

ST449 Artificial Intelligence and Deep Learning

Lecture 2

Introduction to neural networks



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<https://github.com/lse-st449/lectures>

Topics of this lecture

- Single-layer networks
 - Linear discriminant functions
 - XOR problem
 - Perceptron
- Multi-layer perceptron
 - XOR problem solved
- Feedforward neural networks
 - Basic concepts: architecture, neurons, layers, size, width, depth
 - The expressive power of neural networks
 - A brief history of feedforward neural networks

Single-layer networks

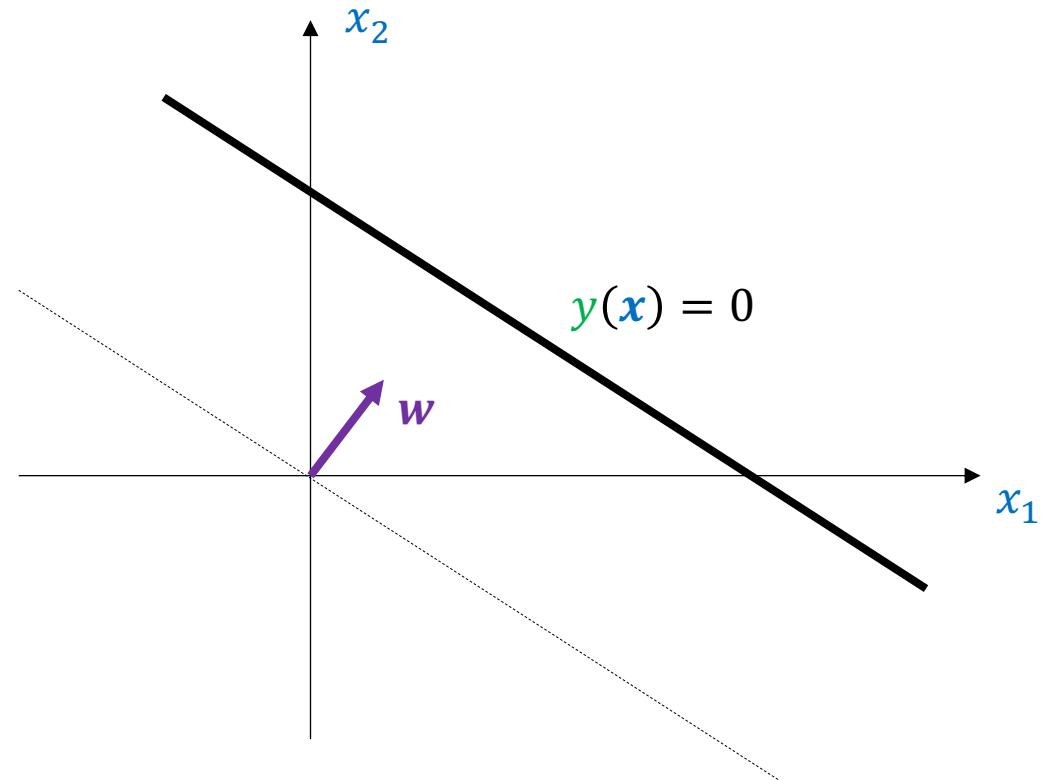
Binary classification problem

- Points $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_m, y_m)$
 - Feature vector: $\mathbf{x}_i \in \mathbf{R}^n$
 - Label: $y_i \in \{0,1\}$

- Linear discriminant function:

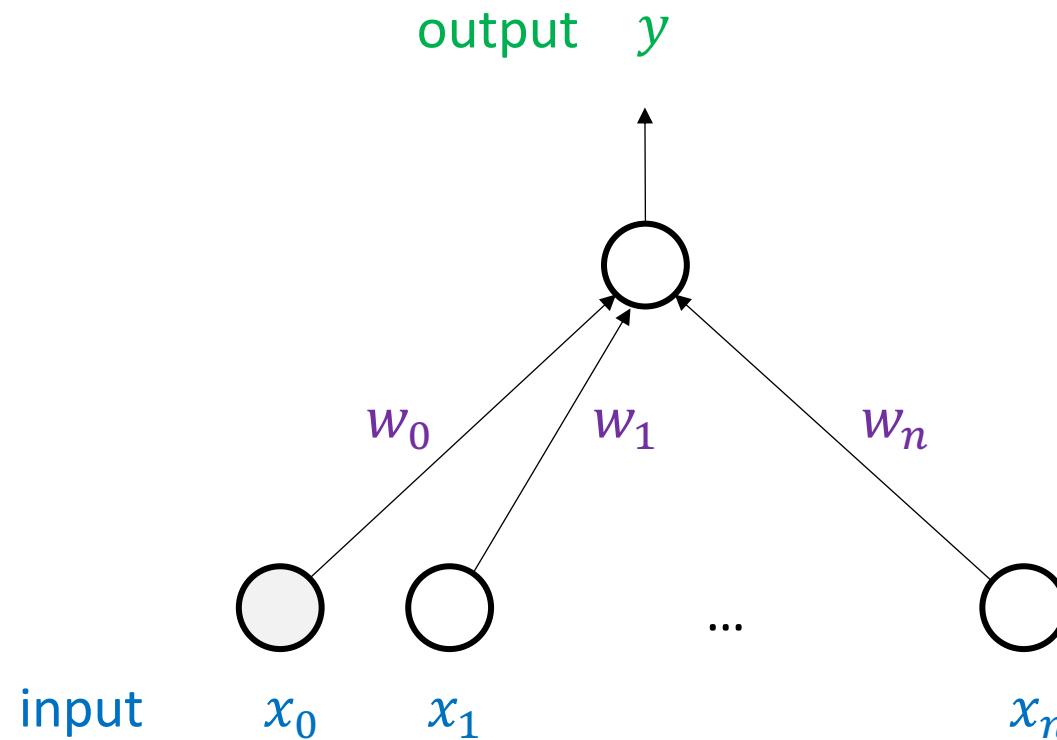
$$y(\mathbf{x}) = \mathbf{x}^\top \mathbf{w} + w_0$$

weight vector bias term



- Linear decision boundary
 - Decision boundary $y(\mathbf{x}) = 0$ is a $(n - 1)$ -dimensional hyperplane

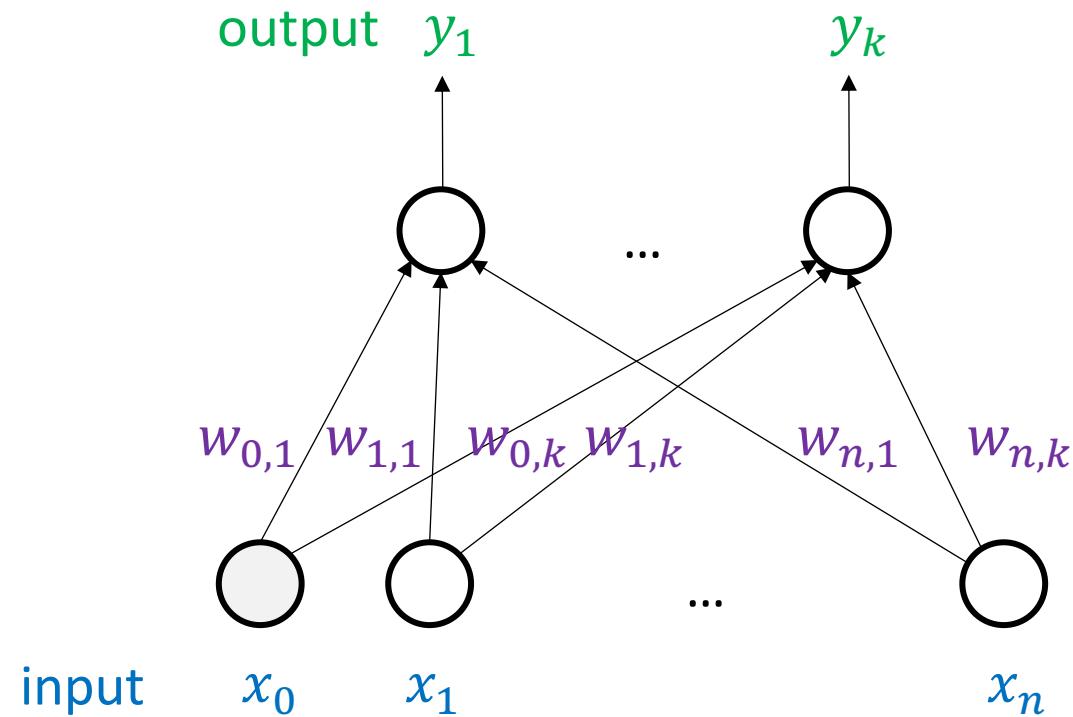
Representation by a neural network diagram



