CS2109S: Introduction to AI and Machine Learning

Lecture 8: Intro to Neural Networks

13 October 2023

Recap

- Overfitting
- Regularization
 - Linear and logistic regression
- Support Vector Machine (SVM)
 - Hard-margin SVM
 - Soft-margin SVM
- Kernel
 - SVM with Kernel Trick

Logistic Regression / SVM With x as features

Logistic Regression / SVM With $\phi(x)$ as features

SVM with Kernel Trick With $\phi(x)$ mapping to finite-dimensional features

SVM with Kernel Trick With $\phi(x)$ mapping to infinite-dimensional features





Linear Regression w/ Regz: Gradient Descent

$$J(w) = \frac{1}{2m} \left[\sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)})^{2} + \lambda \sum_{i=1}^{n} w_{i}^{2} \right]$$
Optimization goal: min $J(w)$

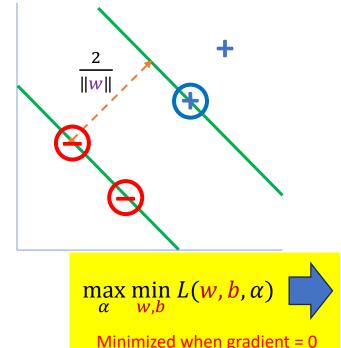
$$Repeat \left\{ w_{0} := w_{0} - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)}) \cdot x_{0}^{(i)} \right\}$$

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

$$w_{n} := w_{n} - \alpha \frac{1}{m} \left[\sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)}) \cdot x_{n}^{(i)} + \lambda w_{n} \right]$$
Why does
$$w_{n} := w_{n} - \alpha \frac{1}{m} \left[\sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)}) \cdot x_{n}^{(i)} + \lambda w_{n} \right]$$
This work?

Support Vector Machines (SVM)





$$\max \frac{2}{\|w\|} \to \max \frac{1}{\|w\|} \to \min \|w\| \to \min \frac{1}{2} \|w\|^2 \quad \text{"Maximize gap"}$$
Assume $x^{(i)}$ in margin

s.t.
$$\bar{y}^{(i)}(w \cdot x^{(i)} + b) - 1 \ge 0$$
 "Classify correctly"

$\mathbf{b} = \bar{y}^{(i)} - \mathbf{w} \cdot \mathbf{x}^{(i)}$

Objective (Lagrange Dual):

Objective (Lagrange Dual).
$$L(w, \mathbf{b}, \alpha) = \frac{1}{2} ||w||^2 - \sum_{i} \alpha^{(i)} [\bar{y}^{(i)}(w \cdot x^{(i)} + b) - 1], \forall_i \alpha^{(i)} \ge 0$$

$$\frac{\partial L(w, \mathbf{b}, \alpha)}{\partial w} = w - \sum_{i} \alpha^{(i)} \bar{y}^{(i)} x^{(i)} = 0$$

$$\frac{\partial L(w, \mathbf{b}, \alpha)}{\partial b} = \sum_{i} \alpha^{(i)} \bar{y}^{(i)} = 0$$
Samples with non-zero $\alpha^{(i)}$ = support vectors

$$\frac{\partial L(\mathbf{w}, \mathbf{b}, \alpha)}{\partial \mathbf{b}} = \sum_{i} \alpha^{(i)} \bar{y}^{(i)} = 0$$

... a few math later ...

Maximize
$$\longrightarrow L(\alpha) = \sum_{i} \alpha^{(i)} - \frac{1}{2} \sum_{i} \sum_{j} \alpha^{(i)} \alpha^{(j)} \overline{y}^{(i)} \overline{y}^{(j)} x^{(i)} \cdot x^{(j)}$$

SVM with Kernel Trick

From Before:
$$w = \sum_{i} \alpha^{(i)} \hat{y}^{(i)} x^{(i)}$$

Objective:

$$L(\mathbf{w}, \mathbf{b}, \alpha) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i} \alpha^{(i)} [\bar{y}^{(i)} (\mathbf{w} \cdot \phi(x^{(i)}) + b) - 1]$$

... a few math later ...

Decision Rule:

$$w \cdot \phi(x) + b \ge 0 \text{ then } +$$

$$\sum_{i} \alpha^{(i)} \hat{y}^{(i)} \phi(x^{(i)}) \cdot \phi(x) + b \ge 0 \text{ then } +$$

$$\sum_{i} \alpha^{(i)} \hat{y}^{(i)} K(x^{(i)}, x) + b \ge 0 \text{ then } +$$

$$\mathbf{L}(\boldsymbol{\alpha}) = \sum_{i} \alpha^{(i)} - \frac{1}{2} \sum_{i} \sum_{j} \alpha^{(i)} \alpha^{(j)} \bar{y}^{(i)} \bar{y}^{(j)} \phi(x^{(i)}) \cdot \phi(x^{(j)})$$

$$L(\alpha) = \sum_{i} \alpha^{(i)} - \frac{1}{2} \sum_{i} \sum_{j} \alpha^{(i)} \alpha^{(j)} \bar{y}^{(i)} \bar{y}^{(j)} \phi(x^{(i)}) \cdot \phi(x^{(j)})$$

$$L(\alpha) = \sum_{i} \alpha^{(i)} - \frac{1}{2} \sum_{i} \sum_{j} \alpha^{(i)} \alpha^{(j)} \bar{y}^{(i)} \bar{y}^{(j)} K(x^{(i)}, x^{(j)})$$

There is <u>no need</u> to compute the transformed features explicitly!

Can have SVM with **infinite-dimensional** features!



Outline

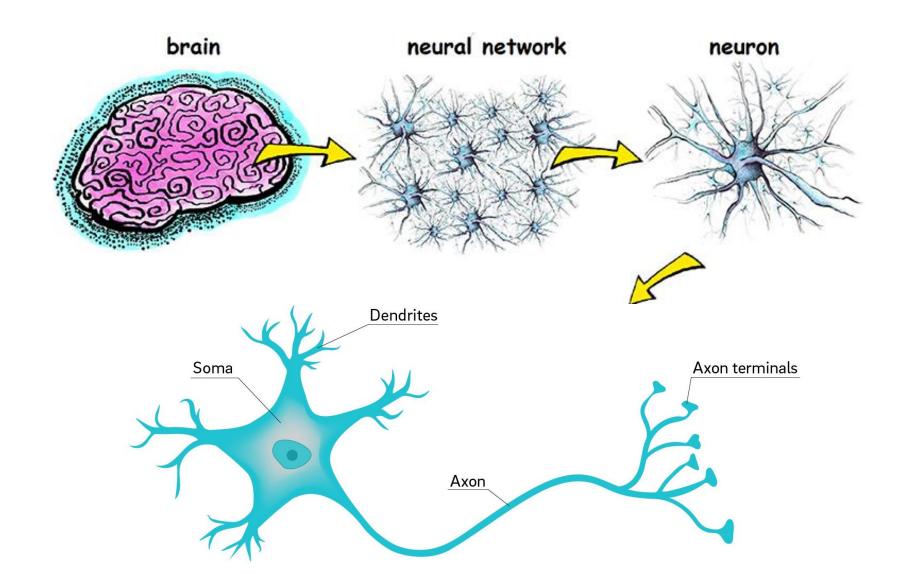
- Perceptron
 - Biological inspiration
 - Perceptron Learning Algorithm
- Neural Networks
 - Single-layer Neural Networks
 - Multi-layer Neural Networks
 - Regression and Classification
- Neural Networks with Gradient Descent
- Neural Networks vs Other Models

