Applied Deep Learning

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Learning objectives of today

Goals: Creating neural networks – from logistic regression to feed-forward networks

- Use what we have learned about linear algebra and calculus to create a logistic regression algorithm from scratch
- Understand how what we learned generalizes to neural networks in general

How will we do this?

- We start with a quick recap on our discussion about logistic regression so far
- We then implement a logistic regression algorithm with numpy only
- Next, we visualize more general neural networks with the TensorFlow playground, before defining the concepts relevant for running our own networks

Taking a step back – logistic regression

What do we actually do when training a logistic regression model?

$$X = \begin{array}{c|c} & 1 \; \cdots \; m \\ 1 & \\ \vdots & \left(\begin{array}{c} x^{(1)} \\ \vdots \\ x^{(n)} \end{array} \right) \\ n & \end{array}$$

$$Y = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{pmatrix}$$

- We are given values $(\boldsymbol{x}^{(i)}, y^{(i)})$, where $\boldsymbol{x}^{(i)} \in \mathbb{R}^m$ and $y^{(i)} \in \{0,1\}$
- Our prediction $\hat{y}^{(i)}$ should reflect the probability that $y^{(i)} = 1$: $\hat{y}^{(i)} = P\left(y^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}\right)$

- We model this probability, using the sigmoid function:

What do we actually do when training a logistic regression model?

$a_0 + a_1 x_1^{(i)} + a_2 x_2^{(i)} \dots + a_m x_m^{(i)}$

$b + w_1 x_1 + w_2 x_2 + \dots + w_m x_m$

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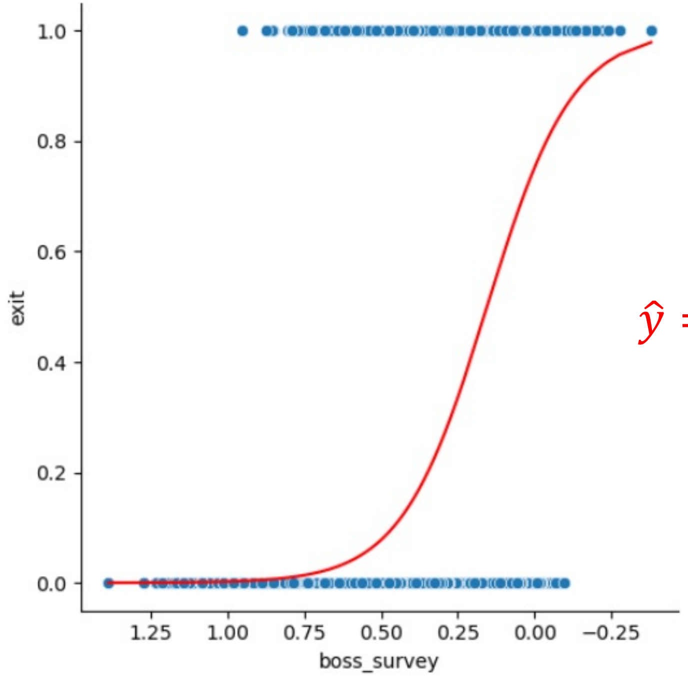
- We model this probability, using the sigmoid function:

$$\underset{(1,m)}{x}\ \underset{(m,1)}{w} + \underset{(1,1)}{b}$$



$$\hat{y} = \frac{1}{1 + e^{-(\boldsymbol{x}\cdot\boldsymbol{w}+\boldsymbol{b})}} = \frac{e^{(\dots)}}{1 + e^{(\dots)}}$$

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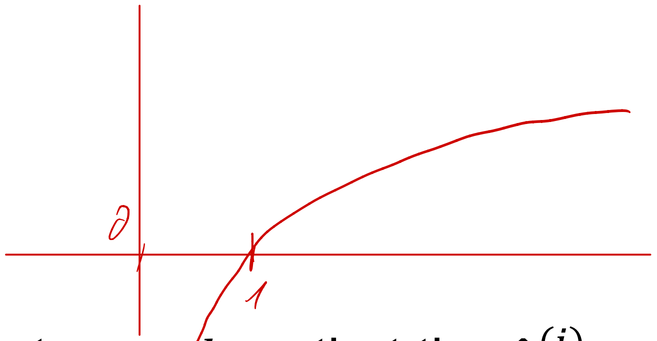

- Remember that $\boldsymbol{w} \in \mathbb{R}^m$ and $b \in \mathbb{R}$
- To get to the "right" model, we optimize our parameters $\boldsymbol{w}, b$ so that the $\hat{y}^{(i)}$s are "as close as possible" to the y^is
- What we do is to minimize the "cost-function" $J(\boldsymbol{w}, b)$, where $\hat{y}^{(i)} = \frac{1}{1+e^{-\left(\boldsymbol{x}^{(i)}\boldsymbol{w}+\boldsymbol{b}\right)}}$:

$$J(\boldsymbol{w}, b) = -\frac{1}{n}\sum_{i=1}^{n}\underbrace{\left[y^{(i)} \ln \hat{y}^{(i)} + \left(1 - y^{(i)}\right)\ln\left(1 - \hat{y}^{(i)}\right)\right]}_{L^{(i)}}$$

$y^{(i)} = 1 : -[\ln \hat{y}^{(i)} + 0]$ $\to 0 : \hat{y}^{(i)} \to 1$; $\to \infty : \hat{y}^{(i)} \to 0$

$y^{(i)} = 0 : -[0 + \ln(1 - \hat{y}^{(i)})]$ $\to 0 : \hat{y}^{(i)} \to 0$; $\to \infty : \hat{y}^{(i)} \to 1$

- Remember that $\boldsymbol{w} \in \mathbb{R}^m$ and $b \in \mathbb{R}$
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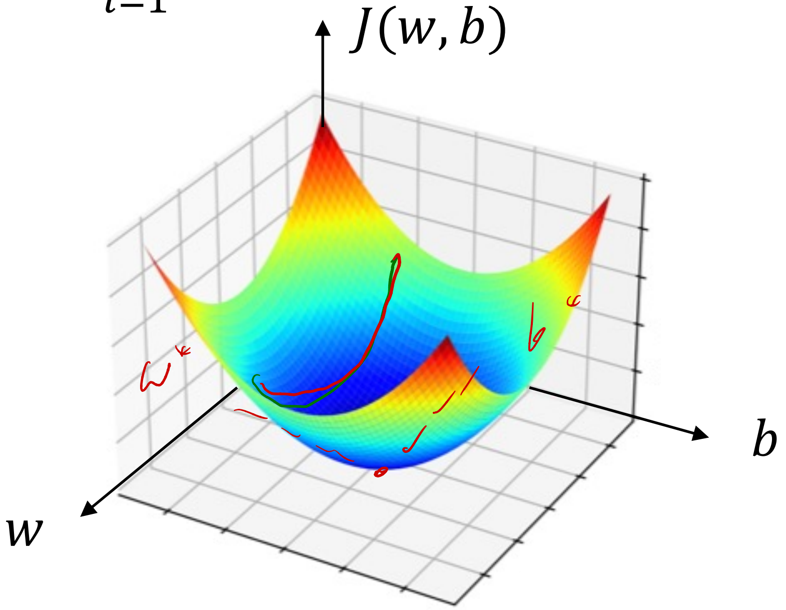

