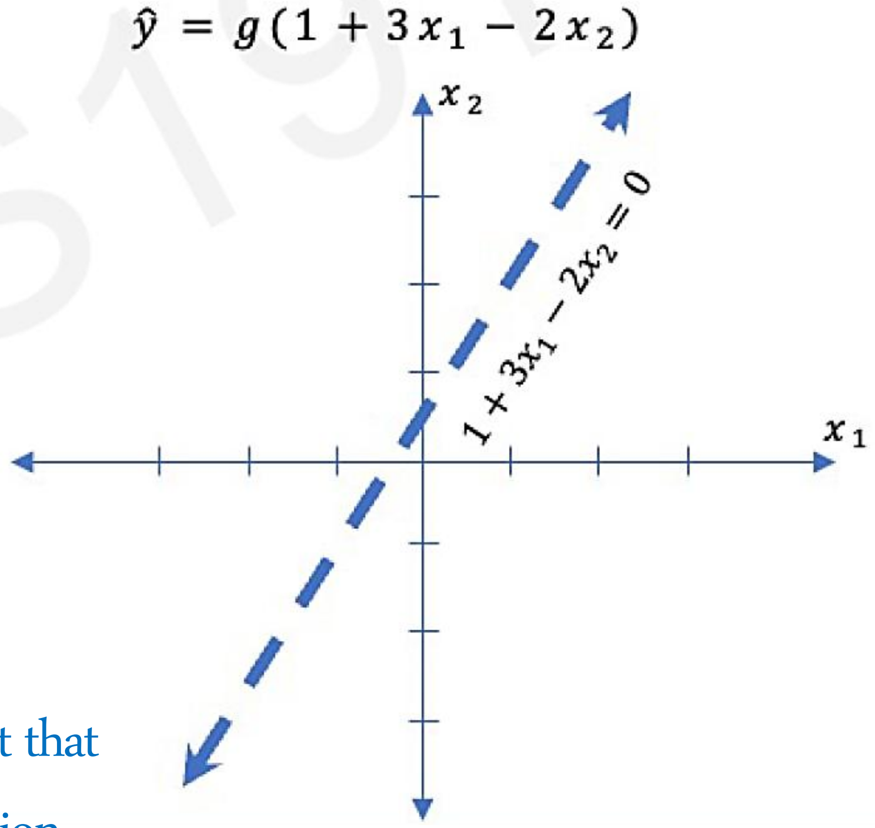


We have: $w_0 = 1$ and $\boldsymbol{W} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$

$$\begin{aligned} \hat{y} &= g(w_0 + \boldsymbol{X}^T \boldsymbol{W}) \\ &= g\left(1 + \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 3 \\ -2 \end{bmatrix}\right) \\ \hat{y} &= g(\underbrace{1 + 3x_1 - 2x_2}_{\text{This is just a line in 2D!}}) \end{aligned}$$

