Lecture 8: Neural Network & Deep Learning Fall 2022

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Announcements

- Quiz 2 is due today
- Hw 1 is due next Tue
 - The definition of F1 score will be covered today
- Midterm postpones to 11/1?
 - The practice exam will be posted

What you will learn today

- Optimization
 - Gradient descent
 - Stochastic gradient descent (SGD)
- Evaluation Metrics
- Neural network / Deep learning
 - Non-linear classifier
 - Feed-forward neural network
 - Deep learning architecture

Gradient Descent

Example $\min f(\boldsymbol{\theta}) = 0.5(\theta_1^2 - \theta_2)^2 + 0.5(\theta_1 - 1)^2$

- **!** Use the following iterative procedure for gradient descent $\nabla f(\theta) = \begin{bmatrix} 2(\theta_1^2 \theta_2)\theta_1 + \theta_1 1 \\ -(\theta_1^2 \theta_2) \end{bmatrix}$
- ① Initialize $\theta_1^{(0)}$ and $\theta_2^{(0)}$, and t=0
- 2 do
 Type equation here.

$$\theta_1^{(t+1)} \leftarrow \theta_1^{(t)} - \eta \left[2(\theta_1^{(t)^2} - \theta_2^{(t)}) \theta_1^{(t)} + \theta_1^{(t)} - 1 \right]$$

$$\theta_2^{(t+1)} \leftarrow \theta_2^{(t)} - \eta \left[-(\theta_1^{(t)^2} - \theta_2^{(t)}) \right]$$

$$t \leftarrow t + 1$$

lacksquare until $f(oldsymbol{ heta}^{(t)})$ does not change much

Remarks

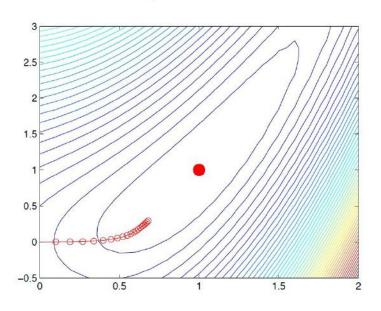
- η is often called step size or learning rate -- how far our update will go along the the direction of the negative gradient
- * With a suitable choice of η , the iterative procedure converges to a stationary point where

$$\frac{\partial f}{\partial \boldsymbol{\theta}} = 0$$

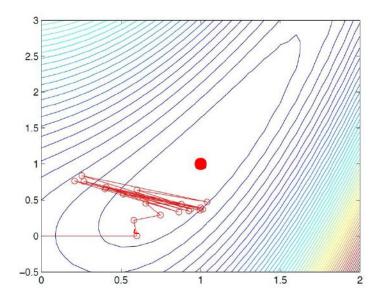
A stationary point is only necessary for being the minimum

Choosing the right learning rate (η) is important

small η is too slow?



large η is too unstable?



Recap: Logistic Regression

- **Training data:** $S = \{(x_i, y_i)\}$, m examples
- Hypothesis space:

$$H = \{ h \mid h : X \to P(Y \mid X), h(x) = \sigma (w^T x + b) \}$$
$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

- i.e., model P(Y|X) by $\sigma(w^Tx + b)$
- \clubsuit How to find the best $h \in H$: maximum log-likelihood

$$\arg \max - \sum_{i=1}^{m} \log(1 + \exp(-y_i(w^T x_i + b)))$$

Gradient Descent for Logistic Regression

Maximum log-likelihood

$$arg \max - \sum_{i=1}^{m} \log(1 + \exp(-y_i(w^T x_i + b)))$$

Equivalent to the following minimization problem

$$\arg\min\sum_{i=1}^{m}\log(1+\exp(-y_i(w^Tx_i+b)))$$

$$L(w,b)$$

 \clubsuit Gradient of L(w, b)

$$\nabla L(w,b) = \sum_{i=1}^{m} \nabla \log(1 + \exp(-y_i(w^T x_i + b)))$$

Recap: Gradient

♣ Let z to be a n-dimensional vector of variables, f(z) is a function of z

$$\nabla f(z) = \begin{bmatrix} \partial f(z)/\partial z_1 \\ \partial f(z)/\partial z_2 \\ \vdots \\ \partial f(z)/\partial z_{n-1} \\ \partial f(z)/\partial z_n \end{bmatrix}$$

Exercise

• Let $z = [z_1, z_2, z_3]^T$ to be a 3-dimensional vector of variables, $a = [3, 2, 4]^T$ $\nabla f(z) = \begin{bmatrix} \frac{\partial f(z)}{\partial z_1} \\ \frac{\partial f(z)}{\partial z_2} \\ \vdots \\ \frac{\partial f(z)}{\partial z_{n-1}} \end{bmatrix}$

$$f(z) = \log(a^T z)$$

= $\log(3z_1 + 2z_2 + 4z_3)$

$$\nabla f(z) = \begin{vmatrix} \partial f(z)/\partial z_1 \\ \partial f(z)/\partial z_2 \\ \partial f(z)/\partial z_3 \end{vmatrix} = ?$$

Exercise

Let $z = [z_1, z_2, z_3]^T$ to be a 3-dimensional vector of variables, $a = [3, 2, 4]^T$

$$f(z) = \log(a^T z)$$

= $\log(3z_1 + 2z_2 + 4z_3)$

$$= \frac{1}{3z_1 + 2z_2 + 4z_3} \begin{bmatrix} 3 \\ 2 \\ 4 \end{bmatrix} = \frac{1}{a^T z} a$$

$$\nabla f(z) = \begin{bmatrix} \frac{\partial f(z)}{\partial z_1} \\ \frac{\partial f(z)}{\partial z_2} \\ \vdots \\ \frac{\partial f(z)}{\partial z_{n-1}} \\ \frac{\partial f(z)}{\partial z_n} \end{bmatrix}$$