$$\underline{y^{(i)}} = \frac{1}{1 + e^{-w^* x^{(i)} + b^*}}$$

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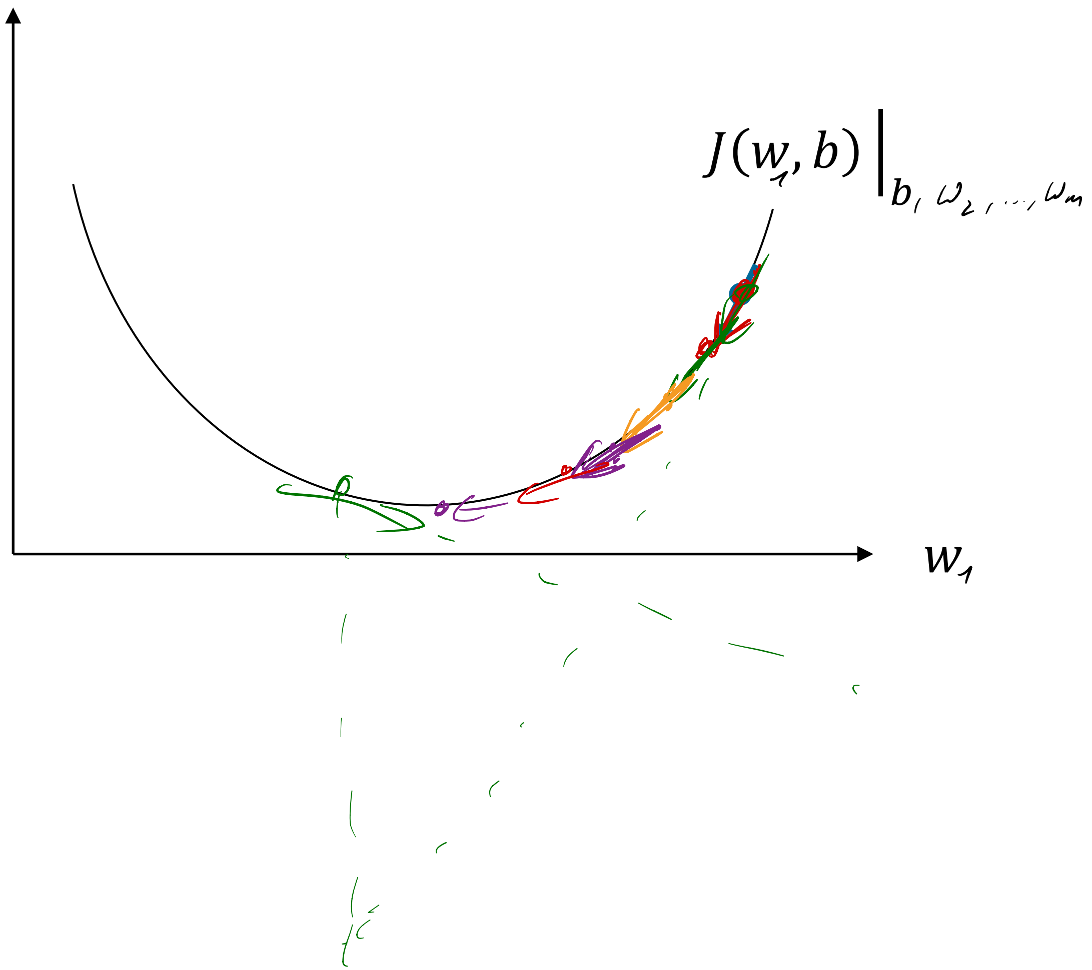
Solving the optimization problem through gradient descent



$w_1 \rightsquigarrow \frac{\partial J}{\partial w_1}$

$w_1 := w_1 - \alpha \frac{\partial J}{\partial w_1}$

$w_1 := w_1 - \alpha \frac{\partial J}{\partial w_1}$ #

Our first optimization algorithm

1. Decide a "learning rate" α
2. Start with some $\boldsymbol{w}$ and b and compute $J(\boldsymbol{w}, b)$
3. Until J "doesn't change" anymore:
   - Let $w_1 := w_1 - \alpha \frac{\partial J(\boldsymbol{w},b)}{\partial w_1}$
   - Let $w_2 := w_2 - \alpha \frac{\partial J(\boldsymbol{w},b)}{\partial w_2}$
   - …
   - Let $w_m := w_m - \alpha \frac{\partial J(\boldsymbol{w},b)}{\partial w_m}$
   - Let $b := b - \alpha \frac{\partial J(\boldsymbol{w},b)}{\partial b}$
   - Recompute $J(\boldsymbol{w}, b)$
4. Enjoy the fruits of your labor: you have fit a logistic regression model manually!

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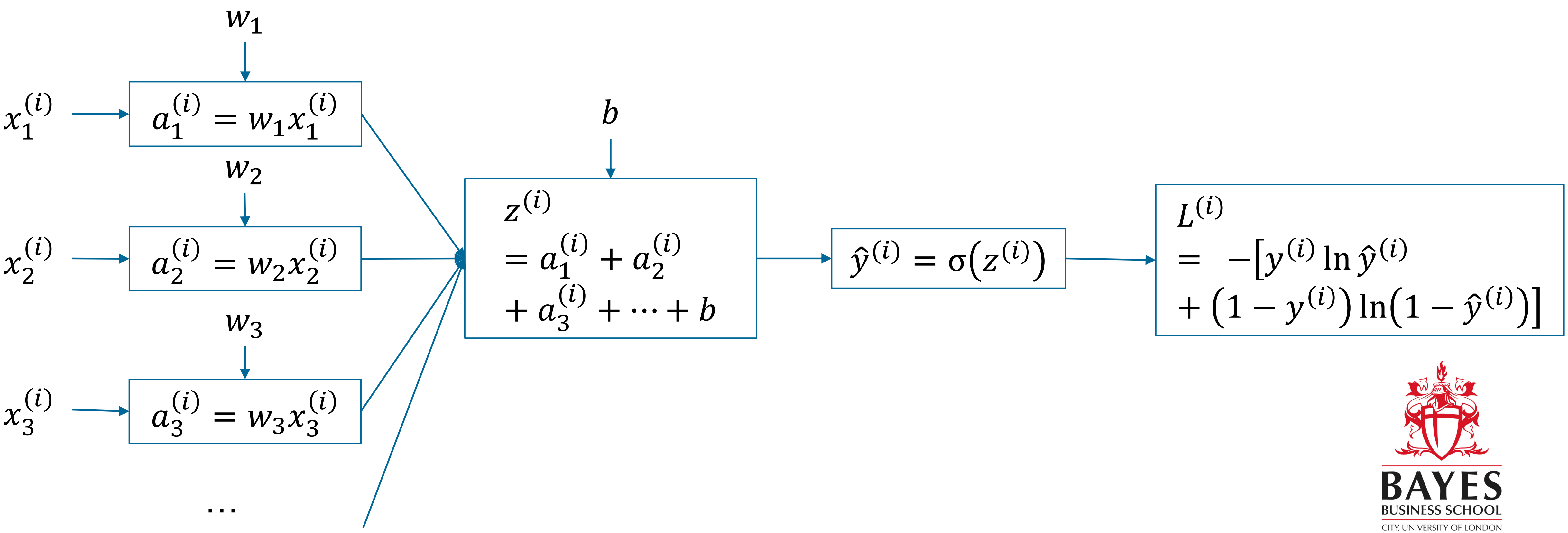
Wait a second, how do we find all those derivatives?

