ST449 Artificial Intelligence and Deep Learning

Lecture 2

Introduction to neural networks



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https://github.com/lse-st449/lectures2021

Topics of this lecture

- Single-layer networks
 - Linear discriminant functions
 - XOR problem
- Perceptron
 - Perceptron criterion and algorithm
 - Multi-layer perceptron
 - XOR problem solved
- Feedforward neural networks
 - Basic concepts: architecture, neurons, layers, size, width, and depth
 - Boolean function case
- Some important concepts for neural networks
 - Size and expressiveness power of neural networks
 - Computation power and algorithmic advancements
 - Choice of activation functions

Single-layer networks

Binary classification problem

Goal: learn a mapping

$$f: \mathbf{R}^n \to \{0,1\}, \ \mathbf{x} \mapsto f(\mathbf{x})$$

where $\mathbf{x} \in \mathbf{R}^n$ is a feature vector
and $\mathbf{y} \in \{0,1\}$ is a label

Supervised learning (learn from given examples)

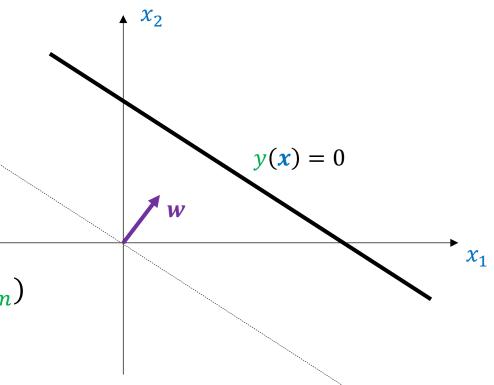
Training dataset:
$$(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)$$

Linear discriminant function:

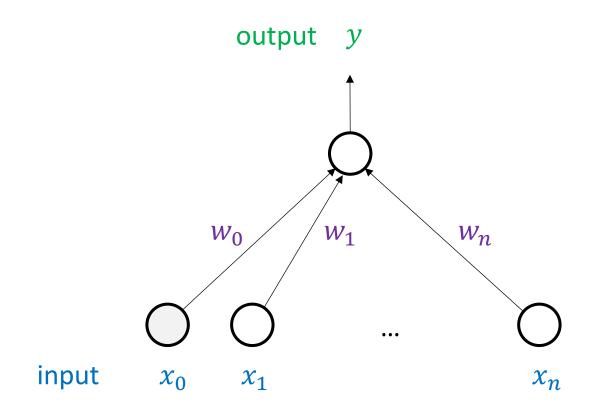
$$y(\mathbf{x}) = \mathbf{x}^\mathsf{T} \mathbf{w} + w_0$$

w weight vector w_0 bias term

- Linear decision boundary y(x) = 0
 - Decision boundary is a (n-1)-dimensional hyperplane



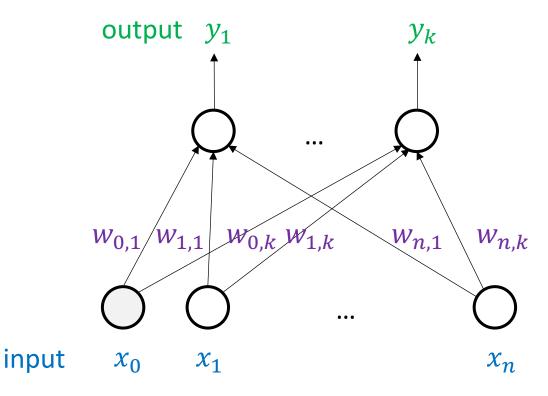
Representation by a neural network diagram



Multiple classes

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

$$y_i(x) = x^T w_i + w_{0,i}$$
 for $i = 1, 2, ..., k$



Non-linear discriminant functions

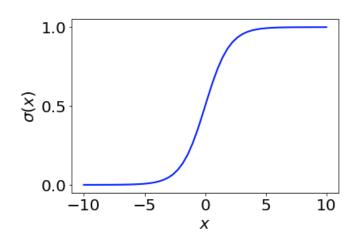
• Here is a way to have a non-linear discriminant function:

