

Neural Networks: Multi-layer Perceptrons

Spring 2021

Review

- ▶ A perceptron is a simplistic model of a single neuron.
- ▶ A perceptron can learn to perform simple classification tasks using an update rule.
- ▶ **Today:** Imagine what a network of millions of perceptrons can learn!

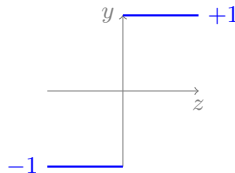
A new activation function

Our simple perceptron computes an intermediate value z using a weighted sum of the inputs

$$z = \mathbf{w} \cdot \mathbf{x}$$

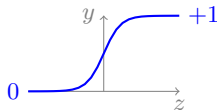
To simulate firing, we used the *sign function* for activation:

$$y = \text{sgn}(z) = \begin{cases} +1, & z > 0 \\ -1, & z < 0 \end{cases}$$



To avoid the discontinuity at zero, let's switch to the *sigmoid function*:

$$y = \sigma(z) = \frac{1}{1 + e^{-z}}$$



Back to logistic regression?

A perceptron with a sigmoid activation function

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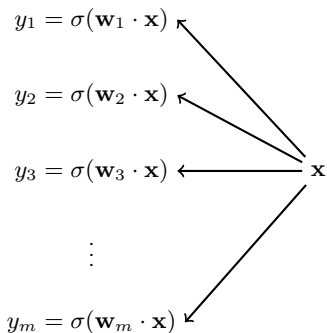
Adding the sigmoid function prevents us from using the Perceptron Update Algorithm. We must use a gradient descent-type method instead (just as we did for logistic regression).

Fortunately, the sigmoid function has a convenient derivative:

$$\frac{d}{dz}\sigma(z) = \sigma(z)[1 - \sigma(z)].$$

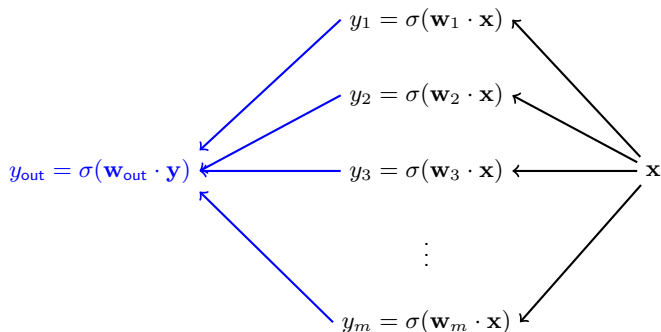
Multi-neuron (wide) perceptrons

Neural networks use multiple neurons to learn different features from the **same inputs**.



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The outputs of each neuron are collected into a single neuron to predict the final class.

A matrix formalism for perceptrons

Consider a stack of m neurons that are all connected to the same input \mathbf{x} .

$$z_1 = \mathbf{w}_1 \cdot \mathbf{x}$$

$$z_2 = \mathbf{w}_2 \cdot \mathbf{x}$$

$$\vdots$$

$$z_m = \mathbf{w}_m \cdot \mathbf{x}$$

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The stack can be written as the product of the input \mathbf{x} and a weight matrix

$$\mathbf{z} = \mathbf{W}\mathbf{x}$$

where each row in \mathbf{W} contains the weights for a single neuron

$$\mathbf{W} = \begin{pmatrix} \leftarrow \mathbf{w}_1 \rightarrow \\ \leftarrow \mathbf{w}_2 \rightarrow \\ \vdots \\ \leftarrow \mathbf{w}_m \rightarrow \end{pmatrix}.$$

Three looks at linear systems

We've studied three classes of linear systems, differing only by what is **known** and **unknown**.

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

matrix multiplication

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}$$

linear models

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neural networks

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Of these problems, neural networks are the most difficult to solve since \mathbf{W} is a *matrix* of unknowns, not a *vector* like \mathbf{y} and $\boldsymbol{\beta}$.

Elementwise activation functions

Let's define an *elementwise* sigmoid activation function

$$\boldsymbol{\sigma}(\mathbf{z}) = \begin{pmatrix} \sigma(z_1) \\ \sigma(z_2) \\ \vdots \\ \sigma(z_n) \end{pmatrix}.$$

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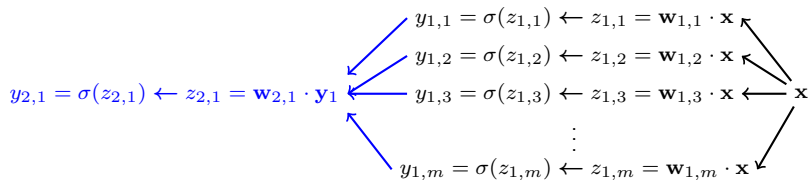
$$\mathbf{y} = \boldsymbol{\sigma}(\mathbf{W}\mathbf{x})$$

where

$$\dim(\mathbf{y}) = m \times 1, \quad \dim(\mathbf{z}) = m \times 1$$

$$\dim(\mathbf{W}) = m \times n, \quad \dim(\mathbf{x}) = n \times 1$$

Completing our matrix formalism



Completing our matrix formalism

Diagram illustrating the forward pass of a neural network layer:

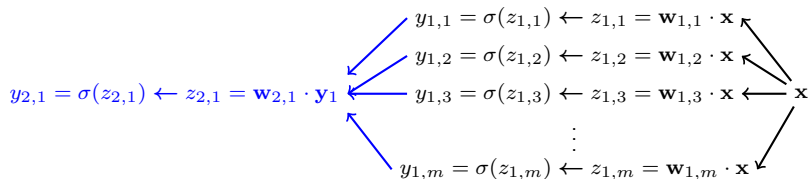
$$\begin{aligned} y_{1,1} &= \sigma(z_{1,1}) \leftarrow z_{1,1} = \mathbf{w}_{1,1} \cdot \mathbf{x} \\ y_{1,2} &= \sigma(z_{1,2}) \leftarrow z_{1,2} = \mathbf{w}_{1,2} \cdot \mathbf{x} \\ y_{1,3} &= \sigma(z_{1,3}) \leftarrow z_{1,3} = \mathbf{w}_{1,3} \cdot \mathbf{x} \\ &\vdots \\ y_{1,m} &= \sigma(z_{1,m}) \leftarrow z_{1,m} = \mathbf{w}_{1,m} \cdot \mathbf{x} \end{aligned}$$

The output y_1 is then used to compute y_2 :

$$y_{2,1} = \sigma(z_{2,1}) \leftarrow z_{2,1} = \mathbf{w}_{2,1} \cdot \mathbf{y}_1$$

$$\mathbf{y}_2 = \boldsymbol{\sigma}(\mathbf{z}_2) \quad \leftarrow \quad \mathbf{z}_2 = \mathbf{W}_2 \mathbf{y}_1 \quad \leftarrow \quad \mathbf{y}_1 = \boldsymbol{\sigma}(\mathbf{z}_1) \quad \leftarrow \quad \mathbf{z}_1 = \mathbf{W}_1 \mathbf{x}$$

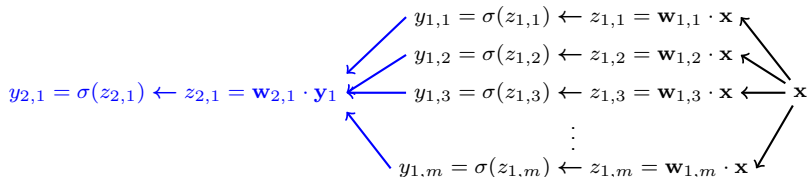
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$$\mathbf{y}_2 = \sigma(\mathbf{W}_2(\sigma(\mathbf{W}_1 \mathbf{x})))$$

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In general, a network with d layers is

$$\mathbf{y}_d = \sigma(\mathbf{W}_d(\sigma(\mathbf{W}_{d-1}(\cdots \sigma(\mathbf{W}_2(\sigma(\mathbf{W}_1 \mathbf{x}))))))).$$

Deep learning with neural networks

$$\mathbf{y}_d = \sigma(\mathbf{W}_d(\sigma(\mathbf{W}_{d-1}(\cdots \sigma(\mathbf{W}_2(\sigma(\mathbf{W}_1\mathbf{x})))))))$$

- ▶ The number of neurons in each layer i is the *width* of the layer.
 - ▶ If the $(i - 1)$ th layer has n outputs and the i th layer has m outputs, the weight matrix \mathbf{W}_i has dimensions $m \times n$.
 - ▶ The dimensions of the inputs \mathbf{x} and outputs \mathbf{y}_d are fixed by the problem.
 - ▶ Layer 1 is called the *input layer*, and layer d is the *output layer*.
 - ▶ We can use as many nodes as we want in the *hidden* layers.

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- ▶ The number of layers d is the *depth* of the neural network.
- ▶ *Deep learning* means $d > 2$.

The importance of nonlinearity

The nonlinear functions (like σ) sandwiched between the layers are critical to deep learning.

Let's imagine what would happen if we removed them:

$$\begin{aligned} \mathbf{y}_d &= \sigma(\mathbf{W}_d(\sigma(\mathbf{W}_{d-1}(\cdots \sigma(\mathbf{W}_2(\sigma(\mathbf{W}_1\mathbf{x}))))))) \\ &= \mathbf{W}_d(\mathbf{W}_{d-1}(\cdots \mathbf{W}_2(\mathbf{W}_1\mathbf{x}))) \\ &= \mathbf{W}_d\mathbf{W}_{d-1}\cdots\mathbf{W}_2\mathbf{W}_1\mathbf{x} \\ &= \widetilde{\mathbf{W}}\mathbf{x} \end{aligned}$$

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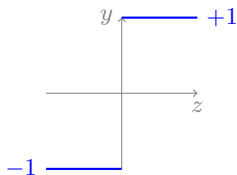
Without the activation functions, the entire neural network reduces to a single linear system!

Any nonlinearity will do

Any nonlinear function can be an activation function.

