Foundations of Data Science, Fall 2020

13. Neural Networks I

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Data • (Systems+Theory)

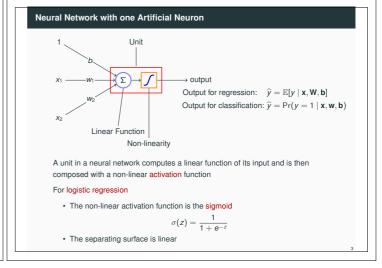
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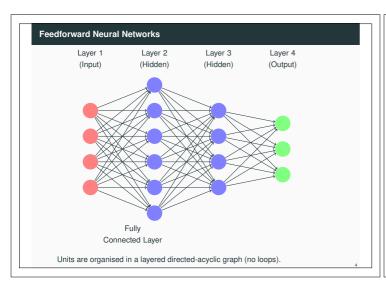
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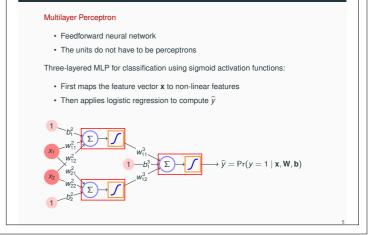
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## Today, we'll study feedforward neural networks • Multi-layer perceptrons • Classification or regression settings • Backpropagation to compute gradients

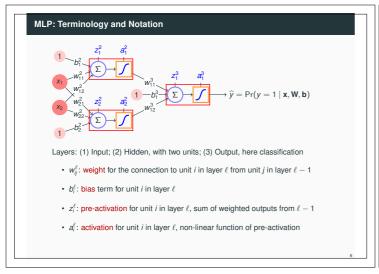
## Recall: The Perceptron Perceptron • Input: Feature vector $\mathbf{x}$ and label $\mathbf{y}$ • Output: $sign(b + \mathbf{w} \cdot \mathbf{x})$ , where b = bias term, $\mathbf{w} = weight$ parameters Artificial neuron (unit): generalisation of perceptron • Activation function $f : \mathbb{R} \to \mathbb{R}$ • Output: $f(b + \mathbf{w} \cdot \mathbf{x})$ • Can be used to build Boolean gates (recall Exercise Sheet 2) Neural Networks: Composition of artificial neurons into networks • Can compute any function that a computer can • The units have continuous activation functions • Suitably chosen loss function for any input-output is a differentiable function

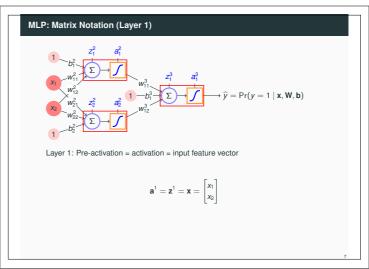


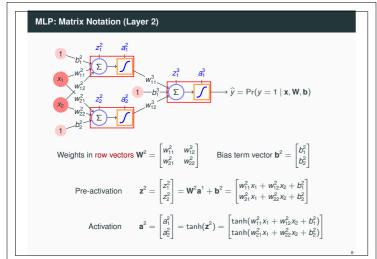


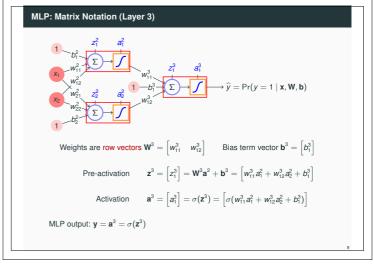


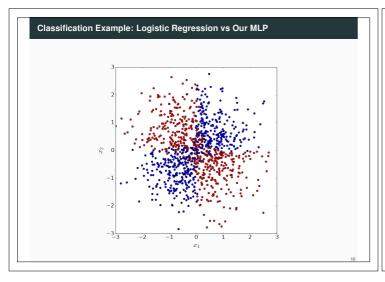
Multilayer Perceptron (MLP)

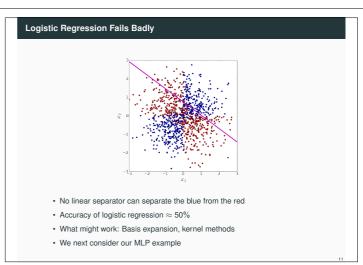


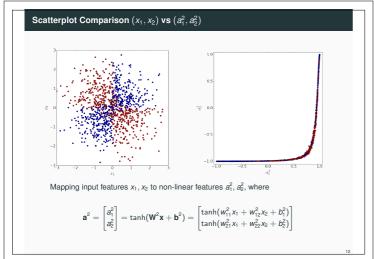


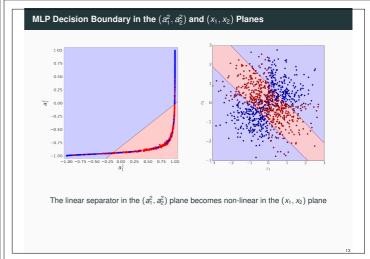


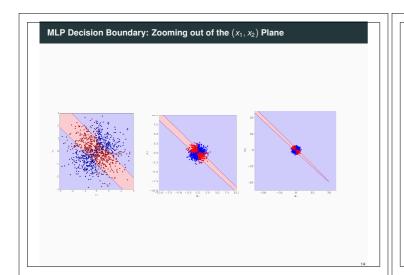












Compute the derivatives for all parameters of the MLP for each data point
 Average the derivatives over the training data points
 Common: Average over a mini-batch instead of the entire dataset
 Perform a gradient descent step to update the model parameters
 Learning the weights is guided by the error at every iteration
 Error at output node gets back propagated to every layer
 Weights adjusted in the next step proportionally to the error and weights
 Larger weights get assigned larger error since they contribute more to the overall error