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

activation function

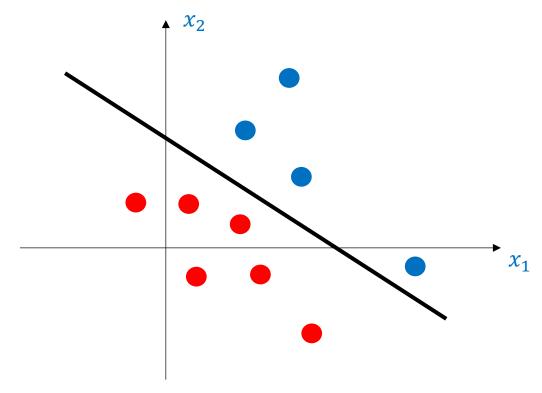
where $a: \mathbf{R} \to \mathbf{R}$ is a monotonic function

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



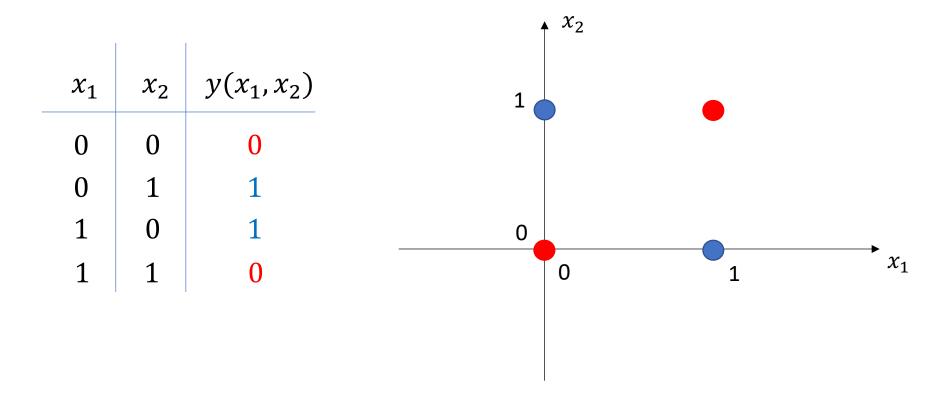
Linear separability

• 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)

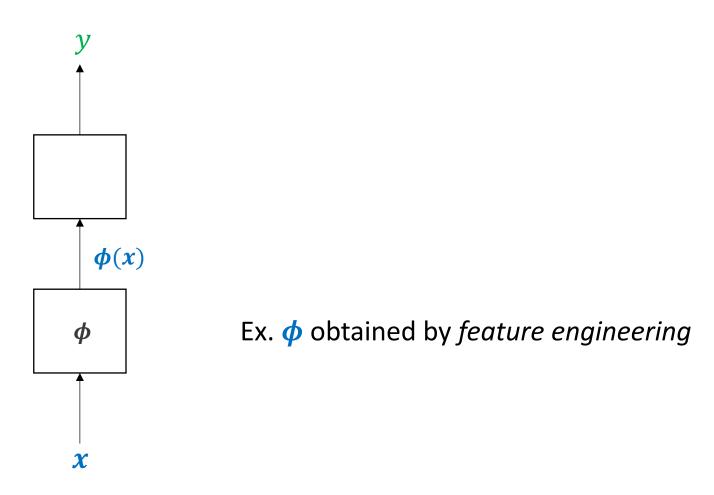
XOR: the exclusive-OR



• Not linearly separable

Input feature transformation

• Instead of using original feature vectors, we may use transformed feature vectors



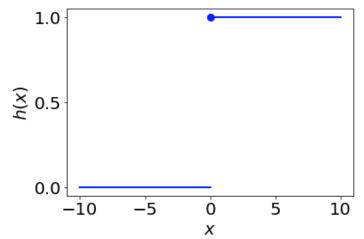
Perceptron

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: $h(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \ge 0 \end{cases}$

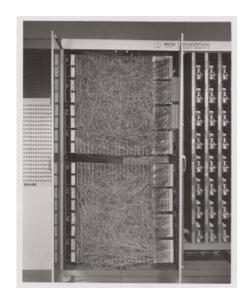


- Also known as the unit step function or the Heaviside step function
- An alternative half-maximum convention: redefine h(0) = 1/2
- In a more compact vector notation: $y(x) = h(\phi(x)^T w)$