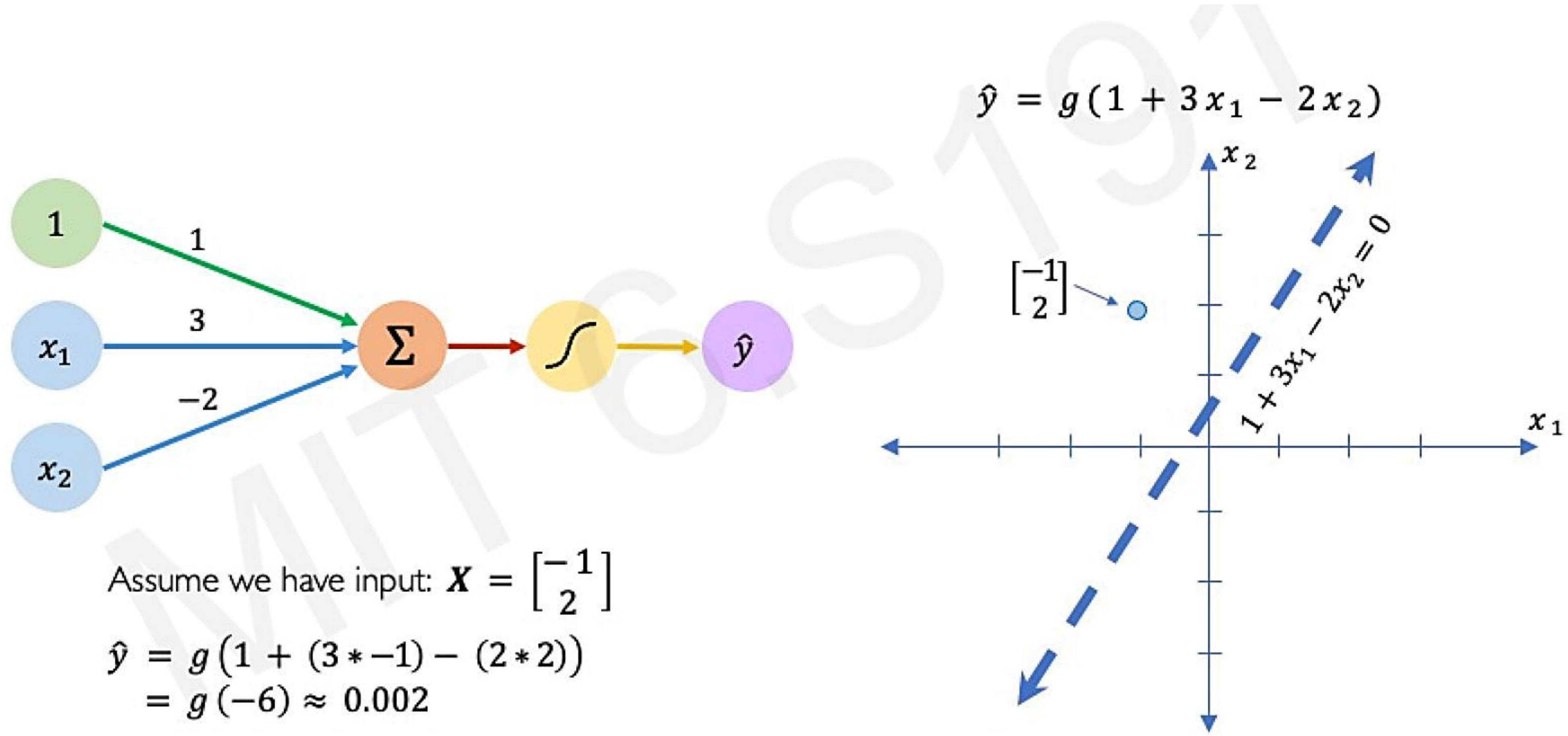
The Perceptron Example



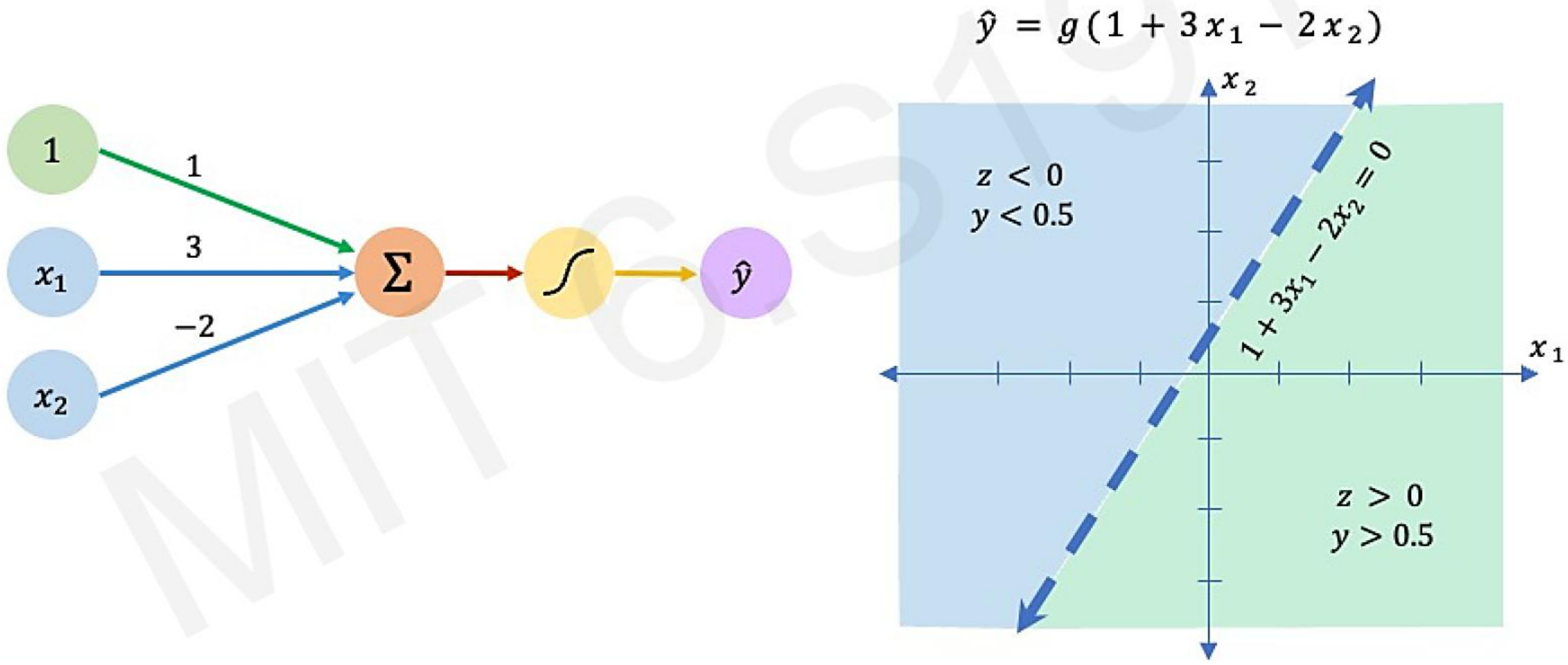


The weight w_i represents how important that input feature is to the classification decision