- We can use again the computation graph!
- Recall that $\hat{y}^{(i)} = \frac{1}{1+e^{-\left(\boldsymbol{x}^{(i)}\boldsymbol{w}+\boldsymbol{b}\right)}} = \sigma\left(\boldsymbol{x}^{(i)}\boldsymbol{w} + b\right)$



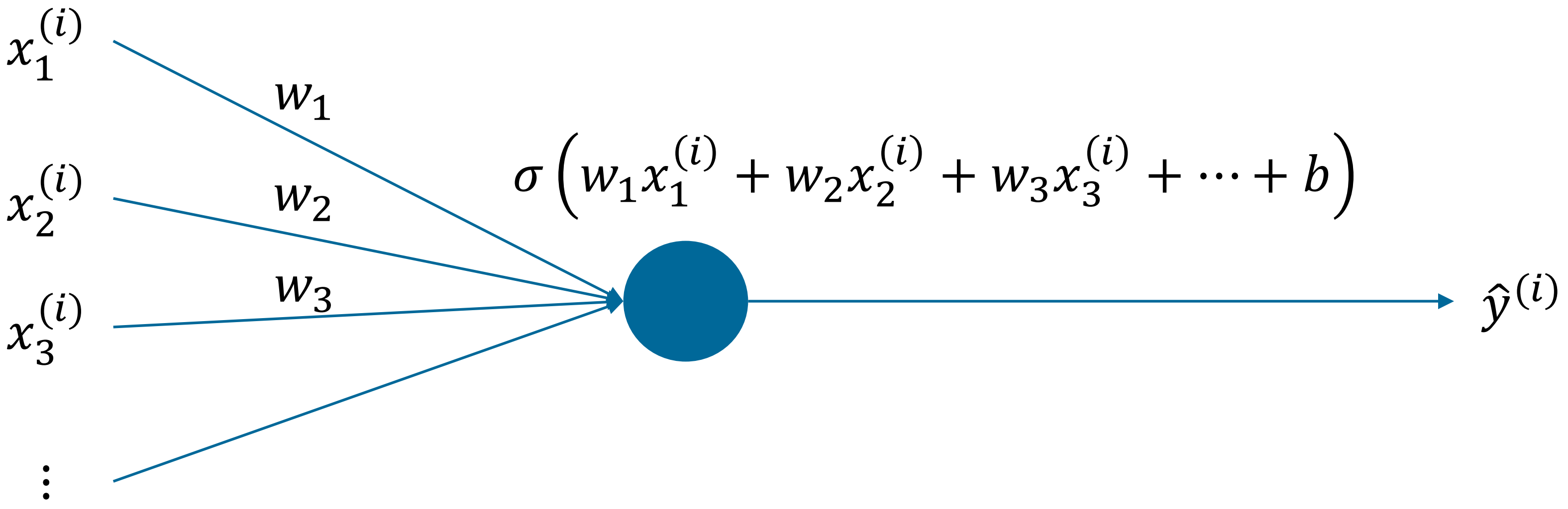
As the same parameters influence all examples, we have to consider one final step

- Recall that $J(\boldsymbol{w}, b) = -\frac{1}{n}\sum_{i=1}^{n}\left[y^{(i)} \ln \hat{y}^{(i)} + \left(1 - y^{(i)}\right) \ln\left(1 - \hat{y}^{(i)}\right)\right] = \frac{1}{n}\sum_{i=1}^{n} L^{(i)}$
- We have that $\frac{\partial J(\boldsymbol{w},b)}{\partial w_j} = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial L^{(i)}}{\partial w_j}$

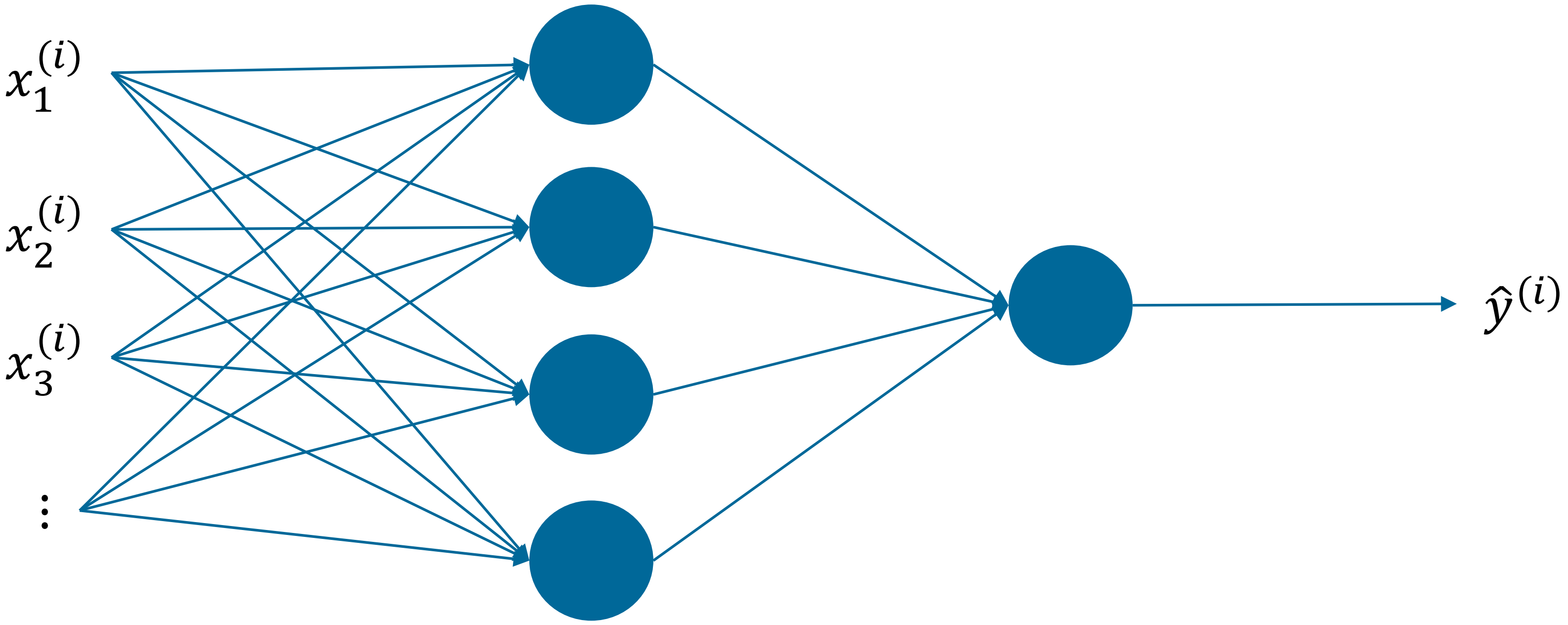
We can now implement a logistic regression