History of perceptron

- The perceptron algorithm was invented by Frank RosenBlatt (psychologist) in 1957 at the Cornell Aeronautical Laboratory
- Intended to be a physical machine rather than a software 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





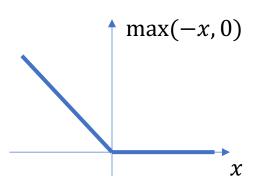
Source: <u>Perceptron</u>, Wikipedia

Perceptron criterion

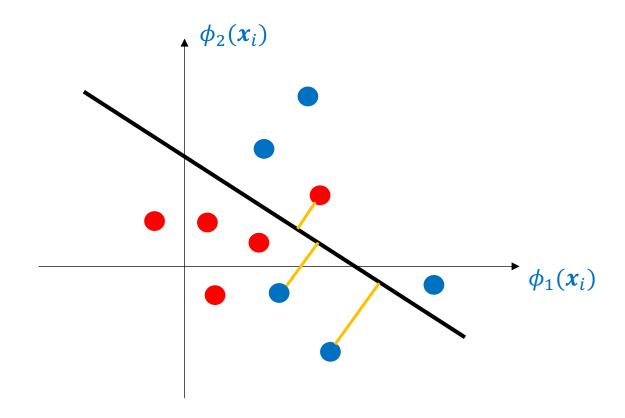
- Convention: $y_i \in \{-1,1\}$ and h(x) = -1 if x < 0, h(x) = 1 otherwise
- Correct classification: $y_i \phi(x_i)^T w > 0$
- False classification: $y_i \phi(x_i)^T w < 0$ same sign as the sign of the prediction label
- Goal: find parameter $\mathbf{w} \in \mathbf{R}^n$ such that for all input points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

$$L(\mathbf{w}) = \sum_{i=1}^{m} \max(-y_i \boldsymbol{\phi}(\mathbf{x}_i)^{\mathsf{T}} \mathbf{w}, 0)$$

A continuous piecewise-linear loss function (positive cost only 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, $\eta > 0$ step size, $\mathbf{w}^{(0)}$ arbitrarily (say null vector)

Repeat until there are no misclassified examples: // i.e. until $\forall (x_i, y_i): y_i \phi(x_i)^T w^{(t)} > 0$

$$\hat{y}_{i(t)} = h(\phi(x_{i(t)})^{\mathsf{T}} w^{(t)}) \qquad //(x_{i(t)}, y_{i(t)}) \text{ is the input example at } t$$

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

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

else

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

end if

$$t \leftarrow t + 1$$

Perceptron convergence property

• Let $L_i(w)$ be the contribution to the loss function of input example (x_i, y_i) for given parameter vector w, i.e.

$$L_i(\mathbf{w}) = \max(-y_i \boldsymbol{\phi}(\mathbf{x}_i)^{\mathsf{T}} \mathbf{w}, 0)$$

• Convergence property: for every t such that $\hat{y}_{i(t)} \neq y_{i(t)}$:

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

Question: can you prove this inequality?

Solution to the question

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

$$L_{i(t)}(\mathbf{w}^{(t+1)}) = \max\left(-y_{i(t)}\boldsymbol{\phi}(\mathbf{x}_{i(t)})^{\mathsf{T}}\mathbf{w}^{(t+1)}, 0\right)$$

$$= \max\left(-y_{i(t)}\boldsymbol{\phi}(\mathbf{x}_{i(t)})^{\mathsf{T}}\mathbf{w}^{(t)} - \eta \|\boldsymbol{\phi}(\mathbf{x}_{i(t)})\|^{2}, 0\right)$$

$$< \max\left(-y_{i(t)}\boldsymbol{\phi}(\mathbf{x}_{i(t)})^{\mathsf{T}}\mathbf{w}^{(t)}, 0\right)$$

$$= L_{i(t)}(\mathbf{w}^{(t)})$$

Perceptron convergence theorem

• Thm Assume that the input sequence of examples to the algorithm consists of misclassified examples 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 (given in the 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:

$$\exists w^*: y_i \phi(x_i)^T w^* > 0 \text{ for all } i = 1, 2, ..., m$$

• Note the identity:

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

where $M_i^{(t)}$ is the number of iterations s such that

$$(x_{i(s)}, y_{i(s)}) = (x_i, y_i), \hat{y}_{i(s)} \neq y_{i(s)} \text{ and } s \leq t$$

- 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)

• We claim that for all *t* until convergence:

$$\left(\min_{i} y_{i} \boldsymbol{\phi}(\boldsymbol{x}_{i})^{\mathsf{T}} \boldsymbol{w}^{*}\right) \boldsymbol{t} \leq \left(\|\boldsymbol{w}^{*}\| \max_{i} \|\boldsymbol{\phi}(\boldsymbol{x}_{i})\|\right) \sqrt{\boldsymbol{t}} \tag{*}$$

- Assume that the algorithm does not converge in a finite number of iterations
- Then, this implies that (\star) holds for all $t \geq 0$ which is a contradiction
- In the next slide we establish claim (*)

Proof of the convergence theorem (cont'd)

• Fact 1:
$$(w^*)^T w^{(t)} = \eta \sum_{i=1}^m M_i^{(t)} y_i \phi(x_i)^T w^* \ge M^{(t)} \eta \min_i y_i \phi(x_i)^T w^*$$

• Fact 2:
$$\|w^{(t)}\| \le \sqrt{M^{(t)}} \eta \max_{i} \|\phi(x_i)\|$$

- Fact 3: $(w^*)^T w^{(t)} \le ||w^*|| ||w^{(t)}||$ (Cauchy-Schwartz)
- Fact 4: $M^{(t)} = t$ (assumption of the theorem)

Note: to check Fact 2 note

$$\|\mathbf{w}^{(t+1)}\|^2 = \|\mathbf{w}^{(t)}\|^2 + 2\eta y_{i(t)} \boldsymbol{\phi}(\mathbf{x}_{i(t)})^{\mathsf{T}} \mathbf{w}^{(t)} + \eta^2 \|\boldsymbol{\phi}(\mathbf{x}_{i(t)})\|^2$$
and $y_{i(t)} \boldsymbol{\phi}(\mathbf{x}_{i(t)})^{\mathsf{T}} \mathbf{w}^{(t)} < 0$

Bound on mistakes theorem

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

Then, for the perceptron learning algorithm, we have

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

where
$$\gamma = \min \left\{ \frac{|\phi(x_i)^T w^*|}{\|w^*\|} : i = 1, 2, ..., m \right\}$$

• 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

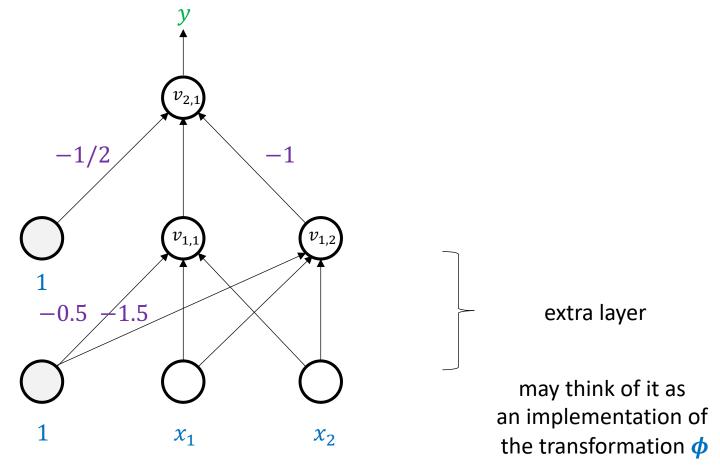
Proof of the theorem

- Similar arguments as for the theorem on slide 18
- Without loss of generality assume that $||w^*|| = 1$
- From Fact 1 [slide 22]: $(\mathbf{w}^*)^T \mathbf{w}^{(t)} \ge \gamma \eta M^{(t)}$
- From Fact 2 [slide 22]: $\|\mathbf{w}^{(t)}\| \le \eta r \sqrt{M^{(t)}}$
- From Fact 3 [slide 22] and $\|\mathbf{w}^*\| = 1$: $(\mathbf{w}^*)^T \mathbf{w}^{(t)} \le \|\mathbf{w}^{(t)}\|$
- The claim of the theorem follows from the last three inequalities

