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

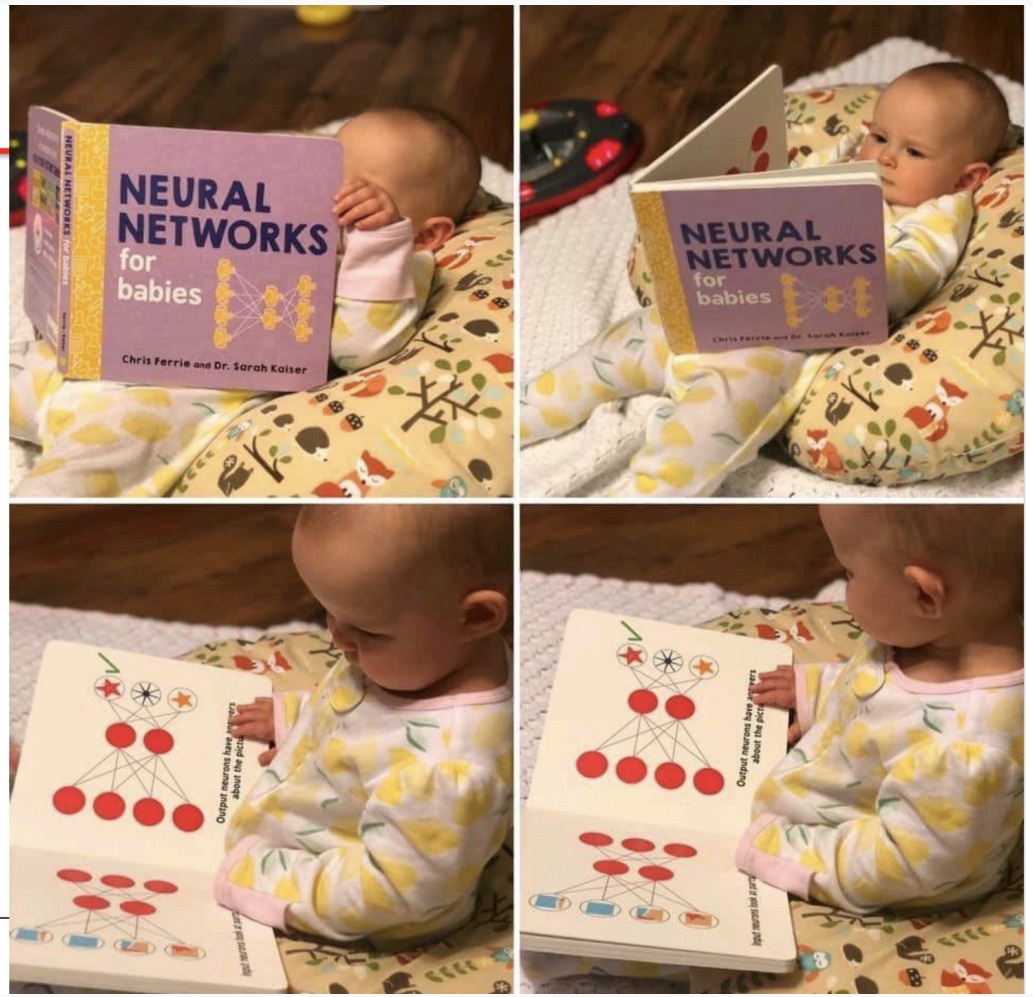
$$\hat{y}_i = \arg \max_{k \in \{1,\ldots,K\}} P(Y = k \mid \mathbf{x}_i, \mathbf{w})$$