Gradient of L(w, b)

$$\nabla L(w,b) = \sum_{i=1}^{m} \nabla \log(1 + \exp(-y_i(w^T x_i + b)))$$

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

$$\nabla \log \frac{1}{\sigma(y_i(w^Tx_i+b))}$$

Gradient of L(w, b)

$$\nabla L(w,b) = \sum_{i=1}^{m} \nabla_{i} \log(1 + \exp(-y_i(w^T x_i + b)))$$

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

$$\nabla \log \frac{1}{\sigma(y_i(w^Tx_i+b))}$$

 $\text{Using } \nabla \log \frac{1}{\sigma(z)} = \sigma(z) - 1$

Partial gradient w.r.t w

$$\nabla_{w}L(w,b) = \sum_{i=1}^{m} \nabla_{w} \log \frac{1}{\sigma(y_{i}(w^{T}x_{i}+b))}$$

$$= \sum_{i=1}^{m} (\sigma(y_{i}(w^{T}x_{i}+b)) - 1)y_{i}x_{i}$$

$$\nabla_{b}L(w,b) = \sum_{i=1}^{m} (\sigma(y_{i}(w^{T}x_{i}+b)) - 1)y_{i}$$

Gradient descent for logistic regression

Given a training data set $S = \{(x_i, y_i)\}, i = 1 \dots m$

- 1. Initialize w (e.g., $w \leftarrow 0 \in \mathbb{R}^n$)
- 2. For epoch 1 ... *T*:

Loop over instance to compute the summation

3. Compute $\nabla_w L(w, b)$ and $\nabla_b L(w, b)$

$$\nabla_{w} L(w, b) = \sum_{i=1}^{m} (\sigma(y_{i}(w^{T}x_{i} + b)) - 1)y_{i}x_{i}$$

$$\nabla_{b} L(w, b) = \sum_{i=1}^{m} (\sigma(y_{i}(w^{T}x_{i} + b)) - 1)y_{i}$$

4. Update w and b

$$w \leftarrow w - \eta \nabla_w L(w, b)$$
$$b \leftarrow b - \eta \nabla_b L(w, b)$$

5. Return w and b

Remark

$$\nabla_w L(w,b) = \sum_{i=1}^m (\sigma(y_i(w^T x_i + b)) - 1) y_i x_i$$

$$\nabla_b L(w,b) = \sum_{i=1}^m (\sigma(y_i(w^T x_i + b)) - 1) y_i$$

- Need to compute $(\sigma(y_i(w^Tx_i + b)) 1)$ for every data point (x_i, y_i)
- Gradient descent usually needs many iterations to converge
- * When size of data (m) is large, computing $\nabla L(w,b)$ is expensive

Stochastic Gradient Descent

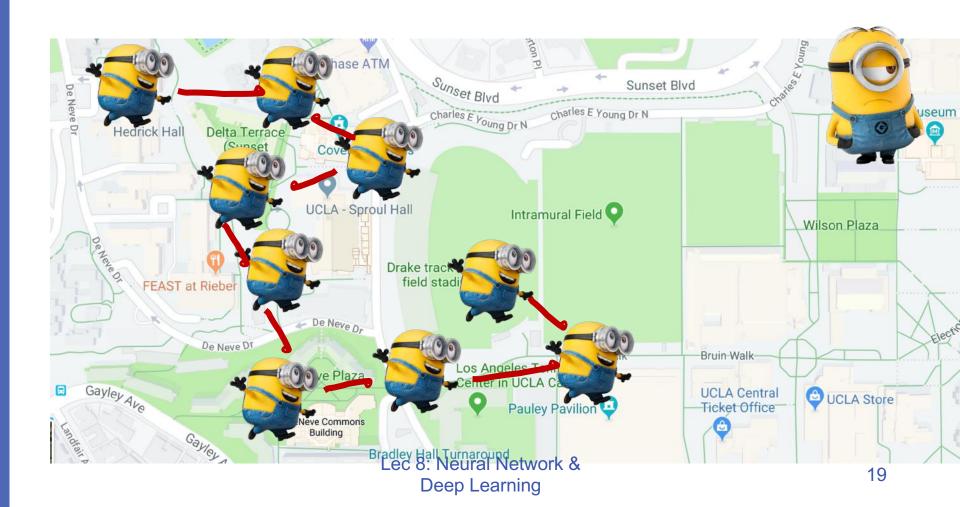
Intuition

Asking direction. Gradient descent: compute gradient of all instances.



Intuition

Asking direction. Stochastic Gradient descent: compute approximate gradient by one instance



Incremental/Stochastic gradient descent

Repeat for each example (**x**_i, y_i)

Use this example to calculate approximate the gradient and update the model

Contrast with *batch gradient descent* which makes one update to the weight vector for every pass over the data

Recap: Gradient Descent

$$\nabla_{w}L(w,b) = \sum_{i=1}^{m} (\sigma(y_{i}(w^{T}x_{i}+b)) - 1)y_{i}x_{i}$$

$$\nabla L_{i}(w,b)$$

Gradient descent update:

$$w \leftarrow w - \eta \sum_{i=1}^{m} \nabla_{\mathbf{w}} L_i(w, b)$$

Alternative way of gradient update

For i = 1 ... m

$$w \leftarrow w - \eta \nabla_w L_i(w, b)$$

Stochastic Gradient Descent

- \star avg $(\nabla_{\mathbf{W}} L_i(w, b)) = E_{(x_i, y_i) \sim S} [\nabla_{\mathbf{W}} L_i(w, b)]$ Average $L_i(w, b)$ over instance
- Gradient descent update:

$$w \leftarrow w - \eta \; \Sigma_{i=1}^m \nabla_{\mathbf{w}} L_i(w, b)$$

Expectation of gradient $L_i(w,b)$ over dataset S

- Stochastic gradient descent
 - Repeat until converge

Sample a data point (x_i, y_i) from S

$$w \leftarrow w - \eta' \nabla_{\mathbf{w}} L_i(w, b)$$

Stochastic Gradient descent for logistic regression

Given a training data set $S = \{(x_i, y_i)\}, i = 1 \dots m$

- 1. Initialize w (e.g., $w \leftarrow 0 \in \mathbb{R}^n$)
- 2. For epoch 1 ... *T*:
- 3. Sample a data point (x_i, y_i) from S
- 4. Compute $\nabla_w L_i(w, b)$ and $\nabla_b L_i(w, b)$ $\nabla_w L_i(w, b) = (\sigma(y_i(w^T x_i + b)) - 1)y_i x_i$ $\nabla_b L_i(w, b) = (\sigma(y_i(w^T x_i + b)) - 1)y_i$
- 5. Update w and b $w \leftarrow w \eta \nabla_w L_i(w, b)$ $b \leftarrow b \eta \nabla_b L_i(w, b)$
- Return w and b

The Perceptron Algorithm [Rosenblatt 1958]

```
Given a training set \mathcal{D} = \{(x,y)\}

1. Initialize w \leftarrow \mathbf{0} \in \mathbb{R}^n

2. For epoch 1 \dots T:

3. For (x,y) in \mathcal{D}:

4. if y(w^Tx) < \mathbf{0}

5. w \leftarrow w + \eta yx
```

Prediction: $y^{\text{test}} \leftarrow \text{sgn}(\mathbf{w}^{\mathsf{T}}\mathbf{x}^{\text{test}})$

6. Return w

The Perceptron Algorithm [Rosenblatt 1958]

Given a training set $\mathcal{D} = \{(x, y)\}$

- 1. Initialize $\mathbf{w} \leftarrow \mathbf{0} \in \mathbb{R}^n$
- 2. For epoch 1...T:
- 3. For (x,y) in \mathcal{D} :
- $4. if y(w^Tx) < 0$
- 5. $w \leftarrow w + \eta y x$
- 6. Return w

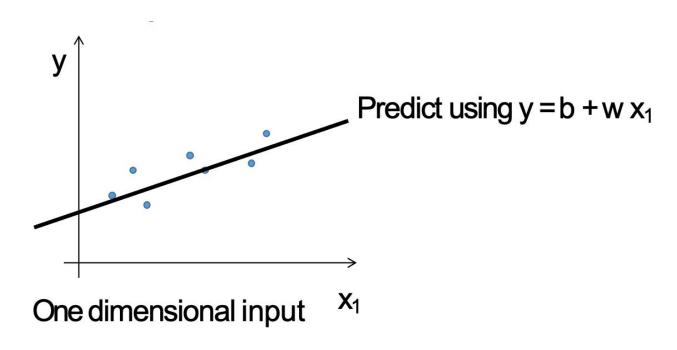
Prediction: y^{test}

Perceptron effectively minimizing:

$$\sum_{i} \max(0, 1 - y_i(\mathbf{w}^T \mathbf{x}_i))$$

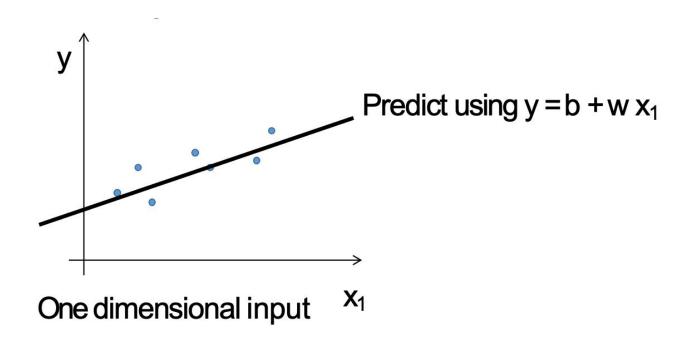
Linear Regression

Find a line $w^T x + b$ to approximate real-value output y based on input x e.g., predict house price next year



Linear Regression

Find a line to approximate real-value output e.g., predict house price next year

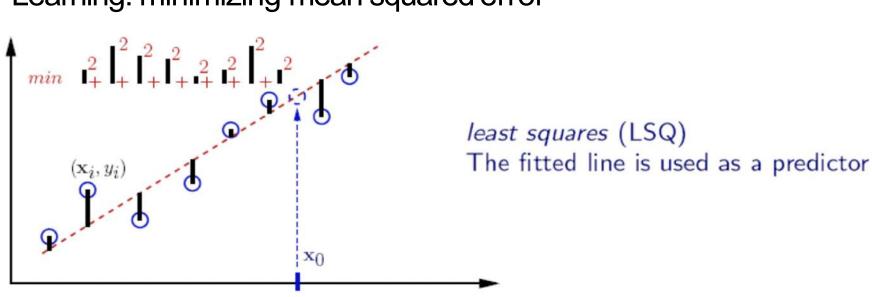


Least Mean Squares (LMS) Regression

Given a dataset $S = \{(x_i, y_i)\}_{i=1..m}, x_i \in \mathbb{R}^n, y \in \mathbb{R}$

$$\arg\min_{w,b} \frac{1}{2} \sum_{i}^{m} (y_i - (w^T x_i + b))^2$$

Learning: minimizing mean squared error



Exercise

Derive the stochastic gradient descent algorithm for solving LMS regression

$$\arg\min_{w,b} \frac{1}{2} \sum_{i}^{m} (y_i - (w^T x_i + b))^2$$

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Accuracy and Error Rate

True label	-	-	-	-	+	-	-	-	-	-	+	-	-	+	-	-
Predicted label	-	-	-	-	+	-	+	-	-	-	-	+	-	+	-	-

