CSE 417T Introduction to Machine Learning

Lecture 19

Instructor: Chien-Ju (CJ) Ho

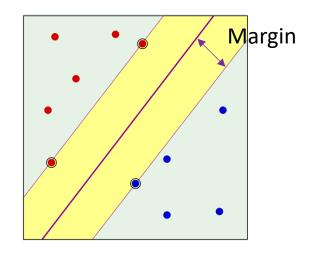
Recap

Support Vector Machines

- Goal: Find the max-margin linear separator
- If the data is linearly separable
 - Hard-Margin SVM (Assume data is linearly separable)

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minimize<sub>\vec{w},b</sub> \frac{1}{2}\vec{w}^T\vec{w} subject to y_n(\vec{w}^T\vec{x}_n + b) \ge 1, \forall n
```

•
$$g(\vec{x}) = sign(\vec{w}^* \vec{x} + b^*)$$



- If the data is not linearly separable
 - Soft-margin SVM
 - Nonlinear transformation Dual Formulation and Kernel Tricks

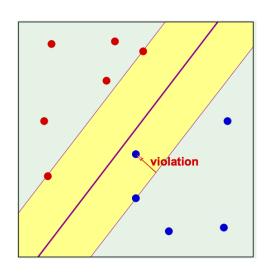
Soft-Margin SVM

- For each point (\vec{x}_n, y_n) , we allow some violation $\xi_n \geq 0$
 - The constraint becomes: $y_n(\vec{w}^T\vec{x}_n + b) \ge 1 \xi_n$
 - We add a penalty for each violation: Total penalty $C \sum_{n=1}^{N} \xi_n$

```
minimize \overrightarrow{w}, b, \overrightarrow{\xi} = \frac{1}{2} \overrightarrow{w}^T \overrightarrow{w} + C \sum_{n=1}^N \xi_n

subject to y_n(\overrightarrow{w}^T \overrightarrow{x}_n + b) \ge 1 - \xi_n, \forall n

\xi_n \ge 0, \forall n
```



Remarks:

- C is a hyper-parameter we can choose, e.g., using validation
 - Larger C => less tolerable to noise => smaller margin
- Soft-margin SVM is still a Quadratic Program, with efficient solvers
- ξ_n^* indicates where \vec{x}_n is with respect to the separator and the margin

Primal-Dual Formulations of Hard-Margin SVM

Primal

minimize
$$_{\overrightarrow{w},b}$$
 $\frac{1}{2}\overrightarrow{w}^T\overrightarrow{w}$ subject to $y_n(\overrightarrow{w}^T\overrightarrow{x}_n+b) \geq 1, \forall n$

Dual

$$\begin{aligned} \text{maximize}_{\overrightarrow{\alpha}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \overrightarrow{x}_n^T \overrightarrow{x}_m \\ \text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0 \\ \alpha_n \geq 0, \forall n \end{aligned}$$

Key messages:

- Both formulations can be efficiently solved using QP solver.
- We can infer the solution from one to the other

Given optimal $\vec{\alpha}^*$:

- $\vec{w}^* = \sum_{\alpha_n^* > 0} \alpha_n^* y_n \vec{x}_n$
- Find a $\alpha_n^* > 0$, $b^* = y_n \vec{x}_n^T \vec{w}^*$

Kernel Functions

- Define kernel function $K_{\Phi}(\vec{x}, \vec{x}') = \Phi(\vec{x})^T \Phi(\vec{x}') (= \vec{z}^T \vec{z}')$
 - The similarity of two vectors in the projected space
- Goal: Compute $K_{\Phi}(\vec{x}, \vec{x}')$ without transforming \vec{x} and \vec{x}'

 Why? This enables us to operate in higher dimensional spaces without really worrying about the computational overhead.

Kernel Trick: Utilize Dual and Kernel Functions

The dual with nonlinear transform

maximize
$$\vec{\alpha} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \vec{z}_n^T \vec{z}_m$$
 subject to $\sum_{n=1}^{N} \alpha_n y_n = 0$ $\alpha_n \geq 0, \forall n$

• Plug in the kernel function $K_{\Phi}(\vec{x}, \vec{x}') = \Phi(\vec{x})^T \Phi(\vec{x}')$

```
\begin{aligned} & \text{maximize}_{\overrightarrow{\alpha}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m K_{\Phi}(\vec{x}_n, \vec{x}_m) \\ & \text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0 \\ & \alpha_n \geq 0, \forall n \end{aligned}
```

- If the kernel can be computed efficiently, we can solve $\vec{\alpha}^*$ efficiently.