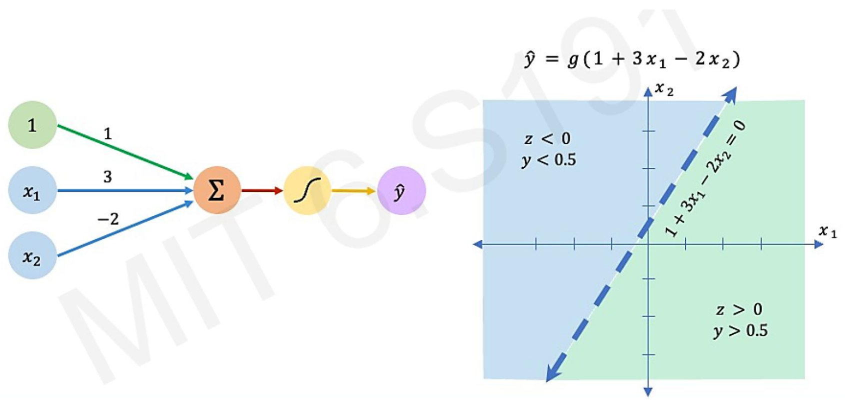
The Perceptron Example

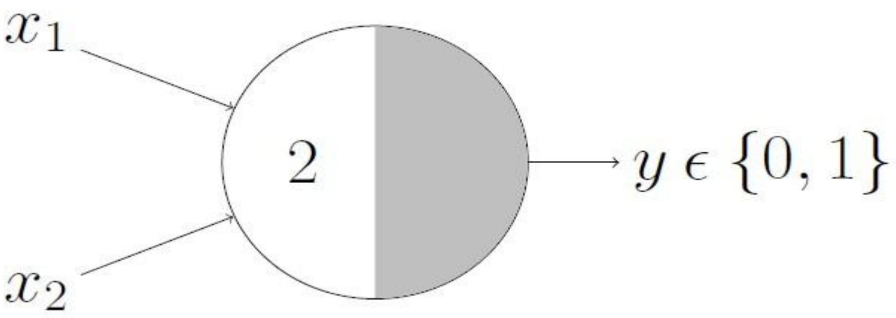


The Perceptron Example



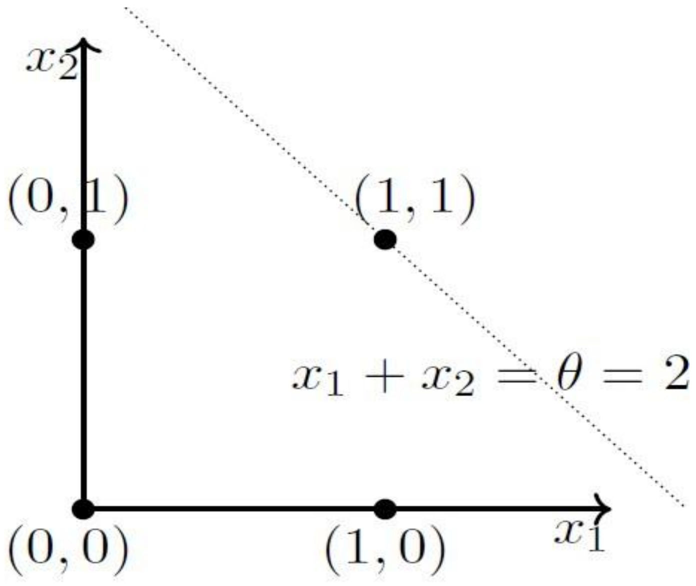
Boolean Functions



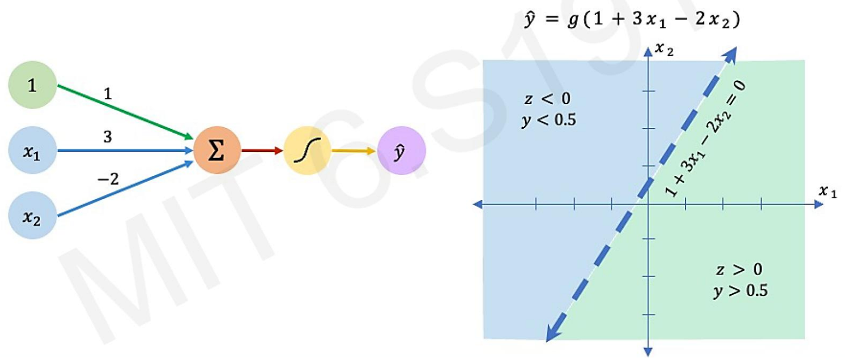


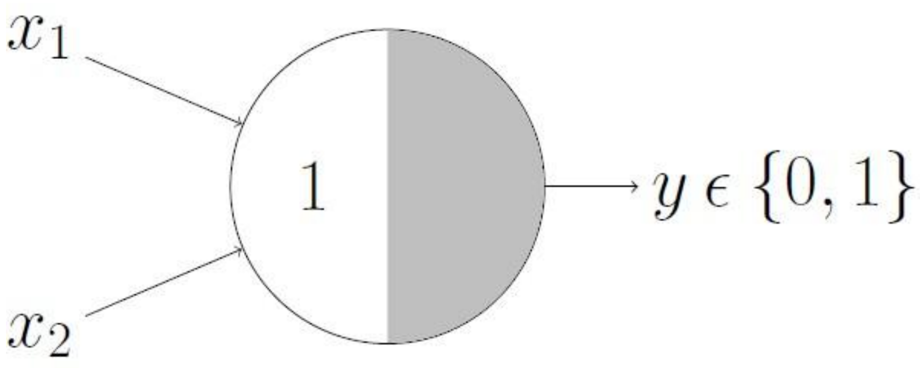
AND function

$$x_1 + x_2 = \sum_{i=1}^{2} x_i \geq 2$$



