

CSE 417T

Introduction to Machine Learning

Lecture 19

Instructor: Chien-Ju (CJ) Ho

Logistics

- No class on Nov 22 (Tuesday): The day before the thanksgiving break
- Homework 4 was due yesterday
- Homework 5 will be announced later today
 - This will be our last assignment
 - Keep track of your own late days
 - Gradescope doesn't allow separate deadlines
 - Your submissions **won't be graded** if you exceed the late-day limit
- Please ask course-related questions on Piazza
 - I have been very behind on emails and don't open all emails
 - However, I'll try to check Piazza regularly

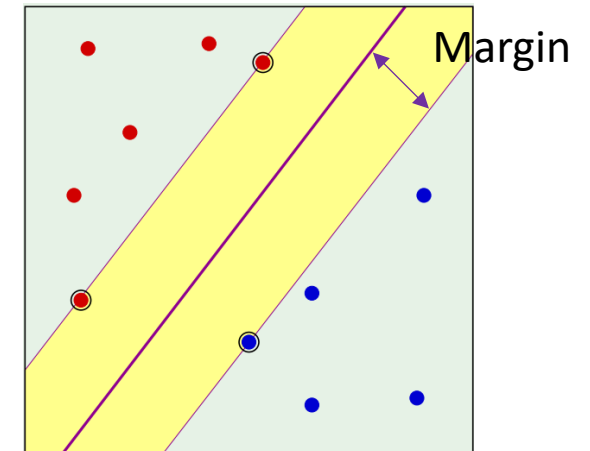
Recap

Support Vector Machines

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

$$\begin{array}{ll} \text{minimize}_{\vec{w}, b} & \frac{1}{2} \vec{w}^T \vec{w} \\ \text{subject to} & y_n (\vec{w}^T \vec{x}_n + b) \geq 1, \forall n \end{array}$$

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

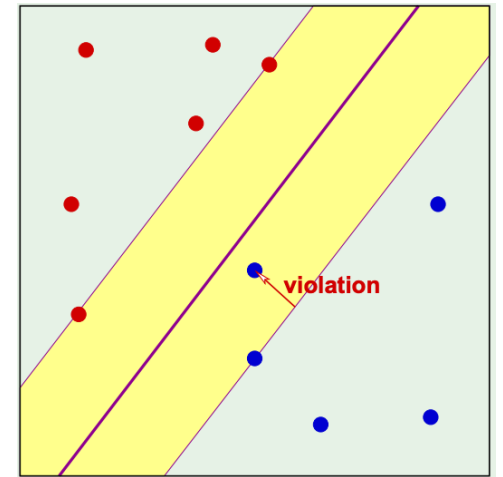


- If the data is not linearly separable
 - **Soft-margin SVM**
 - Nonlinear transformation – **Dual Formulation** and **Kernel Tricks**

Soft-Margin SVM

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

$$\begin{aligned} & \text{minimize}_{\vec{w}, b, \vec{\xi}} \quad \frac{1}{2} \vec{w}^T \vec{w} + C \sum_{n=1}^N \xi_n \\ & \text{subject to} \quad y_n(\vec{w}^T \vec{x}_n + b) \geq 1 - \xi_n, \forall n \\ & \quad \quad \quad \xi_n \geq 0, \forall n \end{aligned}$$



Remarks:

- C is a hyper-parameter we can choose, e.g., using validation
 - Larger $C \Rightarrow$ less tolerable to noise \Rightarrow 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

$$\begin{aligned} & \text{minimize}_{\vec{w}, b} \quad \frac{1}{2} \vec{w}^T \vec{w} \\ & \text{subject to} \quad y_n (\vec{w}^T \vec{x}_n + b) \geq 1, \forall n \end{aligned}$$

- Dual

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

- Key messages:

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

Reminders of definitions in general convex program:

$$\begin{aligned} & \text{minimize}_{\vec{w}} \quad f(\vec{w}) \\ & \text{subject to} \quad g_i(\vec{w}) \leq 0, \quad i = 1, \dots, k \\ & \quad \quad \quad h_j(\vec{w}) = 0, \quad j = 1, \dots, \ell \end{aligned}$$

$$L(\vec{w}, \vec{\alpha}, \vec{\beta}) = f(\vec{w}) + \sum_{i=1}^k \alpha_i g_i(\vec{w}) + \sum_{j=1}^{\ell} \beta_j h_j(\vec{w})$$

$$\text{Primal: } \min_{\vec{w}} \max_{\vec{\alpha}, \vec{\beta}; \alpha_i \geq 0} L(\vec{w}, \vec{\alpha}, \vec{\beta})$$

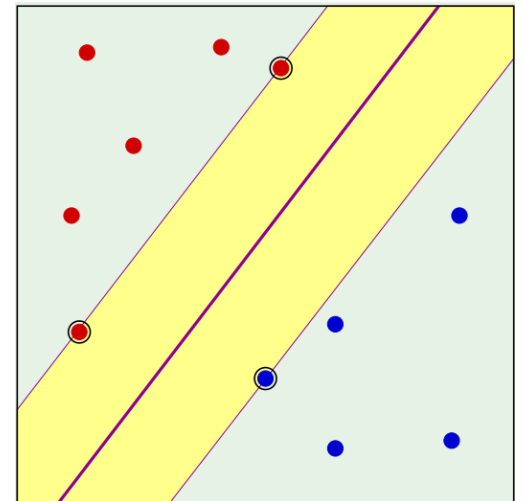
$$\text{Dual: } \max_{\vec{\alpha}, \vec{\beta}; \alpha_i \geq 0} \min_{\vec{w}} L(\vec{w}, \vec{\alpha}, \vec{\beta})$$

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

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

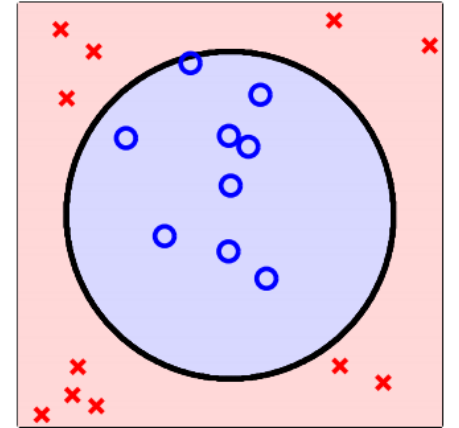
Support Vectors

- Primal point of view
 - We call the points closest to the separator (candidate) support vectors
 - They are the points that the equality holds in the constraints
 - If \vec{x}_n is a support vector, $y_n(\vec{w}^T \vec{x}_n + b) = 1$
 - Removing the non-support vectors will not impact the linear separator
- Dual point of view
 - If $\alpha_n^* > 0 \Rightarrow (\vec{x}_n, y_n)$ is the support vector
 - The optimal separator (\vec{w}^*, b^*)
 - $\vec{w}^* = \sum_{\alpha_n^* > 0} \alpha_n^* y_n \vec{x}_n$
 - $b^* = y_n - \vec{x}_n^T \vec{w}^*$ for some $\alpha_n^* > 0$
 - (\vec{w}^*, b^*) can be defined by “support vectors”
 - Support vector machine!



Nonlinear Transform and Kernel Tricks

- 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

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

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

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

- 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 (\vec{w}^*, b^*) from $\vec{\alpha}^*$ 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 $\alpha_n^* > 0$, $b^* = y_n - \vec{w}^{*T} \Phi(\vec{x}_n)$
- We want to avoid the transformation!

- Let's look at the hypothesis

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

$$\begin{aligned}\vec{w}^{*T} \Phi(\vec{x}) &= \left(\sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n) \right)^T \Phi(\vec{x}) \\ &= \sum_{\alpha_n^* > 0} \alpha_n^* y_n \Phi(\vec{x}_n)^T \Phi(\vec{x}) \\ &= \sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x})\end{aligned}$$

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

$$\begin{aligned}b^* &= y_n - \vec{w}^{*T} \Phi(\vec{x}_n) \\ &= y_n - \left(\sum_{\alpha_m^* > 0} \alpha_m^* y_m \Phi(\vec{x}_m) \right)^T \Phi(\vec{x}_n) \\ &= y_n - \sum_{\alpha_m^* > 0} \alpha_m^* y_m K(\vec{x}_m, \vec{x}_n)\end{aligned}$$

- 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

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

- Example in the last lecture: 2nd order polynomial for 2-d \vec{x}
 - $\vec{x} = (x_1, x_2)$
 - $\vec{z} = \Phi_2(\vec{x}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2)$
 - $\vec{z}' = \Phi_2(\vec{x}') = (1, \sqrt{2}x'_1, \sqrt{2}x'_2, \sqrt{2}x'_1x'_2, x_1'^2, x_2'^2)$
 - $$\begin{aligned}\vec{z}^T \vec{z}' &= 1 + 2x_1x'_1 + 2x_2x'_2 + 2x_1x'_1x_2x'_2 + (x_1x'_1)^2 + (x_2x'_2)^2 \\ &= (1 + x_1x'_1 + x_2x'_2)^2 \\ &= (1 + \vec{x}^T \vec{x}')^2\end{aligned}$$
- General 2nd order polynomial
 - $\vec{x} = (x_1, x_2, \dots, x_d)$
 - $$\begin{aligned}K_{\Phi_2}(\vec{x}, \vec{x}') &= (1 + \vec{x}^T \vec{x}')^2 \\ &= (1 + x_1x'_1 + x_2x'_2 + \dots + x_dx'_d)^2\end{aligned}$$