Multiple classes

- If there are $k \geq 2$ classes, for each class we may use a linear discriminant function:

$$y_i(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}_i + w_{0,i} \text{ for } i = 1, 2, \dots, k$$



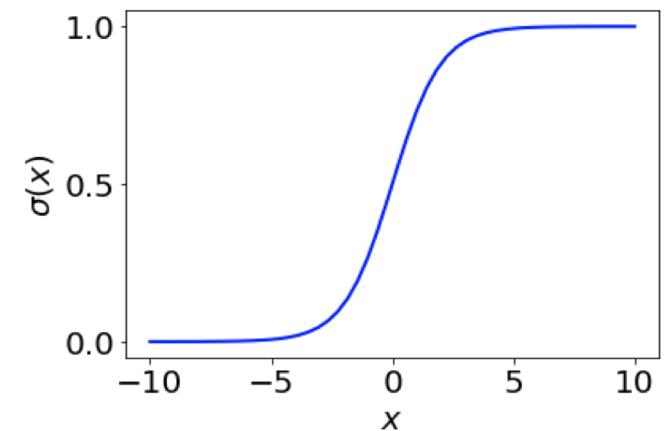
Non-linear discriminant functions

- A way to have a non-linear discriminant function:

$$y(\mathbf{x}) = a(\mathbf{x}^\top \mathbf{w} + w_0)$$

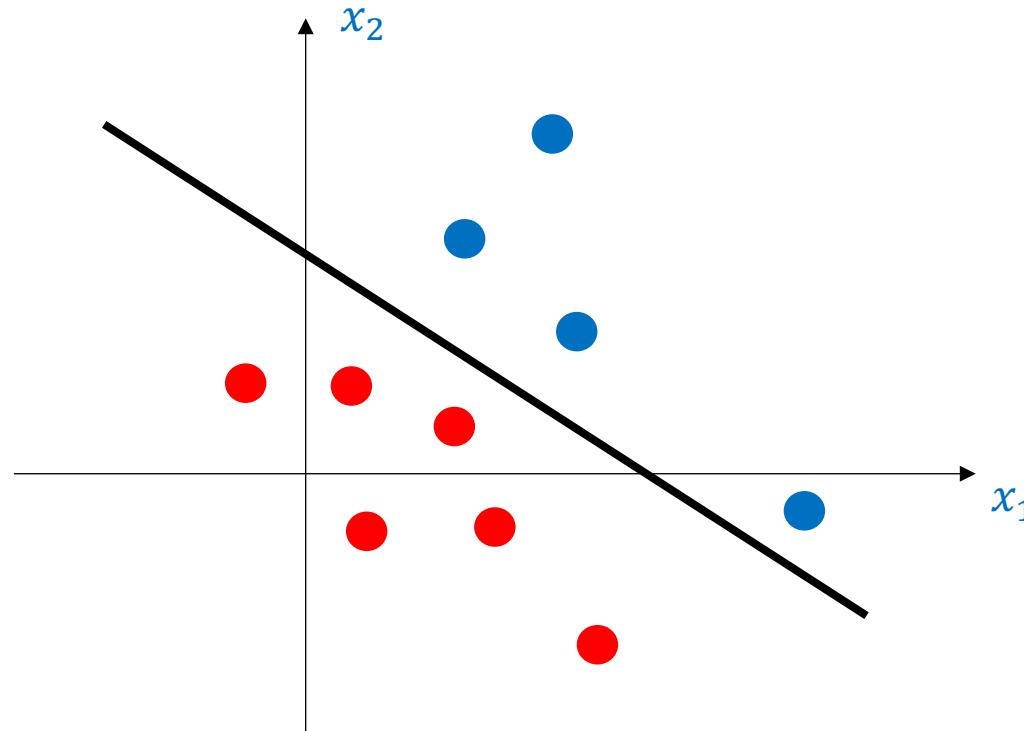
↑
activation function

- $a : \mathbf{R} \rightarrow \mathbf{R}$ is a monotonic function
- Logistic regression example
 - $a(x)$ is the sigmoid function: $\sigma(x) = 1/(1 + e^{-x})$



Linear separability

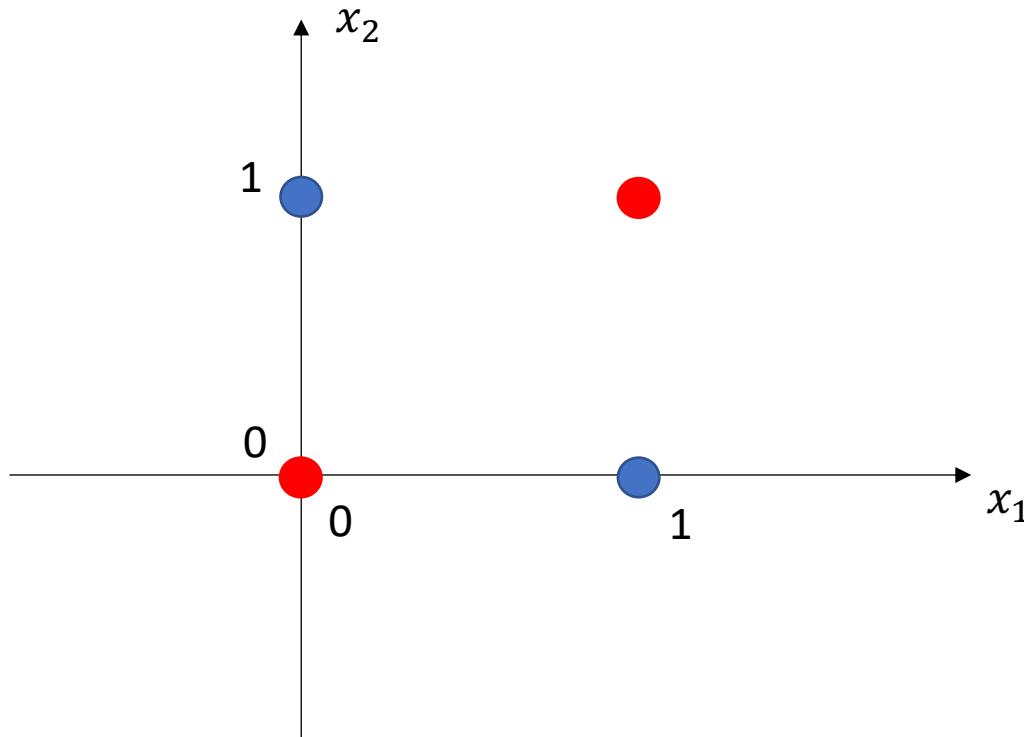
- A set of points is set to be **linearly separable** if the points belonging to different classes can be separated by a linear decision boundary