Visualizing a logistic regression – our first neural network

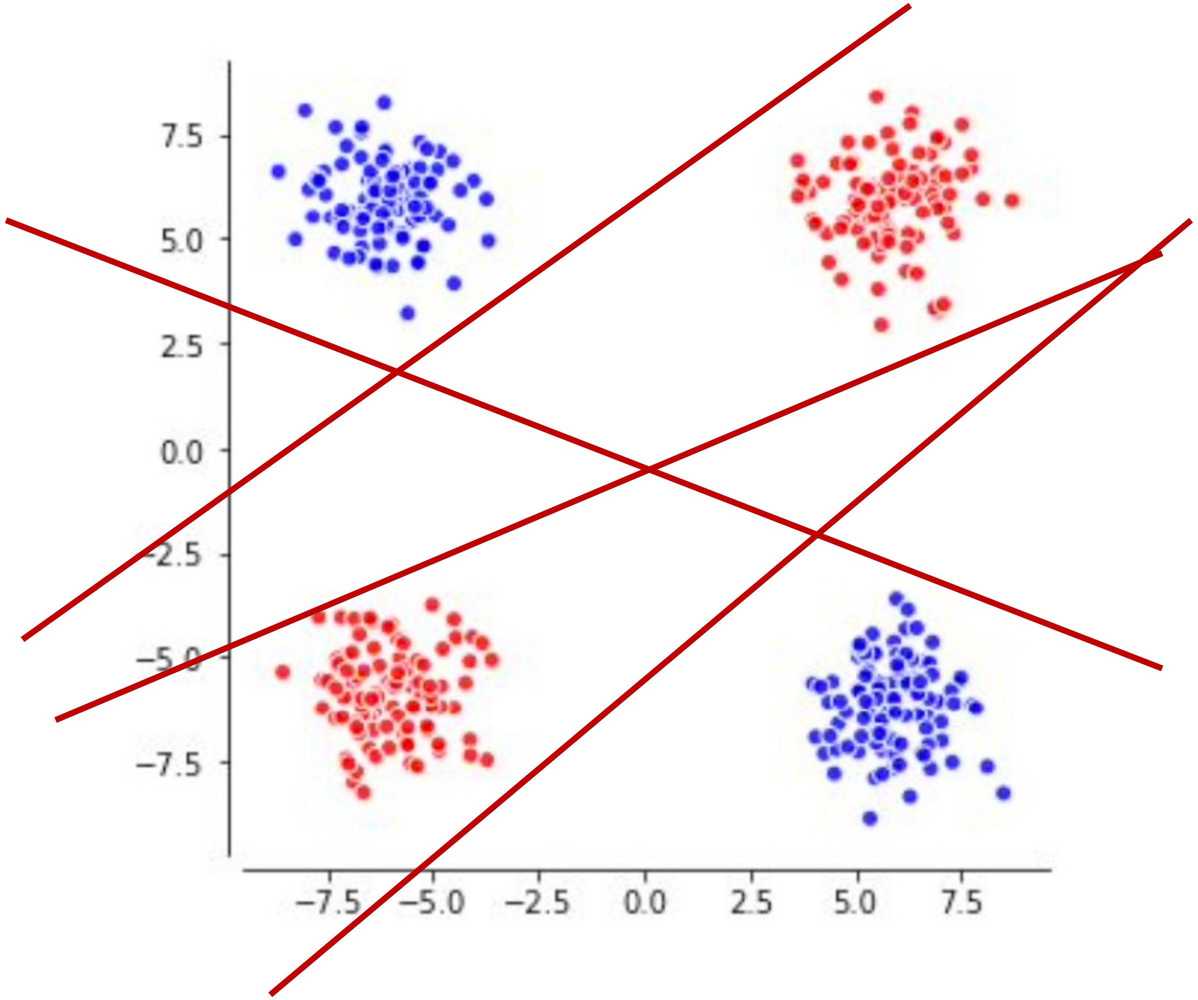
Schema of a logistic regression



Putting multiple neurons together



What neurons learn



Source: Czarnecki

Training neural networks visually

Open https://playground.tensorflow.org/

1. A simple case of binary classification:
   - Change to the pattern on the lower left
   - Set the level of “Noise” to 50
   - Set “Ratio of training to test data” to 50%
   - Set up the neural network: 1 hidden layer, 1 neuron, then press play
   - Answer the following questions:
     - Did the training eventually find a model that seems to capture the pattern in the data?
     - How would you describe the pattern the model captured?
     - Record the “Training loss” and “Test loss”
   - How do your answers change when you select the pattern at the top right? What about setting the noise to 0?

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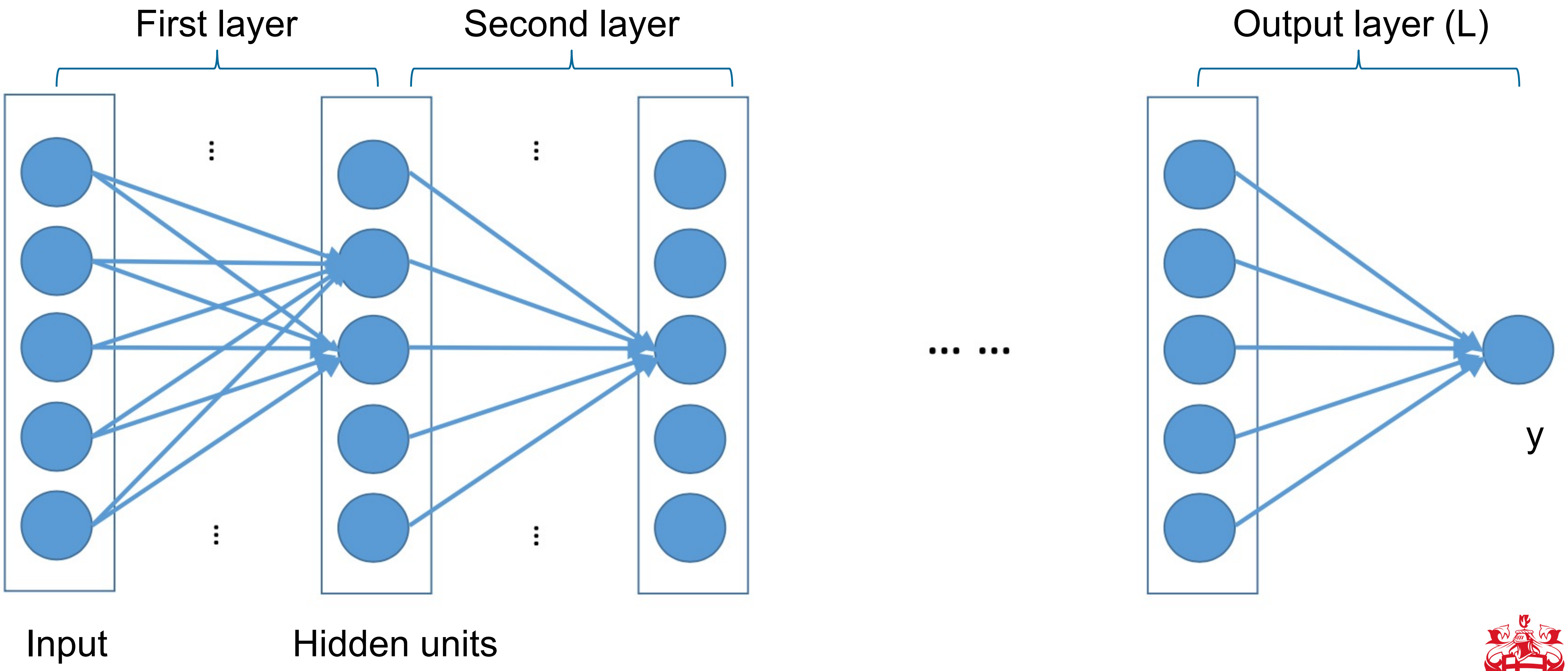
Training neural networks visually

2. A shallow neural network:
- Stick with the pattern at the top right, a noise of 0 and a ratio of 50%
- Now use 3 neurons for your hidden layer
- Answer the three questions from before:
  - Did the training eventually find a model that seems to capture the pattern in the data?
  - How would you describe the pattern the model captured?
  - Record the “Training loss” and “Test loss”
- How do your answers change when you use 6 neurons instead?