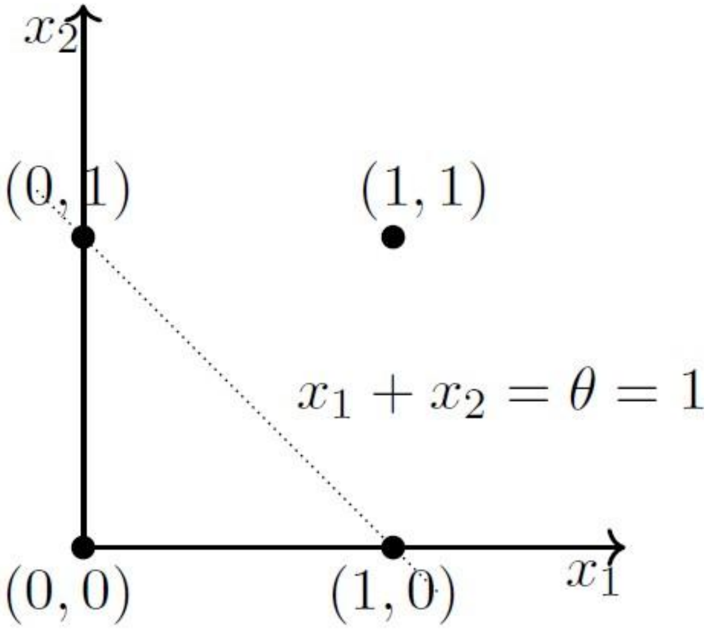
Boolean Functions





OR function

$$x_1 + x_2 = \sum_{i=1}^{2} x_i \geq 1$$



Classification with Logistic Regression

A Document

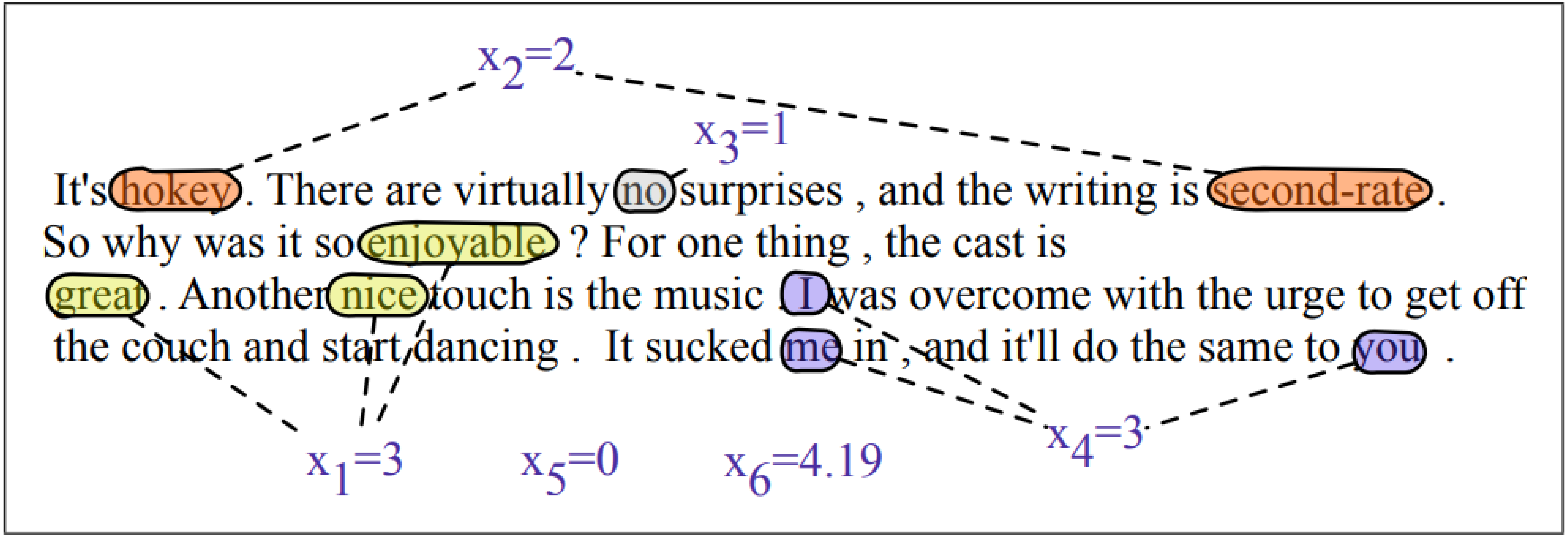


Figure 5.2 A sample mini test document showing the extracted features in the vector *x*.