Sign/step activation

$$\text{sgn}(z) = \begin{cases} +1, & z > 0 \\ -1, & z < 0 \end{cases}$$

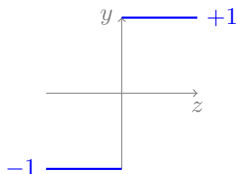


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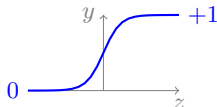
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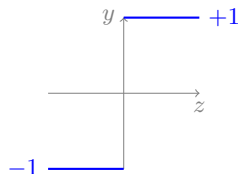


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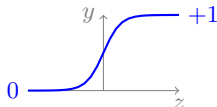
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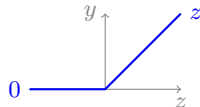
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Rectified linear unit activation

$$\text{ReLU}(z) = \begin{cases} z, & z \geq 0 \\ 0, & z < 0 \end{cases}$$



Why do we want deep networks?

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- ▶ Neural networks are therefore universal function approximators.
- ▶ Unfortunately, the theorem does not tell us how many neurons we need to approximate a given function.
- ▶ For complicated functions, evidence suggests the number is enormous!
- ▶ Our brains are very deep, so it's reasonable to believe that deep networks learn more efficiently than wide ones.
- ▶ In practice this is almost certainly true.
- ▶ Deep learning reduces the total number of neurons needed to learn a function since each of the d layers needs fewer than $1/d$ -times the number of neurons.

Why do deeper networks learn better?

We can understand deep networks using examples from *feature engineering*.

Imagine you wanted to learn a Michaelis-Menten function.

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Single Layer

The diagram illustrates the Michaelis-Menten equation $\frac{V_{\max}[S]}{K_m + [S]}$ as a single-layer model. Three arrows point from the input features to the equation: V_{\max} points to the numerator's coefficient, $[S]$ points to the numerator's variable, and K_m points to the denominator's constant term.

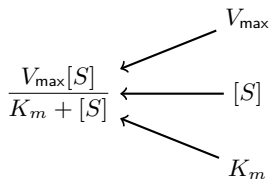
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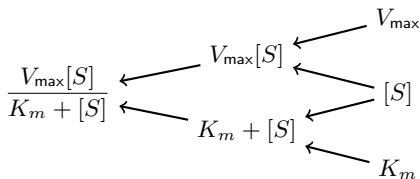
Single Layer



A diagram showing a single layer neural network. On the left is the target function $\frac{V_{\max}[S]}{K_m + [S]}$. Three arrows point from the right towards this function. The top arrow originates from V_{\max} , the middle from $[S]$, and the bottom from K_m .

$$\frac{V_{\max}[S]}{K_m + [S]}$$

Two Layers



A diagram showing a two layer neural network. On the left is the target function $\frac{V_{\max}[S]}{K_m + [S]}$. Three arrows point from the right towards this function. The top arrow originates from $V_{\max}[S]$, the middle from $K_m + [S]$, and the bottom from K_m . To the right of these three intermediate nodes, there is another set of three nodes: V_{\max} , $[S]$, and K_m . Arrows point from these three nodes to the intermediate nodes: from V_{\max} to $V_{\max}[S]$, from $[S]$ to $K_m + [S]$, and from K_m to K_m .

$$\frac{V_{\max}[S]}{K_m + [S]}$$

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Single Layer

A diagram showing a single layer network. On the left is the output expression $\frac{V_{\max}[S]}{K_m + [S]}$. On the right are three inputs: V_{\max} , $[S]$, and K_m . Arrows point from each input to the output expression.

$$\frac{V_{\max}[S]}{K_m + [S]}$$

Two Layers

A diagram showing a two-layer network. On the left is the output expression $\frac{V_{\max}[S]}{K_m + [S]}$. In the middle is an intermediate expression $V_{\max}[S]$. On the right are three inputs: V_{\max} , $[S]$, and K_m . Arrows point from V_{\max} and $[S]$ to the intermediate expression. Arrows point from the intermediate expression and K_m to the final output expression.

$$\frac{V_{\max}[S]}{K_m + [S]}$$

Each layer in the network only needs to improve the features for the next layer.

Summary

- ▶ Deep neural networks are built from layers in artificial neurons.
- ▶ Each neuron has the power of a linear classifier.
- ▶ Layers **must** be separated by nonlinear activation functions.
- ▶ Neural networks can learn nearly any function, but deep networks learn more efficiently.
- ▶ Each layer creates features for the subsequent layers to improve learning.

Preparing for gradient descent

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Similarly, for the k functions f_1, f_2, \dots, f_k ,

$$\frac{d}{dx} f_k(f_{k-1}(\cdots f_2(f_1(x)))) = \frac{df_k}{df_{k-1}} \frac{df_{k-1}}{df_{k-2}} \cdots \frac{df_i}{df_{i-1}} \cdots \frac{df_2}{df_1} \frac{df_1}{dx}$$

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For example, let $f(x) = (2x - 3)^3$. Let $f_1(x) = 2x - 3$ and $f_2(z) = z^3$. Then $f(x) = f_2(f_1(x))$ and

$$\begin{aligned} \frac{df}{dx} &= \frac{df_2}{df_1} \frac{df_1}{dx} \\ &= 3(2x - 3)^2(2) \end{aligned}$$