3. A deep neural network:
- Use a second hidden layer, with 3 neurons each (and the other setups from 2.)
- How do your answers change now?

Key components of a neural network

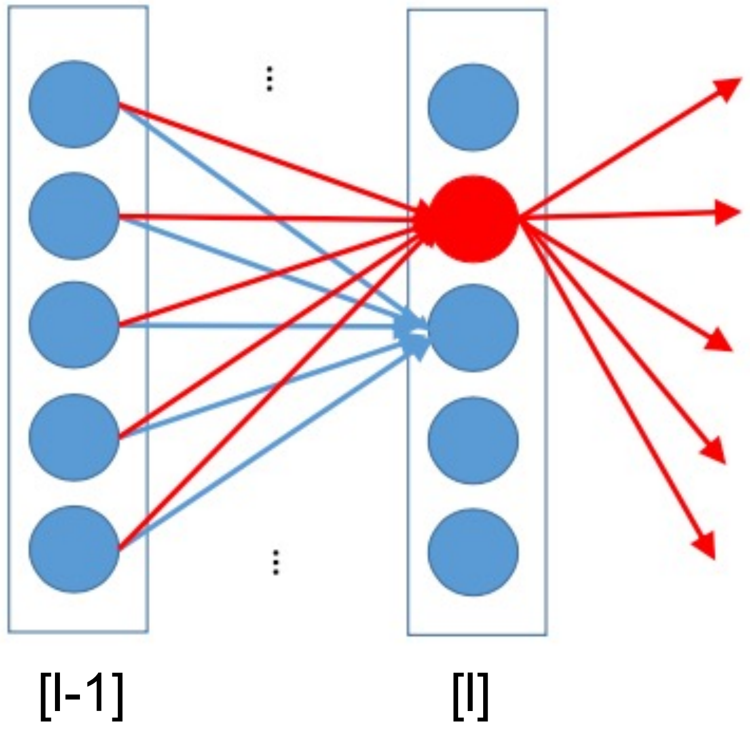
Components



Source: Liang

Hidden layers

$$\text{“}\boldsymbol{x}\text{”} = \boldsymbol{a}^{[l-1]} \qquad z = \boldsymbol{a}^{[\boldsymbol{l}-\mathbf{1}]}\boldsymbol{w} + \boldsymbol{b} \qquad f(\mathrm{z})$$



- f is what we call an “activation function”
- There are many activation functions, and new ones are invented all the time
- Many of these functions do just fine, or slightly better than existing ones

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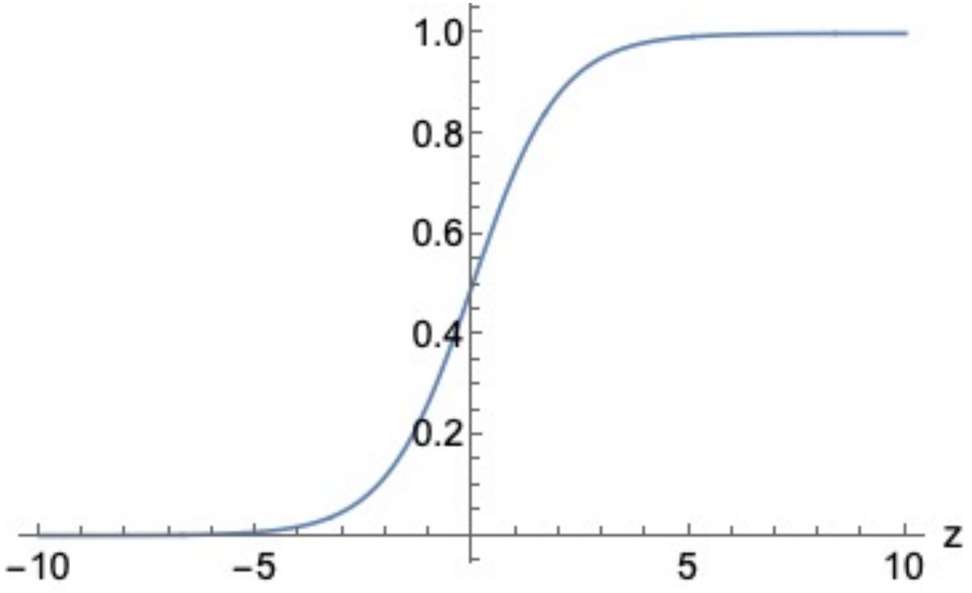
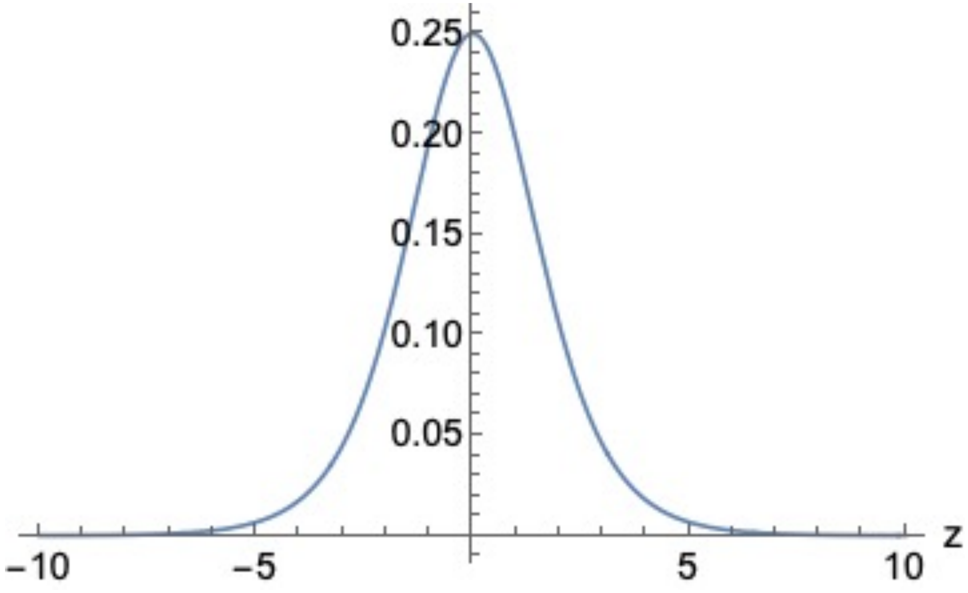
Typical activation functions: logistic (sigmoid) function