Polynomial Kernel

- $\vec{x} = (x_1, x_2, \dots, x_d)$

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 $\Phi_Q(\vec{x})^T \Phi_Q(\vec{x}')$: $O\left(\binom{Q+d}{Q}\right)$

- Computation through kernel $K_{\Phi_Q}(\vec{x}, \vec{x}')$: $O(d)$

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

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

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 illustrative purpose, make $\vec{x} = x$ be 1 dimensional and $\gamma = 1$

$$\begin{aligned} K(\vec{x}, \vec{x}') &= e^{-(x-x')^2} \\ &= e^{-x^2 + 2xx' - x'^2} \\ &= e^{-x^2} e^{-x'^2} e^{2xx'} \\ &= e^{-x^2} e^{-x'^2} \sum_{k=0}^{\infty} \frac{(2xx')^k}{k!} \\ &= \sum_{k=0}^{\infty} e^{-x^2} \sqrt{\frac{2^k}{k!}} x^k e^{-x'^2} \sqrt{\frac{2^k}{k!}} x'^k \end{aligned}$$

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

- 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

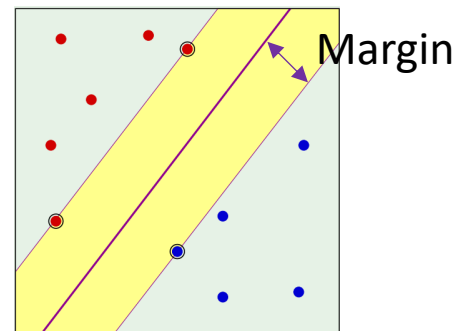
$$\begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \dots & K(\mathbf{x}_1, \mathbf{x}_N) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \dots & K(\mathbf{x}_2, \mathbf{x}_N) \\ \dots & \dots & \dots & \dots \\ K(\mathbf{x}_N, \mathbf{x}_1) & K(\mathbf{x}_N, \mathbf{x}_2) & \dots & K(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

- $K(\vec{x}, \vec{x}')$ 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

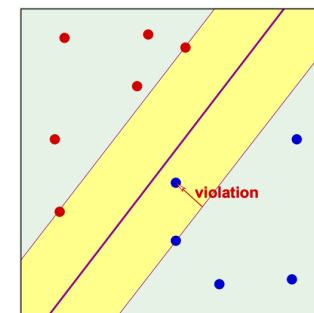
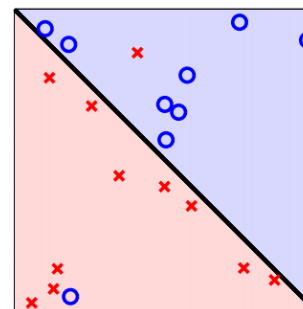
Hard-Margin SVM (Separable Data)

$$\begin{aligned} &\text{minimize}_{\vec{w}, b} \quad \frac{1}{2} \vec{w}^T \vec{w} \\ &\text{subject to} \quad y_n (\vec{w}^T \vec{x}_n + b) \geq 1, \forall n \end{aligned}$$



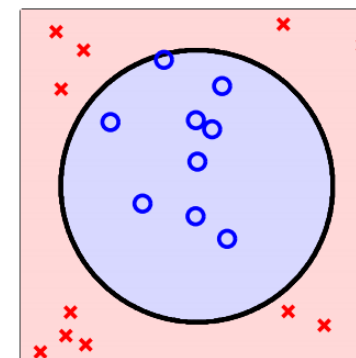
Soft-Margin SVM (Tolerate Noise)

$$\begin{aligned} &\text{minimize}_{\vec{w}, b, \vec{\xi}} \quad \frac{1}{2} \vec{w}^T \vec{w} + C \sum_{n=1}^N \xi_n \\ &\text{subject to} \quad y_n (\vec{w}^T \vec{x}_n + b) \geq 1 - \xi_n, \forall n \\ &\quad \quad \quad \xi_n \geq 0, \forall n \end{aligned}$$



Kernel Formulation of Hard-Margin SVM

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



Kernel Version of Soft-Margin SVM

- Soft-Margin SVM

$$\begin{aligned} & \text{minimize}_{\vec{w}, b, \vec{\xi}} \quad \frac{1}{2} \vec{w}^T \vec{w} + C \sum_{n=1}^N \xi_n \\ & \text{subject to} \quad y_n (\vec{w}^T \vec{x}_n + b) \geq 1 - \xi_n, \forall n \\ & \quad \quad \quad \xi_n \geq 0, \forall n \end{aligned}$$

- Kernel Version of Soft-Margin SVM

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

- 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

- $y_n(\vec{w}^{*T} \vec{x}_n + b^*) = 1 - \xi_n$

- 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 $\alpha_n^* = C$

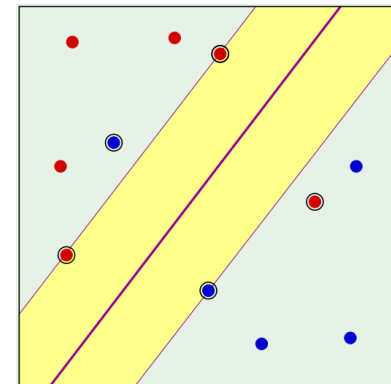
- $\xi_n > 0$

- $y_n(\vec{w}^{*T} \vec{x}_n + b^*) < 1$

- (\vec{x}_n, y_n) is a “non-margin” support vector

$$\begin{aligned} &\text{minimize}_{\vec{w}, b, \vec{\xi}} \quad \frac{1}{2} \vec{w}^T \vec{w} + C \sum_{n=1}^N \xi_n \\ &\text{subject to} \quad y_n(\vec{w}^T \vec{x}_n + b) \geq 1 - \xi_n, \forall n \\ &\quad \quad \quad \xi_n \geq 0, \forall n \end{aligned}$$

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



Another Look at Primal vs. Dual SVM

- Primal

$$\begin{aligned} &\text{minimize}_{\vec{w}, b} \quad \frac{1}{2} \vec{w}^T \vec{w} \\ &\text{subject to} \quad y_n (\vec{w}^T \vec{z}_n + b) \geq 1, \forall n \end{aligned}$$

- Learned hypothesis

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

- 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

- Dual

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

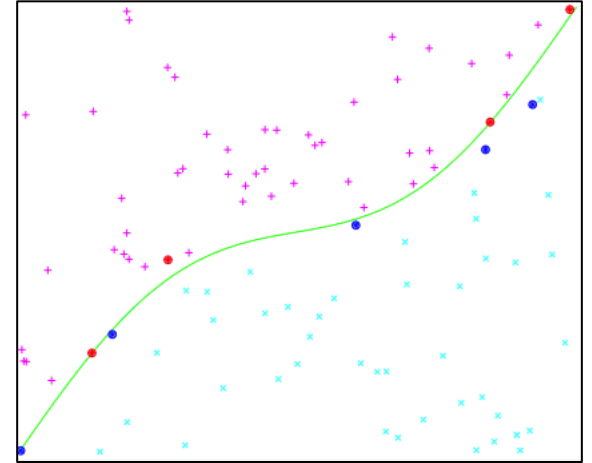
- Learned hypothesis

- $g(\vec{x}) = \text{sign}(\sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x}) + b^*))$
 - $(\alpha_n^* > 0 \Rightarrow \vec{x}_n \text{ is a support vector})$

Kernel SVM and Radial Basis Functions

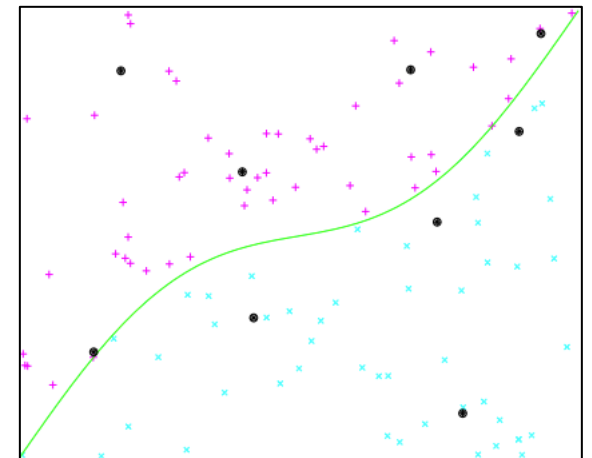
- Kernel SVM

- $g(\vec{x}) = \text{sign}\left(\sum_{\alpha_n^* > 0} \alpha_n^* y_n K(\vec{x}_n, \vec{x}) + b^*\right)$
- Use **support vectors** to characterize a hypothesis



- Radial Basis Functions

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



Neural Networks

Perceptron

- What is a hypothesis in Perceptron

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

- Note that we have reverted back to our original notations

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

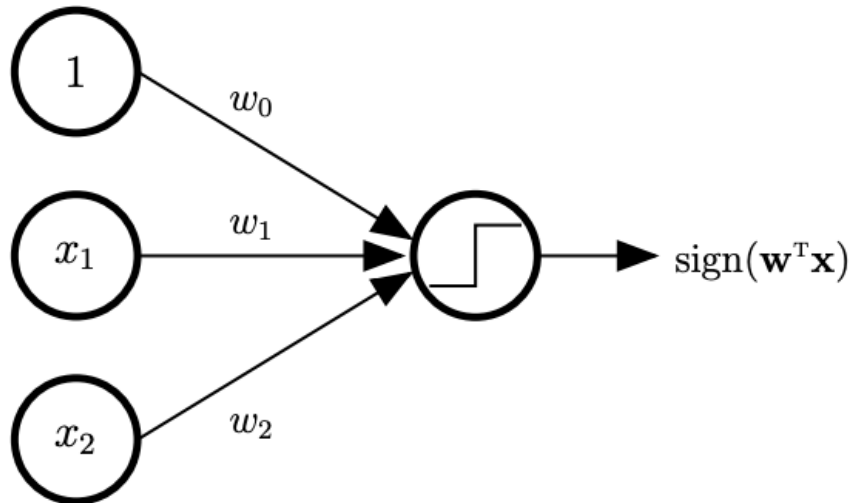
$$h(\vec{x}) = \text{sign}(\vec{w}^T \vec{x})$$