- With kernel tricks, we can avoid the dependency on the dimension of \vec{z}

Recover $(\overrightarrow{w}^*, b^*)$ from $\overrightarrow{\alpha}^*$ with Kernel Tricks

- Note that $\vec{\alpha}^*$ is solved in the \vec{z} space
 - $\vec{w}^* = \sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n)$
 - Find a $\alpha_n^* > 0$, $b^* = y_n \overrightarrow{w}^* \Phi(\overrightarrow{x}_n)$
 - We want to avoid the transformation!
- Let's look at the hypothesis
 - $g(\vec{x}) = sign(\vec{w}^{*T}\Phi(\vec{x}) + b^*)$

$$\vec{w}^{*T} \Phi(\vec{x}) = \left(\sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n)\right)^T \Phi(\vec{x})$$

$$= \sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n)^T \Phi(\vec{x})$$

$$= \sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x})$$

Instead of storing (\vec{w}^*, b^*) , we can store "support vectors" (points with $\alpha_n^* > 0$) and make predictions accordingly.

$$b^* = y_n - \vec{w}^{*T} \Phi(\vec{x}_n)$$

$$= y_n - \left(\sum_{\alpha_m^* > 0} \alpha_m^* y_m \Phi(\vec{x}_m)\right)^T \Phi(\vec{x}_n)$$

$$= y_n - \sum_{\alpha_m^* > 0} \alpha_m^* y_m K(\vec{x}_m, \vec{x}_n)$$

• Still can be computed in the \vec{x} space!

Today's Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook. Let me know if you spot errors.

Kernel Functions

 $K_{\Phi}(\vec{x}, \vec{x}')$: Inner products of two points $\Phi(\vec{x})^T \Phi(\vec{x}')$ in the transformed space Similarity of two points $\Phi(\vec{x})$ and $\Phi(\vec{x}')$ in the transformed space

Polynomial Kernel

Kernel $K(\vec{x}, \vec{x}') = \Phi(\vec{x})^T \Phi(\vec{x}')$

- Example in the last lecture: 2^{nd} order polynomial for 2-d \vec{x}
 - $\vec{x} = (x_1, x_2)$
 - $\vec{z} = \Phi_2(\vec{x}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1, x_2, x_1^2, x_2^2)$
 - $\vec{z}' = \Phi_2(\vec{x}') = (1, \sqrt{2}x'_1, \sqrt{2}x'_2, \sqrt{2}x'_1, x'_2, x'_1, x'_2)$

•
$$\vec{z}^T \vec{z}' = 1 + 2x_1 x_1' + 2x_2 x_2' + 2x_1 x_1' x_2 x_2' + (x_1 x_1')^2 + (x_2 x_2')^2$$

= $(1 + x_1 x_1' + x_2 x_2')^2$
= $(1 + \vec{x}^T \vec{x}')^2$

- General 2nd order polynomial
 - $\vec{x} = (x_1, x_2, ..., x_d)$
 - $K_{\Phi_2}(\vec{x}, \vec{x}') = (1 + \vec{x}^T \vec{x}')^2$ = $(1 + x_1 x_1' + x_2 x_2' + \dots + x_d x_d')^2$

Polynomial Kernel

•
$$\vec{x} = (x_1, x_2, ..., x_d)$$

General form of polynomial kernel:

$$K(\vec{x}, \vec{x}') = (a\vec{x}^T\vec{x}' + b)^Q$$

- 2nd order polynomial kernel $K_{\Phi_2}(\vec{x}, \vec{x}') = (1 + \vec{x}^T \vec{x}')^2$
- Q-th order Polynomial kernel $K_{\Phi_Q}(\vec{x}, \vec{x}') = (1 + \vec{x}^T \vec{x}')^Q$ $= (1 + x_1 x_1' + \dots + x_d x_d')^Q$