Outline

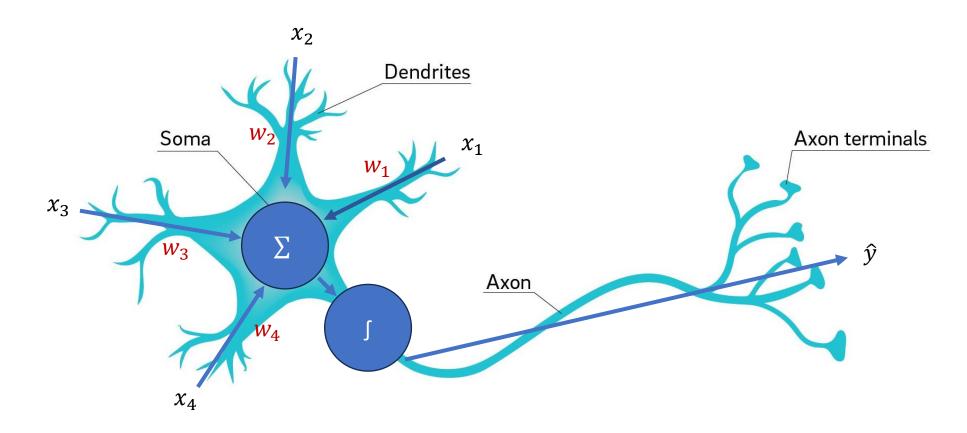
Perceptron

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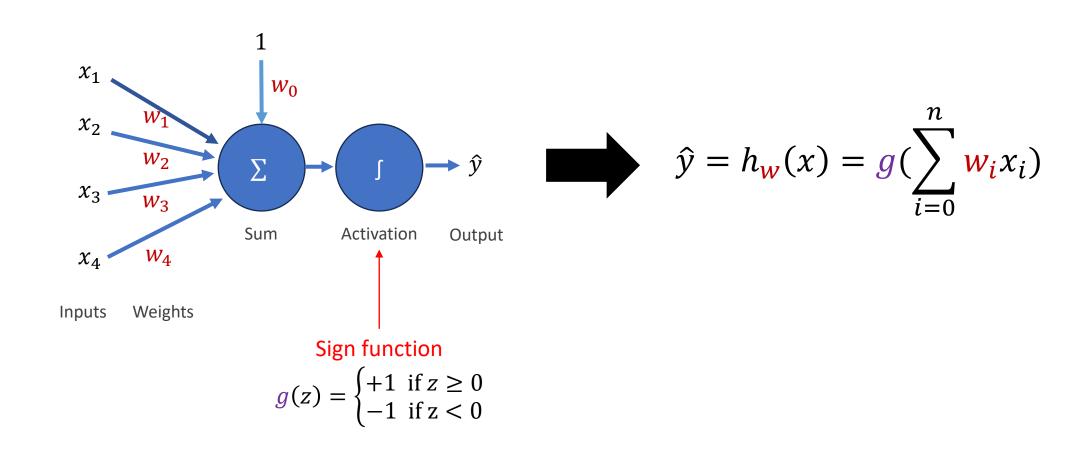
Brain and Neuron



Neuron

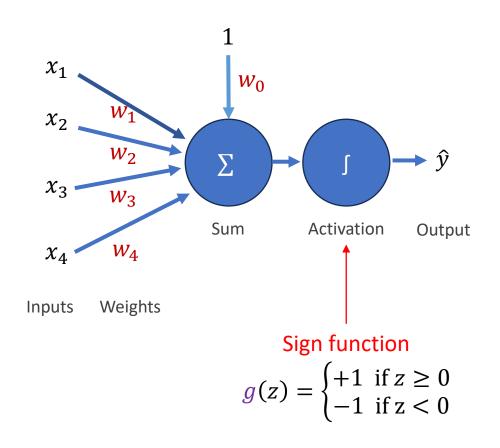


Perceptron

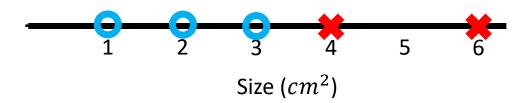


Perceptron: An Example

$$\hat{y} = h_{\mathbf{w}}(x) = g(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

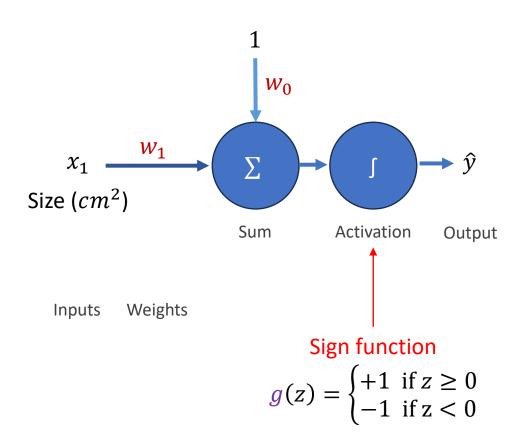


Cancer prediction: benign (-1), malignant (1)



Perceptron: An Example

$$\hat{y} = h_{\mathbf{w}}(x) = g(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$



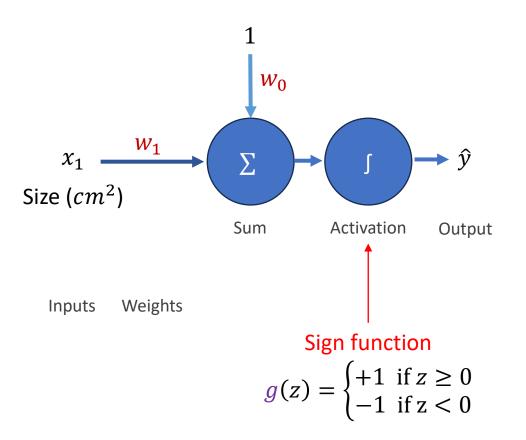
$$h_{\mathbf{w}}(x) = \begin{cases} +1 & \text{if } \mathbf{w}_0 + \mathbf{w}_1 x \ge 0 \\ -1 & \text{otherwise} \end{cases}$$
$$h_{\mathbf{w}}(x) = \begin{cases} +1 & \text{if } -3.5 + 1x \ge 0 \\ -1 & \text{otherwise} \end{cases}$$

Cancer prediction: benign (-1), malignant (1)



Perceptron: An Example

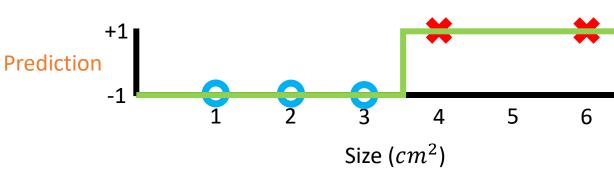
$$\hat{y} = h_{\mathbf{w}}(x) = g(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$



$$h_{\mathbf{w}}(x) = \begin{cases} +1 & \text{if } \mathbf{w}_0 + \mathbf{w}_1 x \ge 0 \\ -1 & \text{otherwise} \end{cases}$$

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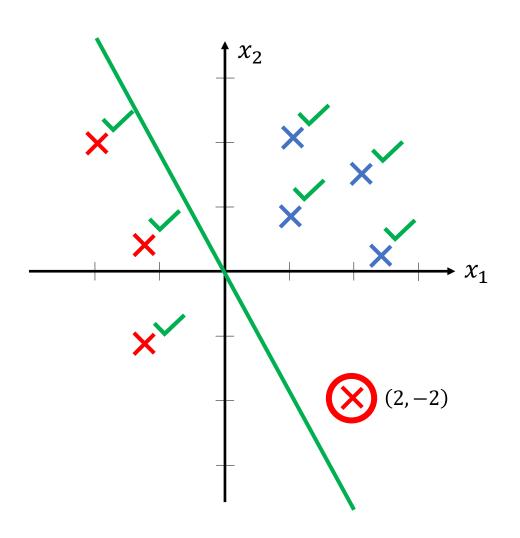
Cancer prediction: benign (-1), malignant (1)



How do we learn *w* **while** g is <u>not</u> differentiable?

