Introduction to Neural Networks

Learning from Scratch

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Course Objectives

The objectives of this lecture would be:

- Recap **regression** and **classification** techniques.
- Understand key ideas from scratch in **neural networks**.
- Build and train simple **neural networks** from scratch and also using **TensorFlow**.
- Bridge **traditional statistical regression methods** with **neural network**.

Some Good References

- Bishop, C. M. (2007). *Pattern Recognition and Machine Learning*. Springer.
- Géron, A. (2022). *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow* (3rd ed.). O'Reilly. [GitHub companion code]
- Goodfellow, I., Bengio, Y., & Courville, A. (2016). *Deep Learning*. MIT Press. [Free online]
- Chollet, F. (2021). *Deep Learning with Python* (2nd ed.). Manning.
- Nielsen, M. A. (2015). *Neural Networks and Deep Learning*. [Free online book]
- Online learning platforms:
  - Coursera - Deep Learning Specialization
  - fast.ai - Practical Deep Learning for Coders
  - DeepLearning.AI

Recap: Regression and Classification

Supervised Learning: General Framework

- **Goal:** Learn (estimate) a function $f(\mathbf{x}; \mathbf{w})$ that maps several input features $\mathbf{x}$ to an output variable y.

$$y \approx f(\mathbf{x}; \mathbf{w}) \quad \text{(there will be some error terms as well)}$$

- **Data:** A collection of input–output pairs

$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$$

  - Inputs (features): $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^\top$
  - Outputs (targets): y_i (numeric or categorical)

- **Learning:** Estimate the unknown parameters (weights in machine learning) $\mathbf{w}$ by minimizing a suitable **loss function** $\mathcal{L}(\mathbf{w})$.
- **Prediction:** Once $\hat{\mathbf{w}}$ is obtained, use

$$\hat{y} = f(\mathbf{x}_0; \hat{\mathbf{w}})$$

  for new input $\mathbf{x}_0$.

Regression Models

- **Task:** Predict a continuous output $y \in \mathbb{R}$.
- **One simpler model (Assume f is linear in w):** Multiple Linear Regression (MLR)

$$y_i = w_0 + w_1 x_{i1} + w_2 x_{i2} + \cdots + w_p x_{ip} + \varepsilon_i$$

- **Loss function (Mean Squared Error):**

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

- **Ordinary Least Squares (OLS) solution:**

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

where

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- **Important Note**: For all regression types of problems, we might not get the closed-form expressions of $\hat{\mathbf{w}}$.

Classification Models

- **Task:** Predict a categorical output $y \in \{1, 2, \ldots, K\}$.
- **Model:** Logistic regression (binary or multinomial)

$$P(Y = k \mid \mathbf{x}, \mathbf{w}) = \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x})}$$

- **Loss function (Cross-Entropy / Log-Loss):**

$$\mathcal{L}(\mathbf{w}) = -\sum_{i=1}^{n} \sum_{k=1}^{K} \mathbf{1}\{y_i = k\} \log P(Y = k \mid \mathbf{x}_i, \mathbf{w})$$

- **Estimation:** No closed-form solution; parameters $\mathbf{w}$ are found using iterative optimization methods (e.g., gradient descent, Adam, Newton–Raphson etc.)
- **Prediction:** Assign the class with the highest predicted probability