- Not all sets of points are linearly separable (e.g. XOR function in the next slide)

XOR: the exclusive-OR

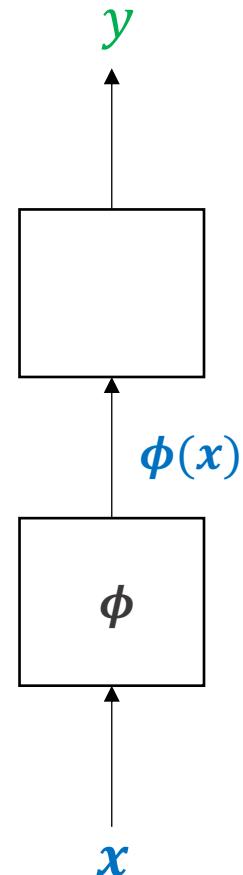
x_1	x_2	$y(x_1, x_2)$
0	0	0
0	1	1
1	0	1
1	1	0



- Not linearly separable

Input feature transformation

- Instead of using original feature vectors use transformed feature vectors
 - Representation for a function learning $x \mapsto y$



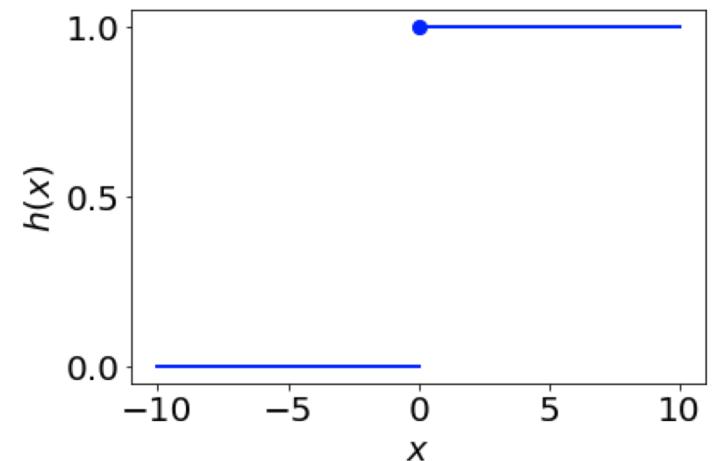
E.g. ϕ obtained by a feature engineering

The perceptron

- Perceptron: a single-layer network with a threshold activation function

$$y(\mathbf{x}) = h(\sum_{i=0}^n \phi_i(\mathbf{x}) w_i)$$

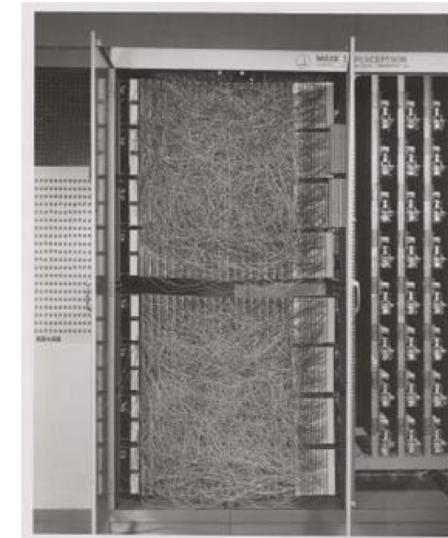
- Threshold function: $h(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$
 - Also known as a **unit step function** or the **Heaviside step function**
 - An alternative half-maximum convention: redefine $h(0) = 1/2$
 - In vector notation: $y(\mathbf{x}) = h(\boldsymbol{\phi}(\mathbf{x})^\top \mathbf{w})$



Note: by convention, $\phi_0(\mathbf{x}) = 1$

History of perceptron

- The perceptron algorithm was invented by Frank RosenBlatt (psychologist) in 1957 at the Cornell Aeronautical Laboratory
- Intended to be a machine rather than a program
- First implementation in software on an IBM system
- Subsequent implementation in a custom-built hardware: Mark 1 perceptron
 - Patchboard for experimenting with different combinations of features
 - Potentiometers for adjusting weights



Source: [Perceptron](#), Wikipedia

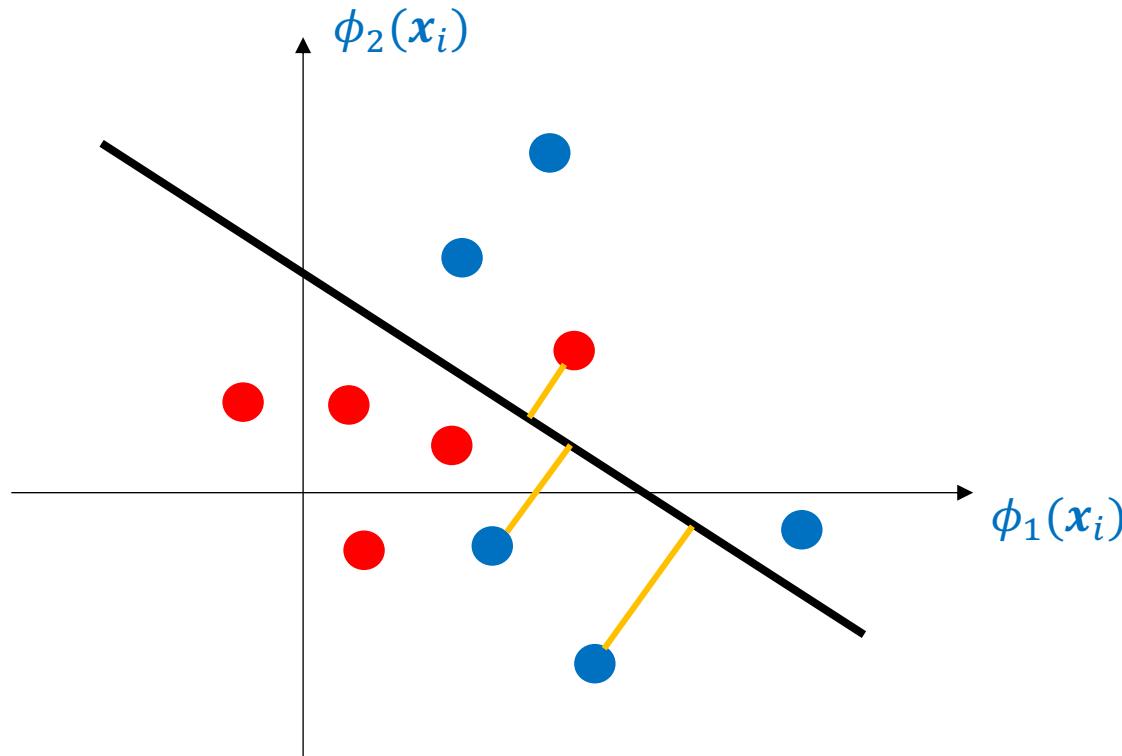
Perceptron criterion

- Convention: $y_i \in \{-1,1\}$ and $h(x) = -1$ if $x < 0$, $h(x) = 1$ otherwise
- Correct classification: $y_i \phi(x_i)^\top w > 0$
- False classification: $y_i \underbrace{\phi(x_i)^\top w}_{\text{same sign as for the predicted label}} < 0$
- Goal: find parameter $w \in \mathbb{R}^n$ such that for all input points $y_i \phi(x_i)^\top w > 0$
- **Perceptron criterion:** loss function

$$L(w) = \sum_{i=1}^m \max(-y_i \phi(x_i)^\top w, 0)$$

A continuous piecewise-linear loss function (positive costs for misclassified examples)