- Computational complexity
 - Dimension of $\Phi_Q(\vec{x})$: $\binom{Q+d}{Q}$
 - Direct computation of $\Phi_Q(\vec{x})^T \Phi_Q(\vec{x}')$: $O\left(\begin{pmatrix} Q+d \\ Q \end{pmatrix}\right)$
 - Computation through kernel $K_{\Phi_O}(\vec{x}, \vec{x}')$: O(d)

We Only Need \vec{z} Space to Exist

- In the discussion of polynomial kernels,
 - We have a target transformation in mind
 - We want to find a corresponding kernel function
- In fact, as long as $K(\vec{x}, \vec{x}')$ is an inner product in some \vec{z} space, we are good
 - Just plug in the kernel in the dual formulation
 - We obtain a linear separator in the corresponding \vec{z} space

```
maximize \vec{\alpha} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m K_{\Phi}(\vec{x}_n, \vec{x}_m) subject to \sum_{n=1}^{N} \alpha_n y_n = 0 \alpha_n \ge 0, \forall n
```

Gaussian RBF Kernel

- $K(\vec{x}, \vec{x}') = e^{-\gamma \|\vec{x} \vec{x}'\|^2}$
- What's the corresponding \vec{z} space? (What is Φ such that $\Phi(\vec{x})^T \Phi(\vec{x}') = e^{-\gamma ||\vec{x} \vec{x}'||^2}$)
 - For simplicity, make $\vec{x} = x$ be 1 dimensional and $\gamma = 1$

•
$$K(\vec{x}, \vec{x}') = e^{-(x-x')^2}$$

 $= e^{-x^2 + 2xx' - x'^2}$
 $= e^{-x^2} e^{-x'^2} e^{2xx'}$
 $= e^{-x^2} e^{-x'^2} \sum_{k=0}^{\infty} \frac{(2xx')^k}{k!}$
 $= \sum_{k=0}^{\infty} e^{-x^2} \sqrt{\frac{2^k}{k!}} x^k e^{-x'^2} \sqrt{\frac{2^k}{k!}} x'^k$

Taylor expansion: $e^{2xx'} = \sum_{k=0}^{\infty} \frac{(2xx')^k}{k!}$

• The corresponding $\Phi(x) = e^{-x^2} \left(1, \sqrt{\frac{2}{1}} x, \sqrt{\frac{2^2}{2!}} x^2, \dots \right)$

Gaussian RBF Kernel

- $K(\vec{x}, \vec{x}') = e^{-\gamma \|\vec{x} \vec{x}'\|^2}$
- The corresponding transform in 1-dim input $\vec{x} = x$

•
$$\Phi(x) = e^{-x^2} \left(1, \sqrt{\frac{2}{1}} x, \sqrt{\frac{2^2}{2!}} x^2, \dots \right)$$

- $K(\vec{x}, \vec{x}')$ is the inner product of two vectors in an infinite dimensional space!
- When we plug in $K(\vec{x}, \vec{x}')$ in dual SVM
 - We are finding the max-margin separator in an infinite dimensional space
 - Seems to introduce infinite generalization error?
 - Maximizing margin help mitigate this issue
 - The number of support vectors provides indicators on the generalization

Design Your Own Kernel? [Safe to Skip]

• Say we design a kernel function, how do we know whether it is valid, i.e., whether there is a corresponding \vec{z} space?

- Mercer's condition (See discussion in LFD 8.3.2)
 - Kernel matrix

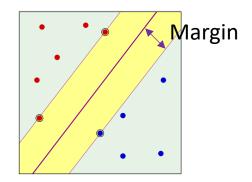