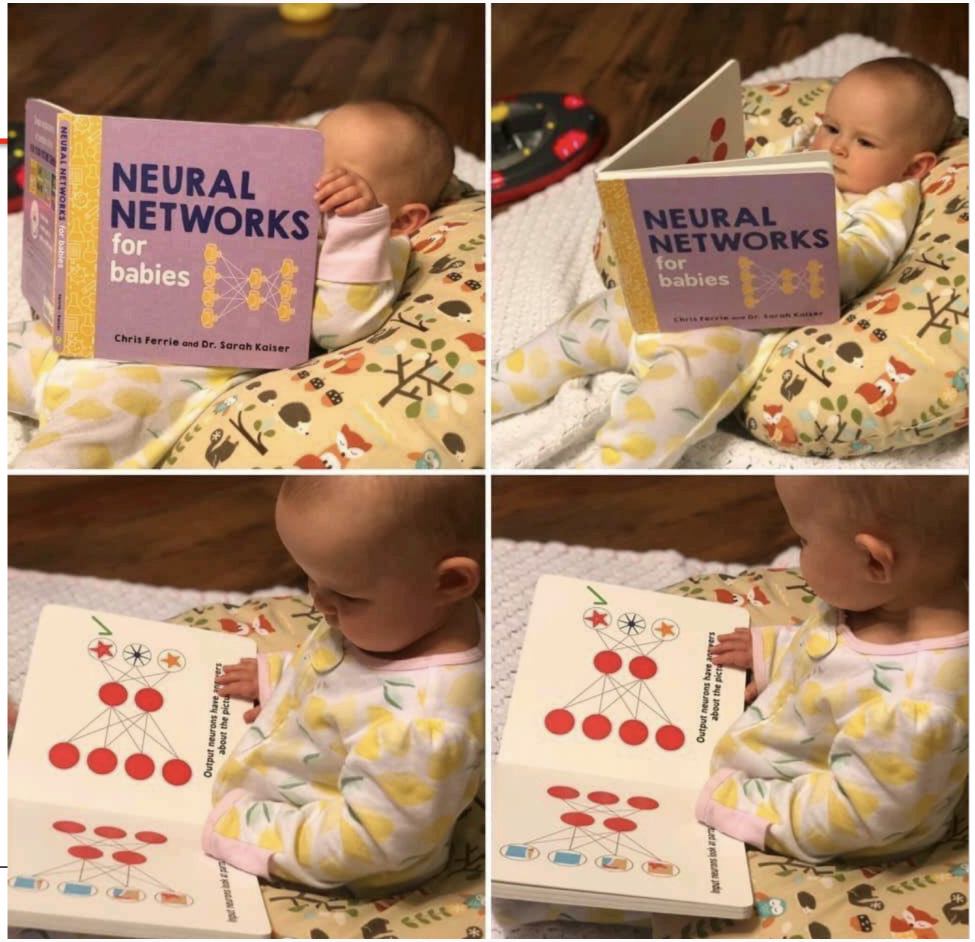
$$\hat{y}_i = \arg \max_{k \in \{1, \ldots, K\}} P(Y = k \mid \mathbf{x}_i, \mathbf{w})$$

Neural Networks

Everybody is learning

Never too late

😀



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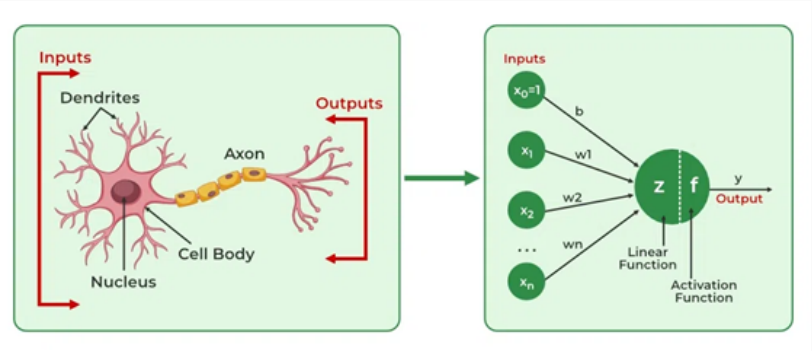
[1] CS 229: Prof. Xiangliang Zhang (KAUST)

Agenda

What is a Neural Network?

- Neural networks mimic how the human brain functions.
- Brain activity occurs when a **stimulus** enters the system; information is processed through the network via neurons that extract relevant information, and this information is passed to another area.
- A **Neural Network** is a computational model inspired by the way biological neural networks in the human brain process information. It consists of **layers** of interconnected **nodes**, or **neurons**, which work together to solve complex problems.