Perceptron Learning Algorithm

- Initialize $\forall_i \mathbf{w}_i = 0$
- Loop (until convergence or max steps reached)
 - For each instance $(x^{(i)}, y^{(i)})$, classify $\hat{y}^{(i)} = h_{\mathbf{w}}(x^{(i)})$
 - Select one misclassified instance $(x^{(j)}, y^{(j)})$
 - Update weights: $\mathbf{w} \leftarrow \mathbf{w} + \gamma (y^{(j)} \hat{y}^{(j)}) x^{(j)}$ Learning rate



Sign function

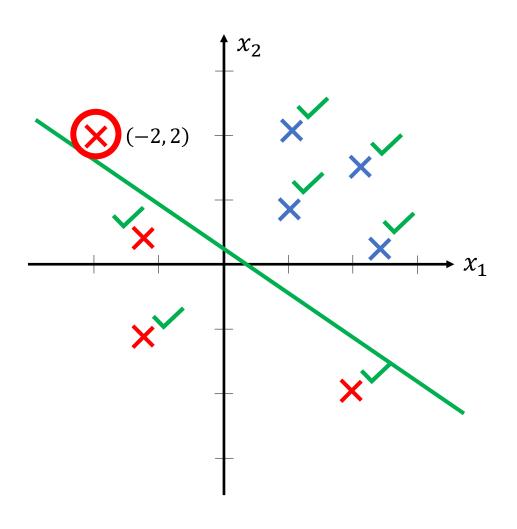
$$g(z) = \begin{cases} +1 & \text{if } z \ge 0 \\ -1 & \text{if } z < 0 \end{cases}$$

$$\hat{y} = h_{w}(x) = g(w_0 + w_1 x_1 + w_2 x_2)$$
$$= g(0 + 1x_1 + 0.5x_2)$$

$$w \leftarrow w + \gamma (y^{(i)} - \hat{y}^{(i)}) x^{(i)}$$

$$\begin{bmatrix} 0 \\ 1 \\ 0.5 \end{bmatrix} + 0.1(-1 - 1) \begin{bmatrix} 1 \\ 2 \\ -2 \end{bmatrix} = \begin{bmatrix} -0.2 \\ 0.6 \\ 0.9 \end{bmatrix}$$

New
$$h_{\mathbf{w}}(x) = g(-0.2 + 0.6x_1 + 0.9x_2)$$



Sign function

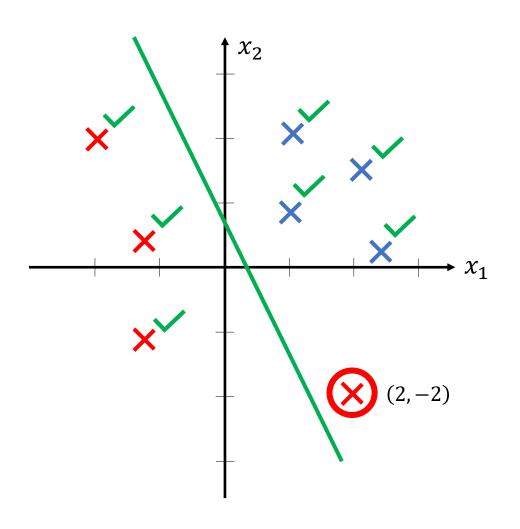
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$$w \leftarrow w + \gamma (y^{(i)} - \hat{y}^{(i)}) x^{(i)}$$

$$\begin{bmatrix} -0.2 \\ 0.6 \\ 0.9 \end{bmatrix} + 0.1(-1 - 1) \begin{bmatrix} 1 \\ -2 \\ 2 \end{bmatrix} = \begin{bmatrix} -0.4 \\ 1 \\ 0.5 \end{bmatrix}$$

New
$$h_{\mathbf{w}}(x) = g(-0.4 + 1x_1 + 0.5x_2)$$



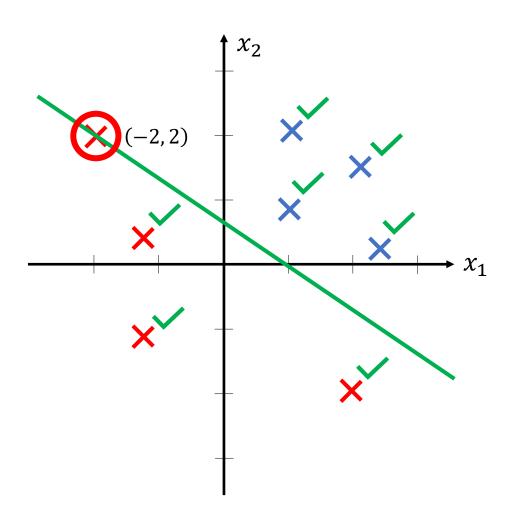
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Sign function

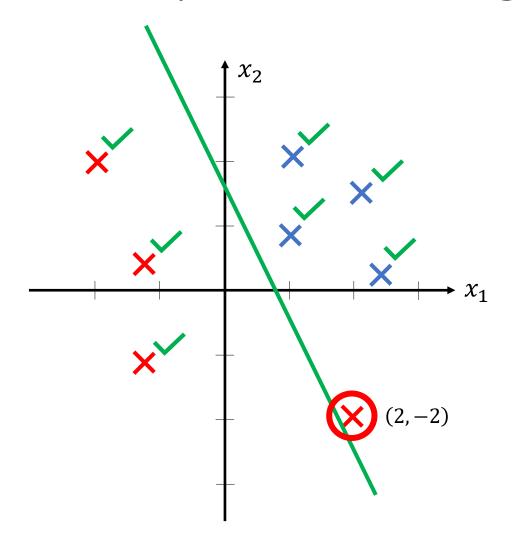
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$$\hat{y} = h_{w}(x) = g(w_0 + w_1 x_1 + w_2 x_2)$$
$$= g(-0.6 + 0.6x_1 + 0.9x_2)$$

$$w \leftarrow w + \gamma (y^{(i)} - \hat{y}^{(i)}) x^{(i)}$$

$$\begin{bmatrix} -0.6 \\ 0.6 \\ 0.9 \end{bmatrix} + 0.1(-1 - 1) \begin{bmatrix} 1 \\ -2 \\ 2 \end{bmatrix} = \begin{bmatrix} -0.8 \\ 1 \\ 0.5 \end{bmatrix}$$

New
$$h_{\mathbf{w}}(x) = g(-0.8 + 1x_1 + 0.5x_2)$$



Sign function

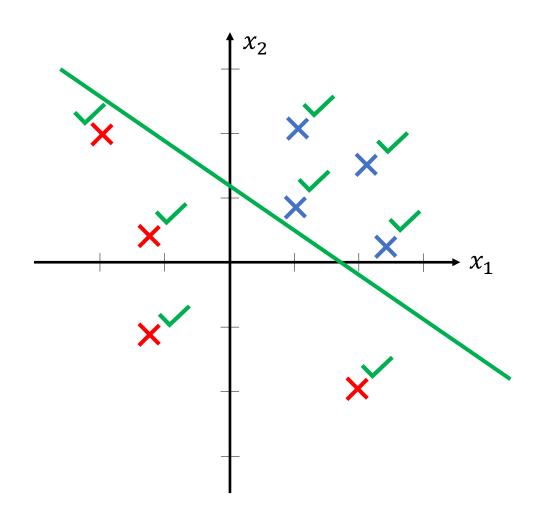
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$$w \leftarrow w + \gamma (y^{(i)} - \hat{y}^{(i)}) x^{(i)}$$

$$\begin{bmatrix} -0.8 \\ 1 \\ 0.5 \end{bmatrix} + 0.1(-1 - 1) \begin{bmatrix} 1 \\ 2 \\ -2 \end{bmatrix} = \begin{bmatrix} -1 \\ 0.6 \\ 0.9 \end{bmatrix}$$

New
$$h_{\mathbf{w}}(x) = g(-1 + 0.6x_1 + 0.9x_2)$$



Sign function

$$g(z) = \begin{cases} +1 & \text{if } z \ge 0 \\ -1 & \text{if } z < 0 \end{cases}$$

$$\hat{y} = h_{w}(x) = g(w_0 + w_1 x_1 + w_2 x_2)$$
$$= g(-1 + 0.6x_1 + 0.9x_2)$$

No misclassifications! Converged!