Perceptron

- What is a hypothesis in Perceptron

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

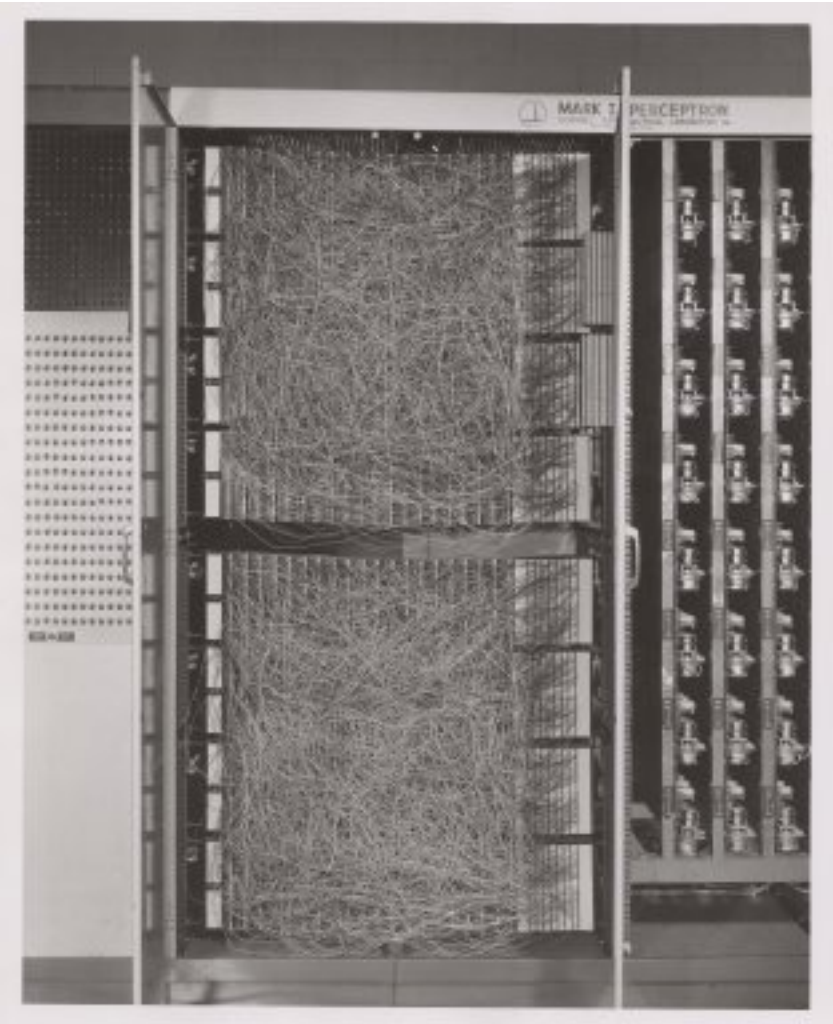
- Graphical representation of Perceptron



Inspired by [neurons](#):

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

The First Perceptron Machine



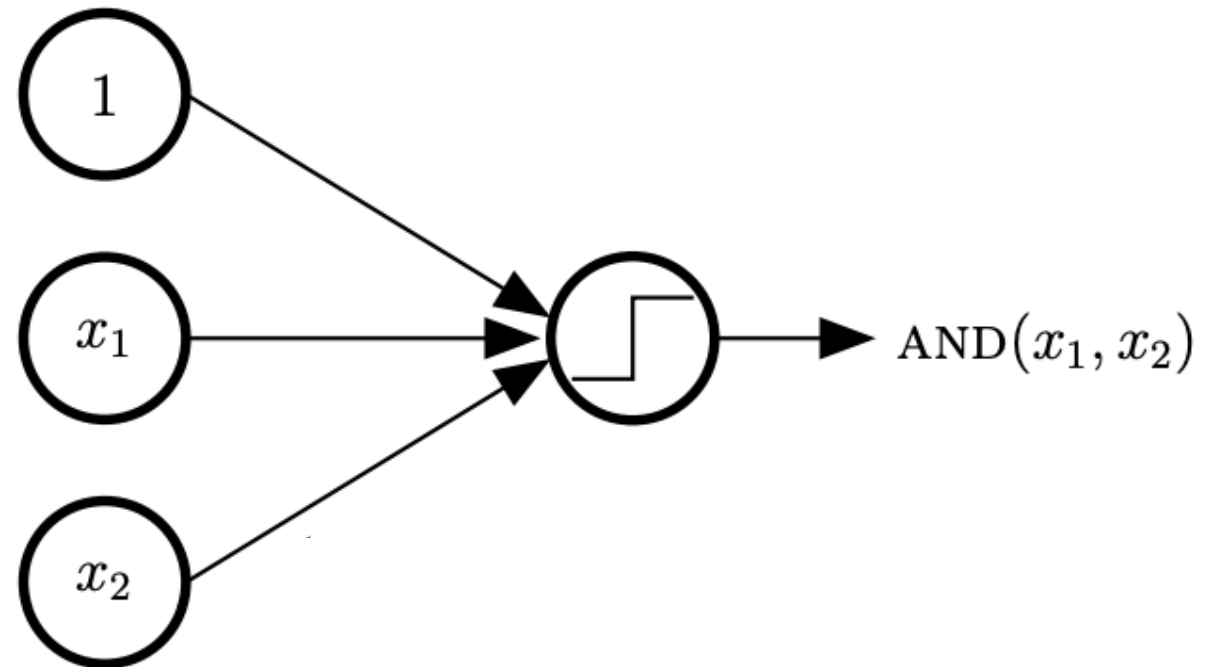
Mark I Perceptron machine, the first implementation of the perceptron algorithm. (From Wikipedia)

“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.” [1958]

Implement Logic Gates with Perceptron

- $\text{AND}(x_1, x_2)$
 - Use +1 to denote “true” and -1 to denote “false”

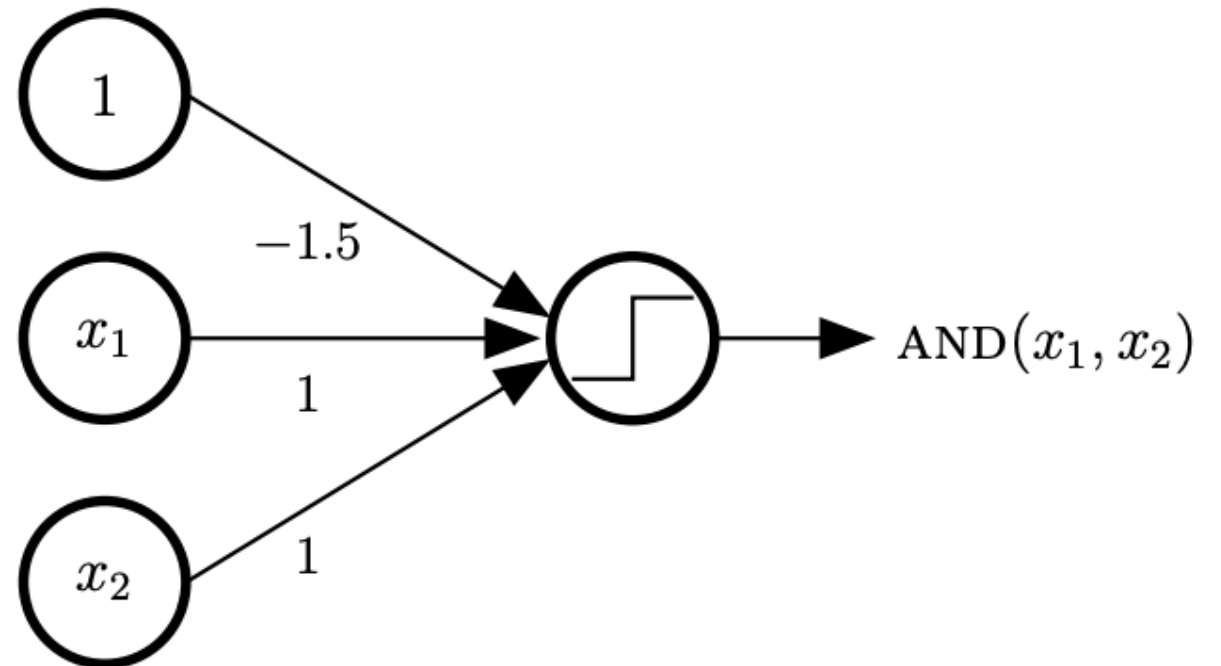
x_1	x_2	$\text{AND}(x_1, x_2)$
+1	+1	+1
+1	-1	-1
-1	+1	-1
-1	-1	-1



Implement Logic Gates with Perceptron

- $\text{AND}(x_1, x_2)$
 - Use +1 to denote “true” and -1 to denote “false”