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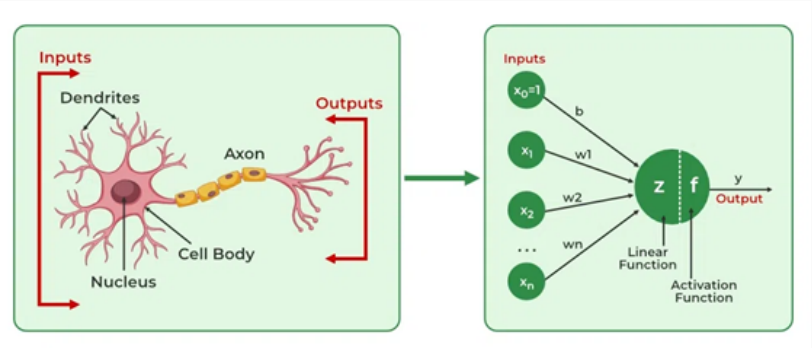
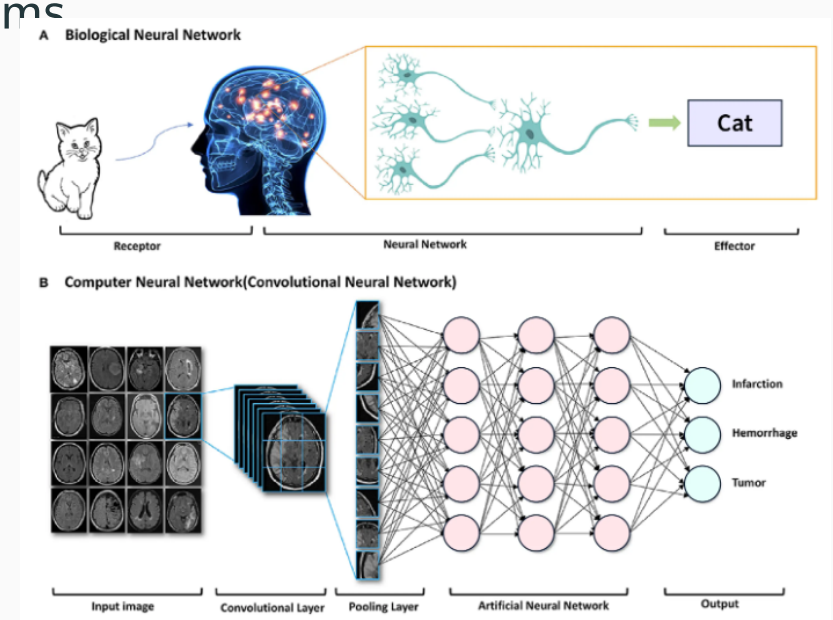




Historical Development of Deep Learning

- **Early Origins (1940s–1960s)**: McCulloch–Pitts (1943): first neuron model, Rosenblatt's Perceptron (1958): first trainable neural network.
- **First AI Winter (1970s)**: Minsky & Papert (1969) show perceptron limits (XOR), Loss of funding & shift to symbolic AI.
- **Backpropagation Revolution (1980s)**: Werbos (1974), Rumelhart–Hinton–Williams (1986) $\rightarrow$ training multi-layer NNs.
- **Second AI Winter (1987–1995)**: Hardware & data insufficient, neural nets sidelined; symbolic/statistical AI rise.
- **Statistical Learning Era (1990s–2000s)**: SVMs (Vapnik), Probabilistic Graphical Models (Pearl), strong math foundations (optimization, RKHS).
- **Deep Learning Boom (2006–2015)**: DBNs (Hinton) in 2006, ImageNet/AlexNet (2012), Word2Vec, GANs.
- **Modern Era (2017–Present)**: Transformers (2017), LLMs (GPT, BERT), AlphaGo, Diffusion Models, Multimodal AI.