What if it's not linearly separable? The algorithm will not converge

Perceptron Learning Algorithm: Why?

$$\hat{y} = g\left(\sum_{i=0}^{n} w_i x_i\right) \qquad g(z) = \begin{cases} +1 & z \ge 0\\ -1 & z < 0 \end{cases}$$

When there is a misclassification: y = +1, $\hat{y} = -1$, or vice versa

Doesn't affect the sign

$$\hat{y} = -1$$

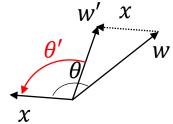
$$w^T x < 0$$

$$w \cdot x < 0$$

$$||w||.||x||\cos\theta<0$$

$$\cos \theta < 0$$

$$\frac{\pi}{2} < \theta < \pi$$



$$w' \leftarrow w + x$$

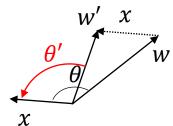
 θ' will be smaller (as required)

What we want:

$$y = +1$$

$$\cos \theta > 0$$

$$0 < \theta < \frac{\pi}{2}$$



What we want:

Doesn't affect

the sign

$$y = -1$$

 $\hat{y} = +1$

 $w^T x > 0$

 $w \cdot x > 0$

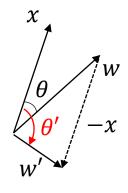
 $\cos \theta > 0$

 $0 < \theta < \frac{\pi}{2}$

||w||. $||x|| \cos \theta > 0$

$$\cos \theta < 0$$

$$\frac{\pi}{2} < \theta < \pi$$



$$w' \leftarrow w - x$$

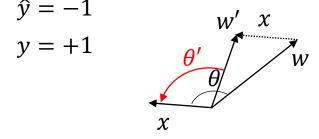
 θ' will be larger
 (as required)

Perceptron Learning Algorithm: Why?

$$\hat{y} = g\left(\sum_{i=0}^{n} w_i x_i\right) \qquad g(z) = \begin{cases} +1 & z \ge 0\\ -1 & z < 0 \end{cases}$$

When there is a misclassification: y = +1, $\hat{y} = -1$, or vice versa

$$\hat{y} = -1$$
$$y = +1$$



$$w' \leftarrow w + x$$

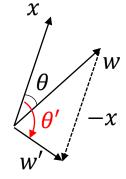
 θ' will be smaller (as required)

$$w \leftarrow w + \gamma(y - \hat{y})x$$

$$\leftarrow w + \gamma(+1 - (-1))x$$

$$\leftarrow w + 2\gamma x$$

$$\hat{y} = +1$$
$$y = -1$$



$$w' \leftarrow w - x$$

 θ' will be larger (as required)

$$w \leftarrow w + \gamma(y - \hat{y})x$$

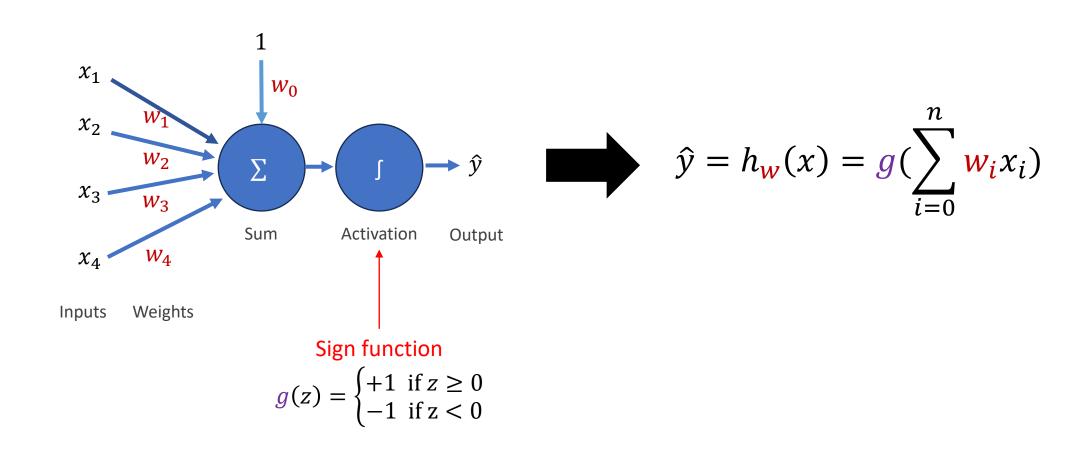
$$\leftarrow w + \gamma(-1 + (-1))x$$

$$\leftarrow w - 2\gamma x$$

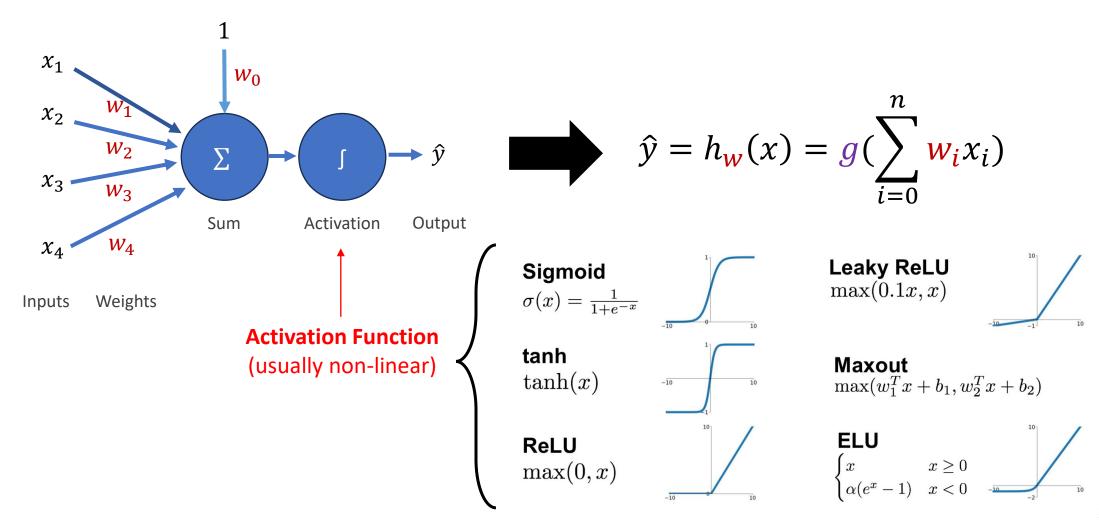
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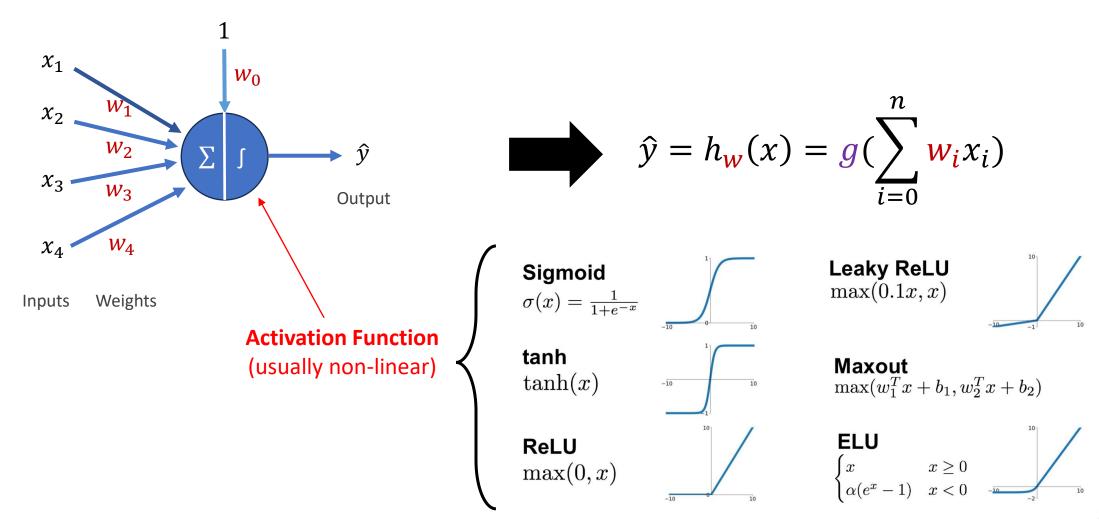
Perceptron