$$\left[egin{array}{ccccc} K(\mathbf{x}_1,\mathbf{x}_1) & K(\mathbf{x}_1,\mathbf{x}_2) & \dots & K(\mathbf{x}_1,\mathbf{x}_N) \ K(\mathbf{x}_2,\mathbf{x}_1) & K(\mathbf{x}_2,\mathbf{x}_2) & \dots & K(\mathbf{x}_2,\mathbf{x}_N) \ & \dots & & \dots & & \dots \ K(\mathbf{x}_N,\mathbf{x}_1) & K(\mathbf{x}_N,\mathbf{x}_2) & \dots & K(\mathbf{x}_N,\mathbf{x}_N) \end{array}
ight]$$

• $K(\vec{x}, \vec{x}')$ is a valid kernel if and only if the kernel matrix is always symmetric positive semi-definite for any $\vec{x}_1, \dots, \vec{x}^N$

Summary of What We Talked About So Far

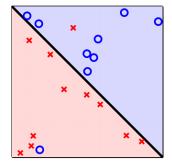
Hard-Margin SVM (Separable Data)

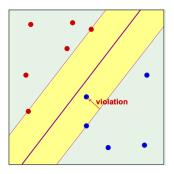
minimize
$$_{\overrightarrow{w},b}$$
 $\frac{1}{2}\overrightarrow{w}^T\overrightarrow{w}$
subject to $y_n(\overrightarrow{w}^T\overrightarrow{x}_n+b) \ge 1, \forall n$



Soft-Margin SVM (Tolerate Noise)

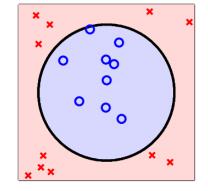
minimize
$$\overrightarrow{w}, b, \overrightarrow{\xi}$$
 $\frac{1}{2} \overrightarrow{w}^T \overrightarrow{w} + C \sum_{n=1}^N \xi_n$
subject to $y_n (\overrightarrow{w}^T \overrightarrow{x}_n + b) \ge 1 - \xi_n, \forall n$
 $\xi_n \ge 0, \forall n$





Kernel Formulation of Hard-Margin SVM

maximize
$$\alpha \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m K_{\Phi}(\vec{x}_n, \vec{x}_m)$$
 subject to $\sum_{n=1}^{N} \alpha_n y_n = 0$ $\alpha_n \ge 0, \forall n$



Kernel Version of Soft-Margin SVM

Soft-Margin SVM

```
minimize \overrightarrow{w}, b, \overrightarrow{\xi} \frac{1}{2}\overrightarrow{w}^T\overrightarrow{w} + C\sum_{n=1}^N \xi_n subject to y_n(\overrightarrow{w}^T\overrightarrow{x}_n + b) \ge 1 - \xi_n, \forall n \xi_n \ge 0, \forall n
```

Kernel Version of Soft-Margin SVM

```
maximize \alpha \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m K_{\Phi}(\vec{x}_n, \vec{x}_m) subject to \sum_{n=1}^{N} \alpha_n y_n = 0 0 \le \alpha_n \le C, \forall n
```

- It can be obtained by similar procedure as hard-margin version
- We can obtain the same relationship between $\vec{\alpha}^*$ and (\vec{w}^*, b^*)

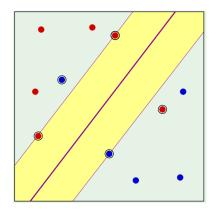
Interpretation of Support Vectors

- $\alpha_n^* > 0 \Rightarrow (\vec{x}_n, y_n)$ is a support vector
 - $y_n(\overrightarrow{w}^*\overrightarrow{x}_n + b^*) = 1 \xi_n$
- Utilizing complementary slackness
 - When $0 < \alpha_n^* < C$
 - $\xi_n = 0$
 - $y_n(\vec{w}^{*T}\vec{x}_n + b^*) = 1$
 - (\vec{x}_n, y_n) is a "margin" support vector
 - When $\alpha_n^* = C$
 - $\xi_n > 0$
 - $y_n(\vec{w}^{*T}\vec{x}_n + b^*) < 1$
 - (\vec{x}_n, y_n) is a "non-margin" support vector

```
minimize \vec{w}, b, \vec{\xi} \frac{1}{2} \vec{w}^T \vec{w} + C \sum_{n=1}^{N} \xi_n subject to y_n (\vec{w}^T \vec{x}_n + b) \ge 1 - \xi_n, \forall n \xi_n \ge 0, \forall n