Logistic (sigmoid) function



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

Derivative



$$f'(z) = \sigma(z)\big(1 - \sigma(z)\big)$$

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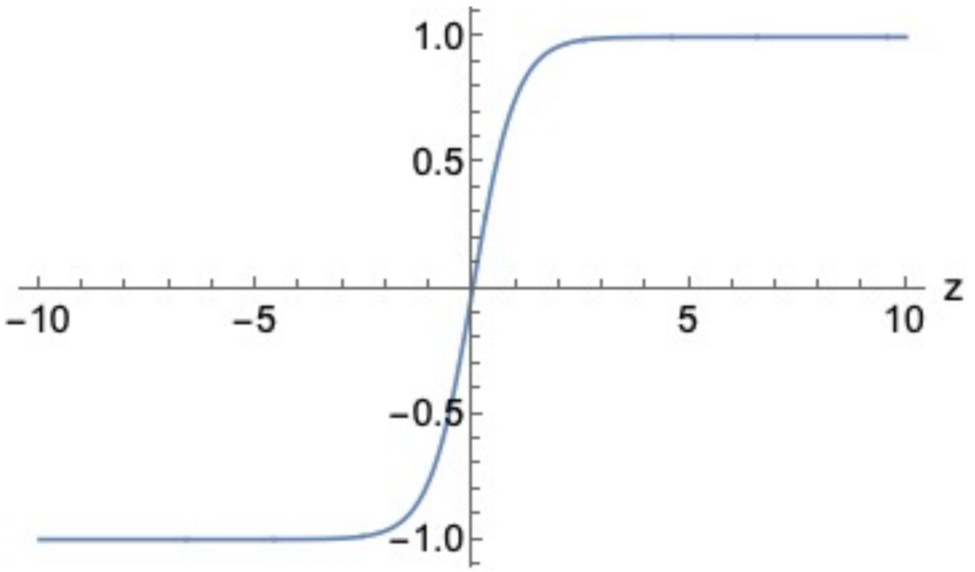
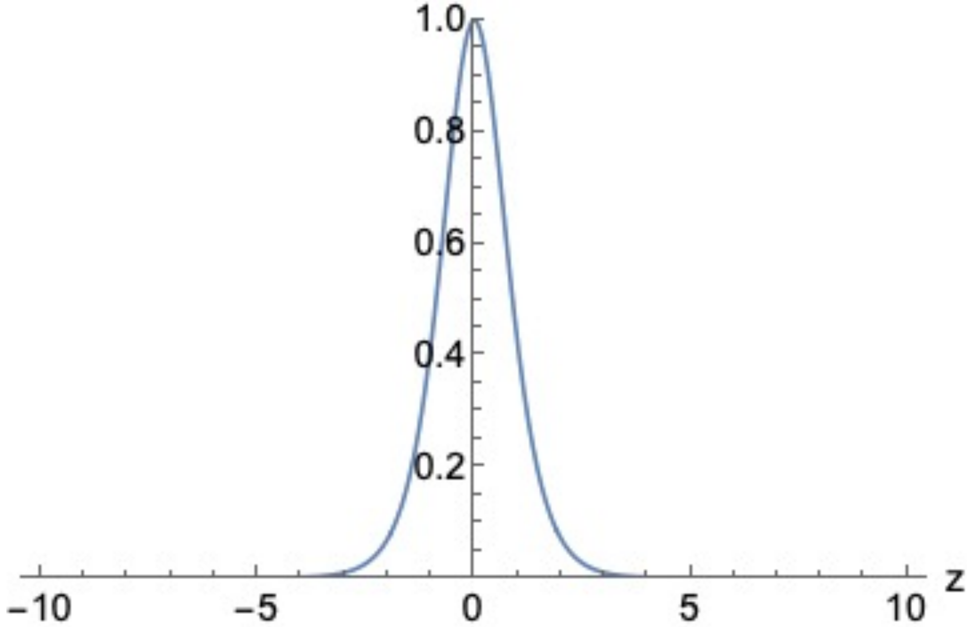
Typical activation functions: hyperbolic tangent

Hyperbolic tangent



$$f(z) = \tanh(z) = \frac{e^{2z} - 1}{e^{2z} + 1}$$

Derivative



$$f'(z) = \operatorname{sech}(z)^2$$

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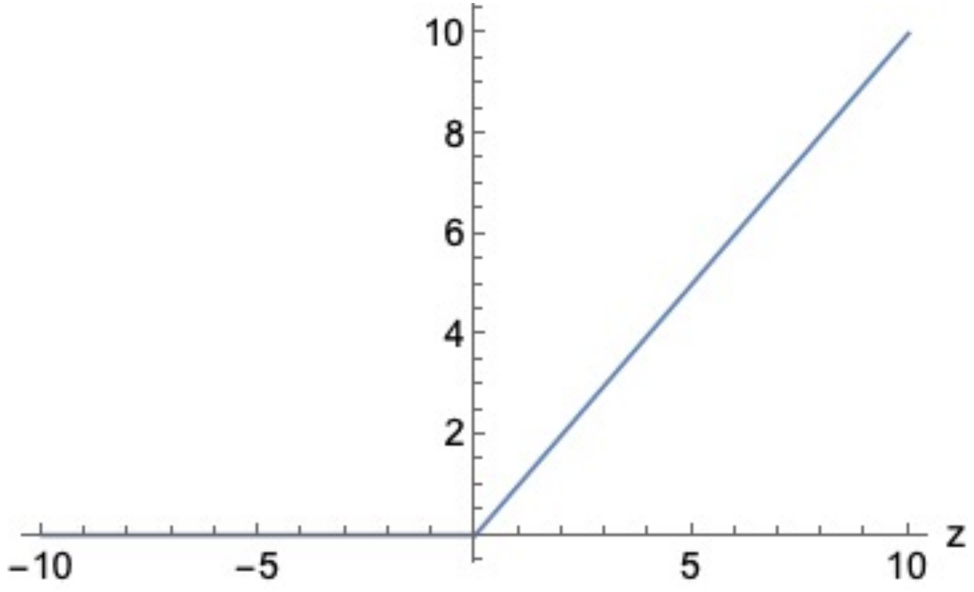
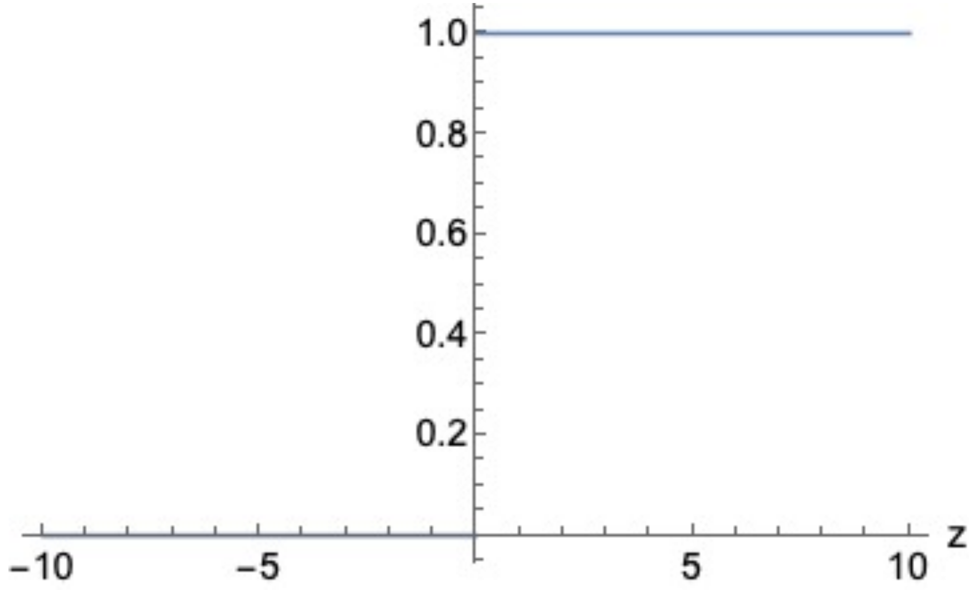
Typical activation functions: Rectified Linear Unit