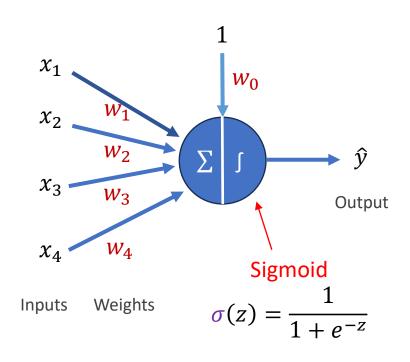
Single-layer Neural Networks



Single-layer Neural Networks

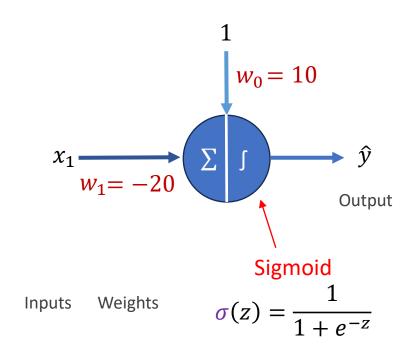


Single-layer Neural Networks



$$\hat{y} = h_{\mathbf{w}}(x) = \sigma(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

Single-layer Neural Networks: NOT

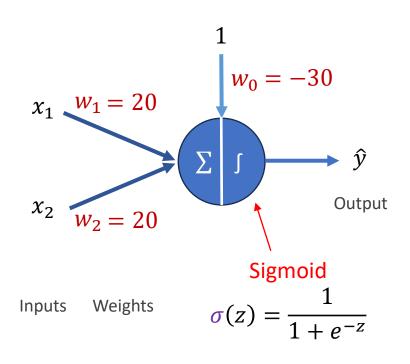


$$\hat{y} = h_{\mathbf{w}}(x) = \sigma(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

Consider $x_1 \in \{1,0\}$

x_1	y	Σ	$\widehat{\mathbf{y}}$
0	1	10	0.999
1	0	-10	0.00004

Single-layer Neural Networks: AND

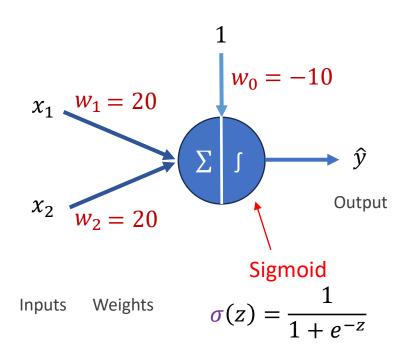


$$\hat{y} = h_{\mathbf{w}}(x) = \sigma(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

Consider $x_1, x_2 \in \{1,0\}$

x_1	x_2	y	Σ	$\widehat{m{y}}$
0	0	0	-30	0.000
0	1	0	-10	0.00004
1	0	0	-10	0.00004
1	1	1	10	0.999

Single-layer Neural Networks: OR

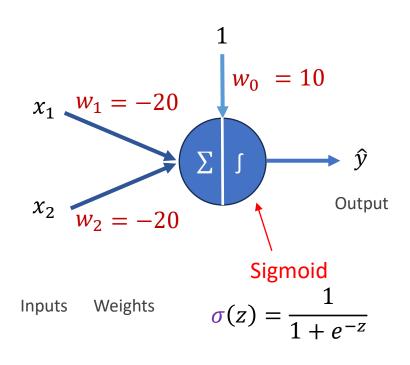


$$\hat{y} = h_{\mathbf{w}}(x) = \sigma(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

Consider $x_1, x_2 \in \{1,0\}$

x_1	x_2	y	Σ	ŷ
0	0	0	-10	0.00004
0	1	1	10	0.999
1	0	1	10	0.999
1	1	1	30	0.999

Single-layer Neural Networks: NOR (NOT x1) AND (NOT x2)



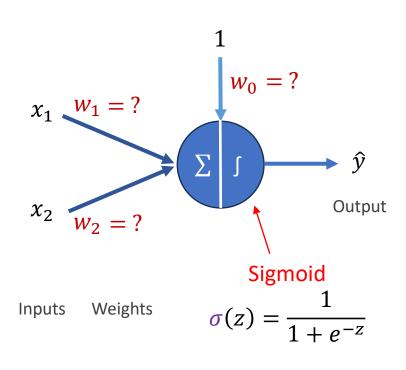
$$\hat{y} = h_{\mathbf{w}}(x) = \sigma(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

Consider $x_1, x_2 \in \{1,0\}$

x_1	x_2	y	Σ	$\widehat{oldsymbol{y}}$
0	0	1	10	0.999
0	1	0	-10	0.00004
1	0	0	-10	0.00004
1	1	0	-30	0.000

Single-layer Neural Networks: XNOR

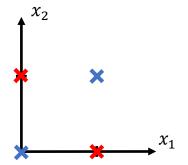
eXclusive Not OR



$$\hat{y} = h_{\mathbf{w}}(x) = \sigma(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

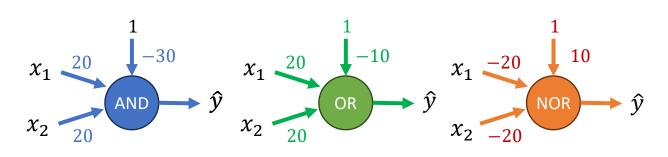
Consider $x_1, x_2 \in \{1,0\}$

x_1	x_2	y
0	0	1
0	1	0
1	0	0
1	1	1



Single-layer Neural Networks: XNOR

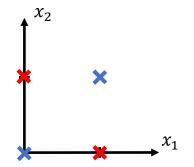
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$$\hat{y} = h_{\mathbf{w}}(x) = \sigma(\sum_{i=0}^{n} \mathbf{w}_{i} x_{i})$$

Consider $x_1, x_2 \in \{1,0\}$

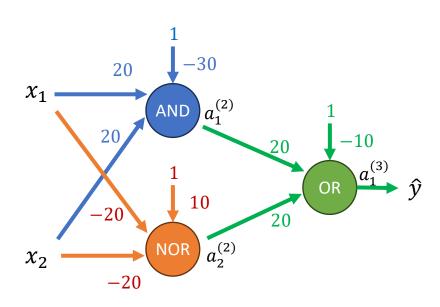
x_1	x_2	y
0	0	1
0	1	0
1	0	0
1	1	1



Multi

Single-layer Neural Networks: XNOR

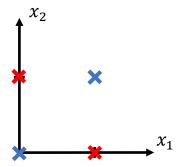
eXclusive Not OR



$$\hat{y} = h_{\cdots}(x) - \sum_{i=0}^{n} w_i x_i$$

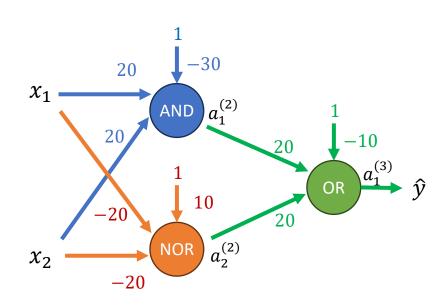
Consider $x_1, x_2 \in \{1,0\}$

x_1	x_2	y
0	0	1
0	1	0
1	0	0
1	1	1



Multi-layer Neural Networks: XNOR

eXclusive Not OR



Output

Layer

Hidden

Layer

Input

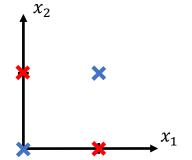
Layer

$$\hat{y} = \sigma\left(\sum_{i=0}^{n} w_{1i}^{(3)} a_i^{(2)}\right) \qquad a_i^{(2)} = \sigma\left(\sum_{j=0}^{n} w_{ij}^{(2)} x_j\right)$$
Function composition
$$a_0^{(2)} = 1$$