Components of Neural Networks

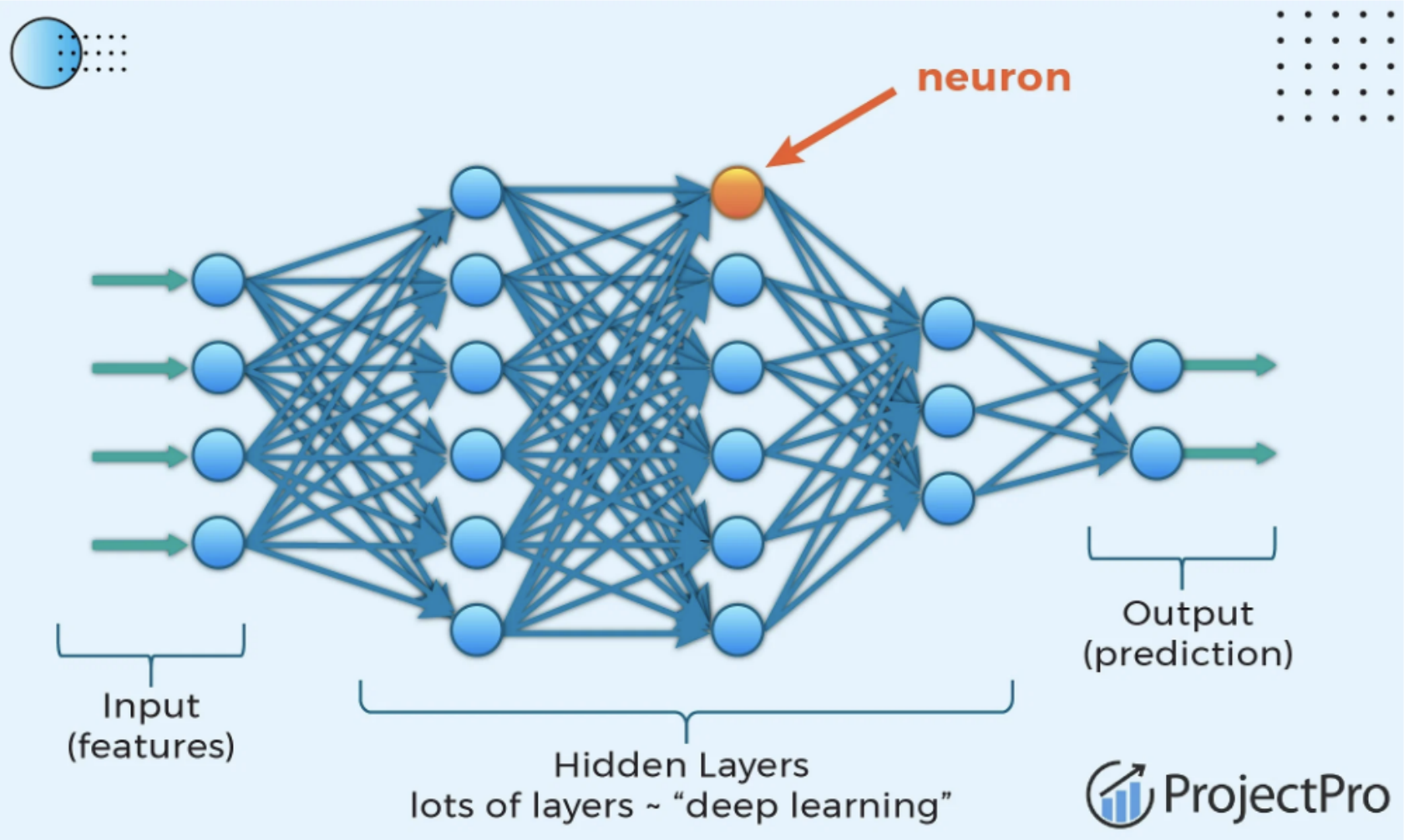
Structural Components

- Layers
- Neurons
- Weights
- Bias
- Activation Functions

Training-Related Components

- Loss Function
- Learning Rate
- Training Data
- Validation and Test Data
- Forward Propagation and Backpropagation