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



- 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:

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

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

Feedforward neural networks

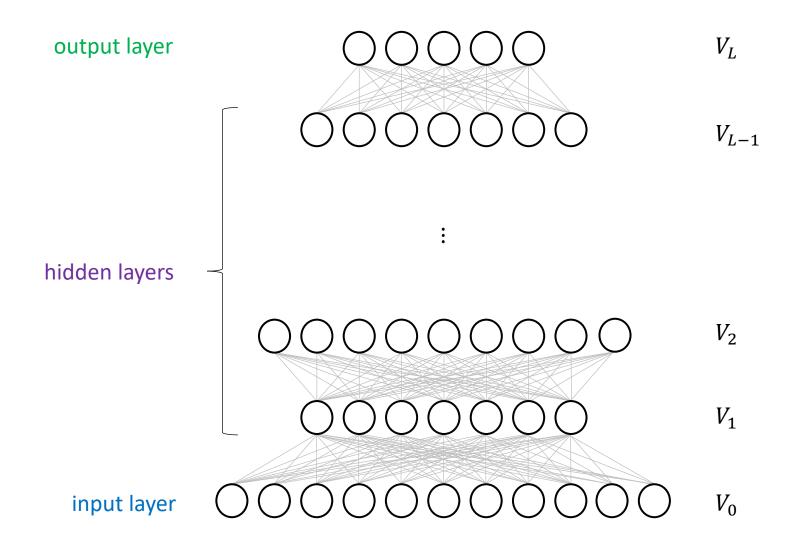
Feedforward networks: basic concepts

- Feedforward network: a network of nodes that can be partitioned in *ordered* layers such that an edge may exist only between two nodes in adjacent layers
 - Defined by a Directed Acyclic Graph (DAG), G = (V, E), where V is the set of nodes and E is the set of edges, and a weight function $w: E \to \mathbf{R}$
- Neuron: each neuron is represented by a node
- Activation function: each neuron has an activation function $a: \mathbf{R} \to \mathbf{R}$
- Network architecture: defined by the triplet (V, E, a)

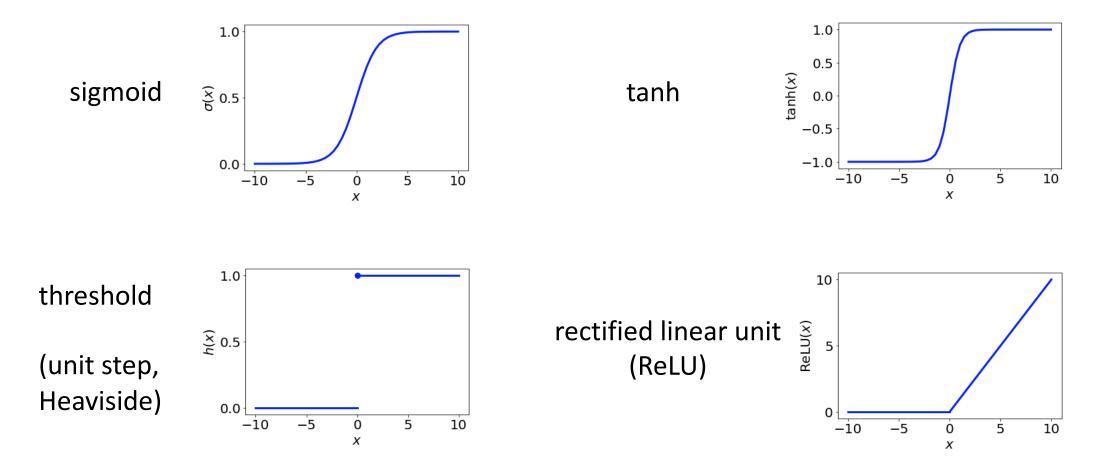
Feedforward networks: basic concepts (cont'd)