Error rate = 3/16Accuracy = 13/16

Accuracy and Error Rate

True label	-	-	-	-	+	-	-	-	-	-	+	-	-	+	-	-
Predicted label	-	-	-	-	+	-	+	-	-	-	-	+	-	+	-	-

Error rate =
$$3/16 = 19\%$$

When data is unbalanced, check the performance of majority baseline

True label	-	-	-	-	+	-	-	-	-	-	+	-	-	+	-	-
Predicted label	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Confusion Matrix

True label	-	-	-	-	+	-	-	-	-	-	+	-	-	+	-	-	
Predicted label	-	-	-	-	+	-	+	-	-	-	-	+	-	+	-	-	

	True Label Positive	True Label Negative
Predicted Label Positive	2 True Positive (TP)	2 False Positive (FP)
Predicted Label Negative	1 False Negative (FN)	16 True Negative (TN)

Accuracy = (TP+TN)/(TP+TN+FN+FP)

Precision, Recall

True label	-	-	-	-	+	-	-	-	-	-	+	-	-	+	-	-
Predicted label	-	-	-	-	+	-	+	-	-	-	-	+	-	+	-	-

	True Label Positive	True Label Negative
Predicted Label Positive	2 True Positive (TP)	2 False Positive (FP)
Predicted Label Negative	1 False Negative (FN)	16 True Negative (TN)

Accuracy = (TP+TN)/(TP+TN+FN+FP)

Precision = (TP)/(TP+FP)

Recall = (TP)/(TP+FN)

F1 Score

Harmonic mean of precision and recall:

$$\frac{1}{F_1} = \left(\frac{1}{P} + \frac{1}{R}\right)/2$$

$$F_1 = \frac{2TP}{2TP + FP + FN}$$

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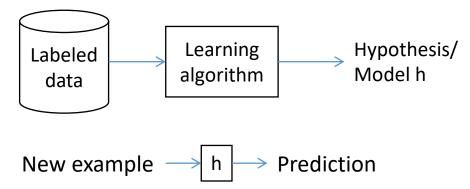
Checkpoint: The bigger picture

Supervised learning: instances, concepts, and hypotheses

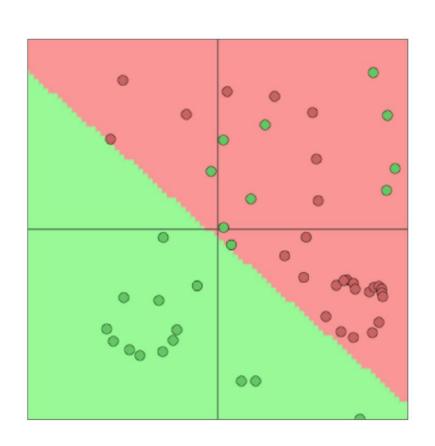
Specific learners

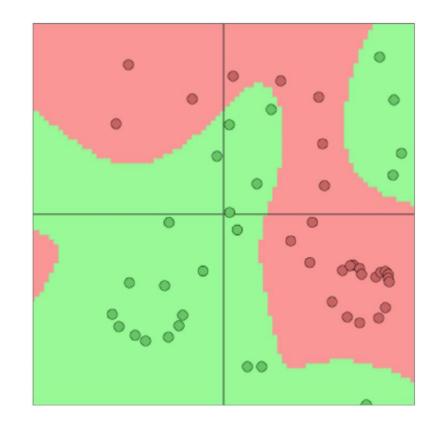
Decision trees

- K-NN
- Perceptron
- Logistic regression
- General ML ideas
 - Feature vectors
 - Overfitting
 - Probabilistic model



Non-Linear Decision Boundary

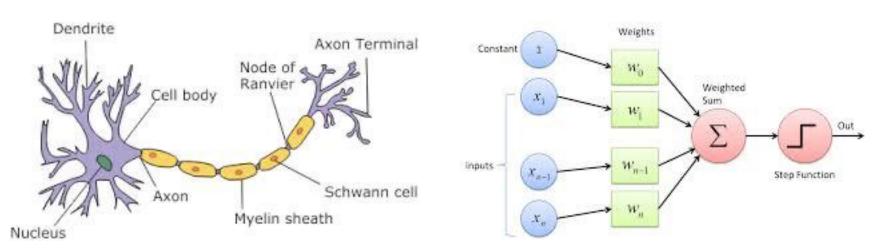




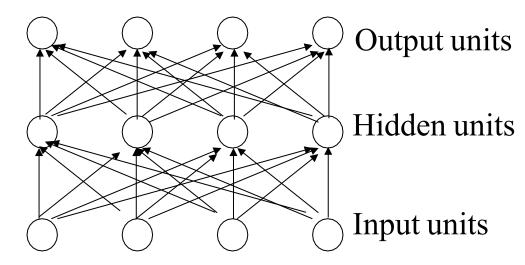
Neural Networks

Design to mimic the brain.