Perceptron criterion (cont'd)



- Perceptron criterion loss function is equal to the sum of absolute distances of misclassified examples to the decision boundary

Perceptron learning algorithm

Initialization: $t = 0$, η step size to a positive value, $\mathbf{w}^{(0)}$ arbitrarily (say null vector)

Repeat until there are any misclassified examples: // i.e. $\exists (\mathbf{x}_i, y_i)$: $y_i \boldsymbol{\phi}(\mathbf{x}_i)^\top \mathbf{w}^{(t)} < 0$

$$\hat{y}_{(i)} = h(\boldsymbol{\phi}(\mathbf{x}_{i(t)})^\top \mathbf{w}^{(t)}) \quad // (\mathbf{x}_{i(t)}, y_{i(t)}) \text{ is the input example at } t$$

If $\hat{y}_{i(t)} \neq y_{i(t)}$ **then**

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \eta y_{i(t)} \boldsymbol{\phi}(\mathbf{x}_{i(t)})$$

else

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)}$$

end for

$$t \leftarrow t + 1$$

Perceptron convergence property

- Let $L_i(\mathbf{w}) = \max(-\mathbf{y}_i \boldsymbol{\phi}(\mathbf{x}_i)^\top \mathbf{w}, 0)$ be the contribution to the loss function by an input example $(\mathbf{x}_i, \mathbf{y}_i)$ for given parameter vector \mathbf{w}
- Convergence property: for every t such that $\hat{\mathbf{y}}_{i(t)} \neq \mathbf{y}_{i(t)}$:

$$L_{i(t)}(\mathbf{w}^{(t+1)}) < L_{i(t)}(\mathbf{w}^{(t)})$$

- Exercise: prove this inequality

Solution to the question

- Recall that $L(\mathbf{w}) = \sum_{i=1}^m L_i(\mathbf{w})$ where $L_i(\mathbf{w}) = \max(-\mathbf{y}_i \boldsymbol{\phi}(\mathbf{x}_i)^\top \mathbf{w}, 0)$
- For every iteration t such that $\hat{y}_{i(t)} \neq y_{i(t)}$ we have

$$\begin{aligned}L_{i(t)}(\mathbf{w}^{(t+1)}) &= \max\left(-\mathbf{y}_{i(t)} \boldsymbol{\phi}(\mathbf{x}_{i(t)})^\top \mathbf{w}^{(t+1)}, 0\right) \\&= \max\left(-\mathbf{y}_{i(t)} \boldsymbol{\phi}(\mathbf{x}_{i(t)})^\top \mathbf{w}^{(t)} - \eta \|\boldsymbol{\phi}(\mathbf{x}_{i(t)})\|^2, 0\right) \\&< \max\left(-\mathbf{y}_{i(t)} \boldsymbol{\phi}(\mathbf{x}_{i(t)})^\top \mathbf{w}^{(t)}, 0\right) \\&= L_{i(t)}(\mathbf{w}^{(t)})\end{aligned}$$

Perceptron convergence theorem

- **Thm** Assume that the algorithm receives a sequence of input examples that are misclassified according to the current parameter vector estimate.
For any linearly separable set of input examples, the algorithm finds a solution in a finite number of steps.
- Proof is by contradiction (see next slide)

Note: the condition of the theorem can be relaxed by allowing for a bounded number of iterations between any two consecutive misclassified examples input to the algorithm

Proof of the convergence theorem

- Assume that examples are linearly separable:

$$\exists \mathbf{w}^* : y_i \boldsymbol{\phi}(\mathbf{x}_i)^\top \mathbf{w}^* > 0 \text{ for all } i = 1, 2, \dots, m$$

- Note the identity:

$$\mathbf{w}^{(t)} = \eta \sum_{i=1}^m M_i^{(t)} y_i \boldsymbol{\phi}(\mathbf{x}_i)$$

where $M_i^{(t)}$ is the number of iterations s such that $(\mathbf{x}_{i(s)}, y_{i(s)}) = (\mathbf{x}_i, y_i)$, $\hat{y}_{i(s)} \neq y_{i(s)}$ and $s \leq t$

- Define $M^{(t)}$ to be the number of iterations s such that $\hat{y}_{i(s)} \neq y_{i(s)}$ and $s \leq t$
 - Indeed, $M^{(t)} = \sum_{i=1}^m M_i^{(t)}$

Proof of the convergence theorem (cont'd)

- Fact 1: $(\mathbf{w}^*)^\top \mathbf{w}^{(t)} = \eta \sum_{i=1}^m M_i^{(t)} y_i \phi(x_i)^\top \mathbf{w}^* \geq M^{(t)} \eta \min_i y_i \phi(x_i)^\top \mathbf{w}^*$
- Fact 2: $\|\mathbf{w}^{(t)}\| \leq \sqrt{M^{(t)}} \eta \max_i \|\phi(x_i)\|$
- Fact 3: $(\mathbf{w}^*)^\top \mathbf{w}^{(t)} \leq \|\mathbf{w}^*\| \|\mathbf{w}^{(t)}\|$ (Cauchy-Schwartz)
- Fact 4: $M^{(t)} = t$ (assumption of the theorem)
- From Facts 1 to 4,

$$C_1 t \leq C_2 \sqrt{t} \quad (*)$$

where $C_1 = \min_i y_i \phi(x_i)^\top \mathbf{w}^*$ and $C_2 = \|\mathbf{w}^*\| \max_i \|\phi(x_i)\|$ are positive constants

- To contradict, assume that the algorithm does not converge in a finite number of iterations: this means that $(*)$ holds for all $t \geq 0$ which is a contradiction

Note: to check Fact 2 use: $\|\mathbf{w}^{(t+1)}\|^2 = \|\mathbf{w}^{(t)}\|^2 + 2\eta y_{i(t)} \phi(x_{i(t)})^\top \mathbf{w}^{(t)} + \eta^2 \|\phi(x_{i(t)})\|^2$
and $y_{i(t)} \phi(x_{i(t)})^\top \mathbf{w}^{(t)} < 0$

Bound on mistakes theorem

- **Thm.** Assume that training examples are consistent with a separating hyperplane defined by \mathbf{w}^* , i.e. $y_i \phi(\mathbf{x}_i)^\top \mathbf{w}^* > 0$ for all $i = 1, 2, \dots, m$, and assume that $\|\phi(\mathbf{x}_i)\| \leq r$ for all $i = 1, 2, \dots, m$

Then, for the perceptron learning algorithm, we have

$$M^{(t)} \leq \frac{r^2}{\gamma^2}$$

$$\text{where } \gamma = \min \left\{ \frac{|\phi(\mathbf{x}_i)^\top \mathbf{w}^*|}{\|\mathbf{w}^*\|} : i = 1, 2, \dots, m \right\}$$

- Note: if the algorithm receives input examples such that each is misclassified according to the current parameter vector, then $M^{(t)} = t$ and thus in this case the algorithm provides a bound on the number of iterations until convergence