- 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: $\max\{|V_0|, |V_1|, ..., |V_L|\}$
- Comments:
 - Width of the input layer for an n dimensional input space: $|V_0| = n + 1$
 - Each edge $e \in E$ connects a node in V_{l-1} and a node in V_l for some layer l

Feedforward networks: basic concepts (cont'd)



Common activation functions



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

Function composition representation

• Function mapping $x \mapsto h(x)$ can be expressed as:

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

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

$$\vdots$$

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

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

• 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 $h_{V,E,a,w}: \mathbf{R}^{|V_0|-1} \to \mathbf{R}^{|V_L|}$
- Hypothesis class of functions:

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

- Fundamental questions on 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 $g: \{-1,1\}^p \to \{-1,1\}^q$
- The expressiveness power question:
 - What Boolean functions can be implemented by $H_{V,E,si,gn}$?
- Understanding Boolean functions is of practical interest
 - Every computer that stores real numbers using b bits, calculating function $f: \mathbb{R}^n \to \mathbb{R}$ corresponds to calculating a Boolean function mapping from $\{-1,1\}^{nb}$ to $\{-1,1\}^b$

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 $\{-1,1\}^n$ to $\{-1,1\}$

Proof

- Let $f: \{-1,1\}^n \to \{-1,1\}$ be a Boolean function
- Let $u_1, u_2, ..., u_k$ be all vectors in $\{-1,1\}^n$ for which f outputs 1
- Fact: for every $x \in \{-1,1\}^n$

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

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

Proof cont'd

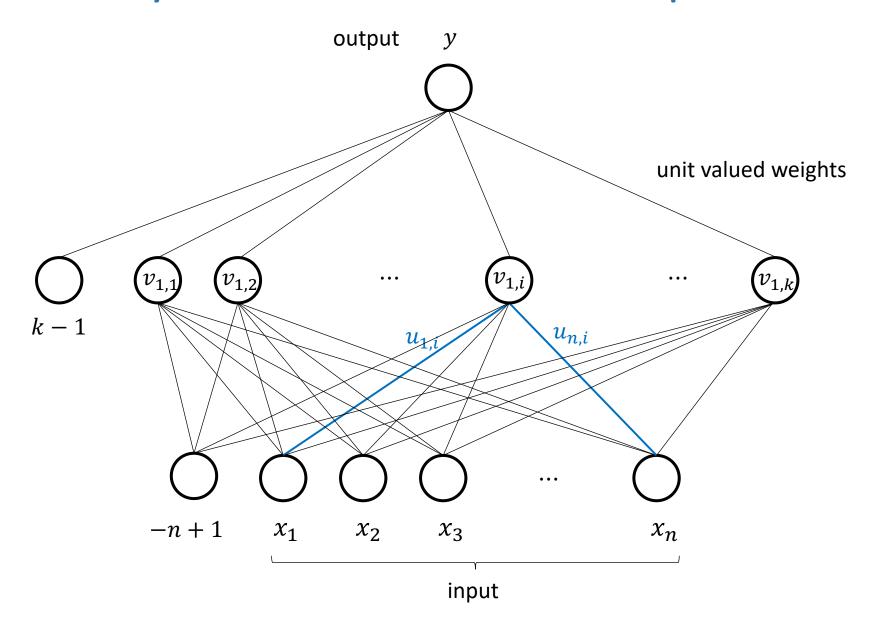
- The neural network weight parameters between layers 0 and 1 can be chosen such that each neuron $v_{1,i}$ implements g_i
- f is a disjunction of functions g_1, \dots, g_k :

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

• Therefore, f can be written as

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

The two-layer network used in the proof



Some important concepts for neural networks

What does the result for Boolean functions mean?

- It means that any Boolean function can be correctly represented by a neural network
- Note, however, that this is a weak property as the network size can be exponentially large in the input dimension n!
- 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 $\{-1,1\}^n$

$$|V_2| = 1$$

Lower bound (theory)

• Thm: For every input dimension 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 $H_{V,E,sign}$ contains all Boolean functions from $\{-1,1\}^n$ to $\{-1,1\}$.