Neural Networks

Everybody is learning

Never too late

😀



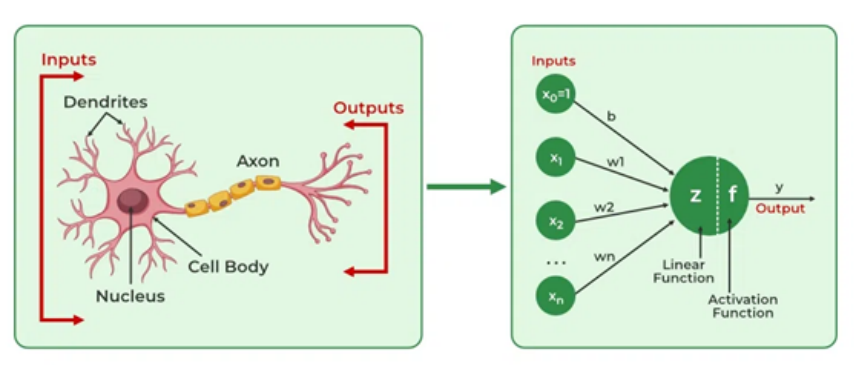
[1]

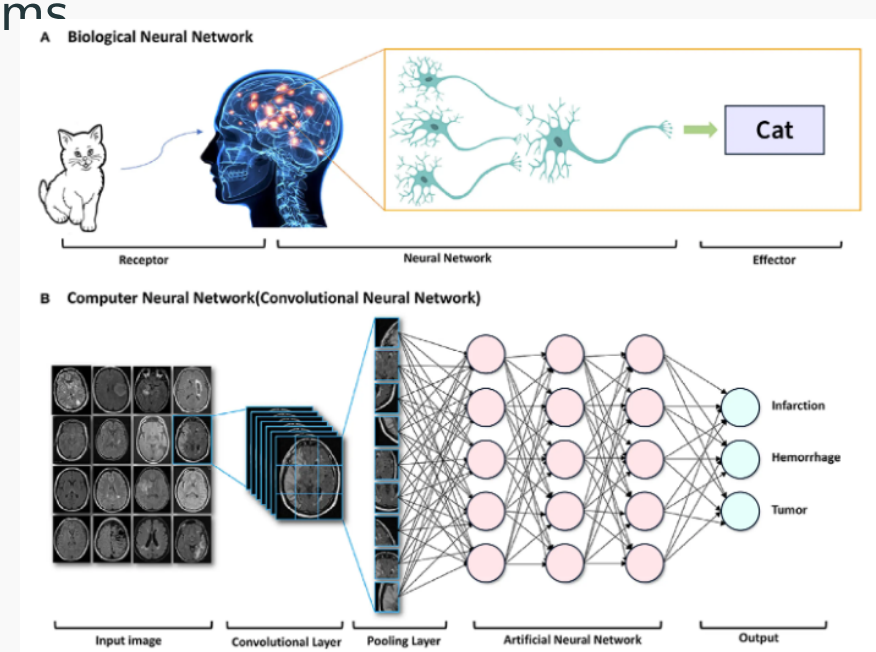
[1] CS 229: Prof. Xiangliang Zhang (KAUST)

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.