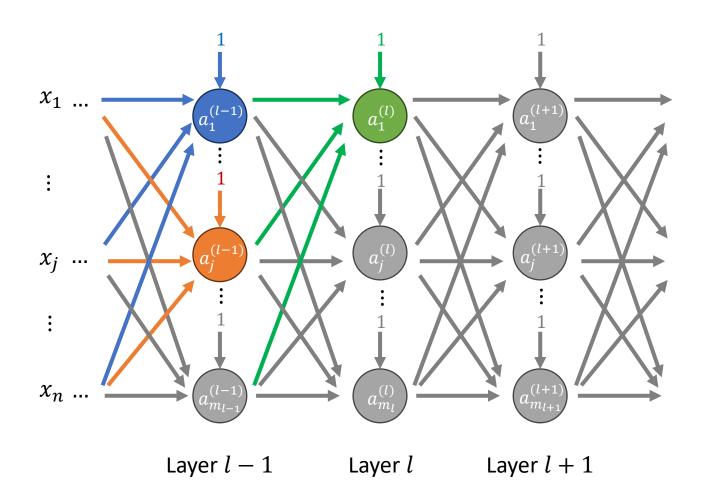
Consider $x_1, x_2 \in \{1,0\}$

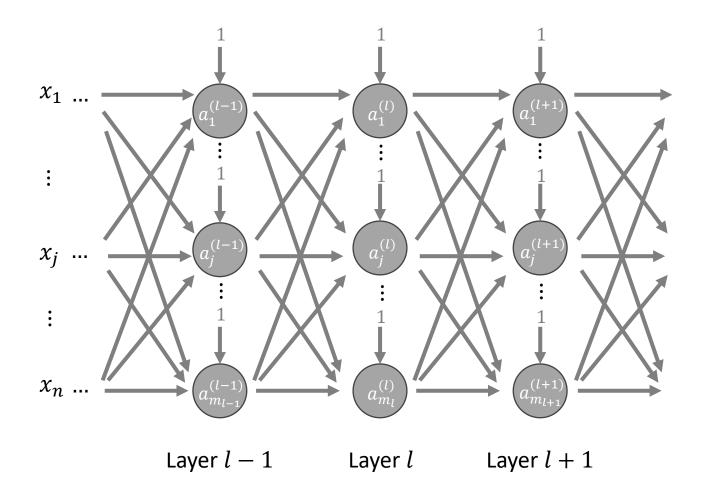
x_1	x_2	у
0	0	1
0	1	0
1	0	0
1	1	1

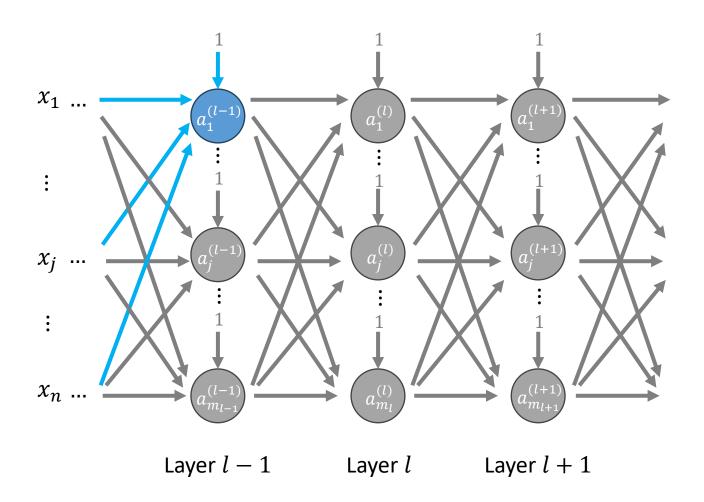
$a_1^{(2)}$	$a_2^{(2)}$	$\widehat{\mathbf{y}}$
0	1	1
0	0	0
0	0	0
1	0	1