```

maximize
$$\vec{\alpha} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m K_{\Phi}(\vec{x}_n, \vec{x}_m)$$

subject to $\sum_{n=1}^{N} \alpha_n y_n = 0$
 $0 \le \alpha_n \le C$, $\forall n$



Another Look at Primal vs. Dual SVM

Primal

minimize
$$_{\overrightarrow{w},b}$$
 $\frac{1}{2}\overrightarrow{w}^T\overrightarrow{w}$ subject to $y_n(\overrightarrow{w}^T\overrightarrow{z}_n+b)\geq 1, \forall n$

Learned hypothesis

•
$$g(\vec{x}) = sign(\vec{w}^{*T}\Phi(\vec{x}) + b^{*})$$

Dual

$$\begin{aligned} & \text{maximize}_{\overrightarrow{\alpha}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \vec{\boldsymbol{z}}_n^T \vec{\boldsymbol{z}}_m \\ & \text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0 \\ & \quad \alpha_n \geq 0, \forall n \end{aligned}$$

Learned hypothesis

•
$$g(\vec{x}) = sign(\sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x}) + b^*))$$

• $(\alpha_n^* > 0 \Rightarrow \vec{x}_n \text{ is a support vector})$

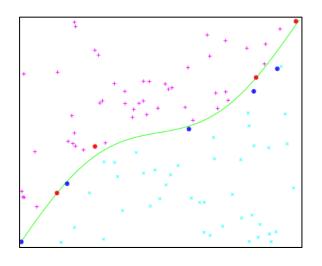
- Primal view of SVM (parametric)
 - We are learning the weights for SVM, i.e., (\vec{w}^*, b^*)
 - When using RBF Kernel, there are infinite number of parameters
- Dual kernel view of SVM (nonparametric)
 - We are learning the support vectors, and use those for prediction

Kernel SVM and Radial Basis Functions

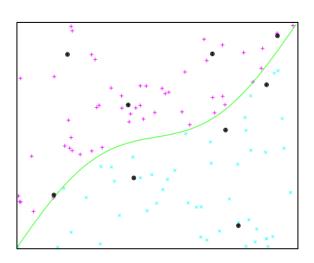
Kernel SVM

•
$$g(\vec{x}) = sign(\sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x}) + b^*))$$

• Use support vectors to characterize a hypothesis



- Radial Basis Functions
 - $h(\vec{x}) = \sum_{k=1}^{K} w_k \, \phi\left(\frac{\|\vec{x} \vec{\mu}_k\|}{r}\right)$
 - Use cluster centers to characterize a hypothesis



Neural Networks

Perceptron

What is a hypothesis in Perceptron

$$h(\vec{x}) = sign(\vec{w}^T \vec{x})$$

Note that we have reverted back to our original notations

- $\vec{x} = (x_0, x_1, ..., x_d)$ $\vec{w} = (w_0, w_1, ..., w_d)$

 - Linear separator

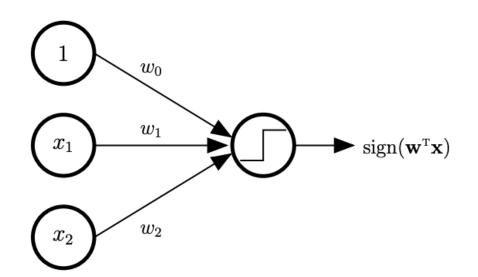
$$h(\vec{x}) = sign(\vec{w}^T \vec{x})$$

Perceptron

What is a hypothesis in Perceptron

$$h(\vec{x}) = sign(\vec{w}^T \vec{x})$$

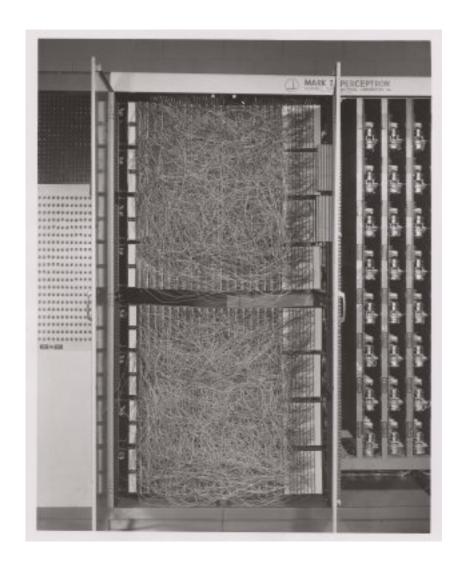
Graphical representation of Perceptron



Inspired by neurons:

The output signal is triggered when the weighted combination of the inputs is larger than some threshold

The First Perceptron Machine

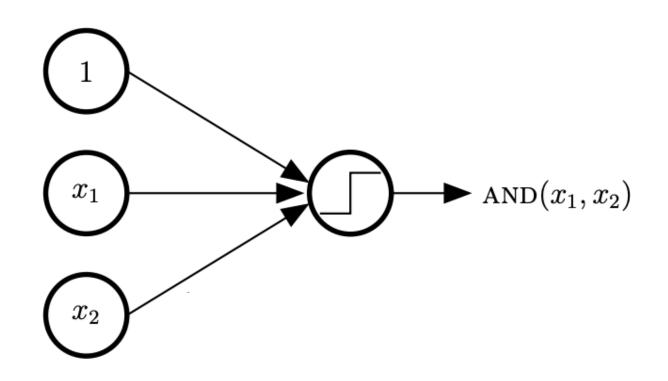


Mark I Perceptron machine, the first implementation of the perceptron algorithm. (From Wikipedia)

"the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence."