Features

Var	Definition	Value in Fig. 5.2
x_1	count(positive lexicon words $\in$ doc)	3
x_2	count(negative lexicon words $\in$ doc)	2
x_3	$\begin{cases} 1 & \text{if “no”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	1
x_4	count(1st and 2nd pronouns $\in$ doc)	3
x_5	$\begin{cases} 1 & \text{if “!”} \in \text{doc} \\ 0 & \text{otherwise} \end{cases}$	0
x_6	$\ln(\text{word count of doc})$	$\ln(66) = 4.19$

Weights and Biases

- Let’s assume the 6 weights corresponding to the 6 features are

```
w = [2.5,-5.0,-1.2,0.5,2.0,0.7]
```

```
b = [0.1]
```

The weight w_i represents how important that input feature is to the classification decision

Classification with Logistic Regression

$$
\begin{aligned}
p(+|x) = P(y=1|x) &= \sigma(\mathbf{w}\cdot\mathbf{x}+b) \\
&= \sigma([2.5,-5.0,-1.2,0.5,2.0,0.7]\cdot[3,2,1,3,0,4.19]+0.1) \\
&= \sigma(.833) \\
&= 0.70 \\
p(-|x) = P(y=0|x) &= 1-\sigma(\mathbf{w}\cdot\mathbf{x}+b) \\
&= 0.30
\end{aligned}
$$

Processing many examples at once

$$\textbf{foreach} \quad x^{(i)} \quad \text{in input } [x^{(1)}, x^{(2)}, \ldots, x^{(m)}]$$
$$y^{(i)} = \sigma(\mathbf{w} \cdot \mathbf{x}^{(\mathbf{i})} + b)$$

$$\begin{aligned}
P(y^{(1)} = 1|x^{(1)}) &= \sigma(\mathbf{w} \cdot \mathbf{x}^{(\mathbf{1})} + b) \\
P(y^{(2)} = 1|x^{(2)}) &= \sigma(\mathbf{w} \cdot \mathbf{x}^{(\mathbf{2})} + b) \\
P(y^{(3)} = 1|x^{(3)}) &= \sigma(\mathbf{w} \cdot \mathbf{x}^{(\mathbf{3})} + b)
\end{aligned}$$

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \ldots & x_f^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \ldots & x_f^{(2)} \\ x_1^{(3)} & x_2^{(3)} & \ldots & x_f^{(3)} \\ \ldots & & & \end{bmatrix}$$

$$\hat{y}^{(1)} = [x_1^{(1)}, x_2^{(1)}, \ldots, x_f^{(1)}] \cdot [w_1, w_2, \ldots, w_f] + b$$

$$\underset{(m \times 1)}{\mathbf{y}} = \underset{(m \times f)}{\mathbf{X}} \; \underset{(f \times 1)}{\mathbf{w}} + \underset{(m \times 1)}{\mathbf{b}}$$

Cost Function

Cost Function

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

m examples $\quad x \in \begin{bmatrix} x_0 \\ x_1 \\ \cdots \\ x_n \end{bmatrix} \quad x_0 = 1, y \in \{0, 1\}$

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

How to choose parameters θ ?

Cost Function

$L(\hat{y}, y)$ = How much $\hat{y}$ differs from the true y.

A good cost function?

1. Punish incorrect answers with high cost

y=1, $h\theta(x) \longrightarrow 0$

y=0, $h\theta(x) \longrightarrow 1$

2. Reward correct answers with a low cost

y=1, $h\theta(x) \longrightarrow 1$

y=0, $h\theta(x) \longrightarrow 0$

The cross-entropy loss function

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

L(ŷ, y) = How much ŷ differs from the true y.

- Rewards $\mathrm{y} = 1, h_{\theta}(x)$ = 1, with cost = 0
- Rewards $\mathrm{y} = 1, h_{\theta}(x)$ → 0 even further with asymptotically smaller costs

y=1

cost = $\log(h_{\theta}(x))$

- Rewards $\mathrm{y} = 1, h_{\theta}(x)$ = 1, with cost = 0
- Punishes $\mathrm{y} = 1, h_{\theta}(x)$ → 0 with asymptotically higher costs

y=1

cost = $-\log(h_{\theta}(x))$

- Rewards $\mathrm{y} = 0, h_\theta\,(x)$ = 0, with cost = 0
- Rewards $\mathrm{y} = 0, h_\theta\,(x)$ → 1 even further with asymptotically smaller costs

y=0

cost = $\log(1 - h_\theta\,(x))$

- Rewards $\mathrm{y} = 0, h_\theta\,(x)$ = 0, with cost = 0
- Punishes $\mathrm{y} = 0, h_\theta\,(x)$ → 1 with asymptotically higher costs

y=0

cost = $-\log(1 - h_\theta\,(x))$

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

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

$$\boldsymbol{cost(h_\theta(x), y) = -y\, log\big(h_\theta(x)\big) - (1-y)\, log\big(1-h_\theta(x)\big)}$$

$$L_{\mathrm{CE}}(\hat{y}, y) = -[y \log \sigma(\mathbf{w} \cdot \mathbf{x} + b) + (1-y) \log (1 - \sigma(\mathbf{w} \cdot \mathbf{x} + b))]$$