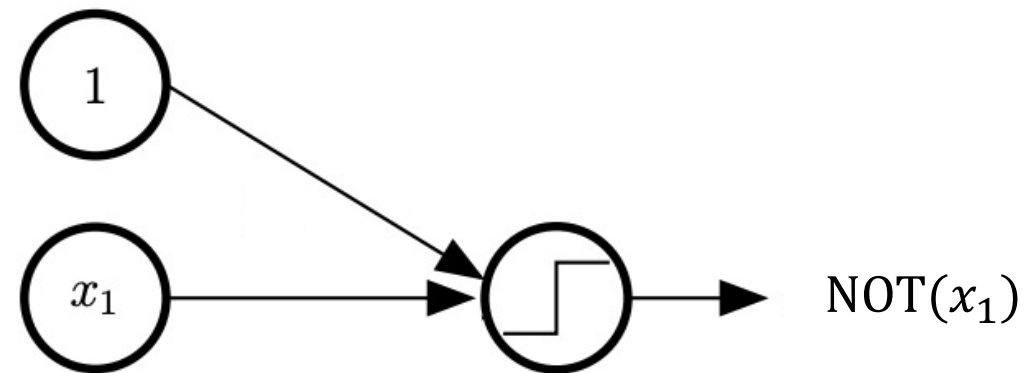
x_1	x_2	$\text{AND}(x_1, x_2)$
+1	+1	+1
+1	-1	-1
-1	+1	-1
-1	-1	-1



Implement Logic Gates with Perceptron

- $\text{NOT}(x_1)$
 - Use $+1$ to denote “true” and -1 to denote “false”

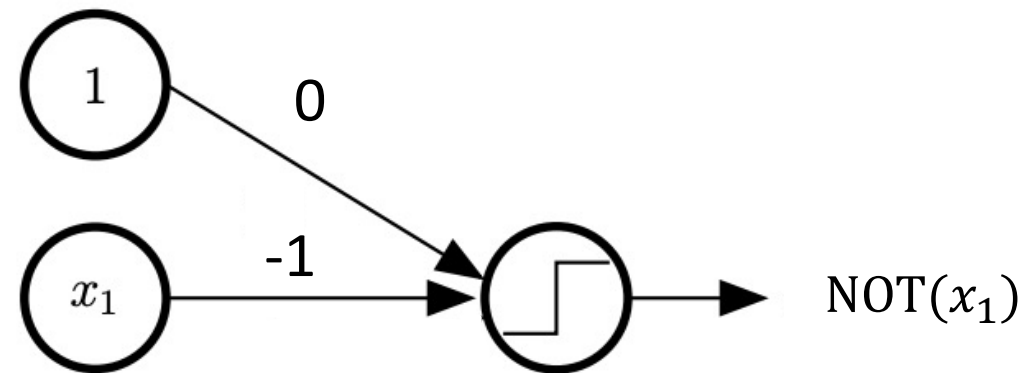
x_1	$\text{NOT}(x)$
$+1$	-1
-1	$+1$



Implement Logic Gates with Perceptron

- $\text{NOT}(x_1)$
 - Use $+1$ to denote “true” and -1 to denote “false”

x_1	$\text{NOT}(x)$
$+1$	-1
-1	$+1$



Practice: How to Implement OR and XOR?

- Use $+1$ to denote “true” and -1 to denote “false”

- $\text{OR}(x_1, x_2)$

x_1	x_2	$\text{OR}(x_1, x_2)$
$+1$	$+1$	$+1$
$+1$	-1	$+1$
-1	$+1$	$+1$
-1	-1	-1

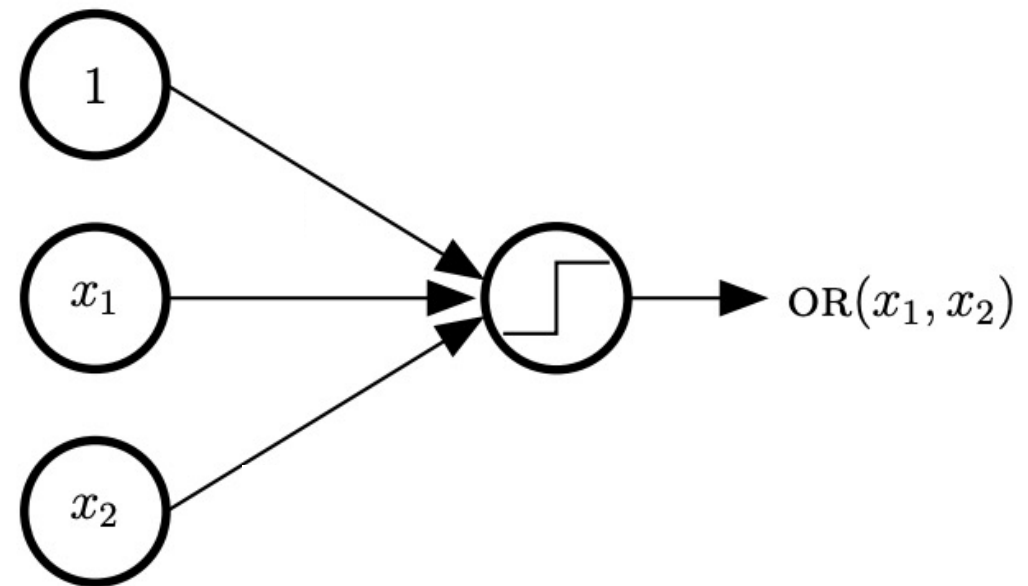
- $\text{XOR}(x_1, x_2)$

x_1	x_2	$\text{XOR}(x_1, x_2)$
$+1$	$+1$	-1
$+1$	-1	$+1$
-1	$+1$	$+1$
-1	-1	-1

Implement Logic Gates with Perceptron

- $\text{OR}(x_1, x_2)$
 - Use +1 to denote “true” and -1 to denote “false”

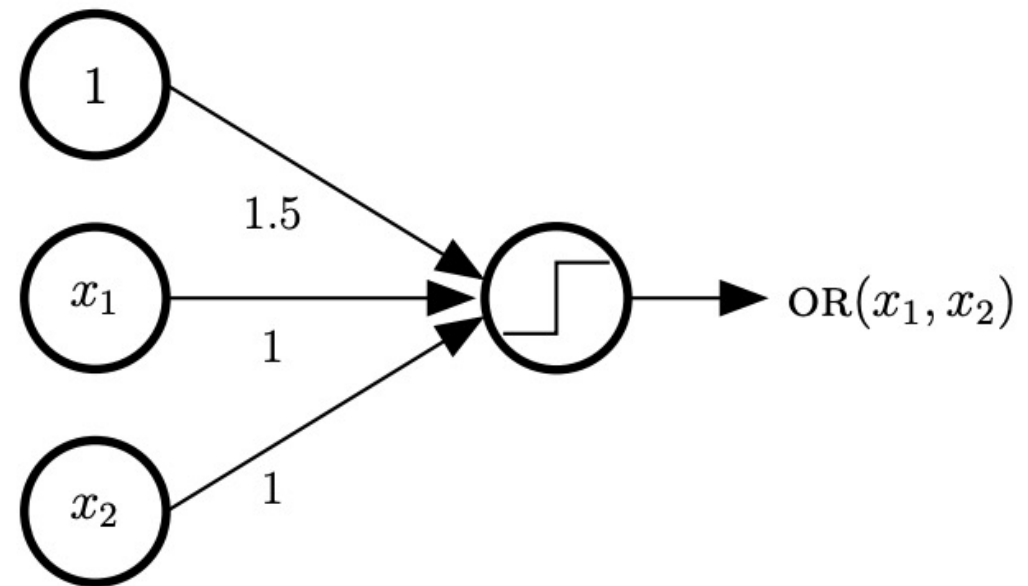
x_1	x_2	$\text{OR}(x_1, x_2)$
+1	+1	+1
+1	-1	+1
-1	+1	+1
-1	-1	-1



Implement Logic Gates with Perceptron

- $\text{OR}(x_1, x_2)$
 - Use +1 to denote “true” and -1 to denote “false”

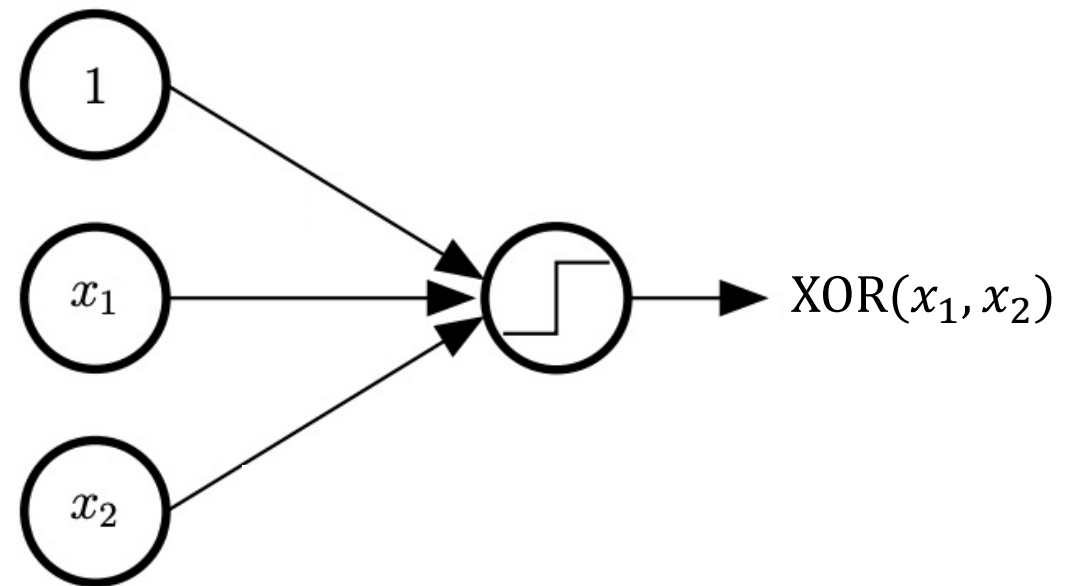
x_1	x_2	$\text{OR}(x_1, x_2)$
+1	+1	+1
+1	-1	+1
-1	+1	+1
-1	-1	-1