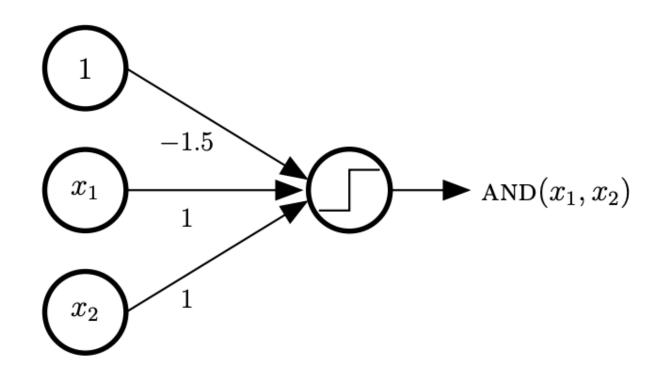
- AND(x_1, x_2)
 - Use +1 to denote "true" and -1 to denote "false"

x_1	x_2	$AND(x_1,x_2)$
+1	+1	+1
+1	-1	-1
-1	+1	-1
-1	-1	-1



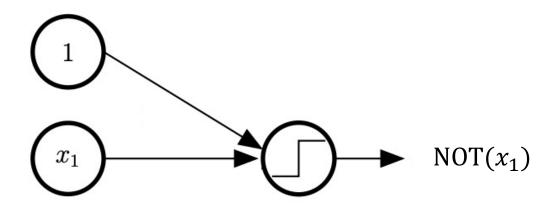
- AND(x_1, x_2)
 - Use +1 to denote "true" and -1 to denote "false"

x_1	x_2	$AND(x_1,x_2)$
+1	+1	+1
+1	-1	-1
-1	+1	-1
-1	-1	-1



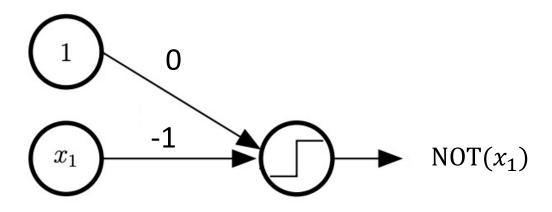
- NOT(x_1)
 - Use +1 to denote "true" and -1 to denote "false"

x_1	OR(x)
+1	-1
-1	+1



- NOT(x_1)
 - Use +1 to denote "true" and -1 to denote "false"

x_1	OR(x)
+1	-1
-1	+1



Practice: How to Implement OR and XOR?

• Use +1 to denote "true" and -1 to denote "false"

• $OR(x_1, x_2)$

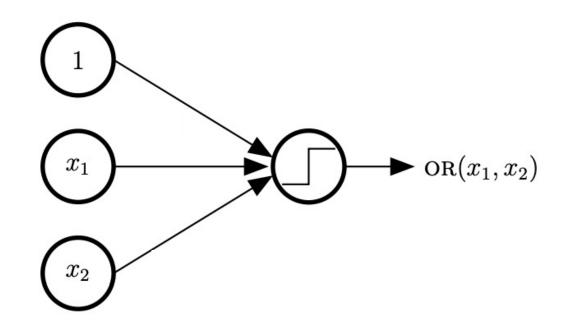
x_1	x_2	$OR(x_1, x_2)$
+1	+1	+1
+1	-1	+1
-1	+1	+1
-1	-1	-1

• $XOR(x_1, x_2)$

x_1	x_2	$XOR(x_1, x_2)$
+1	+1	-1
+1	-1	+1
-1	+1	+1
-1	-1	-1

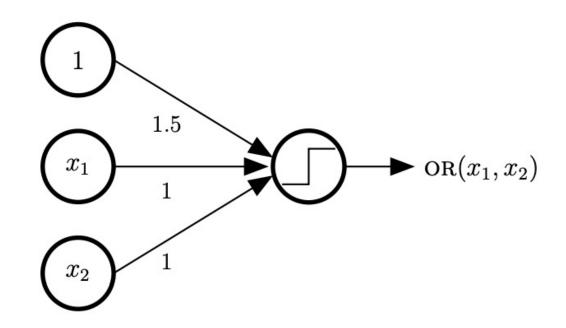
- $OR(x_1, x_2)$
 - Use +1 to denote "true" and -1 to denote "false"

x_1	x_2	$OR(x_1, x_2)$
+1	+1	+1
+1	-1	+1
-1	+1	+1
-1	-1	-1



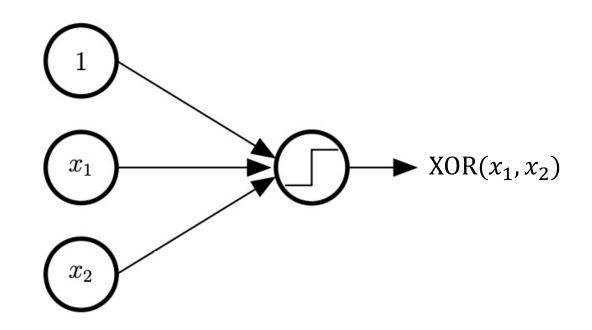