## **Background: Computing Derivatives**

• Vector  $\mathbf{z} \in \mathbb{R}^n$ , function  $f : \mathbb{R}^n \to \mathbb{R}$ . Then  $\frac{\partial f}{\partial \mathbf{z}} \in \mathbb{R}^n$  is the row vector

$$\frac{\partial f}{\partial \mathbf{z}} = \begin{bmatrix} \frac{\partial f}{\partial z_1} & \cdots & \frac{\partial f}{\partial z_n} \end{bmatrix}$$

• Function  $f: \mathbb{R}^n \to \mathbb{R}^m$ , where  $(f(\mathbf{z}))_i = f_i(\mathbf{z})$ . Then  $\frac{\partial f}{\partial \mathbf{z}}$  is the  $m \times n$  Jacobian

$$\frac{\partial f}{\partial \mathbf{z}} = \begin{bmatrix} \frac{\partial f_1}{\partial z_1} & \cdots & \frac{\partial f_1}{\partial z_n} \\ \vdots & \vdots & \vdots \\ \frac{\partial f_m}{\partial z_1} & \cdots & \frac{\partial f_m}{\partial z_n} \end{bmatrix}$$

• Matrix  $\mathbf{W} \in \mathbb{R}^{n \times m}$ , function  $f : \mathbb{R}^{n \times m} \to \mathbb{R}$ . Then  $\frac{\partial f}{\partial \mathbf{z}} \in \mathbb{R}^{n \times m}$  is the matrix

$$\frac{\partial f}{\partial \mathbf{W}} = \begin{bmatrix} \frac{\partial f}{\partial w_{11}} & \cdots & \frac{\partial f}{\partial w_{1m}} \\ \vdots & \vdots & \vdots \\ \frac{\partial f}{\partial w_{n1}} & \cdots & \frac{\partial f}{\partial w_{nm}} \end{bmatrix}$$

**Background: Chain Rule for Multivariate Calculus** 

Functions 
$$f: \mathbb{R}^n \to \mathbb{R}^k, g: \mathbb{R}^k \to \mathbb{R}^m, h = g \circ f: \mathbb{R}^n \to \mathbb{R}^m$$
  
For  $\mathbf{x} \in \mathbb{R}^n$ , let  $\mathbf{z} = f(\mathbf{x})$ 

$$\frac{\partial h}{\partial \mathbf{x}} = \frac{\partial h}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{x}}$$

•  $\frac{\partial h}{\partial \mathbf{x}}$  is an  $m \times n$  Jacobian matrix

•  $\frac{\partial h}{\partial x}$  is an  $m \times k$  Jacobian matrix

•  $\frac{\partial \mathbf{z}}{\partial \mathbf{x}}$  is an  $k \times n$  Jacobian matrix

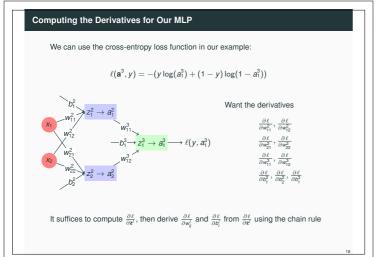
Chain rule is the core technique behind the backpropagation algorithm

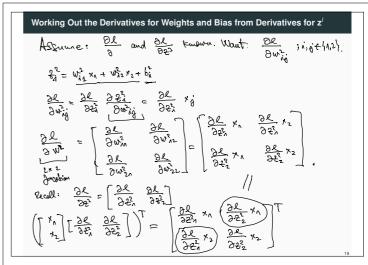
Modular computation of derivatives of neural networks

• Efficient: Decompose derivatives into reusable building blocks

Alternative approach: Ad-hoc computation of derivatives for arbitrary functions

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Working Out the Derivatives for Weights and Bias from Derivatives for 
$$z'$$

$$\frac{\partial \mathcal{L}}{\partial u^{1}} = \left(x \frac{\partial \mathcal{L}}{\partial z^{2}}\right)^{T}$$
Similarly, 
$$\frac{\partial \mathcal{L}}{\partial u^{1}} = \left(a^{1} \frac{\partial \mathcal{L}}{\partial z^{2}}\right)^{T}$$

$$\frac{\partial \mathcal{L}}{\partial u^{1}} = \left(a^{1} \frac{\partial \mathcal{L}}{\partial z^{2}}\right)^{T}$$

$$\frac{\partial \mathcal{L}}{\partial u^{2}} = \left(a^{1} \frac{\partial \mathcal{L}}{\partial z^{2}}\right)^{T}$$

$$\frac{\partial \mathcal{L}}{\partial u^{2}} = \frac{\partial \mathcal{L}}{\partial z^{2}}$$