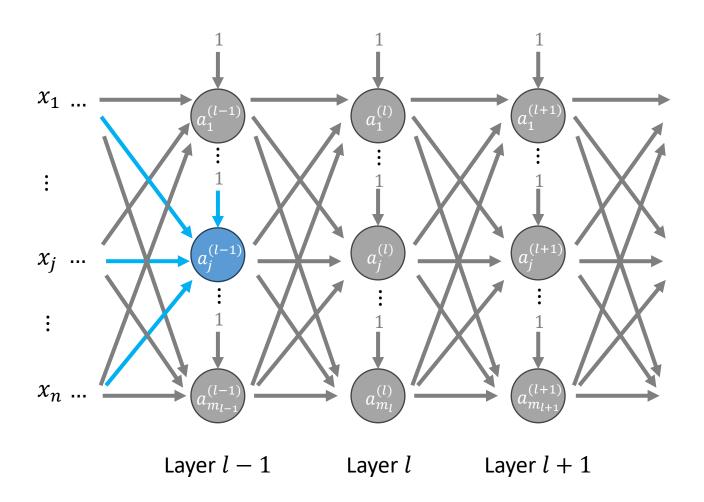


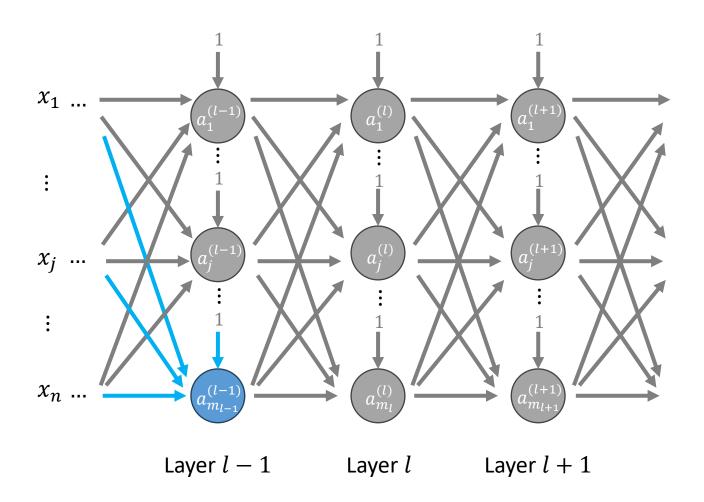
Multi-layer Neural Networks

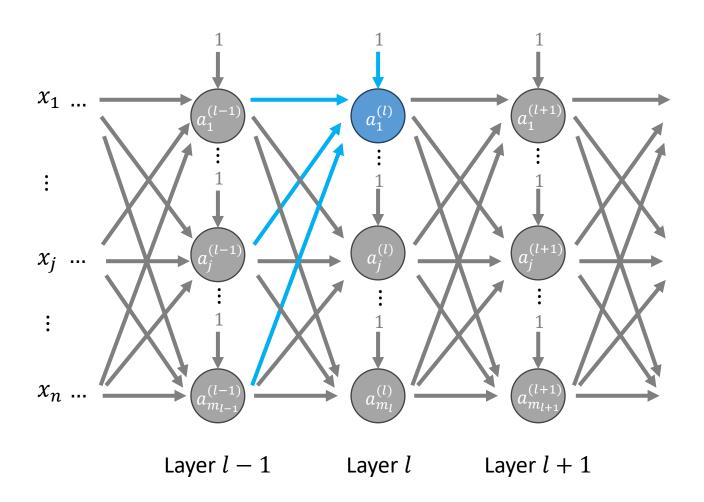


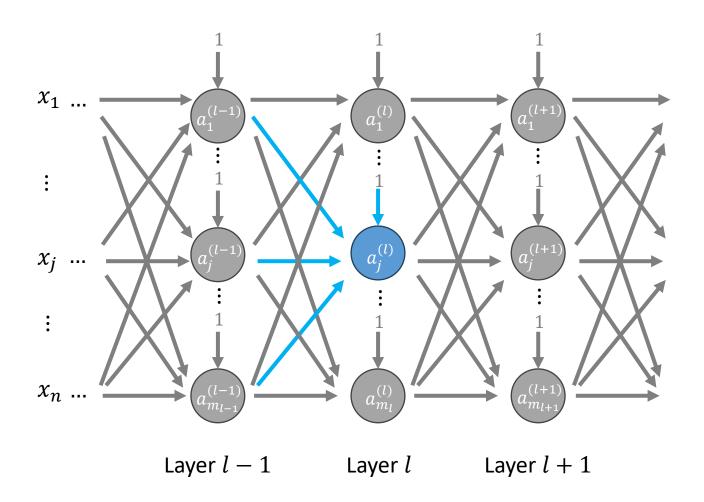


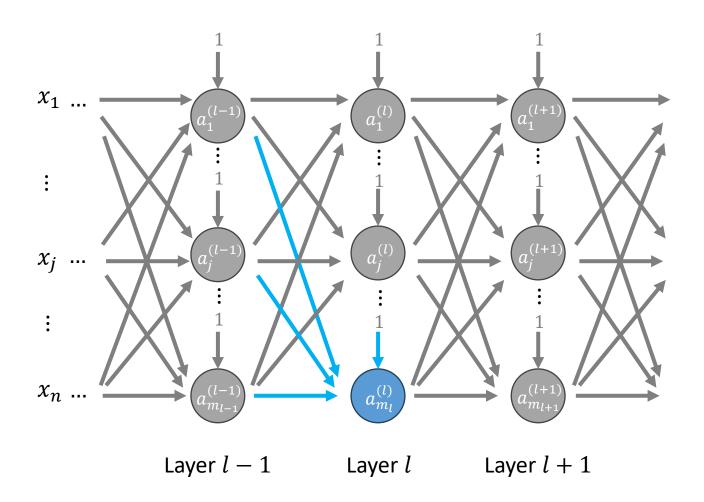


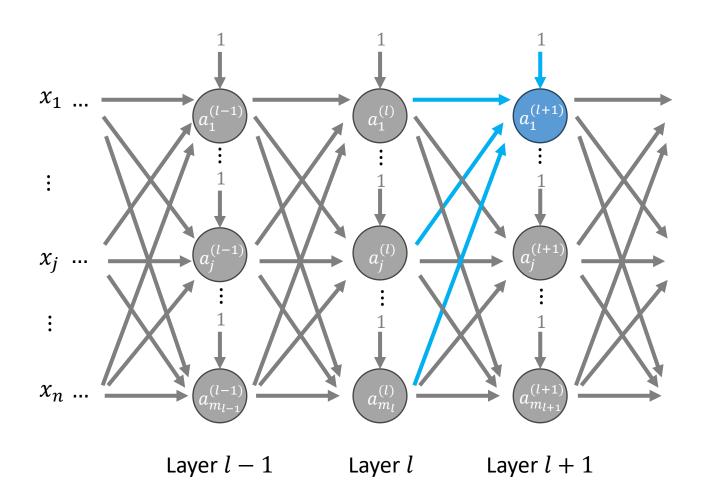


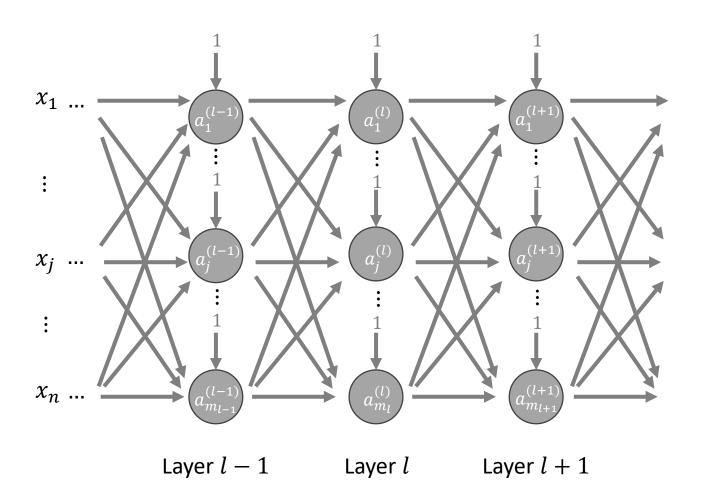










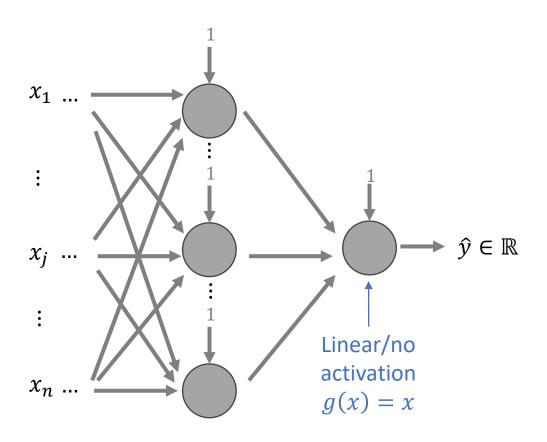


Universal Function Approximation Theorem

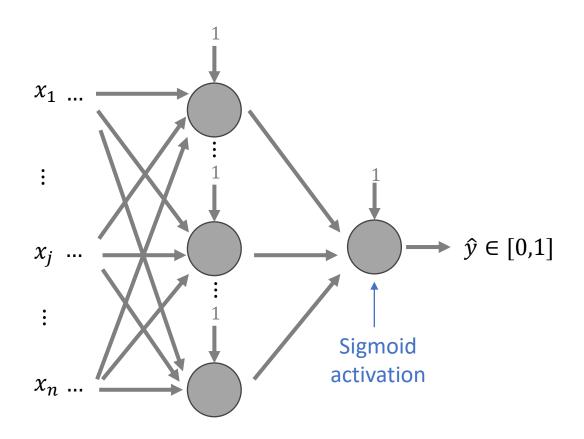
Neural networks can *represent* a wide variety of interesting functions with appropriate weights

 A <u>single hidden layer</u> network can approximate any continuous function within a specific range

Regression and Classification



Regression

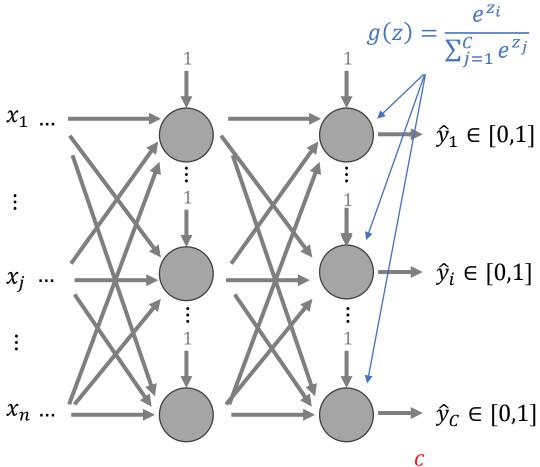


Binary Classification

Regression and Classification

$\hat{y} \in \mathbb{R}$ Linear/no activation g(x) = x

Regression



Multi-class Classification with C classes

$$\sum_{i=1}^{C} \hat{y}_i = 1$$

Softmax activation

Outline

- Perceptron
 - Biological inspiration
 - Perceptron Learning Algorithm
- Neural Networks
 - Single-layer Neural Networks
 - Multi-layer Neural Networks
 - Regression and Classification
- Gradient Descent with Neural Networks
- Neural Networks vs Other Models