Implement Logic Gates with Perceptron

- $\text{XOR}(x_1, x_2)$
 - Use +1 to denote “true” and -1 to denote “false”

x_1	x_2	$\text{XOR}(x_1, x_2)$
+1	+1	-1
+1	-1	+1
-1	+1	+1
-1	-1	-1



Implement Logic Gates with Perceptron

- $\text{XOR}(x_1, x_2)$
 - Use +1 to denote “true” and -1 to denote “false”

x_1	x_2	$\text{XOR}(x_1, x_2)$
+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



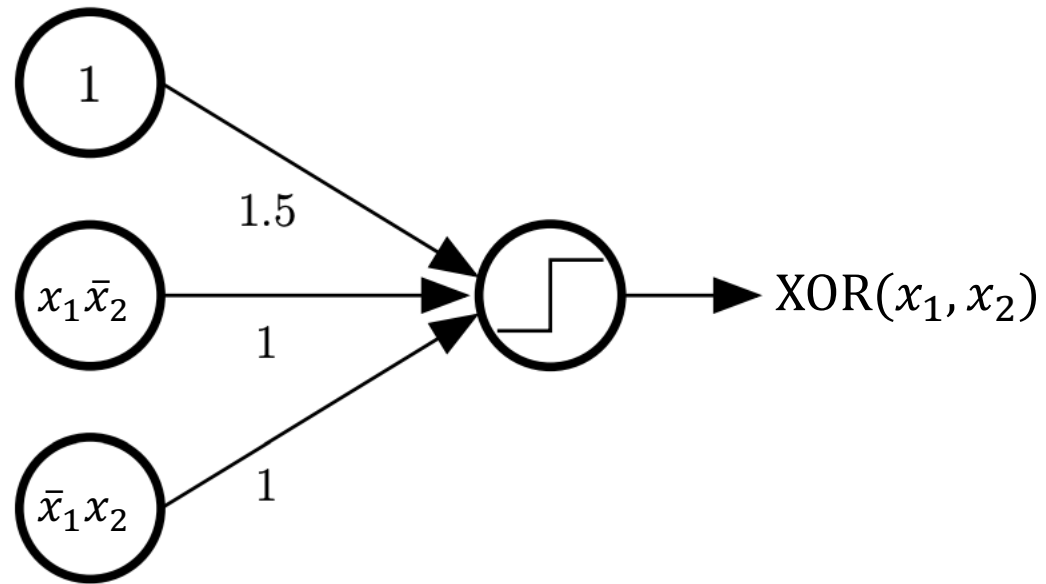
Representing Boolean Operations

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

x_1	x_2	$\text{XOR}(x_1, x_2)$
+1	+1	-1
+1	-1	+1
-1	+1	+1
-1	-1	-1

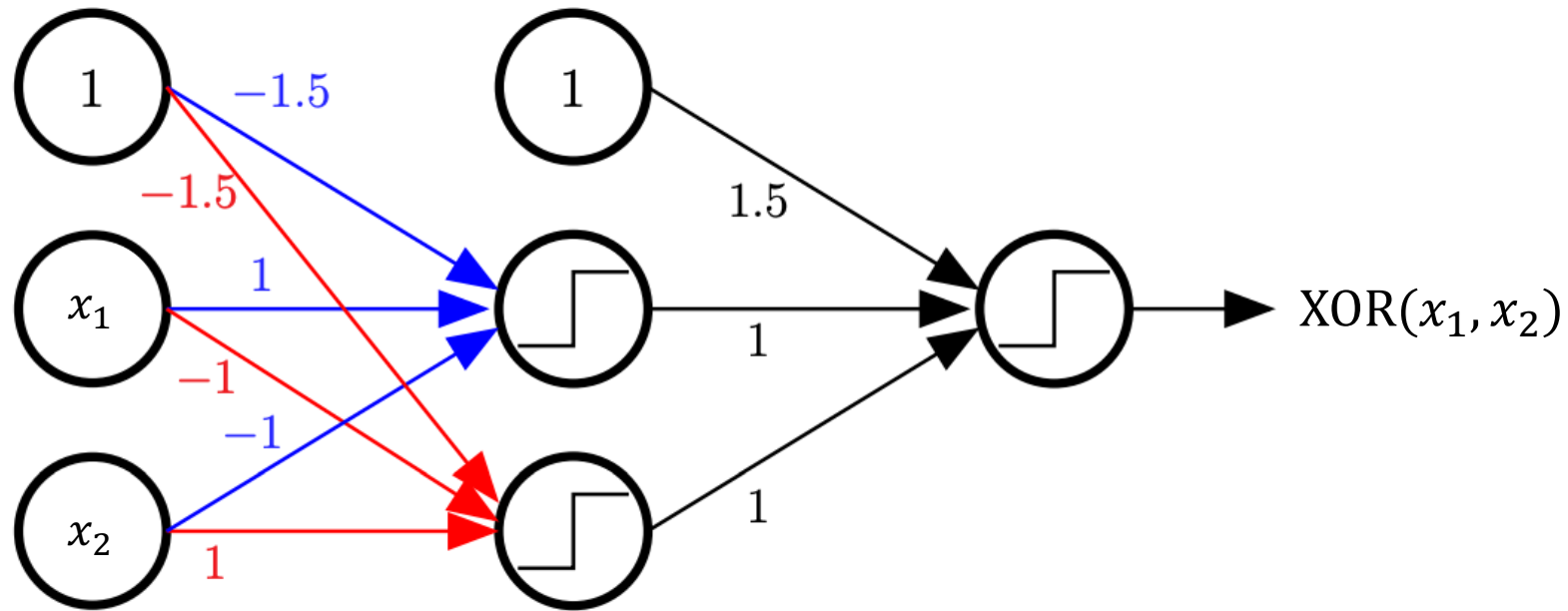
Implementing XOR

- $\text{XOR}(x_1, x_2) \rightarrow x_1\bar{x}_2 + \bar{x}_1x_2$

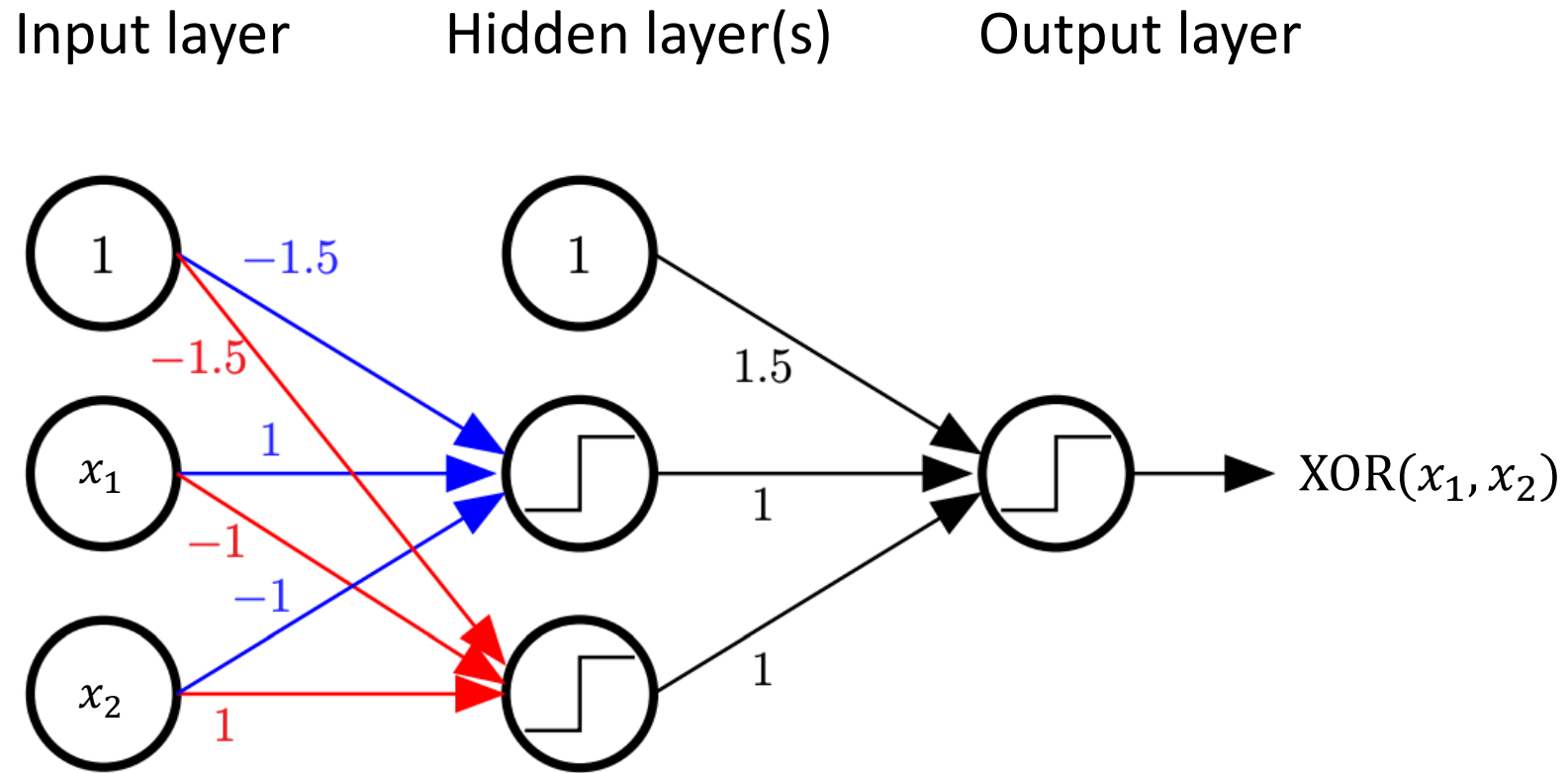


Implementing XOR

- $\text{XOR}(x_1, x_2) \rightarrow x_1\bar{x}_2 + \bar{x}_1x_2$



Multi-Layer Perceptron (MLP)