A Basic Architectures of Neural Networks



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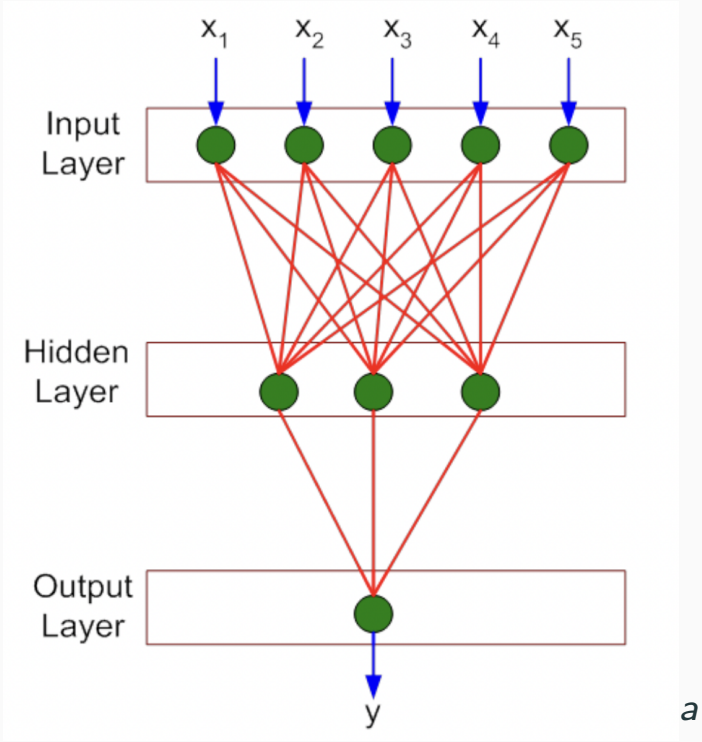
Layers

Neural computing requires a number of neurons, to be connected together into a neural network. Neurons are arranged in layers.

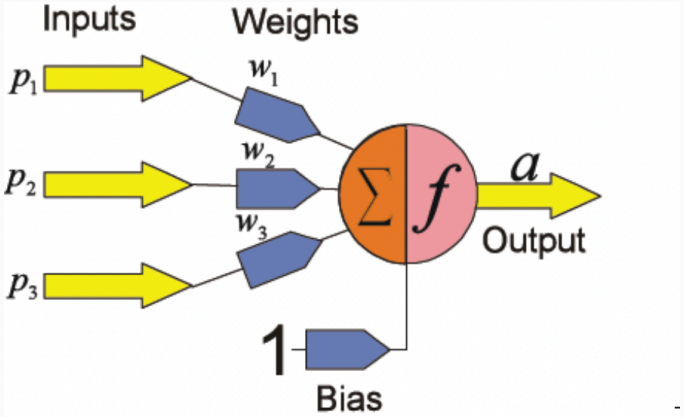
- **Input Layer**
  - First layer of neurons.
  - Receives raw data directly from the input features.
- **Hidden Layers**
  - Layers between the input and output layers.
  - Perform computations.
  - Can have one or many hidden layers.
- **Output Layer**
  - Final layer.
  - Produces the network's output.
  - Structure depends on the specific task (e.g., classification, regression).



[a] CS 229: Prof. Xiangliang Zhang (KAUST)

Neurons, Weights, and Biases

- **Neurons**:
  - Basic units of a neural network.
  - Receive input, process it, and pass it to other neurons.
  - Apply a mathematical function to generate an output.
- **Weights**:
  - Parameters that transform input data within the network.
  - Each connection between neurons has an associated weight.
- **Biases**:
  - Additional parameters in a neuron that allow to fit the data better.
  - Provide ability to each neuron have output not 0 when inputs are 0.



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[3] CS 229: Prof. Xiangliang Zhang (KAUST)

Activation Functions (1)

- Activation functions introduce nonlinearity into the output of a neuron, allowing neural networks to model complex and non-linear relationships.
- While many activation functions exist, they generally satisfy two essential properties:
  - **Nonlinearity**: Without nonlinear activations, the entire network reduces to a pure linear model, regardless of the number of layers.
  - **Continuous differentiability**: Required for gradient-based optimization methods such as backpropagation.
- Activation functions also act similarly to **link functions** in generalized linear models (GLMs), transforming the linear predictor into a scale appropriate for the output.

A single-layer neural network(no hidden layers) is mathematically equivalent to a generalized linear model (GLM).