 Artificial neural networks are not nearly as complex or intricate as the actual brain structure



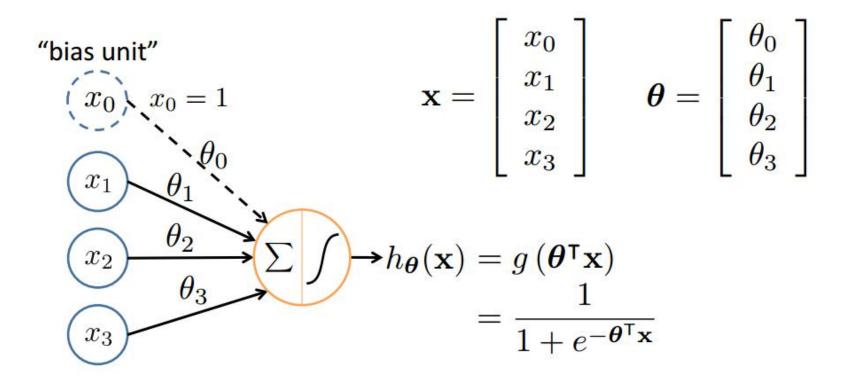
Feed-forward neural network



Layered feed-forward network

- Neural networks are made up of nodes or units, connected by links
- Each link has an associated weight and activation level
- Each node has an **input function** (typically summing over weighted inputs), an **activation function**, and an **output**

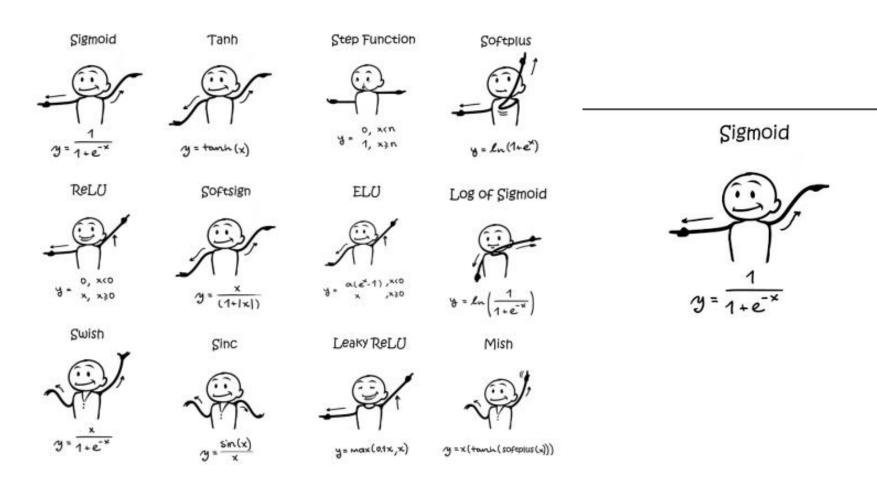
Neuron Model Example: Logistic Unit



Sigmoid (logistic) activation function:
$$g(z) = \frac{1}{1 + e^{-z}}$$

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Activation function



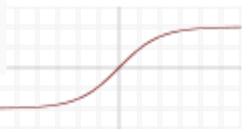
https://sefiks.com/2020/02/dance-moves-of-deep-learning-activation-functions/ by Sefik Ilkin Serengil

Activation functions

* sigmoid function $f(x) = \frac{1}{1 + e^{-x}}$

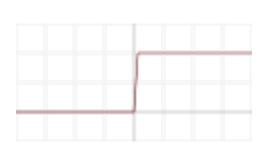
$$f(x)=rac{1}{1+e^{-x}}$$





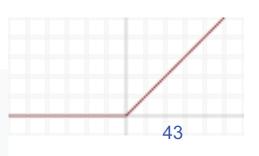
step function

$$\left\{egin{array}{ll} 0 & ext{if } x < 0 \ 1 & ext{if } x \geq 0 \end{array}
ight.$$

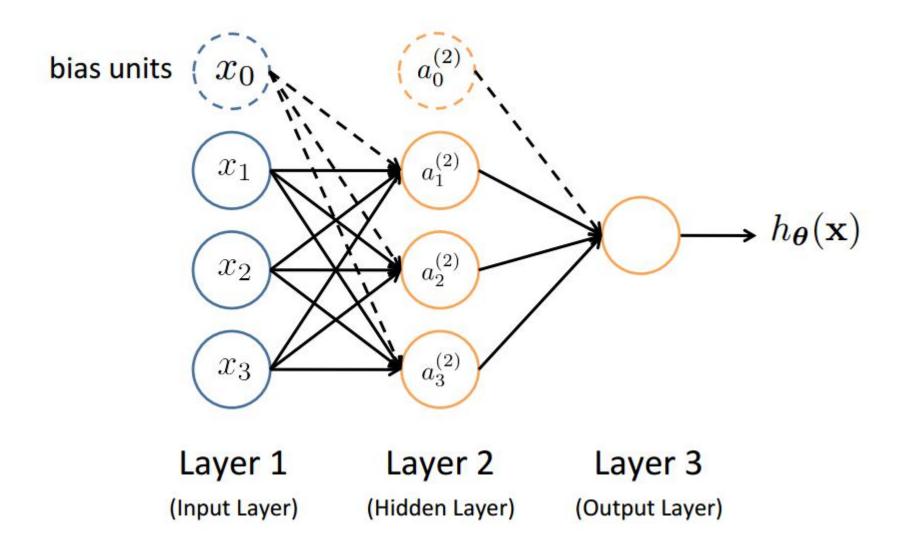


Rectified linear unit (ReLU)

$$(x)^+ \doteq \left\{egin{array}{ll} 0 & ext{if } x \leq 0 \ x & ext{if } x > 0 \end{array}
ight.$$