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

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

To fit parameters θ:

$$\min_\theta J(\theta)$$

To make a prediction given new x:

Output $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$ gives $p(y = 1|x; \theta)$

$$
\begin{aligned}
L_{\mathrm{CE}}(\hat{y},y) &= -[y\log\sigma(\mathbf{w}\cdot\mathbf{x}+b)+(1-y)\log(1-\sigma(\mathbf{w}\cdot\mathbf{x}+b))] \\
&= -[\log\sigma(\mathbf{w}\cdot\mathbf{x}+b)] \\
&= -\log(.70) \\
&= .36
\end{aligned}
$$

$$
\begin{aligned}
L_{\mathrm{CE}}(\hat{y},y) &= -[y\log\sigma(\mathbf{w}\cdot\mathbf{x}+b)+(1-y)\log(1-\sigma(\mathbf{w}\cdot\mathbf{x}+b))] \\
&= -[\log(1-\sigma(\mathbf{w}\cdot\mathbf{x}+b))] \\
&= -\log(.30) \\
&= 1.2
\end{aligned}
$$

Gradient Descent

Gradient Descent

The goal is to find the set of weights which minimizes the loss function, averaged over all examples:

$$\hat{\theta} \;=\; \underset{\theta}{\operatorname{argmin}} \frac{1}{m} \sum_{i=1}^{m} L_{\mathrm{CE}}(f(x^{(i)};\theta), y^{(i)})$$