Activation Functions (2)

Classical Forms

Function	Expression	Pros	Cons	Uses
Sigmoid	$\frac{1}{1+e^{-x}}$	Smooth, bounded, probabilistic output	Vanishing gradients, not zero-centered	Binary classification
Softmax	$\frac{e^{x_i}}{\sum_j e^{x_j}}$	Probabilistic output vector	Sensitive to large logits	Multi-class output
Tanh	$\frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$	Zero-centered, stronger gradients	Saturates, vanishing gradients	RNNs, classical MLPs
ReLU	$\max(0, x)$	Fast, simple, no saturation for $x > 0$	Dying ReLU, unbounded output	CNNs, deep MLPs

Modern Variants

Function	Expression	Pros	Cons	Uses
Leaky ReLU	$\begin{cases} x, & x > 0 \\ \alpha x, & x \leq 0 \end{cases}$	Fixes dying ReLU, small negative slope	Slope α arbitrary	CNNs, MLPs
ELU	$\begin{cases} x, & x > 0 \\ \alpha(e^{x}-1), & x \leq 0 \end{cases}$	Negative outputs stabilize training	Expensive, may saturate	Deep CNNs
Swish	$x\,\sigma(x)$	Smooth, strong empirical performance	Slightly slower	Transformers, modern vision

[4] https://www.analytixlabs.co.in/blog/activation-function-in-neural-network/

Agenda

Notation

- $\mathbf{x} \in \mathbb{R}^d$: d-dimensional input vector (features)
- $\mathbf{W}^{(l)}$: Weight matrix for layer l
- $\mathbf{b}^{(l)}$: Bias vector for layer l
- $\mathbf{z}^{(l)}$: Pre-activation (linear part)
- $\mathbf{a}^{(l)}$: Activation (output) of layer l
- $\sigma(\cdot)$: Activation function (ReLU, sigmoid, etc.)
- Total number of hidden layers will be denoted by H, and dimensions of output would be K.

We define $a^{(0)} = x$ as the input layer.

General Overview

- Forward propagation computes the output of the neural network by passing inputs through each layer.
- Each layer performs:

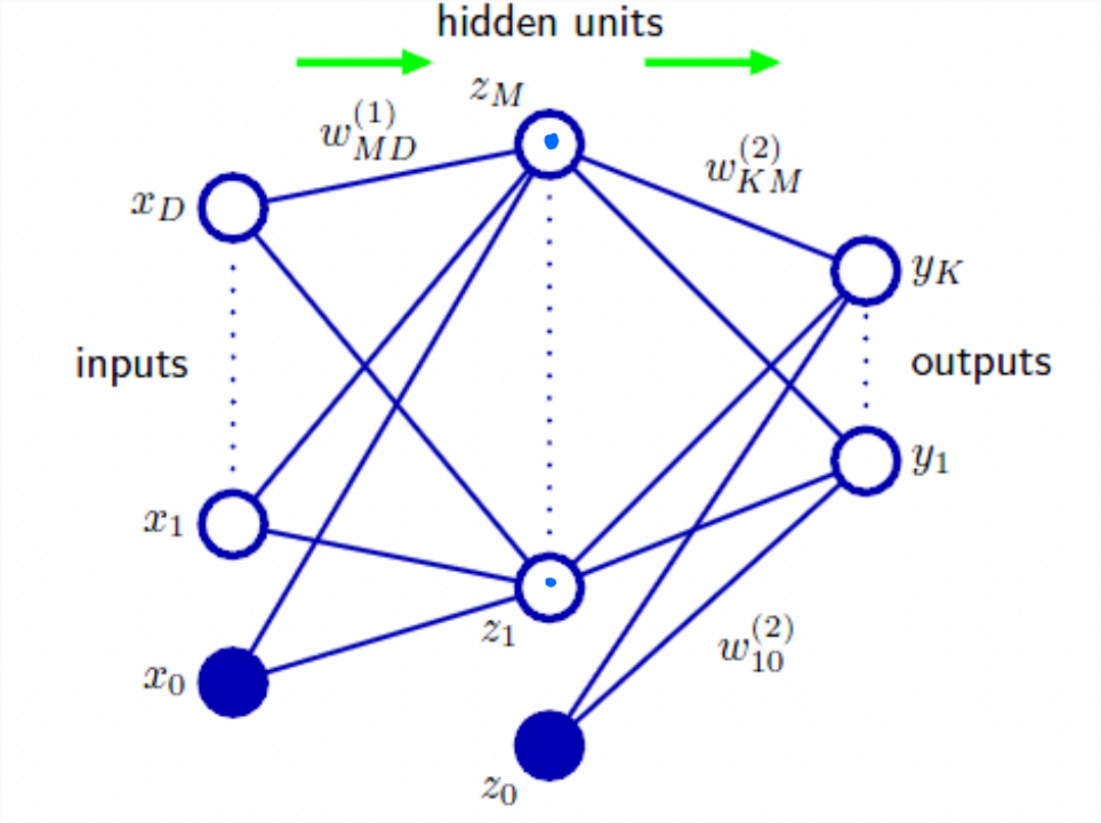
$$\mathbf{z}^{(l)} = \mathbf{W}^{(l)}\mathbf{a}^{(l-1)} + \mathbf{b}^{(l)}$$