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

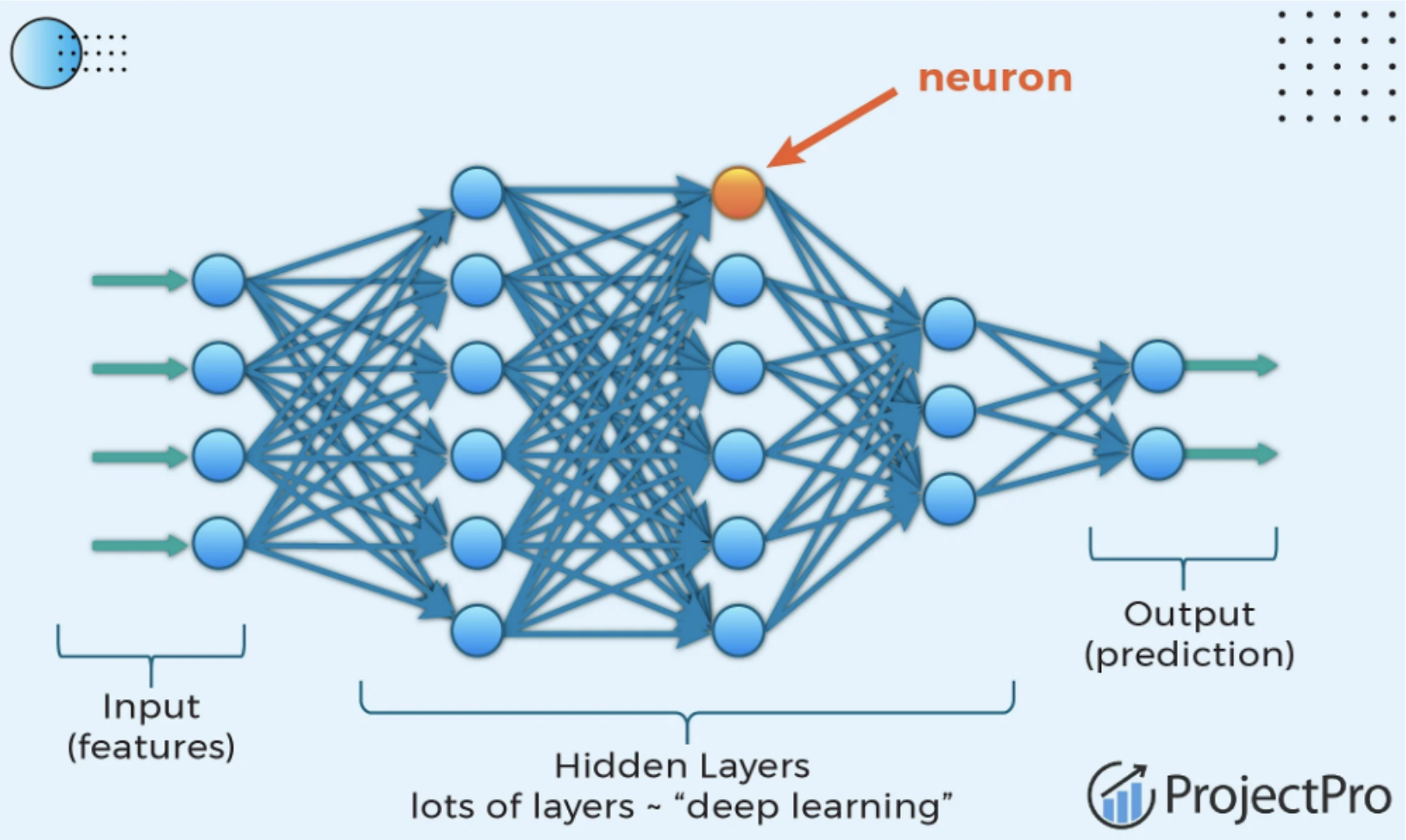
Structural Components

- 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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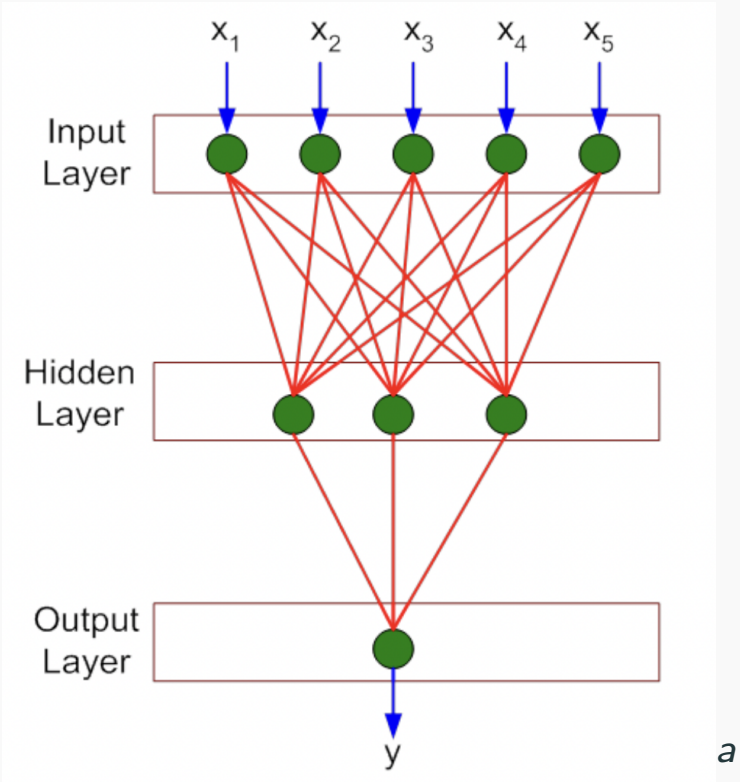
[2] ProjectPro