- $OR(x_1, x_2)$
 - Use +1 to denote "true" and -1 to denote "false"

x_1	x_2	$OR(x_1, x_2)$
+1	+1	+1
+1	-1	+1
-1	+1	+1
-1	-1	-1



- $XOR(x_1, x_2)$
 - Use +1 to denote "true" and -1 to denote "false"

x_1	x_2	$XOR(x_1, x_2)$
+1	+1	-1
+1	-1	+1
-1	+1	+1
-1	-1	-1



- $XOR(x_1, x_2)$
 - Use +1 to denote "true" and -1 to denote "false"

x_1	x_2	$XOR(x_1, x_2)$
+1	+1	-1
+1	-1	+1
-1	+1	+1
-1	-1	-1

It is impossible to implement XOR using a single perceptron (draw the points in the 2-D space, you will see they are not linearly separable)

Stronger version:

It is impossible to implement XOR using a single layer of perceptrons

Multi-Layer Perceptron

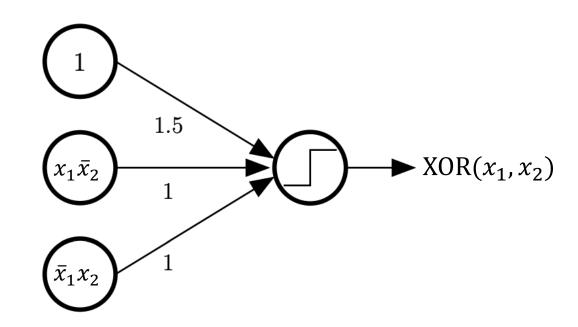


Representing Boolean Operations

- AND $(x_1, x_2) \rightarrow x_1 x_2$
- $OR(x_1, x_2) \to x_1 + x_2$
- NOT $(x_1) \rightarrow \bar{x}_1$
- $XOR(x_1, x_2) \to x_1 \bar{x}_2 + \bar{x}_1 x_2$

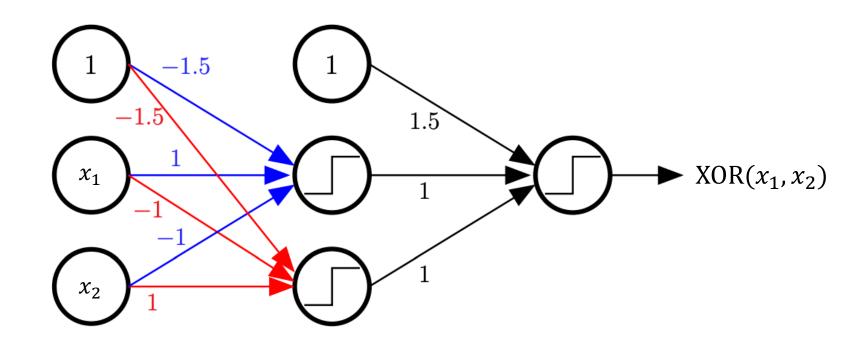
Implementing XOR

• $XOR(x_1, x_2) \to x_1 \bar{x}_2 + \bar{x}_1 x_2$

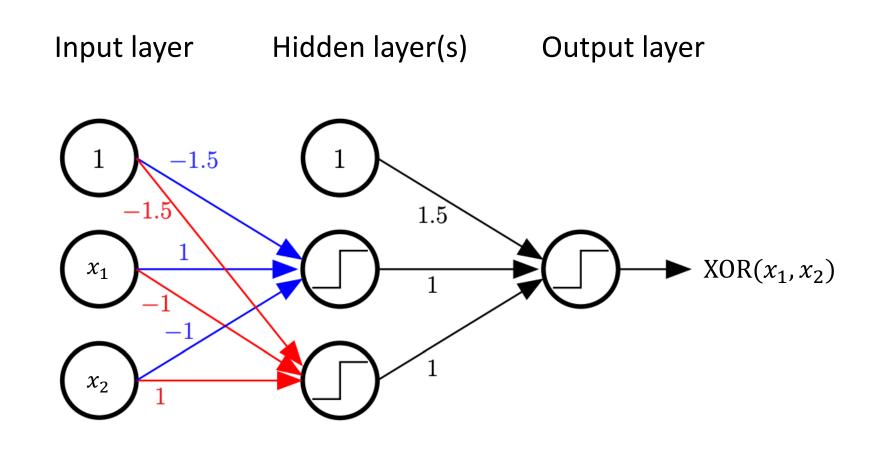


Implementing XOR