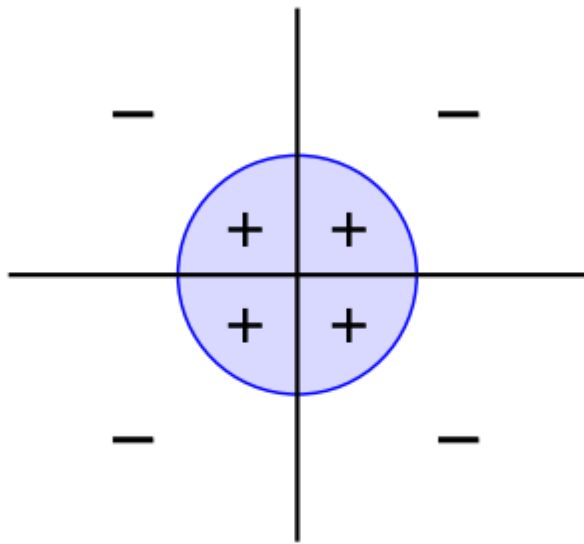
Feed-forward network

The Power of Multi-Layer Perceptron (MLP)

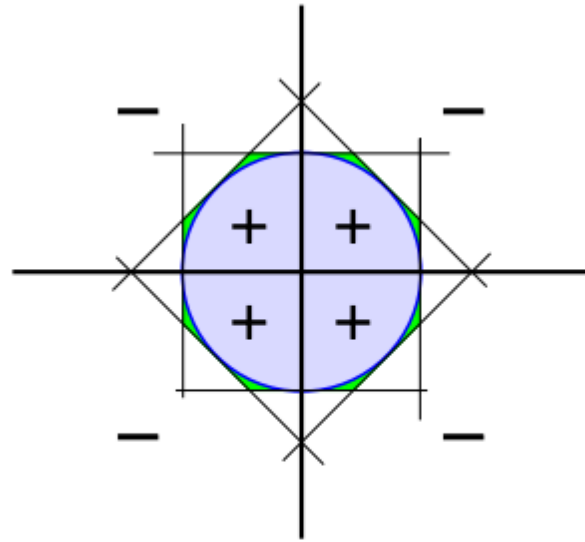
- We now know that we can implement XOR by introducing the hidden layer in MLP. But generally how powerful is MLP?
- Universal approximation theorem
 - a feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of \mathbb{R}^n , under mild assumptions on the activation function.
- Three-layer MLP can approximate ANY continuous target function!

Informal Intuitions of Universal Approximation

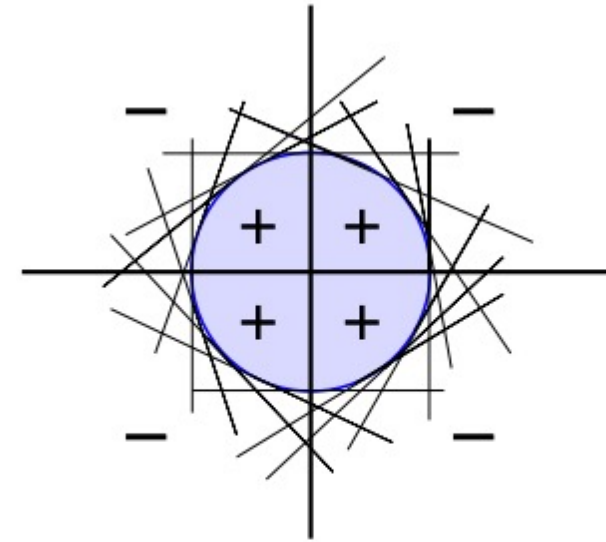
- A continuous separator can be "decomposed" into linear separators



Target



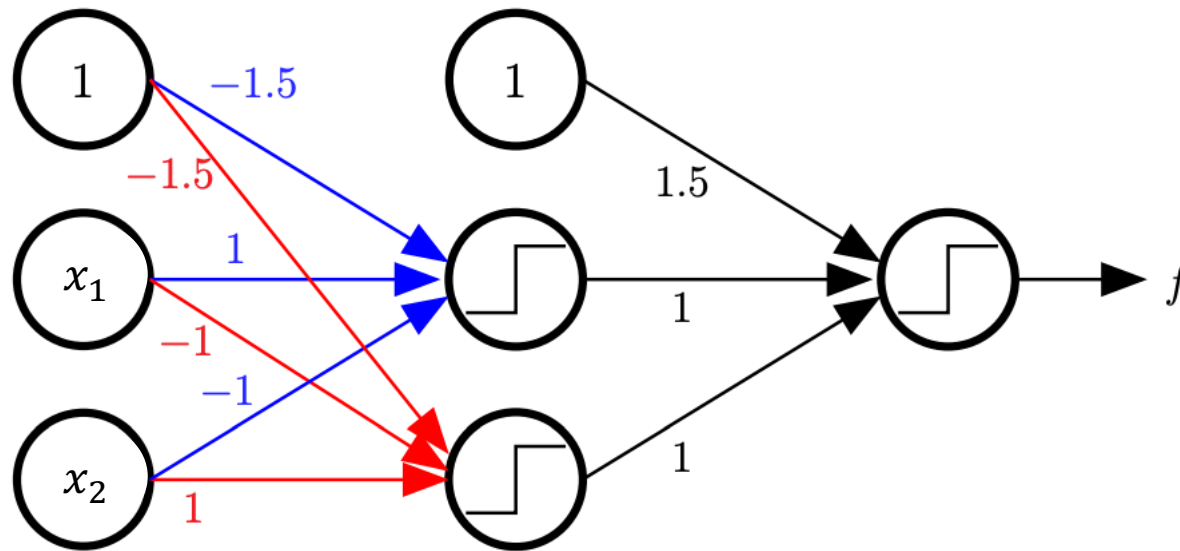
8 perceptrons



16 perceptrons

How to Learn MLP From Data?

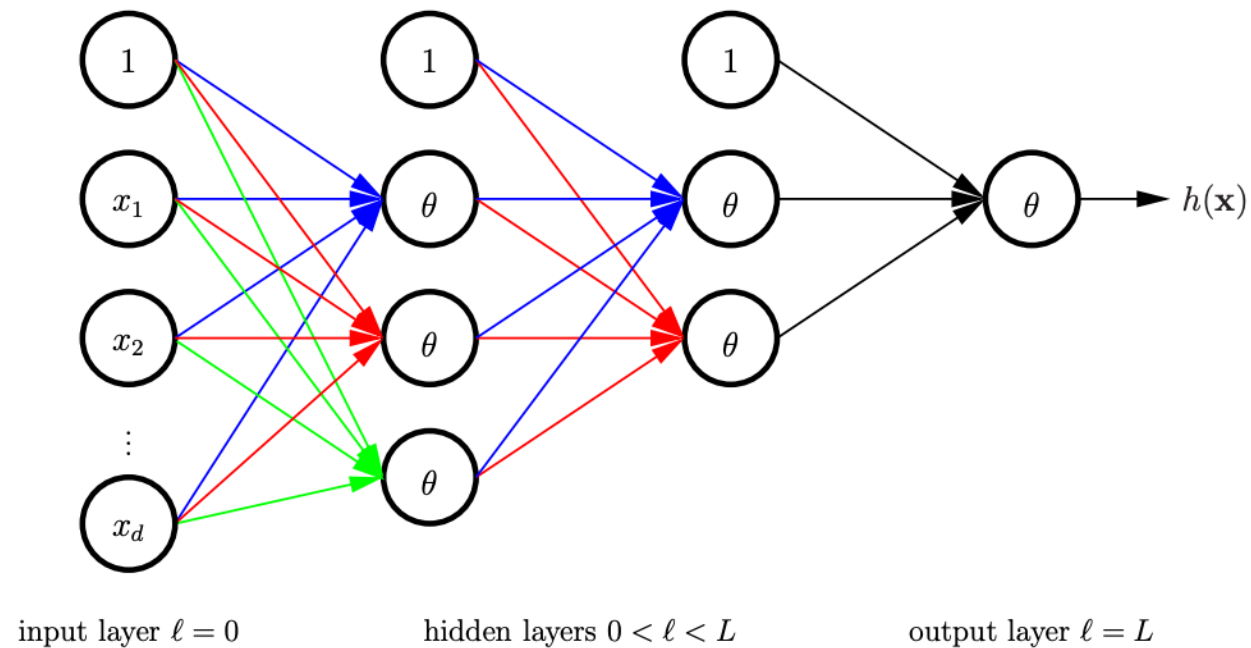
- Given D and the network structure, how to learn the “weights” (i.e., the weight vectors of every Perceptron)?