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

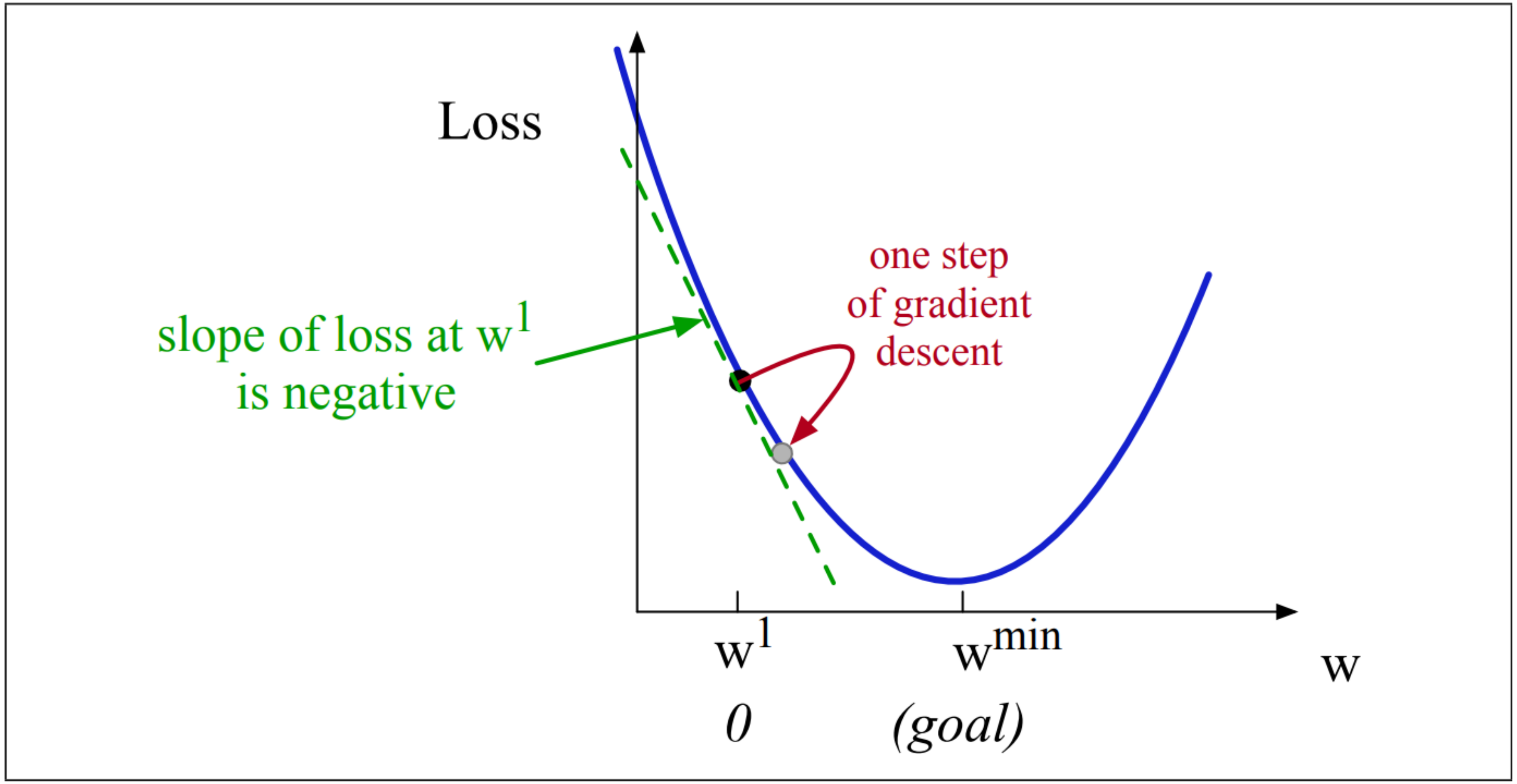
Repeat $\{$

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

$\}$ (simultaneously update all θ_j)

$$w^{t+1} = w^t - \eta \frac{d}{dw} L(f(x;w), y)$$

Gradient Descent



function STOCHASTIC GRADIENT DESCENT($L()$, $f()$, x, y) **returns** θ
where: L is the loss function
f is a function parameterized by θ
x is the set of training inputs $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$
y is the set of training outputs (labels) $y^{(1)}, y^{(2)}, \ldots, y^{(m)}$

$\theta \leftarrow 0$ # (or small random values)
repeat til done   # see caption
  For each training tuple $(x^{(i)}, y^{(i)})$ (in random order)
    1. Optional (for reporting):   # How are we doing on this tuple?
      Compute $\hat{y}^{(i)} = f(x^{(i)};\theta)$ # What is our estimated output $\hat{y}$?
      Compute the loss $L(\hat{y}^{(i)}, y^{(i)})$ # How far off is $\hat{y}^{(i)}$ from the true output $y^{(i)}$?
    2. $g \leftarrow \nabla_\theta L(f(x^{(i)};\theta), y^{(i)})$ # How should we move θ to maximize loss?
    3. $\theta \leftarrow \theta - \eta\, g$ # Go the other way instead
return θ

Batch Gradient Descent

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

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

Repeat $\{$

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

$\}$ (simultaneously update all θ_j)

$$\frac{\partial L_{\mathrm{CE}}(\hat{y}, y)}{\partial w_j} = [\sigma(\mathbf{w} \cdot \mathbf{x} + b) - y] x_j$$
$$= (\hat{y} - y) x_j$$

(see SLP3 for derivation)

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

Batch Gradient Descent

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

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

Repeat $\{$

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

(simultaneously update all θ_j)

$\}$

$$\nabla L(f(x;\boldsymbol{\theta}), y) = \begin{bmatrix} \frac{\partial}{\partial w_1} L(f(x;\boldsymbol{\theta}), y) \\ \frac{\partial}{\partial w_2} L(f(x;\boldsymbol{\theta}), y) \\ \vdots \\ \frac{\partial}{\partial w_n} L(f(x;\boldsymbol{\theta}), y) \\ \frac{\partial}{\partial b} L(f(x;\boldsymbol{\theta}), y) \end{bmatrix}$$

Algorithm looks identical to linear regression!

Gradient Descent Example

$$
\begin{aligned}
x_1 &= 3 \quad \text{(count of positive lexicon words)} \\
x_2 &= 2 \quad \text{(count of negative lexicon words)}
\end{aligned}
$$

$$
\begin{aligned}
w_1 = w_2 = b &= 0 \\
\eta &= 0.1
\end{aligned}
$$

$$\theta^{t+1} = \theta^t - \eta \nabla_\theta L(f(x^{(i)}; \theta), y^{(i)})$$

$$\nabla_{w,b}L = \begin{bmatrix} \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_1} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial w_2} \\ \frac{\partial L_{\mathrm{CE}}(\hat{y},y)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(\mathbf{w}\cdot\mathbf{x}+b)-y)x_1 \\ (\sigma(\mathbf{w}\cdot\mathbf{x}+b)-y)x_2 \\ \sigma(\mathbf{w}\cdot\mathbf{x}+b)-y \end{bmatrix} = \begin{bmatrix} (\sigma(0)-1)x_1 \\ (\sigma(0)-1)x_2 \\ \sigma(0)-1 \end{bmatrix} = \begin{bmatrix} -0.5x_1 \\ -0.5x_2 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

$$\theta^1 = \begin{bmatrix} w_1 \\ w_2 \\ b \end{bmatrix} - \eta \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix} = \begin{bmatrix} .15 \\ .1 \\ .05 \end{bmatrix}$$

So, after one step of gradient descent, the weights have shifted to be: w1 = .15, w2 = .1, and b = .05

Softmax

Softmax

- For a vector z of dimensionality K, the softmax is defined as:

$$\text{softmax}(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^{K} \exp(z_j)} \quad 1 \leq i \leq K$$