Agenda

Layers

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

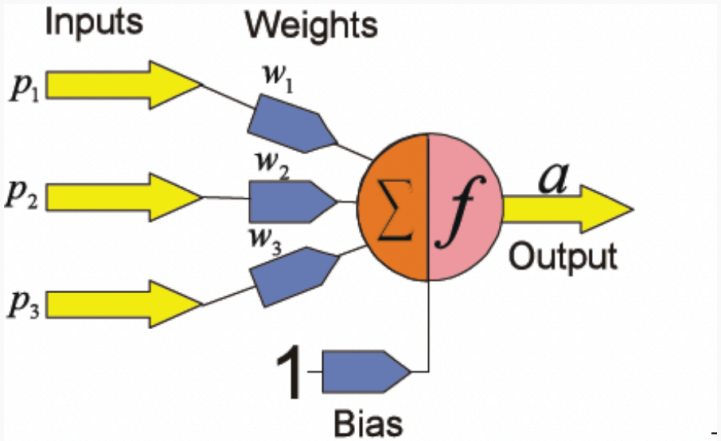
- **Input Layer**
  - First layer of neurons.
  - Receives raw data directly from the input features.
- **Hidden Layers**
  - Layers between the input and output layers.
  - Perform computations.
  - Can have one or many hidden layers.
- **Output Layer**
  - Final layer.
  - Produces the network's output.
  - 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