- Computationally challenging due to the “sign” function 

Neural Networks

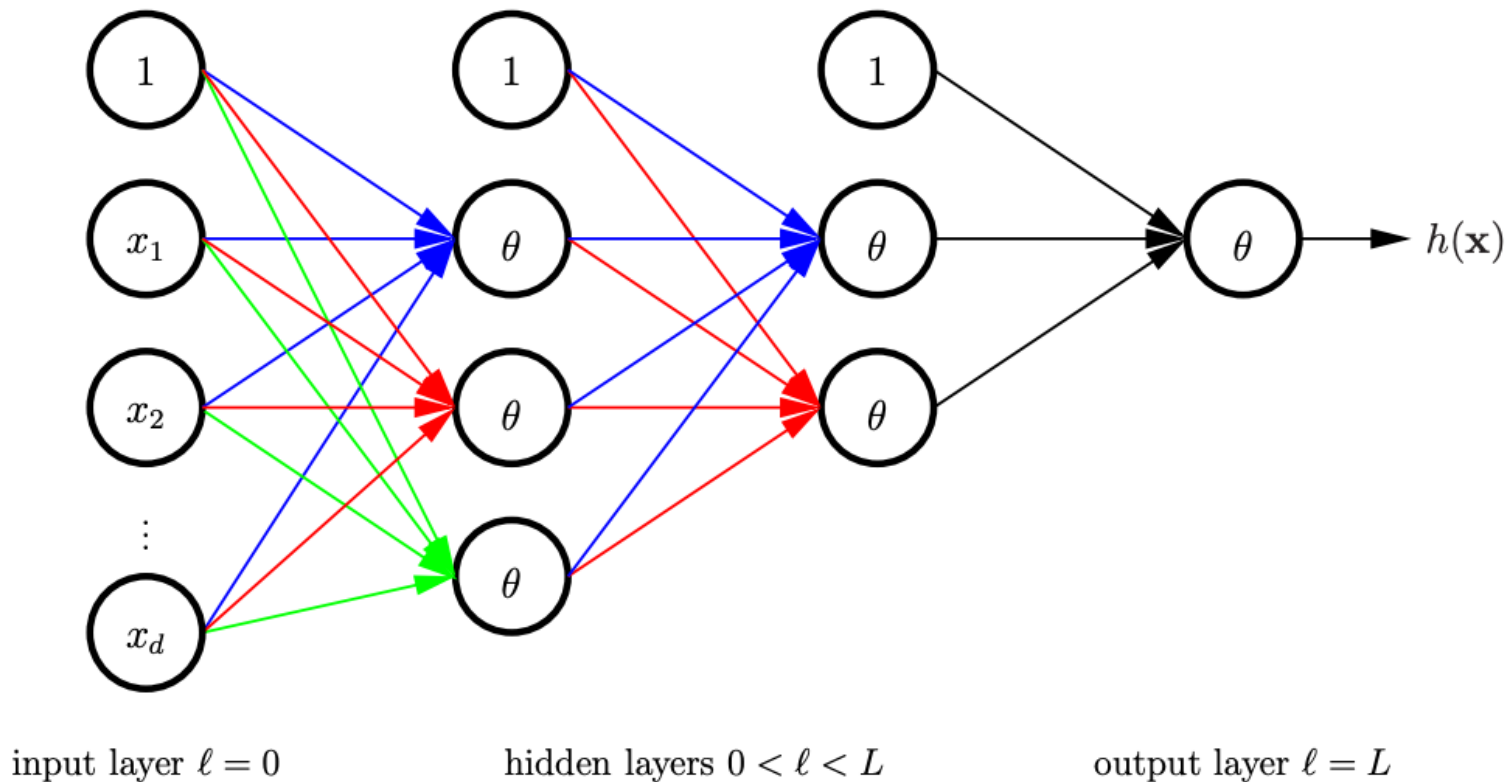
- A softened version of multi-layer Perceptron (MLP)



θ : **activation function**
(Specify the “activation” of the neuron)

Notations of Neural Networks (NN)

Neural Networks

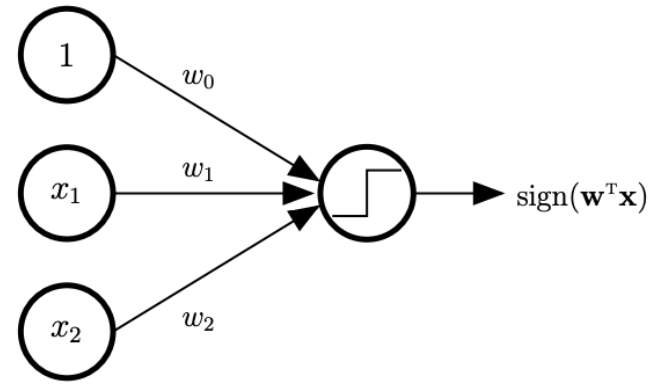


θ : **activation function**
(Specify the “activation” of the neuron)



We mostly focus on **feed-forward** network structure

Activation Function



- Think about a single neuron (**linear model**)
 - Compute the linear signal $s = \vec{w}^T \vec{x}$
 - Transform it to what we need in the output (sign, linear, or sigmoid)

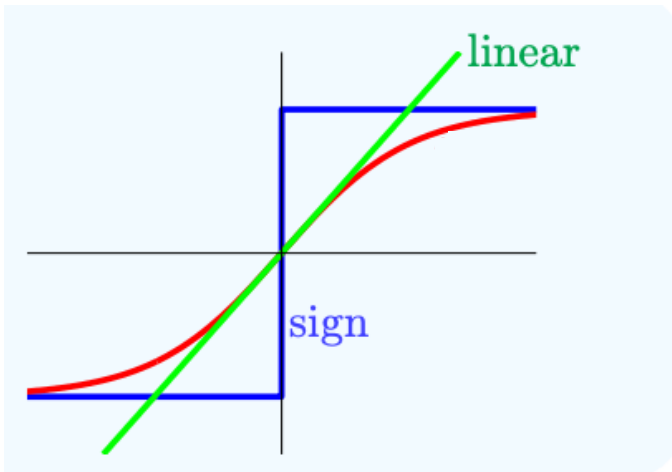
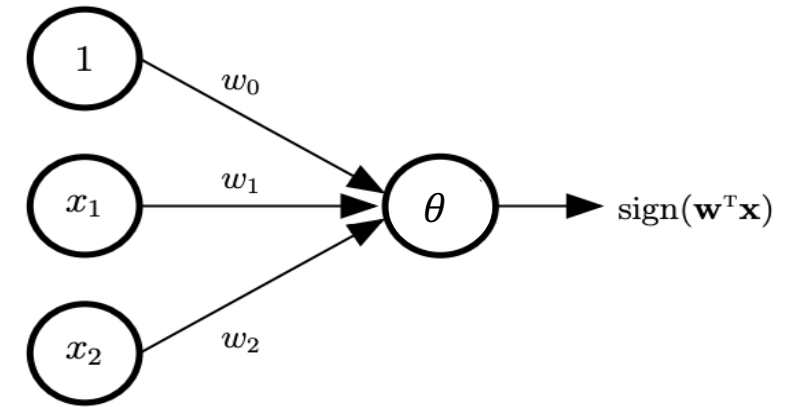
	Domain	Model
Linear Classification	$y \in \{-1, +1\}$	$H = \{h(\vec{x}) = \text{sign}(\vec{w}^T \vec{x})\}$
Linear Regression	$y \in \mathbb{R}$	$H = \{h(\vec{x}) = \vec{w}^T \vec{x}\}$
Logistic Regression	$y \in [0,1]$	$H = \{h(\vec{x}) = \theta(\vec{w}^T \vec{x})\}$

$$\theta(s) = \frac{e^s}{1 + e^s}$$

- In Neural networks, outputs of some nodes are inputs of some others
 - Activation function decides how to do this transformation

Activation Function

- Activation functions in Neural Networks
 - sign function:
 - hard to optimize
 - linear function:
 - the entire neural network is linear
 - One potential option: having a “softened” version of sign function



Activation Function

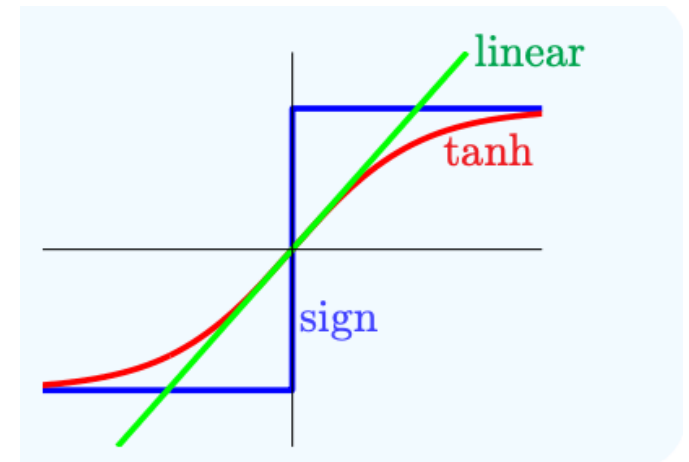
- Activation functions in Neural Networks
 - sign function: hard to optimize
 - linear function: the entire neural network is linear
 - tanh: a softened version of sign