  where $\mathbf{W}^{(l)}$ and $\mathbf{b}^{(l)}$ are the learnable parameters.
- The activation function transforms the linear output:

$$\mathbf{a}^{(l)} = \sigma\left(\mathbf{z}^{(l)}\right)$$

- This process continues layer by layer until the final output is produced.

Example: Unfolding a Single-Hidden-Layer (Two-Layer) Neural Network



- D input variables
- M number of hidden neurons
- K outputs
- Use the two activation functions onthe weights sum on hidden layers and output layers

A Two-Layer Neural Network (2)

Construct M linear combinations of the inputs $x_1, \ldots, x_d$

$$z_j^{(1)} = \sum_{i=0}^{D} w_{ji}^{(1)} x_i, \qquad x_0 = 1.$$

- $z_j^{(1)}$ are the pre-activations on j^{th} neurons of hidden layers, $j = 1, \ldots, M$.
- $w_{ji}^{(1)}$ are the layer one weights, $i = 1, \ldots, D$.
- $w_{j0}^{(1)}$ are the layer one biases.

Each linear combination $z_j^{(1)}$ is transformed by a (non-linear differentiable) activation function,

$$a_j^{(1)} = h(z_j^{(1)}),$$

which will be the activation now at the j^{th} neurons of the hidden layer and act as an input for the next layers (here output).

A Two-Layer Neural Network (3)

The hidden outputs $a_j^{(1)} = h(z_j^{(1)})$ are linearly combined in layer two:

$$z_k^{(2)} = \sum_{j=0}^{M} w_{kj}^{(2)} a_j^{(1)}, \qquad z_0 = 1.$$

- $z_k^{(2)}$ are the output pre-activations at the k^{th} output neurons, $k = 1, \ldots, K$.
- $w_{kj}^{(2)}$ are the layer two weights, $j = 1, \ldots, M$.
- $w_{k0}^{(2)}$ are the layer one biases.

The output pre-activations $z_k^{(2)}$ are transformed by the output (non-linear differentiable) activation function

$$y_k = \sigma(z_k^{(2)}).$$

- y_k are the final outputs.
- $\sigma(\cdot)$ is like $h(\cdot)$, but often sigmoid function for classification and linear function for Regressions.

A Two-Layer Neural Network (4)

After substituting $y_k = \sigma(z_k^{(2)})$;

$$y_k(\boldsymbol{x}, \boldsymbol{w}) = \sigma\left(\sum_{i=0}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right).$$

Evaluation of this is called **forward propagation**.

- Here, $h(\cdot)$ and $\sigma(\cdot)$ are activation functions.
- There could be several possibilities of activation function; for example:
  - If If $\sigma(\cdot)$ is the sigmoid function, then a binary classification model is obtained, despite any choice of activation $h(\cdot)$
  - If $\sigma(\cdot)$ is the identity function, then a regression model is obtained.
  - If $\sigma(\cdot)$ $h(\cdot)$ both are identity functions, then we get a Linear regression; for example, MLR