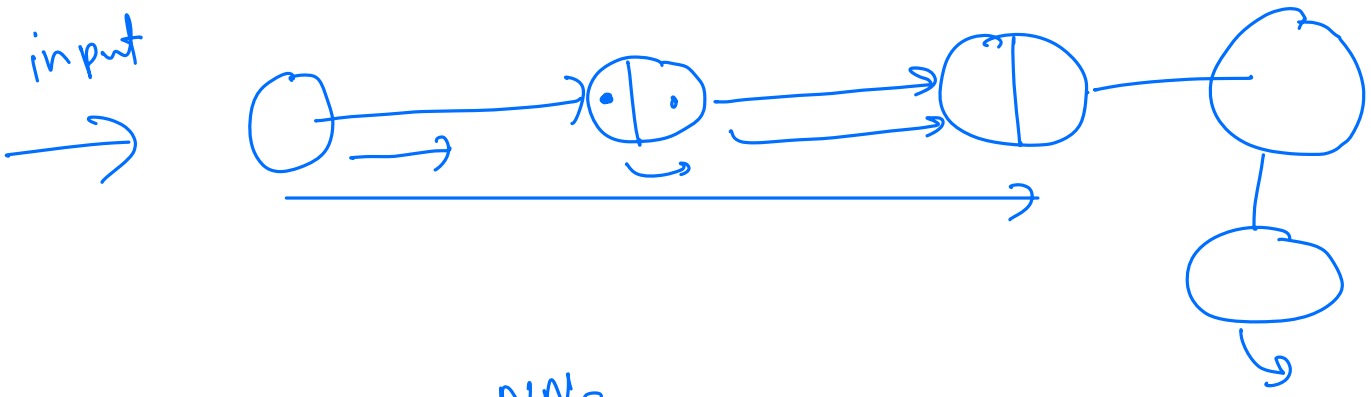
Modern Variants

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/

Recall

NNs → Brain

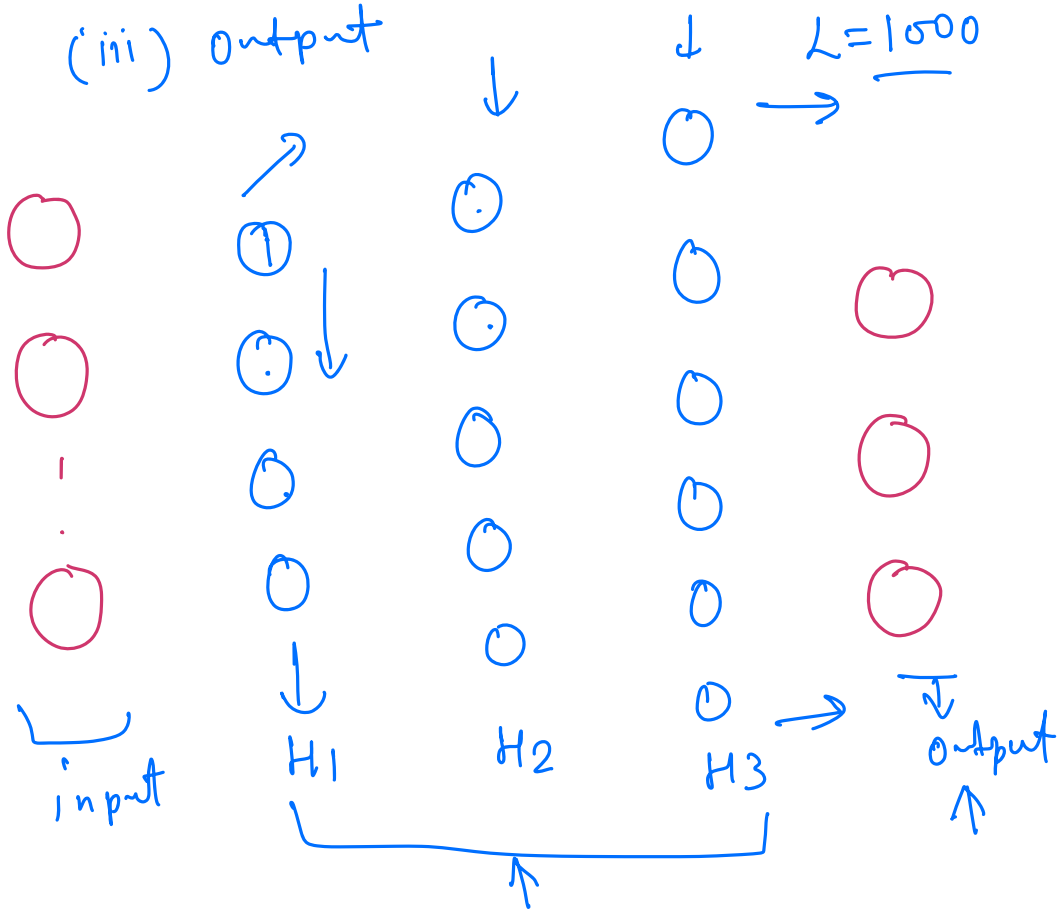


NNs

(i) input Layers

(ii) Hidden L

(iii) output



detect Image

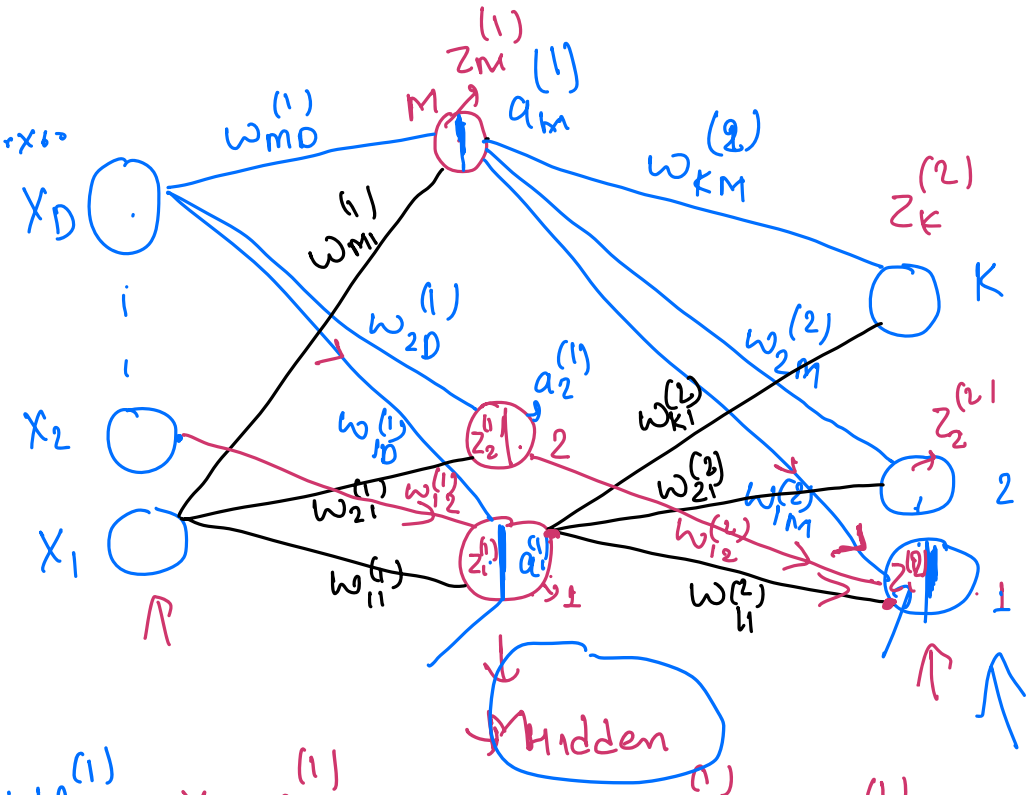
$D = 3600$

x_1: some

x_2: →

x_3: →

!



pre-activation $z^{(1)}$

$$\Rightarrow z_1 = x_1 w_{11}^{(1)} + x_2 w_{12}^{(1)} + \cdots x_D w_{1D}^{(1)} + w_{10}^{(1)}$$

$$z_1^{(1)} = \sum_{i=0}^{D} x_i \cdot w_{1i}^{(1)} \qquad x_0 = 1$$

pre-activation

$$z_J^{(1)} = \sum_{i=0}^{D} x_i \cdot w_{Ji}^{(1)} \qquad x_0 = 1$$

post-activation → h

pre-activation → $a_J^{(1)} = h\left(z_J^{(1)}\right), \quad J = 1 \cdots M$