• $XOR(x_1, x_2) \to x_1 \bar{x}_2 + \bar{x}_1 x_2$



Multi-Layer Perceptron (MLP)



Feed-forward network

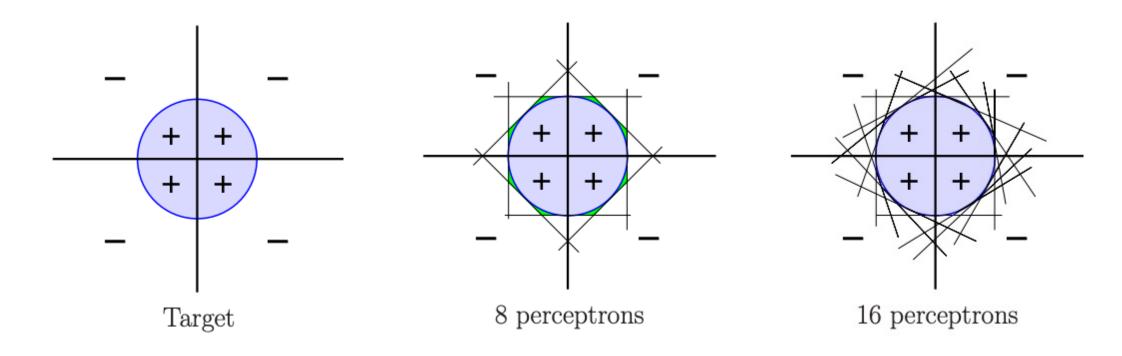
The Power of Multi-Layer Perceptron (MLP)

 We now know that we can implement XOR by introducing the hidden layer in MLP. But generally how powerful is MLP?

- Universal approximation theorem
 - a feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of \mathbb{R}^n , under mild assumptions on the activation function.
- Three-layer MLP can approximate ANY continuous target function!

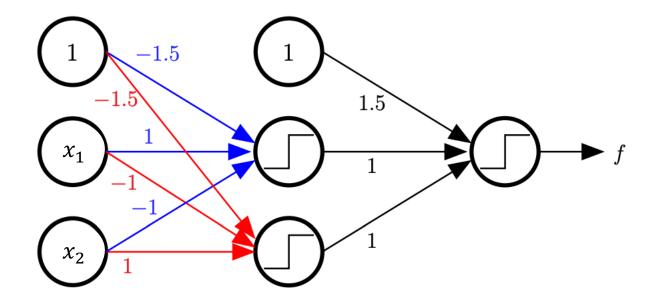
Informal Intuitions of Universal Approximation

A continuous separator can be "decomposed" into linear separators



How to Learn MLP From Data?

• Given D and the network structure, how to learn the "weights" (i.e., the weight vectors of every Perceptron)?

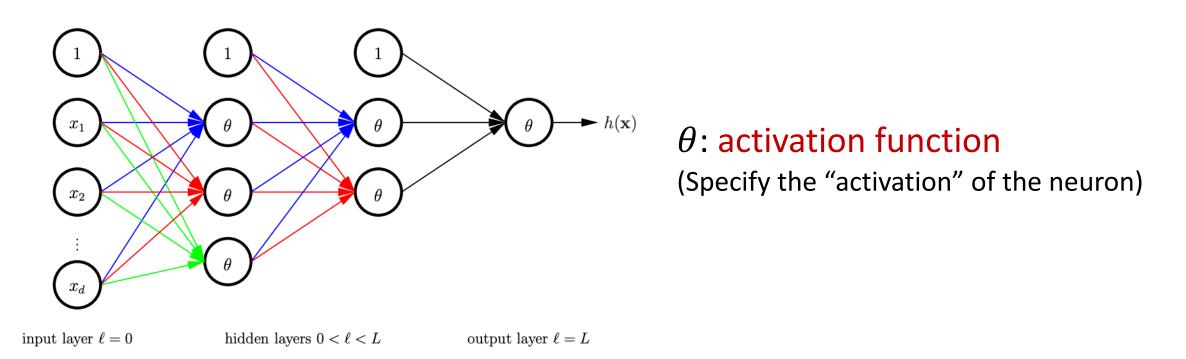


• Computationally challenging due to the "sign" function (\Box)



Neural Networks

A softened version of multi-layer Perceptron (MLP)



Next lecture: formally introduce neural networks and how to learn it from data