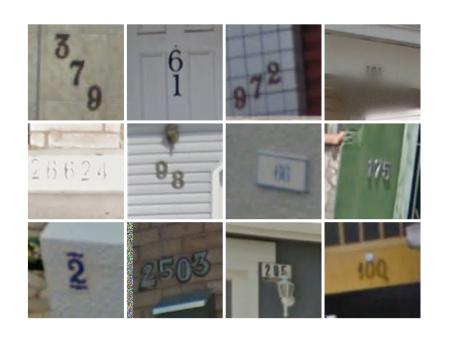
Then, s(n) is exponential in n.

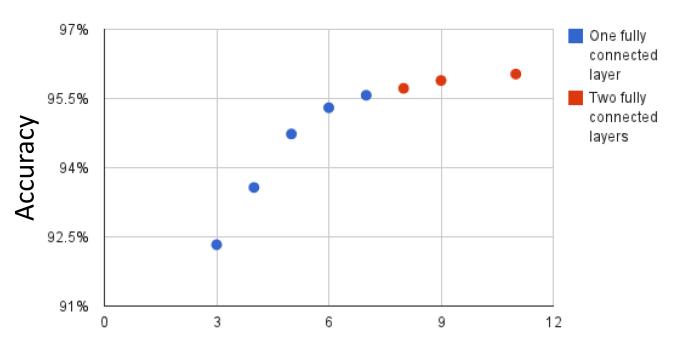
- Similar result also holds for $H_{V,E,\sigma}$ where σ is the sigmoid function
- Proof uses advanced concepts such as VC dimension

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, ...]
 - Again, the required size of such networks can be exponential in the dimension (impractical and prone to overfitting)
- Fundamental 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?
 - How is the depth important for deep learning?
- Empirical evidence and intuition: having depth in a neural network is beneficial

Empirical evidence: depth increases accuracy





Number of hidden layers

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

Some recent separation results (theory)

• There are 3-layer networks of the width polynomial in the dimension n which cannot be arbitrarily well approximated by a 2-layer network unless its 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 the 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: choice of the loss function

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

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

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

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

Exercise solution

• For the mean squared error loss function:

$$\frac{\partial}{\partial w_j} f_{\text{MSE}}(\mathbf{w}, b) = -\sum_{i=1}^m a'(\mathbf{x}_i^{\mathsf{T}} \mathbf{w} + b) \left(y_i - a(\mathbf{x}_i^{\mathsf{T}} \mathbf{w} + b) \right) \mathbf{x}_{i,j}$$

diminishing to zero for $|\mathbf{x}_i^{\mathsf{T}}\mathbf{w} + b|$ large

For the cross-entropy loss function:

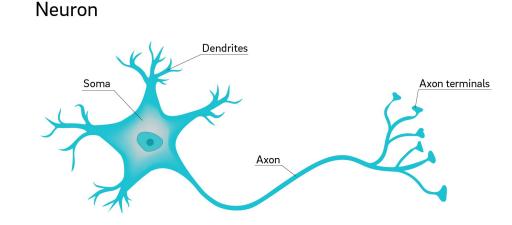
$$\frac{\partial}{\partial w_i} f_{\text{CE}}(\mathbf{w}, b) = -\sum_{i=1}^m \left(y_i - a(\mathbf{x}_i^{\mathsf{T}} \mathbf{w} + b) \right) x_{i,j}$$

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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- Ronen Eldan and Ohad Shamir, The power of depth for feedforward neural networks, Journal of Machine Learning Research, vol 49:1-34, 2016
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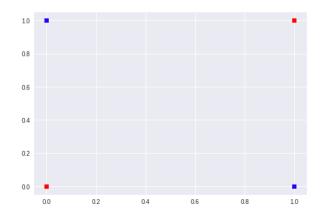
^{*} Theoretical papers

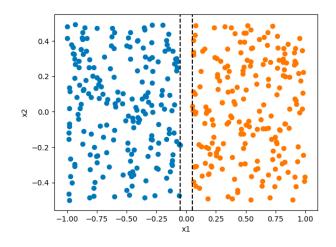
Seminar 2 preview

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