- The softmax of an input vector $z = [z_1, z_2, ..., z_K]$ is thus a vector itself:

$$\text{softmax}(\mathbf{z}) = \left[\frac{\exp(z_1)}{\sum_{i=1}^{K} \exp(z_i)}, \frac{\exp(z_2)}{\sum_{i=1}^{K} \exp(z_i)}, ..., \frac{\exp(z_K)}{\sum_{i=1}^{K} \exp(z_i)} \right]$$

Softmax

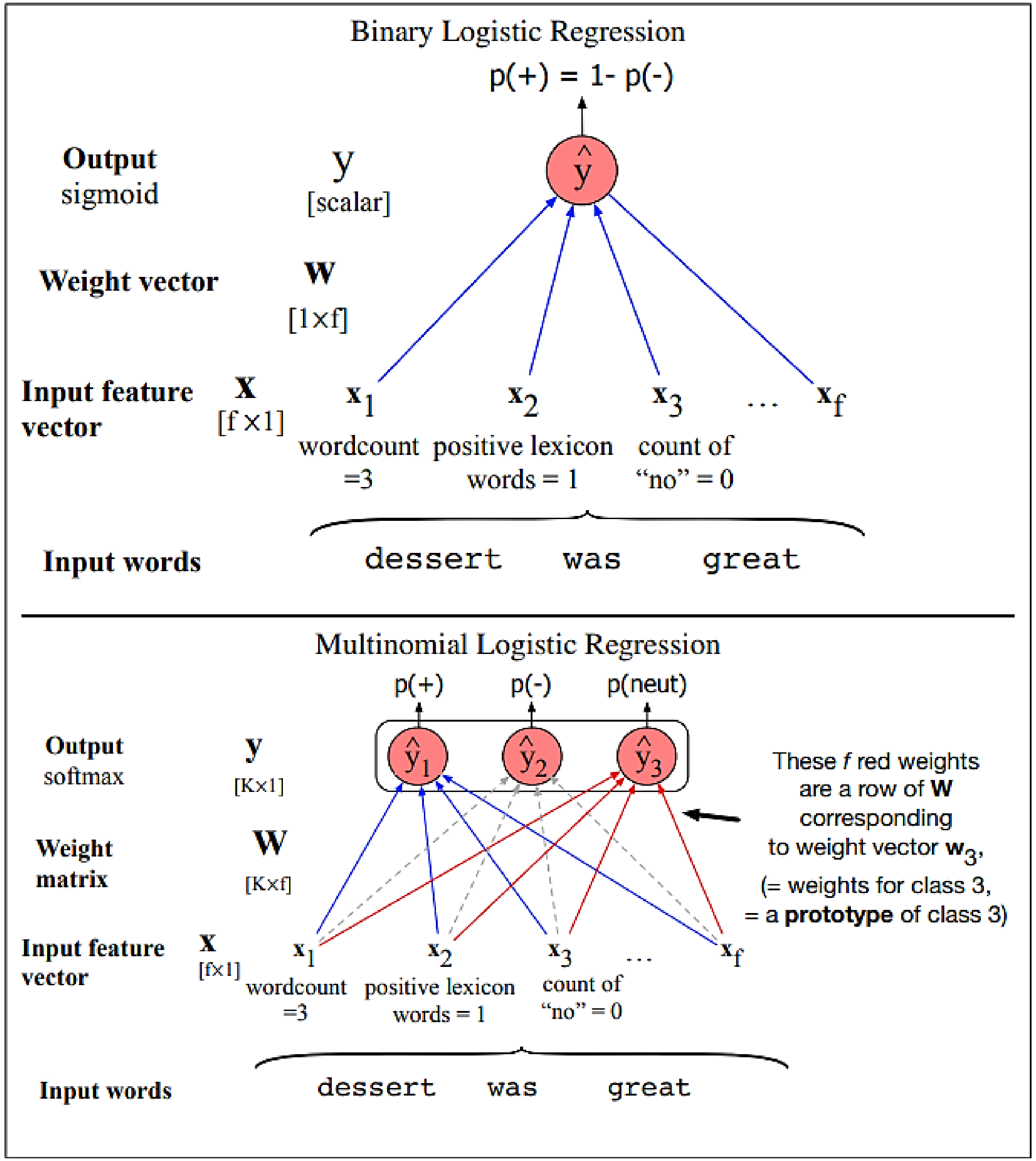
$$\mathrm{softmax}(\mathbf{z}) = \left[\frac{\exp(z_1)}{\sum_{i=1}^{K}\exp(z_i)}, \frac{\exp(z_2)}{\sum_{i=1}^{K}\exp(z_i)}, \ldots, \frac{\exp(z_K)}{\sum_{i=1}^{K}\exp(z_i)}\right]$$

$$\mathbf{z} = [0.6, 1.1, -1.5, 1.2, 3.2, -1.1]$$

The resulting (rounded) softmax(z) is:

$$[0.05, 0.09, 0.01, 0.1, 0.74, 0.01]$$

A neural network can be viewed as a series of logistic regression classifiers stacked on top of each other



Sources

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- https://web.stanford.edu/~jurafsky/slp3/3.pdf
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