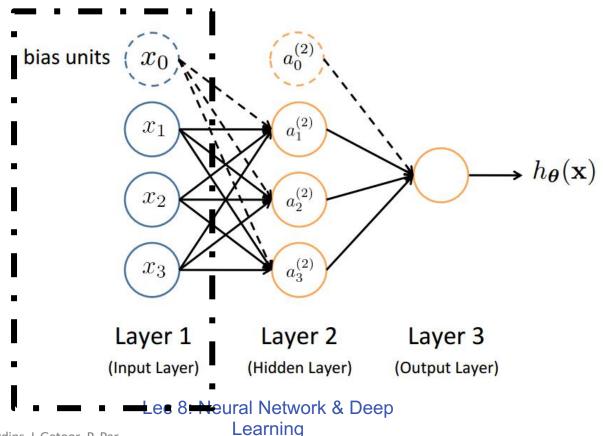


Neural Network



Feed-Forward Process

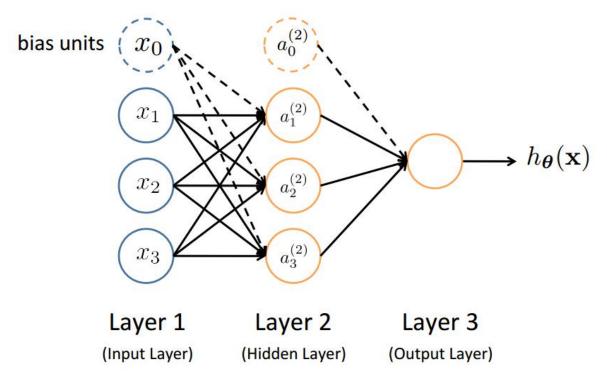
• Input layer units are set by some exterior function (think of these as **sensors**), which causes their output links to be **activated** at the specified level



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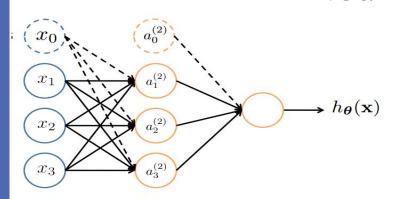
Feed-Forward Process

- Working forward through the network, the **input function** of each unit is applied to compute the input value
- The **activation function** transforms this input function into a final value



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Neural Network



 $a_i^{(j)}$ = "activation" of unit i in layer j

 $oldsymbol{\Theta}^{(j)} = ext{weight matrix controlling function}$ mapping from layer j to layer j + 1

$$a_{1}^{(2)} = g(\Theta_{10}^{(1)}x_{0} + \Theta_{11}^{(1)}x_{1} + \Theta_{12}^{(1)}x_{2} + \Theta_{13}^{(1)}x_{3})$$

$$a_{2}^{(2)} = g(\Theta_{20}^{(1)}x_{0} + \Theta_{21}^{(1)}x_{1} + \Theta_{22}^{(1)}x_{2} + \Theta_{23}^{(1)}x_{3})$$

$$a_{3}^{(2)} = g(\Theta_{30}^{(1)}x_{0} + \Theta_{31}^{(1)}x_{1} + \Theta_{32}^{(1)}x_{2} + \Theta_{33}^{(1)}x_{3})$$

$$h_{\Theta}(x) = a_{1}^{(3)} = g(\Theta_{10}^{(2)}a_{0}^{(2)} + \Theta_{11}^{(2)}a_{1}^{(2)} + \Theta_{12}^{(2)}a_{2}^{(2)} + \Theta_{13}^{(2)}a_{3}^{(2)})$$

If network has s_j units in layer j and s_{j+1} units in layer j+1, then $\Theta^{(j)}$ has dimension $s_{j+1}\times(s_j+1)$.

$$\Theta^{(1)} \in \mathbb{R}^{3 \times 4}$$

$$\Theta^{(1)} \in \mathbb{R}^{3 \times 4} \qquad \Theta^{(2)} \in \mathbb{R}^{1 \times 4}$$

Vectorization

$$a_{1}^{(2)} = g\left(\Theta_{10}^{(1)}x_{0} + \Theta_{11}^{(1)}x_{1} + \Theta_{12}^{(1)}x_{2} + \Theta_{13}^{(1)}x_{3}\right) = g\left(z_{1}^{(2)}\right)$$

$$a_{2}^{(2)} = g\left(\Theta_{20}^{(1)}x_{0} + \Theta_{21}^{(1)}x_{1} + \Theta_{22}^{(1)}x_{2} + \Theta_{23}^{(1)}x_{3}\right) = g\left(z_{2}^{(2)}\right)$$

$$a_{3}^{(2)} = g\left(\Theta_{30}^{(1)}x_{0} + \Theta_{31}^{(1)}x_{1} + \Theta_{32}^{(1)}x_{2} + \Theta_{33}^{(1)}x_{3}\right) = g\left(z_{3}^{(2)}\right)$$

$$h_{\Theta}(\mathbf{x}) = g\left(\Theta_{10}^{(2)}a_{0}^{(2)} + \Theta_{11}^{(2)}a_{1}^{(2)} + \Theta_{12}^{(2)}a_{2}^{(2)} + \Theta_{13}^{(2)}a_{3}^{(2)}\right) = g\left(z_{1}^{(3)}\right)$$



 $\rightarrow h_{\theta}(\mathbf{x})$

Feed-Forward Steps:

$$\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{x}$$

$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

$$\text{Add } a_0^{(2)} = 1$$

$$\mathbf{z}^{(3)} = \Theta^{(2)}\mathbf{a}^{(2)}$$

$$h_{\Theta}(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$



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 x_2

 x_3

 $a_1^{(2)}$

 $a_2^{(2)}$

 $a_3^{(2)}$

Exercise

- Why do we need non-linear activation functions?
 - ***** What happen if g(z) = z

Feed-Forward Steps:

$$\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{x}$$

$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

$$Add \ a_0^{(2)} = 1$$

$$\mathbf{z}^{(3)} = \Theta^{(2)}\mathbf{a}^{(2)}$$

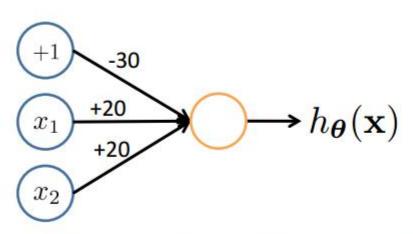
$$h_{\Theta}(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