Rectified Linear Unit (ReLU)



$$f(z) = \max\{0, z\}$$

“Derivative”



$$f'(z) = \begin{cases} 0, if\ z < 0 \\ 1, if\ z > 0 \end{cases}$$

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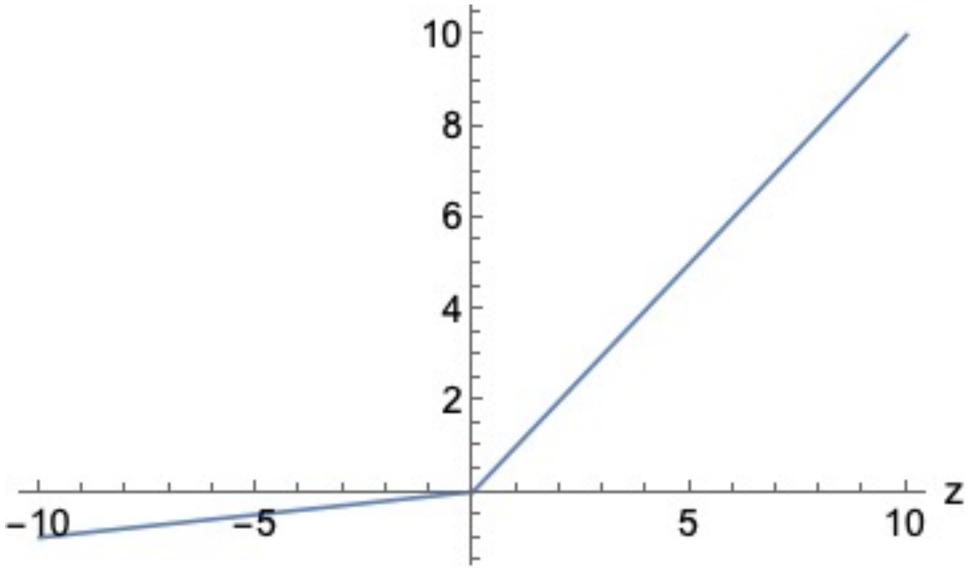
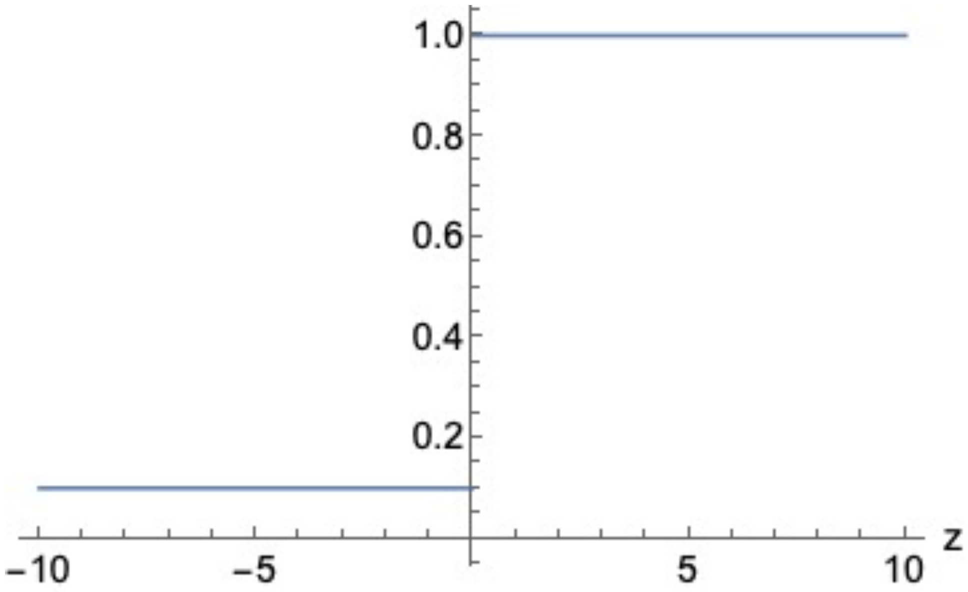
Typical activation functions: Leaky ReLU

Leaky ReLU



$$f(z) = \max\{0.1, z\}$$

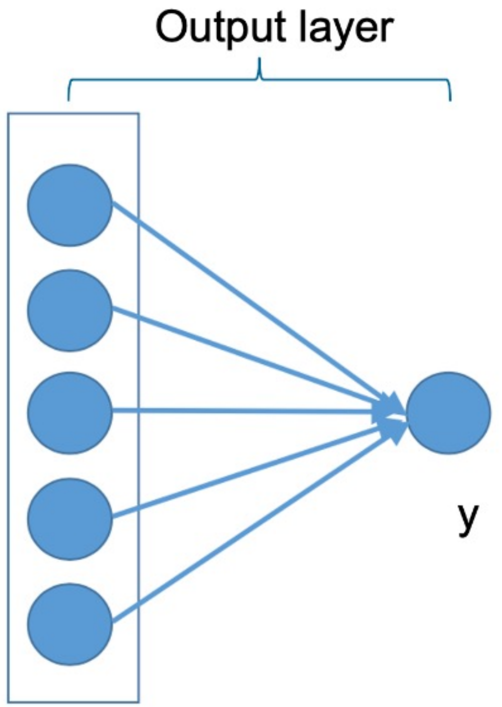
"Derivative"



$$f'(z) = \begin{cases} 0.1, if\ z < 0 \\ 1, if\ z > 0 \end{cases}$$

Binary classification

- Input: $\boldsymbol{a}^{[L-1](i)}$
- As usual, we make a linear transformation: $z^{[L](i)} = \boldsymbol{a}^{[L-1](i)}\boldsymbol{w}^{[L]} + b^{[L]}$
- We then use the logistic sigmoid function $\hat{y}^{(i)} = f\left(z^{[L](i)}\right) = \sigma(z^{[L](i)}) = \frac{1}{1+e^{-z^{[L](i)}}}$
- We can interpret the output as the probability of $y^{(i)} = 1$