Proof of the theorem

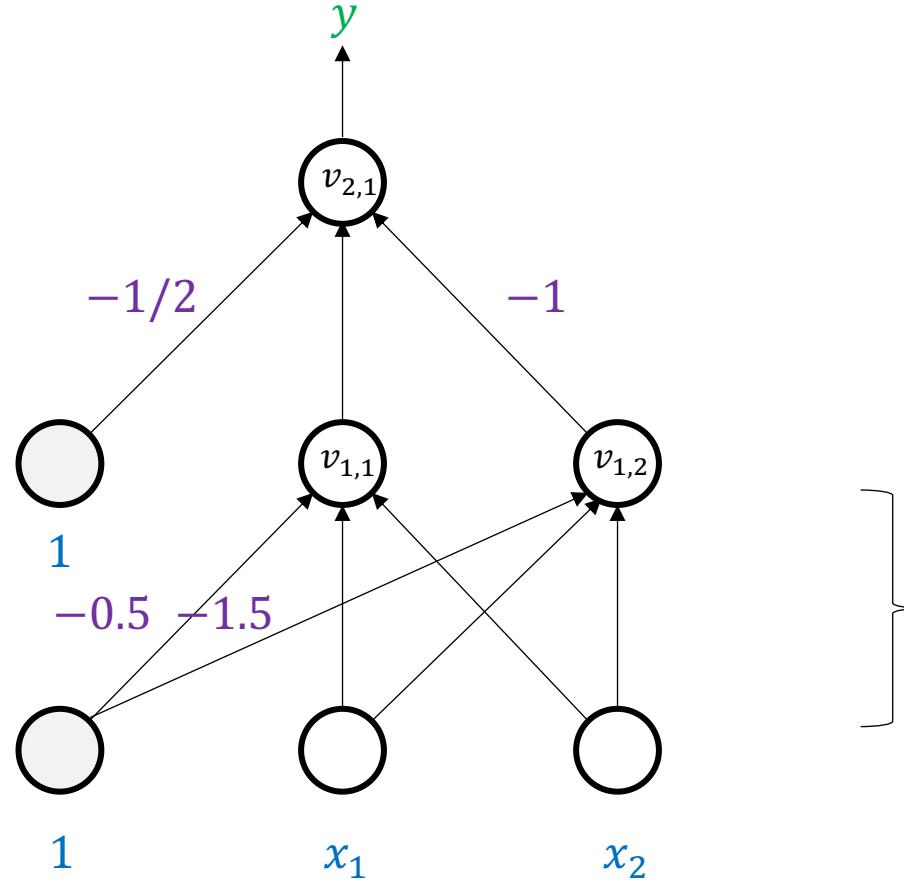
- Similar arguments as for the theorem on slide 18
- Without loss of generality assume that $\|\mathbf{w}^*\| = 1$
- From Fact 1 [slide 20]: $(\mathbf{w}^*)^T \mathbf{w}^{(t)} \geq \gamma \eta M^{(t)}$
- From Fact 2 [slide 20]: $\|\mathbf{w}^{(t)}\| \leq \eta r \sqrt{M^{(t)}}$
- From Fact 3 [slide 20] and $\|\mathbf{w}^*\| = 1$: $(\mathbf{w}^*)^T \mathbf{w}^{(t)} \leq \|\mathbf{w}^{(t)}\|$
- The claim of the theorem follows from the last three inequalities

Multi-layer perceptron

Multi-layer perceptron

- Single-layer perceptron can only discriminate linearly separable data points
- Extension to non linearly separable data points by adding additional layers
- We next show that a multi-layer perceptron can solve the XOR problem
 - By adding one layer to a single-layer perceptron

The XOR problem solved



extra layer

may think of it as
an implementation of
the transformation ϕ

- Edge weights are equal to 1 unless otherwise indicated
- Activation function a is the threshold function mapping to $\{0,1\}$, applied by all non-input nodes
- **Exercise:** check that this two-layer network solves the XOR problem

Exercise solution

- Output of node $v_{1,1}$:

$$a(x_1 + x_2 - 0.5)$$

- Output of node $v_{1,2}$:

$$a(x_1 + x_2 - 1.5)$$

- Output of the network:

$$y(x_1, x_2) = a(1 \times a(x_1 + x_2 - 0.5) - 1 \times a(x_1 + x_2 - 1.5) - 0.5)$$

- Easy to check for each of four possible inputs that y is the XOR function

Feedforward neural networks

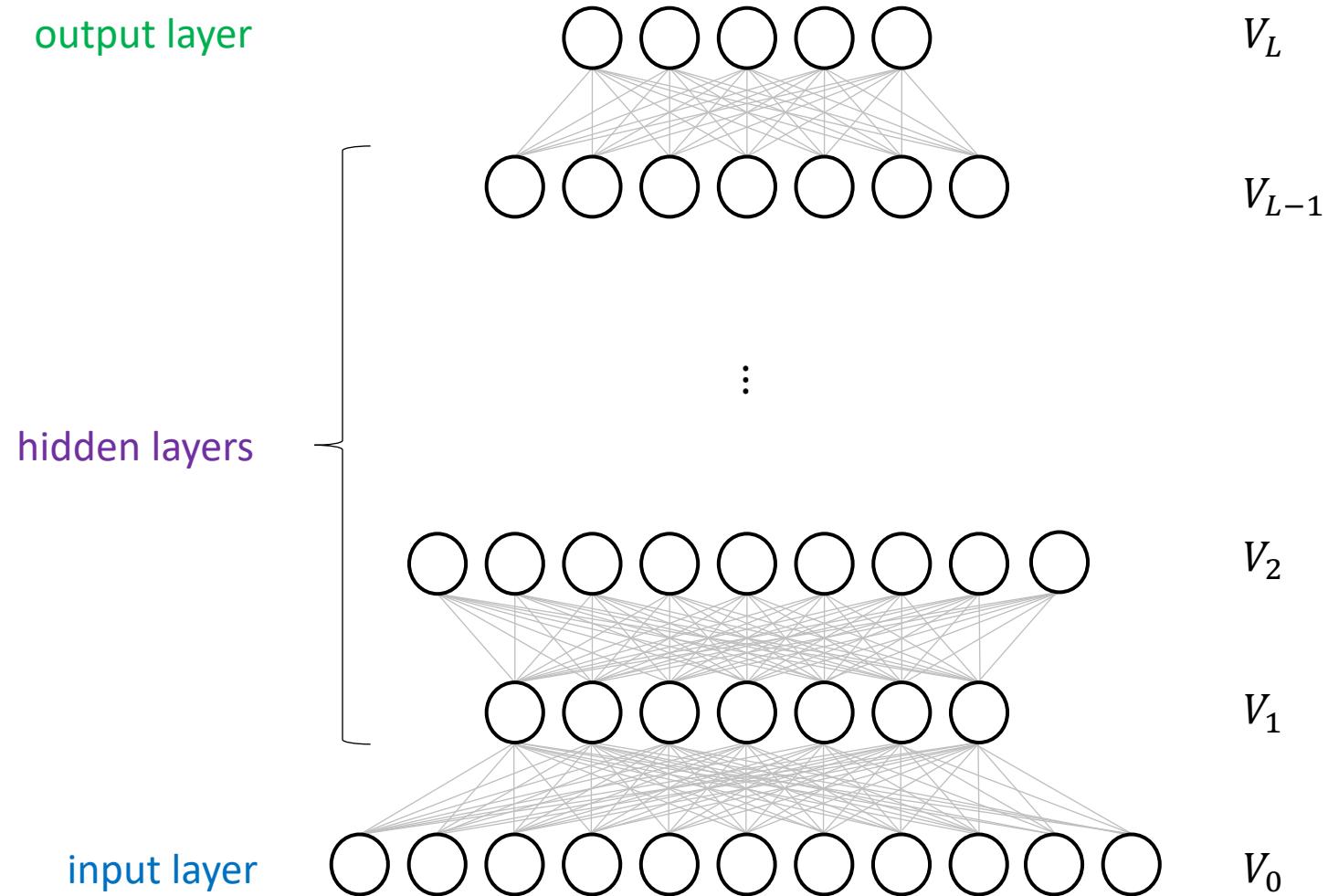
Feedforward networks: basic concepts

- A feedforward network is a network of nodes that can be partitioned in ordered layers such that there may be an edge between two nodes only if they belong to successive layers
- **Feedforward network**: defined by a direct acyclic graph $G = (V, E)$ and a weight function $w: E \rightarrow \mathbf{R}$
- **Neuron**: represented by a node
- **Activation function**: each neuron has an activation function $a: \mathbf{R} \rightarrow \mathbf{R}$
- **Network architecture**: defined by the triplet (V, E, a)