Non-Linear Representations

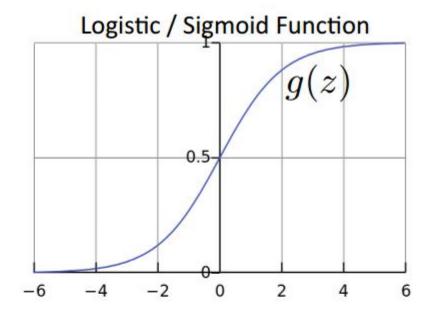
Simple example: AND

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

 $y = x_1 \text{ AND } x_2$

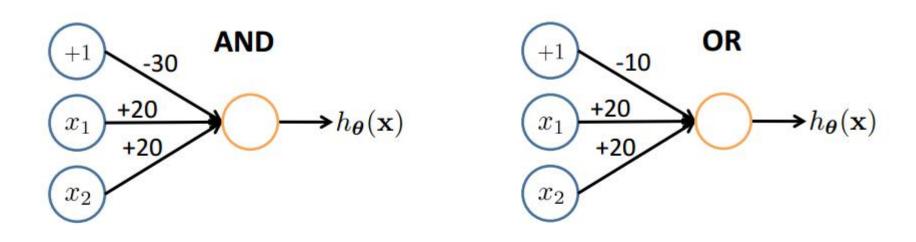


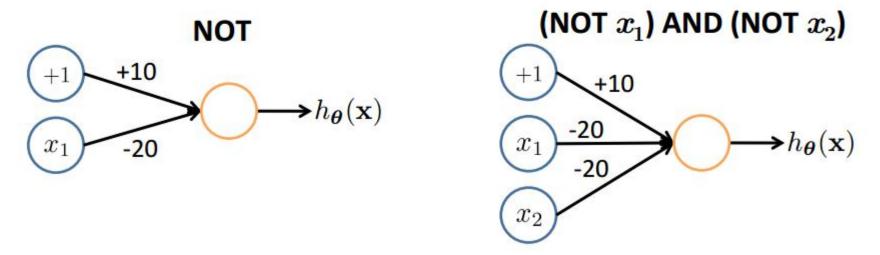
$$h_{\Theta}(\mathbf{x}) = g(-30 + 20x_1 + 20x_2)$$



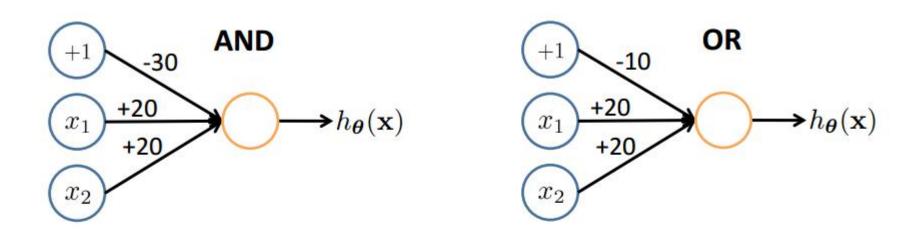
x_{1}	x_2	$h_{\Theta}(\mathbf{x})$
0	0	g(-30) ≈ 0
0	1	$g(-10) \approx 0$
1	0	g(-10) ≈ 0
1	1	$g(10) \approx 1$

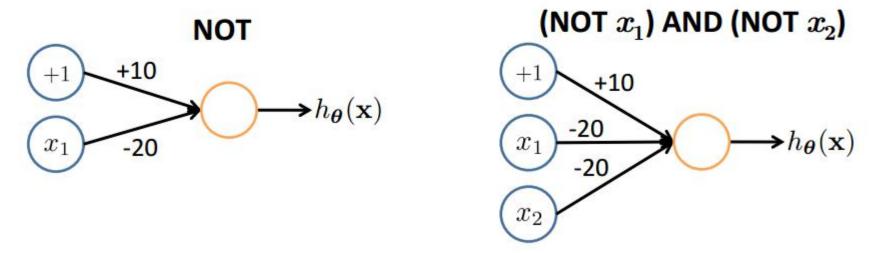
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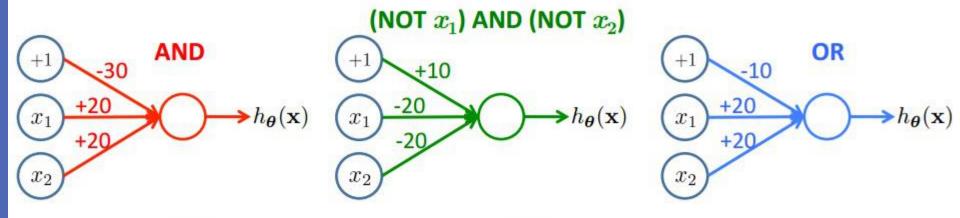
Lec 8: Neural Network & Deep Learning

