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!

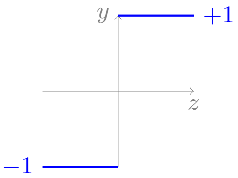
A new activation function

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

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

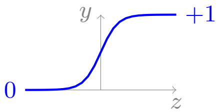
To simulate firing, we used the *sign function* for activation:

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



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

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



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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**.

$$y_1 = \sigma(\mathbf{w}_1 \cdot \mathbf{x}) \longleftarrow \mathbf{x}$$

$$y_2 = \sigma(\mathbf{w}_2 \cdot \mathbf{x}) \longleftarrow \mathbf{x}$$

$$y_3 = \sigma(\mathbf{w}_3 \cdot \mathbf{x}) \longleftarrow \mathbf{x}$$

$$\vdots$$

$$y_m = \sigma(\mathbf{w}_m \cdot \mathbf{x}) \longleftarrow \mathbf{x}$$

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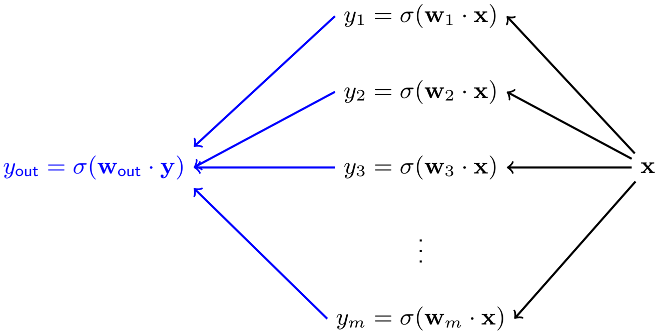

The outputs of each neuron are collected into a single neuron to predict the final class.

A matrix formalism for perceptrons

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

$$
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z_1 &= \mathbf{w}_1 \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 $\mathbf{W}$ contins 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
$\mathbf{y} = \mathbf{X}\beta$	linear models
$\mathbf{z} = \mathbf{W}\mathbf{x}$	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 β.

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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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

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

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

$$y_{2,1} = \sigma(z_{2,1}) \leftarrow z_{2,1} = \mathbf{w}_{2,1} \cdot \mathbf{y}_1 \leftarrow y_{1,3} = \sigma(z_{1,3}) \leftarrow z_{1,3} = \mathbf{w}_{1,3} \cdot \mathbf{x} \leftarrow \mathbf{x}$$

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$$y_{1,m} = \sigma(z_{1,m}) \leftarrow z_{1,m} = \mathbf{w}_{1,m} \cdot \mathbf{x}$$

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

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In general, a network with d layers is

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

Deep learning with neural networks

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

- 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 ith 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*.
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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 $\boldsymbol{\sigma}$) sandwiched between the layers are critical to deep learning.

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

$$\begin{aligned}
\mathbf{y}_d &= \boldsymbol{\sigma}(\mathbf{W}_d(\boldsymbol{\sigma}(\mathbf{W}_{d-1}(\cdots \boldsymbol{\sigma}(\mathbf{W}_2(\boldsymbol{\sigma}(\mathbf{W}_1\mathbf{x}))))))) \\
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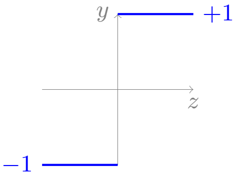
Without the activation functions, the entire neural network reduces to a single linear system!

Any nonlinearity will do

Any nonlinear function can be an activation function.

Sign/step activation

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



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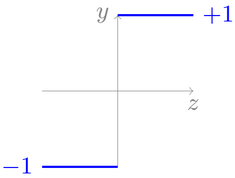

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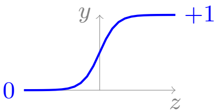

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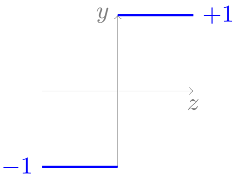

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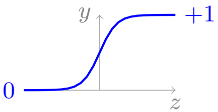
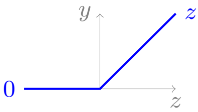


Rectified linear unit activation

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



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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.

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

Imagine you wanted to learn a Michaelis-Menten function.

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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.

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Similarly, for the k functions f_1, f_2, ..., 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

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