Feedforward networks: basic concepts (cont'd)

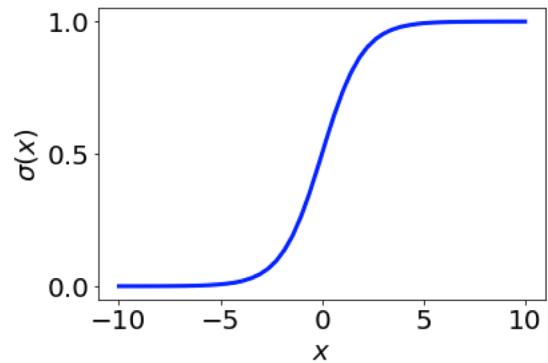
- Network layers defined by a partition of the nodes: V_0, V_1, \dots, V_L
 - **Input layer:** V_0
 - **Hidden layers:** V_1, V_2, \dots, V_{L-1}
 - **Output layer:** V_L
- Key network properties:
 - **Depth:** L
 - **Size:** $|V|$
 - **Width:** $\max\{|V_0|, |V_1|, \dots, |V_L|\}$
- Comments:
 - Width of the input layer for an n dimensional input space: $|V_0| = n + 1$
 - Each edge $e \in E$ connects some nodes in V_{l-1} and V_l for some layer l

Feedforward networks: basic concepts (cont'd)

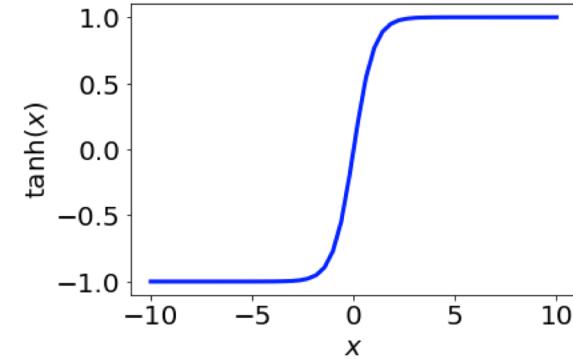


Common activation functions

sigmoid

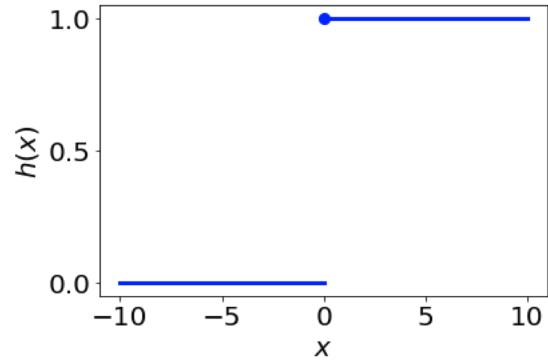


tanh

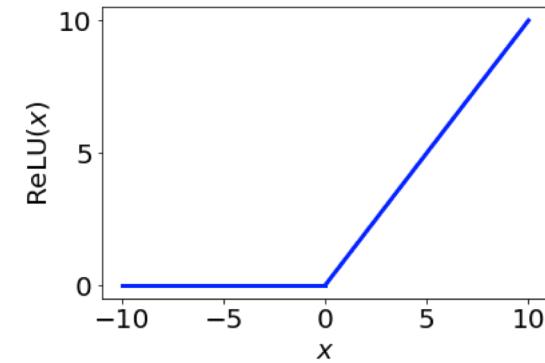


threshold

[unit step,
Heaviside]



rectified linear unit
(ReLU)



Note: $\tanh(x) = 2\sigma(2x) - 1$

Function composition representation

- Function $h(\mathbf{x})$ can be expressed as follows:

$$\mathbf{y}^{(1)} = a_1(\mathbf{W}^{(0)}\mathbf{x} + \mathbf{b}^{(0)})$$

$$\mathbf{y}^{(2)} = a_2(\mathbf{W}^{(1)}\mathbf{y}^{(1)} + \mathbf{b}^{(1)})$$

⋮

$$\mathbf{y}^{(L-1)} = a_{L-1}(\mathbf{W}^{(L-2)}\mathbf{y}^{(L-2)} + \mathbf{b}^{(L-2)})$$

$$\mathbf{y} = \mathbf{W}^{(L-1)}\mathbf{y}^{(L-1)} + \mathbf{b}^{(L-1)}$$

- Using the notation $h_l(\mathbf{x}) = a_l(\mathbf{W}^{(l-1)}\mathbf{x} + \mathbf{b}^{(l-1)})$, we have

$$h(\mathbf{x}) = h_1 \circ h_2 \circ \cdots \circ h_L(\mathbf{x})$$

Expressiveness of neural networks

- Function $h_{V,E,a,w}: \mathbf{R}^{|V_0|-1} \rightarrow \mathbf{R}^{|V_L|}$

- Hypothesis class of functions:

$$H_{V,E,a} = \{h_{V,E,a,w}: w \text{ is a mapping from } E \text{ to } \mathbf{R}\}$$

- The expressive power of neural networks:

- What classes of functions can be implemented by using a neural network?
 - For a given network architecture (V, E, a) what functions can be implemented as a function of the network size?

Boolean functions

- Special class of functions: Boolean functions $g: \{\pm 1\}^p \rightarrow \{\pm 1\}^q$
- The expressiveness power question:
 - What type of Boolean functions can be implemented by $H_{V,E,sign}$?
- For every computer that stores real numbers using b bits, calculating function $f: \mathbf{R}^n \rightarrow \mathbf{R}$ corresponds to calculating a Boolean function from $\{\pm 1\}^{nb}$ to $\{\pm 1\}^b$
 - Boolean functions are of practical interest

Boolean functions by neural networks

- **Thm.** For every n there exists a graph (V, E) of depth 2 such that $H_{V,E,\text{sign}}$ contains all functions from $\{\pm 1\}^n$ to $\{\pm 1\}$

Proof

- Let $f: \{\pm 1\}^n \rightarrow \{\pm 1\}$ be a Boolean function
- Let $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k$ be all vectors in $\{\pm 1\}^n$ for which f outputs 1
- Fact: for every $\mathbf{x} \in \{\pm 1\}^n$

$$\mathbf{u}_i^\top \mathbf{x} \begin{cases} \leq n - 2 & \text{if } \mathbf{x} \neq \mathbf{u}_i \\ = n & \text{if } \mathbf{x} = \mathbf{u}_i \end{cases}$$

$$\Rightarrow g_i(\mathbf{x}) = \text{sign}(\mathbf{u}_i^\top \mathbf{x} - n + 1) = 1 \iff \mathbf{x} = \mathbf{u}_i$$