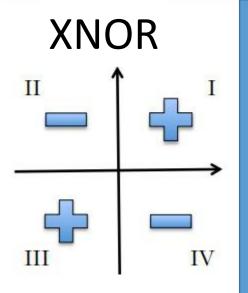




Lec 8: Neural Network & Deep Learning

Combining Representations to Create Non-Linear Functions



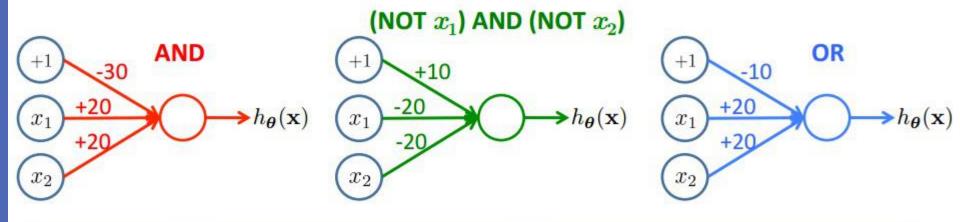


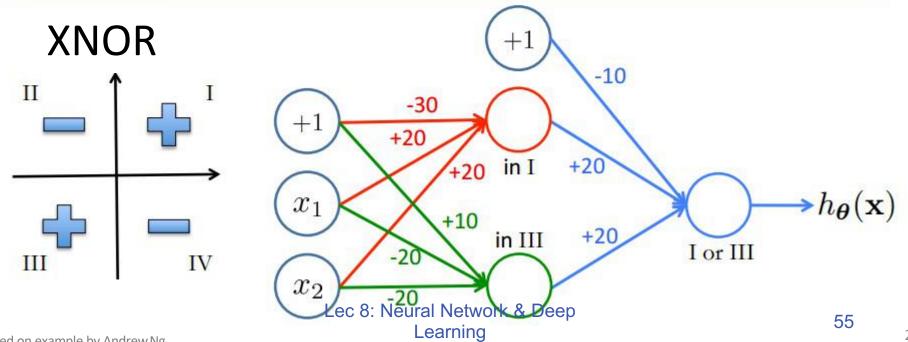
XNOR

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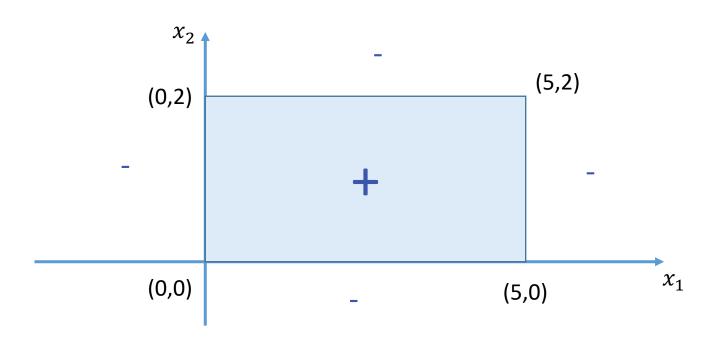
Learning

Combining Representations to Create Non-Linear Functions





Exercise



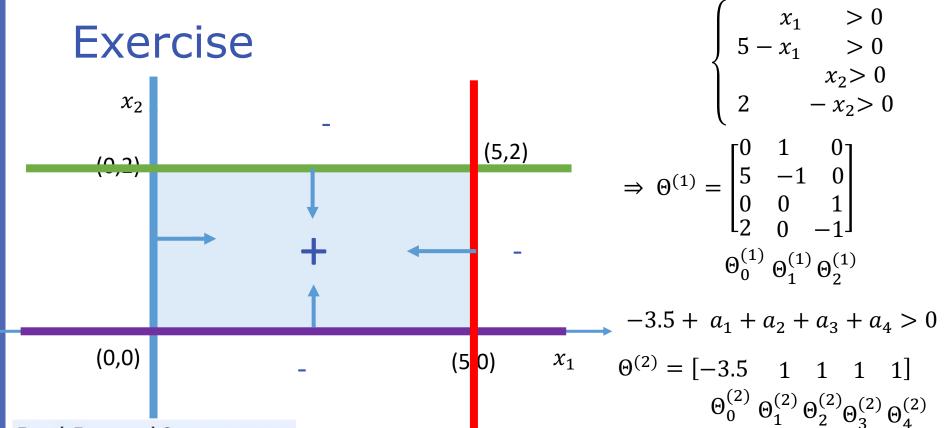
Feed-Forward Steps:

$$\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{x}$$
$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$
Add $a_0^{(2)} = 1$

$$\mathbf{z}^{(3)} = \Theta^{(2)} \mathbf{a}^{(2)}$$

$$h_{\Theta}(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

If all the samples inside the rectangle are positive; otherwise are negative Show a feedforward NN can classify all the samples correctly For simplicity, we assume g(z) is a step function. What are $\Theta^{(1)}$ and $\Theta^{(2)}$



Feed-Forward Steps:

$$\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{x}$$

$$\mathbf{a}^{(2)} = q(\mathbf{z}^{(2)})$$

Add
$$a_0^{(2)} = 1$$

$$\mathbf{z}^{(3)} = \Theta^{(2)} \mathbf{a}^{(2)}$$

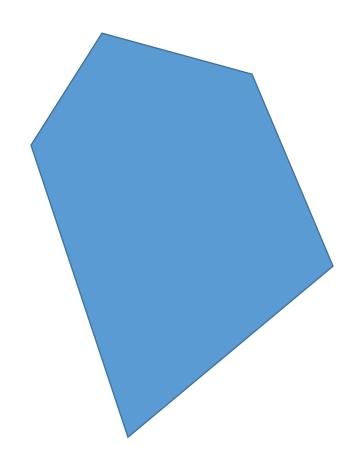
$$h_{\Theta}(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

If all the samples inside the rectangle are positive; otherwise are negative

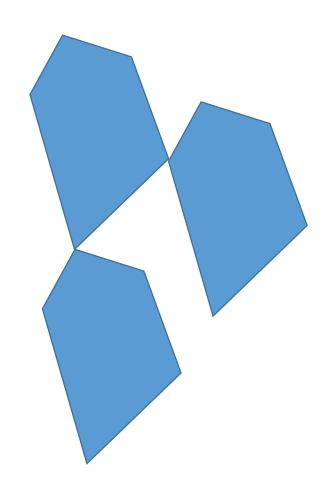
Show a feedforward NN can classify all the samples correctly For simplicity, we assume g(z) is a step function.

What are $\Theta^{(1)}$ and $\Theta^{(2)}$

Arbitrary Decision Boundary



Arbitrary Decision Boundary



Neural Network Training Animation

https://playground.tensorflow.org/