- $\tanh(s) = \frac{e^s - e^{-s}}{e^s + e^{-s}}$

- Examine $\tanh(s)$

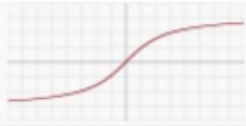




- $\tanh(s) = \begin{cases} 1 & \text{when } s \rightarrow \infty \\ 0 & \text{when } s = 0 \\ -1 & \text{when } s \rightarrow -\infty \end{cases}$

- For $\theta(s) = \tanh(s)$, $\theta'(s) = 1 - \theta(s)^2$



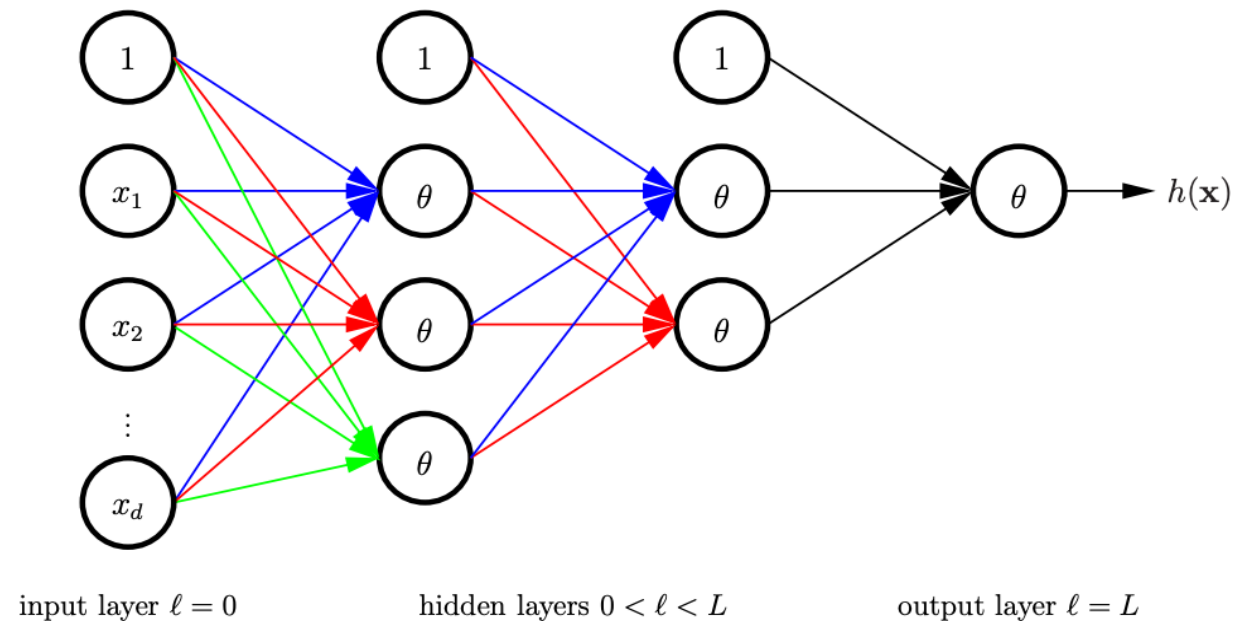
Activation Function

- There are other activation functions with different benefits. However, it doesn't impact our discussions, and we'll focus on `tanh()` as the activation function
- A few more examples

ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2 + 1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$

Notations of Neural Networks (NN)

- Layers $\ell = 0$ to L
 - Layer 0: input layer
 - Layer 1 to $L - 1$: hidden layers
 - Layer L : output layer
- $d^{(\ell)}$: dimension of layer ℓ
 - # nodes (excluding 1s) in the layer
- $\vec{x}^{(\ell)}$: the nodes in layer ℓ
 - $\vec{x}^{(0)}$ is the input feature \vec{x}
 - $x_i^{(\ell)}$ is the i -th node in layer ℓ



Notations of Neural Networks (NN)

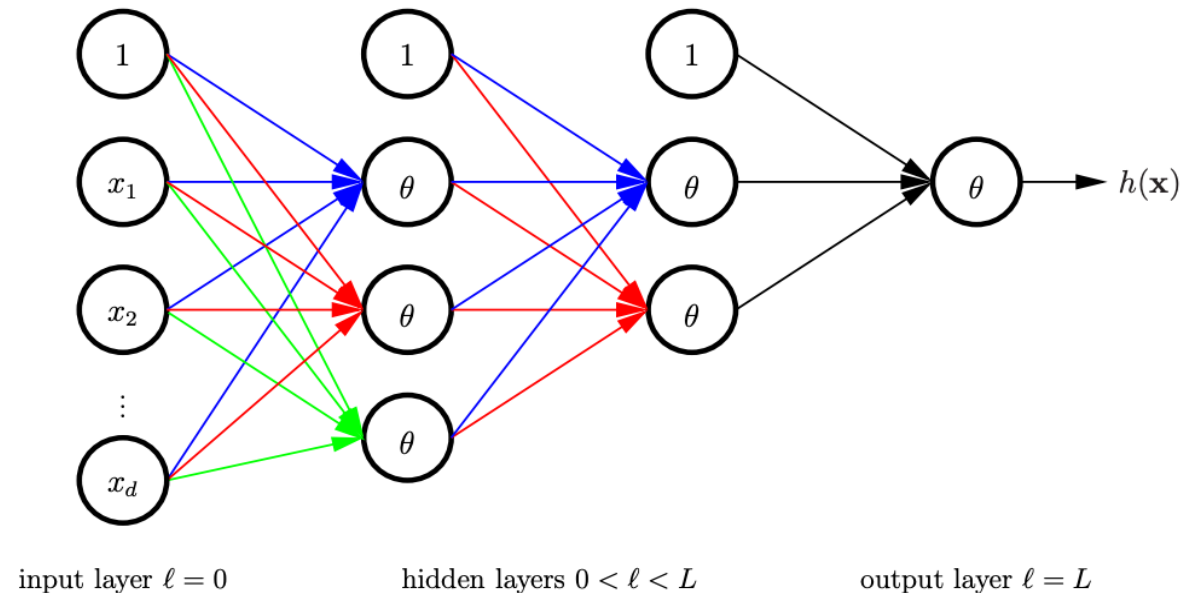
- A hypothesis in linear model is specified by the weights $\{w_i\}$
- Similarly, a hypothesis in NN is characterized by the weights $\{w_{i,j}^{(\ell)}\}$

- $1 \leq \ell \leq L$
- $0 \leq i \leq d^{(\ell-1)}$
- $1 \leq j \leq d^{(\ell)}$

layers

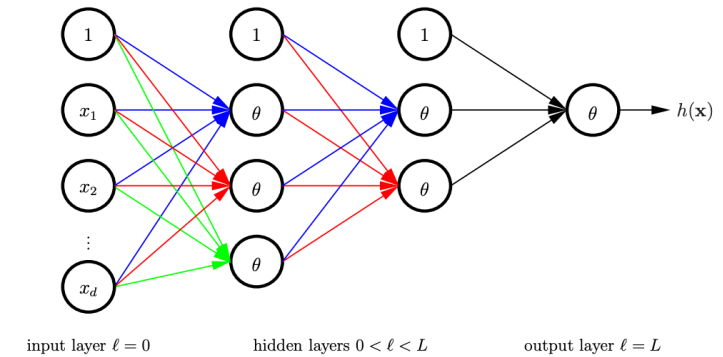
inputs

outputs



Notations of Neural Networks (NN)

- Notations so far:
 - $d^{(\ell)}$: dimension of layer ℓ
 - $\vec{x}^{(\ell)}$: the nodes in layer ℓ
 - $w_{i,j}^{(\ell)}$: weights; characterize hypothesis in NN

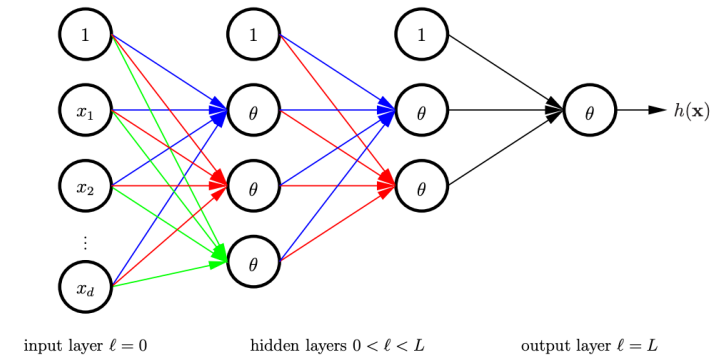


- Lastly, linear signal $s_j^{(\ell)} = \sum_{i=0}^{d^{(\ell-1)}} w_{i,j}^{(\ell)} x_i^{(\ell-1)}$
 - By definition: $x_j^{(\ell)} = \theta(s_j^{(\ell)})$

$$\mathbf{s}^{(\ell)} \xrightarrow{\theta} \mathbf{x}^{(\ell)}$$

Notations of Neural Networks (NN)

- Notations so far:
 - $d^{(\ell)}$: dimension of layer ℓ
 - $\vec{x}^{(\ell)}$: the nodes in layer ℓ
 - $w_{i,j}^{(\ell)}$: weights; characterize hypothesis in NN



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