Background: Chain Rule

$$z(x) = h\left(g(f(x))\right)$$

$$\frac{dz}{dx} = \frac{dz}{dh} \frac{dh}{dg} \frac{dg}{df} \frac{df}{dx}$$

Aside: Derivative of Sigmoid Function

$$\sigma(x) = \frac{1}{1 + e^{-x}} \qquad \sigma'(x) = \frac{d\left(\frac{1}{1 + e^{-x}}\right)}{dx}$$

$$= \frac{d\left((1 + e^{-x})^{-1}\right)}{dx}$$

$$= -(1 + e^{-x})^{-2} (-e^{-x})$$

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

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

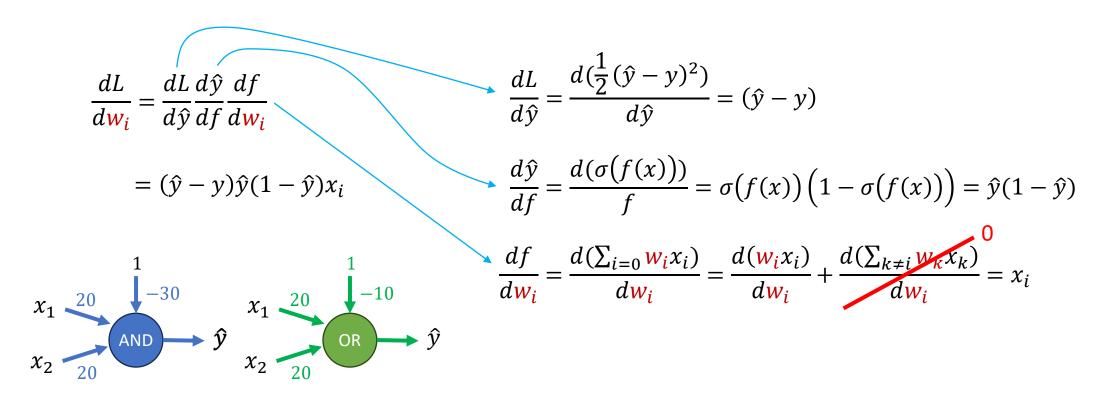
$$= \frac{1}{1 + e^{-x}} \left(1 - \frac{1}{1 + e^{-x}}\right)$$

$$= \sigma(x) \left(1 - \sigma(x)\right)$$

Gradient Descent on Single-layer NN

$$\hat{y} = \sigma(f(x)) \qquad f(x) = \sum_{i=0}^{n} w_i x_i \qquad L = \frac{1}{2} (\hat{y} - y)^2 \qquad \qquad w_i \leftarrow w_i - \gamma \frac{dL}{dw_i}$$

$$\text{Mean-squared Error} \qquad \qquad w_i \leftarrow w_i - \gamma (\hat{y} - y) \hat{y} (1 - \hat{y}) x_i$$



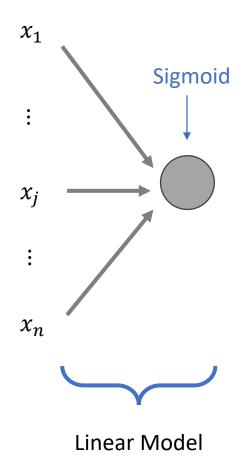
Gradient Descent on Multi-layer NN

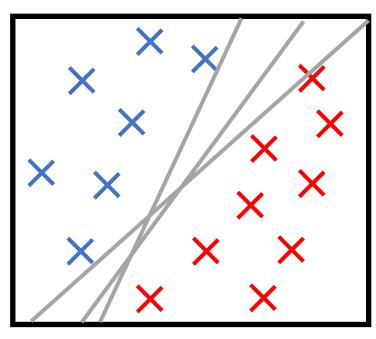
Backpropagation is covered in the next Lecture!

Outline

- Perceptron
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Neural Networks vs Logistic Regression



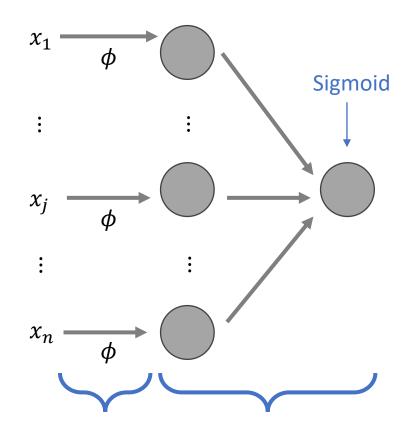


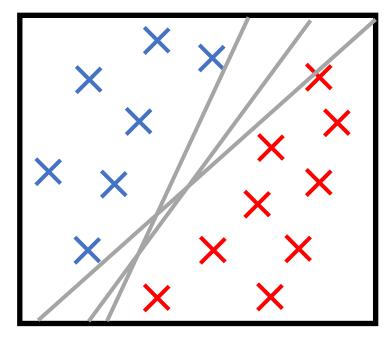
Linear, non-robust decision boundary

Prone to misclassification since the decision boundary can be **too close to data points**

Neural Networks vs Logistic Regression

With Feature Mapping



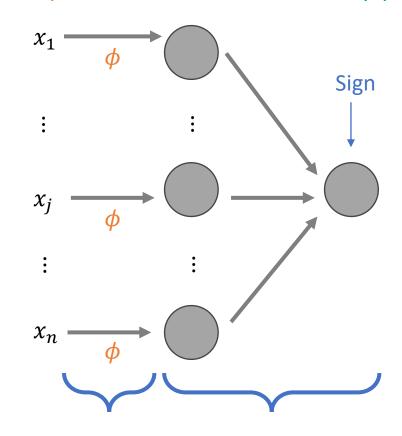


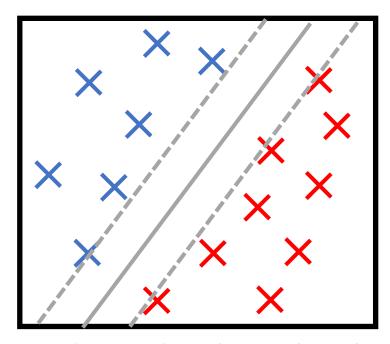
Non-linear, non-robust decision boundary

Prone to misclassification since the decision boundary can be **too close to data points**

Neural Networks vs Support Vector Machines

Implicit with Kernel: can have many, possibly infinite dimensional features





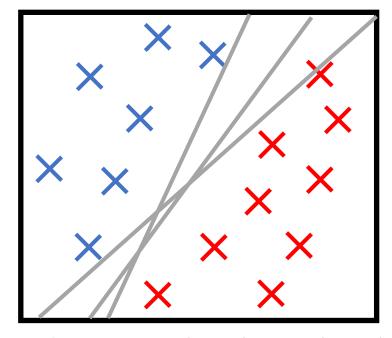
Non-linear, robust decision boundary

Decision boundary is guaranteed to be far from the data points

Neural Networks vs Other Methods

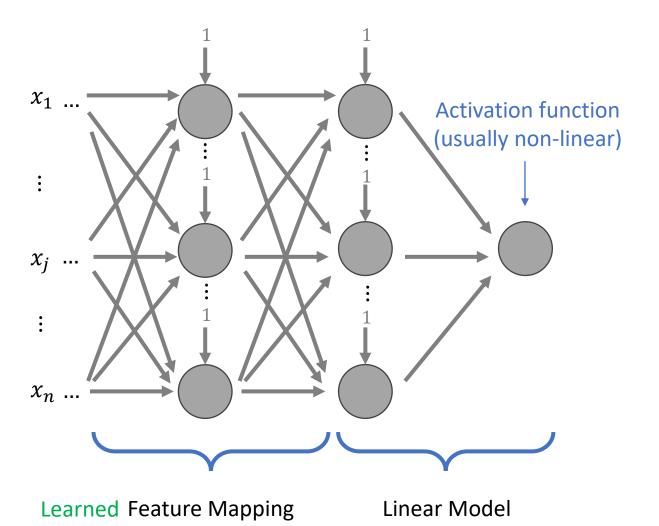


Credit: Internet meme, original source unknown



Non-linear, non-robust decision boundary

Prone to misclassification since the decision boundary can be **too close to data points**



Summary

- Perceptron
 - Biological inspiration: brain, neural network, neuron
 - Perceptron Learning Algorithm:
 - $w \leftarrow w + \gamma (y^{(j)} \hat{y}^{(j)}) x^{(j)}$ on a misclassified instance
- Neural Networks
 - Single-layer Neural Networks: AND, OR, NOR
 - Multi-layer Neural Networks: XNOR, Universal Approximation Theorem
 - Regression and Classification
- Neural Networks with Gradient Descent
- Neural Networks vs Other Models: learned feature mapping!

Coming Up Next Week

Math revision

- Linear algebra: scalar, vector, matrix, and their operations
- Calculus: partial derivative, matrix calculus, chain rule
- Backpropagation
- Introduction to PyTorch
 - Training neural networks with gradient descent

To Do

- Lecture Training 8
 - +100 Free EXP
 - +50 Early bird bonus
- **PS5**
 - Due **tomorrow** (Saturday, 21st October) 23:59
- PS6 is out today!
 - May need some knowledge from the next lecture (Lecture 9)