Proof cont'd

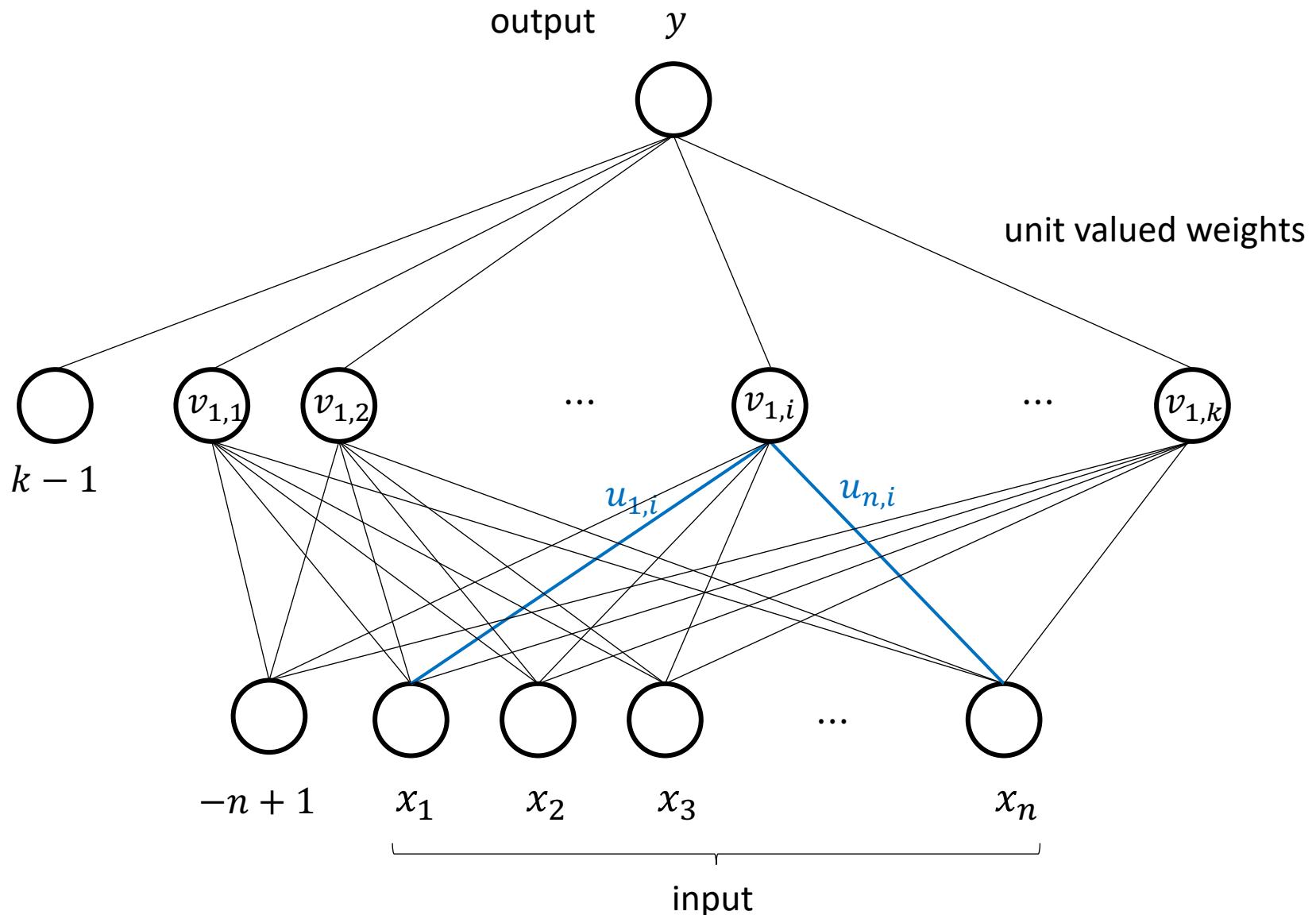
- The neural network weight parameters between layers 0 and 1 can be chosen such that each neuron $v_{1,i}$ implements g_i
- f is a disjunction of functions g_1, \dots, g_k :

$$f(\mathbf{x}) = \begin{cases} -1 & \text{if } g_1(\mathbf{x}) = g_2(\mathbf{x}) = \dots = g_k(\mathbf{x}) = -1 \\ 1 & \text{otherwise} \end{cases}$$

- Therefore, f can be written as

$$f(\mathbf{x}) = \text{sign}\left(\sum_{i=1}^k g_i(\mathbf{x}) + k - 1\right)$$

The two-layer network used in the proof



Comments

- The last theorem shows that neural networks can implement any Boolean function
- This is a weak property as the network might be exponentially large !
- The proof used a network of depth 2 with

$$|V_0| = n + 1$$

$|V_1|$ = exponential in n if f outputs 1 for a constant fraction of elements in $\{\pm 1\}^n$

$$|V_2| = 1$$

Lower bound

- **Thm:** For every n , let $s(n)$ be the minimal integer such that there exists a graph (V, E) with $|V| = s(n)$ such that the hypothesis class $H_{V,E,\text{sign}}$ contains all Boolean functions from $\{\pm 1\}^n$ to $\{\pm 1\}$

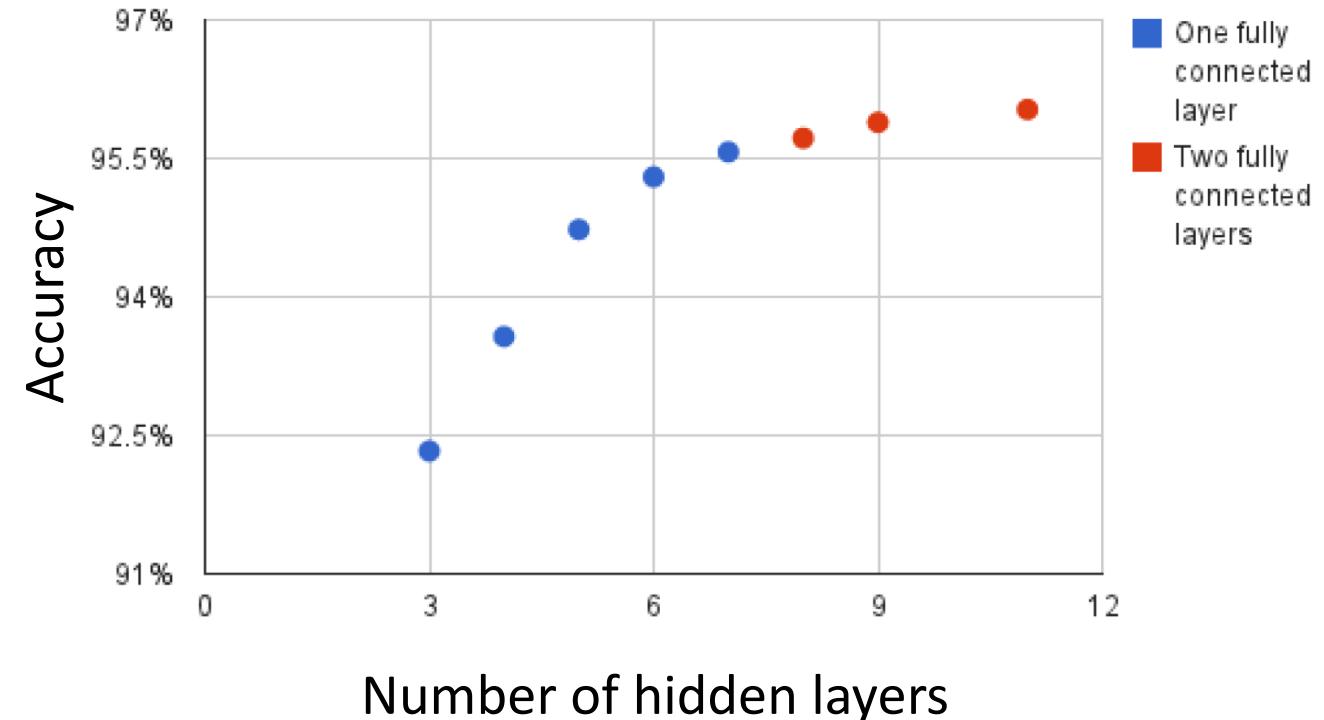
Then, $s(n)$ is exponential in n

- Similar result also holds for $H_{V,E,\sigma}$ where σ is the sigmoid function
- Proof uses advanced concepts such as VC dimension