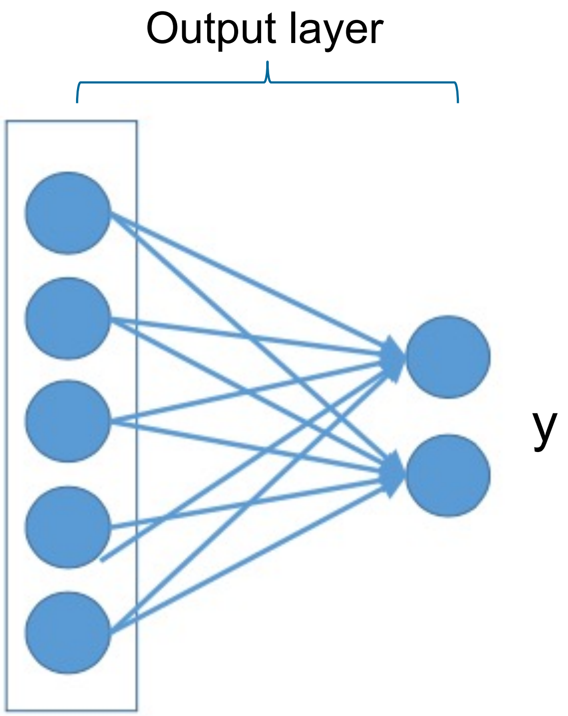
Source: Liang

Multi-class classification

- We again make a linear transformation with a matrix of weights: $\boldsymbol{z}^{[L](i)} = \boldsymbol{a}^{[L-1](i)}\boldsymbol{W}^{[L]} + \boldsymbol{b}^{[L]}$
- Note that $\boldsymbol{z}^{[L](i)} = \begin{pmatrix} z_1^{[L](i)} & z_2^{[L](i)} & \cdots & z_K^{[L](i)} \end{pmatrix}$
- We then use the softmax function on each of the outputs:

$$\hat{y}_k^{(i)} = f\left(\boldsymbol{z}^{[L](i)}\right) = \frac{e^{-z_k^{[L](i)}}}{\sum_{k=1}^{K} e^{-z_k^{[L](i)}}}$$

- This implies that $\hat{y}_k^{(i)} \in (0,1)$ and $\sum_{k=1}^{K} \hat{y}_k^{(i)} = 1$
- Hence, we can interpret $\hat{y}_k^{(i)}$ as the probability that $y^{(i)} = k$ ("belongs to class k")



Source: Liang

Cost functions

- Recall from logistic regression:

$$J(\boldsymbol{w}, b) = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} = -\frac{1}{n}\sum_{i=1}^{n}\left[y^{(i)} \ln \hat{y}^{(i)} + \left(1 - y^{(i)}\right) \ln\left(1 - \hat{y}^{(i)}\right)\right]$$

- Generally, to learn parameters $\boldsymbol{\theta}$, we define the cross-entropy

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L^{(i)} = -\frac{1}{n}\sum_{i=1}^{n} \ln p_{\boldsymbol{\theta}}\left(y^{(i)} \middle| \boldsymbol{x}^{(i)}\right)$$

- Also known as "maximum likelihood estimator"

- Mean square error tends to perform poorly, especially when we have activation functions with e^z

Generalizing our optimization algorithm

1. Decide a "learning rate" α
2. Start with some parameters $\boldsymbol{\theta}$ and compute $J(\boldsymbol{\theta})$ (forward propagation)
3. Until J "doesn't change" anymore:
   - Let $\boldsymbol{\theta} := \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ (back-propagation)
   - Recompute $J(\boldsymbol{\theta})$ (forward propagation)

Initializing parameters

- Initialize weights to small random values (e.g., *np.random.randn(**shape of W**) * 0.01*)

- Bias terms can be initialized randomly, but can also just be initialized to zero (e.g., *np.zeros(**shape of b**)*)

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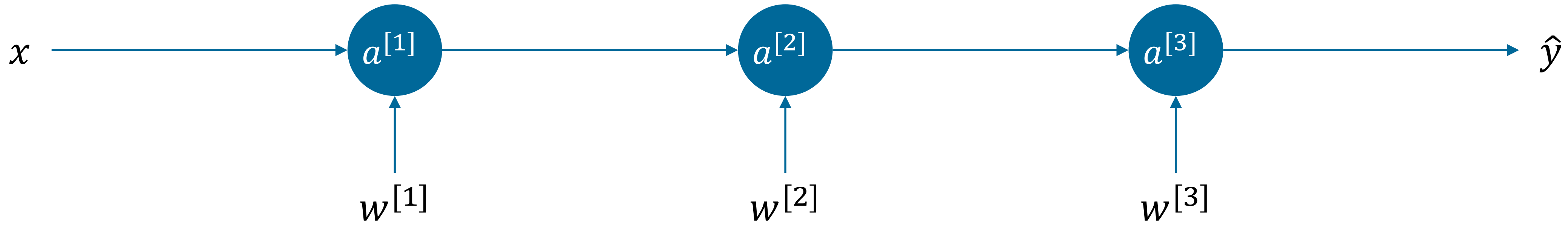
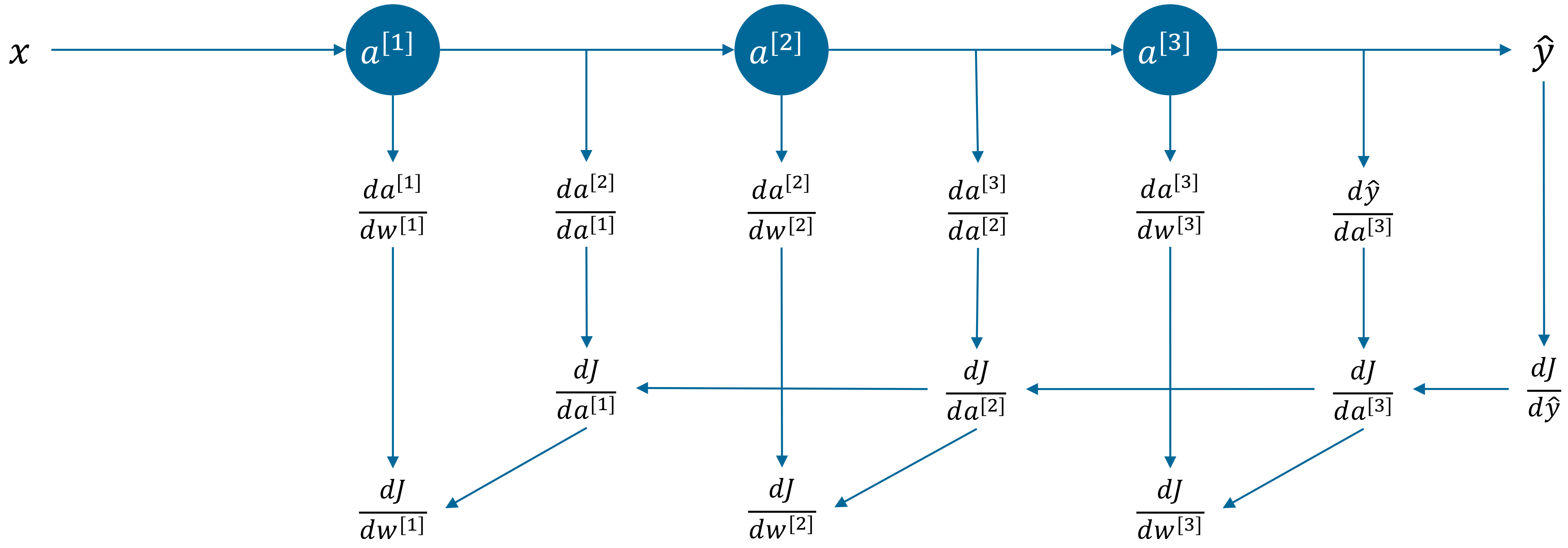
Step 1: Forward propagation through the computational graph



Step 2: Back-propagation through the computational graph



See you next week!