On the expressiveness power of neural networks

- **Universal approximation:** sufficiently large depth-2 neural networks, using reasonable activation functions, can approximate any continuous function on a bounded domain [Hornik et al, 1989, ...]
 - The required size of such networks can be exponential in the dimension (impractical and prone to overfitting)
- The basic architectural questions for networks of bounded size:
 - How to trade-off between a network width and depth?
 - Should we use networks that are narrow and deep (many layers with a small number of neurons per layer), or shallow and wide?
 - Is the depth really important in deep learning?
- Empirical evidence and intuition: having depth in a neural network is beneficial

Empirical evidence: depth increases accuracy



- Goodfellow et al, Multi-digit Number Recognition from Street View Imagery using Deep Convolutional Neural Networks, ICLR 2014

Some recent separation results

- There are 3-layer networks of width polynomial in the dimension n which cannot be arbitrarily well approximated by 2-layer networks unless their width is exponential in n
[Eldan and Shamir, JMLR 2016]
- For any positive integer k , there exist neural networks with $\Theta(k^3)$ layers, $\Theta(1)$ width, and $\Theta(1)$ distinct parameters which cannot be approximated by networks with $\Theta(k)$ layers unless they are exponentially large of size $\Omega(2^k)$
[Telgarsky, COLT 2016]
- For any positive integer k , there exists a function representable by a ReLU neural network with k^2 hidden layers and total size k^3 such that any ReLU neural network with at most k hidden layers requires at least $\Omega(k^{k+1})$ total size
[Arora et al, ICLR 2018]

Historical remarks

- 1940s: function approximation used to motivate ML models such as perceptron
 - Early models based on linear models
 - Minsky's critique: inability of linear models to learn the XOR function
- The need to learn nonlinear functions led to
 - Multi-layer perceptron
 - Backpropagation: algorithm for computing a loss function gradient [LeCun (1985), Parker (1985), Rumelhart et al (1986)]
- 1980s: feedforward networks gained in popularity
 - Established the core ideas behind modern feedforward neural networks

* Backpropagation algorithm: next week

Historical remarks (cont'd)

- Most improvements in neural network performance attributed to:
 - Large datasets: allowing for generalization
 - Computing power and software: allowing to train larger neural networks
- Algorithmic developments also improved neural network performance:
 - Choice of the loss function: replacement of mean squared error with cross-entropy loss functions
 - Choice of activation functions: replacement of sigmoid activation functions with piecewise linear activation functions (ex. ReLUs)

Exercise: the choice of the loss function

- Consider a binary classifier using a single neural unit with activation function a :

$$\Pr[y_i = 1] = 1 - \Pr[y_i = 0] = p_{\theta} = a(\mathbf{x}_i^T \mathbf{w} + b)$$

where $\theta^T = (\mathbf{w}^T, b)$ is the parameter vector

- Loss functions:
 - Mean squared error: $f_{\text{MSE}}(\theta) = \frac{1}{2} \sum_{i=1}^m (y_i - p_{\theta})^2$
 - Cross-entropy: $f_{\text{CE}}(\theta) = - \sum_{i=1}^m y_i \log(p_{\theta}) + (1 - y_i) \log(1 - p_{\theta})$
- Compute the gradient vectors for the mean squared error loss function and the cross-entropy loss function (assume a is sigmoid function)
 - Why the gradient of the cross-entropy loss function may be preferred?

Exercise solution

- For the mean squared error loss function:

$$\frac{\partial}{\partial w_j} f_{\text{MSE}}(\mathbf{w}, b) = - \sum_{i=1}^m \underbrace{a'(\mathbf{x}_i^\top \mathbf{w} + b)}_{\text{diminishing to zero for } |\mathbf{x}_i^\top \mathbf{w} + b| \text{ large}} \left(y_i - a(\mathbf{x}_i^\top \mathbf{w} + b) \right) x_{i,j}$$

- For the cross-entropy loss function:

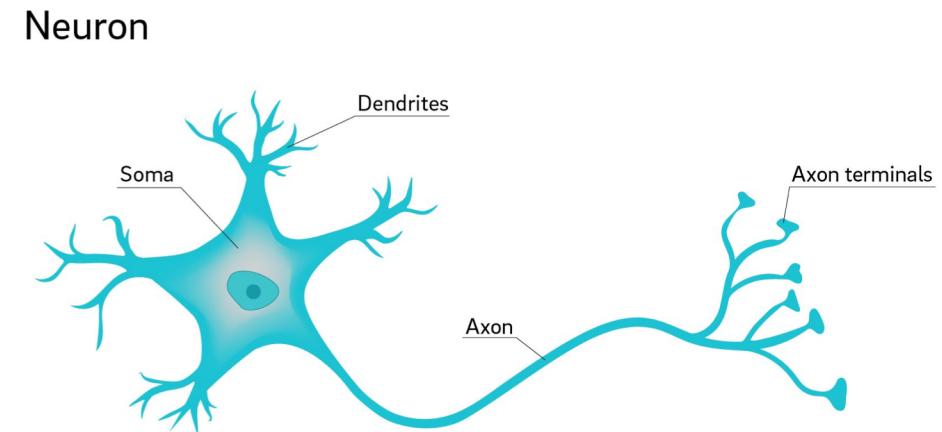
$$\frac{\partial}{\partial w_j} f_{\text{CE}}(\mathbf{w}, b) = - \sum_{i=1}^m \left(y_i - a(\mathbf{x}_i^\top \mathbf{w} + b) \right) x_{i,j}$$

Use of ReLU activation functions

- ReLUs used in early neural networks
 - Cognitron and neocognitron [Fukushima, 1975, 1980]
- Largely replaced by sigmoid function in 1980s
 - Perhaps sigmoids perform better for small neural networks
- Avoided until early 2000s
 - Preference for differentiable functions
- [Jarrett et al, 2009] found ReLUs to perform better than some other commonly used activation functions
- [Glorot et al, 2011] deep neural network easier with ReLU than with using activation with saturation

Biological justification of ReLUs

- Properties of biological neurons:
 - For some inputs biological neurons are completely inactive
 - For some inputs, the outputs of biological neurons are proportional to their inputs
 - Most of the time biological neurons operate in a region in which they are inactive (sparse activation)
- These properties are captured by ReLUs



References

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References: expressiveness of neural networks

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* Theoretical papers

Seminar 2 preview

- Solving the XOR problem in TensorFlow
- Learning new TensorFlow concepts such as scope
- HW: implementation and evaluation of the perceptron learning algorithm

Next lecture

- Training neural networks
 - Gradient descent algorithms
 - Stochastic gradient descent algorithms
 - Backpropagation algorithm
 - Acceleration by momentum
 - Adaptive moment estimation
 - Dropout
 - Batch normalization