$$z_1^{(2)} = a_1^{(1)} w_{11}^{(2)} + a_2^{(1)} w_{12}^{(2)} + \cdots + a_M^{(1)} w_{1M} + w_{10}^{(2)}$$

$$= \sum_{J=0}^{M} a_J^{(1)} w_{1J}^{(2)} \qquad a_0^{(1)} = 1$$

$$z_K^{(2)} = \sum_{J=0}^{M} a_J^{(1)} w_{KJ}^{(2)}, \quad K = 1 \cdots k$$

Hidden

$$\Rightarrow z_1^{(1)} = x_1 w_{11}^{(1)} + x_2 w_{12}^{(1)} + \cdots + x_D w_{1D}^{(1)} + w_{10}^{(1)}$$

$$z_1^{(1)} = \sum_{i=0}^{D} x_i w_{1i}^{(1)} \qquad x_0 = 1$$

pre-activation

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

$a_i^{(0)}$

post-activation → h

pre-activation → $a_j^{(1)} = h(z_j^{(1)})$, $j = 1 \cdots M$

$$z_1^{(2)} = a_1^{(1)} w_{11}^{(2)} + a_2^{(1)} w_{12}^{(2)} + \cdots + a_M^{(1)} w_{1n}^{(2)}$$

$$= \sum_{j=0}^{M} a_j^{(1)} w_{1j}^{(2)} \qquad a_0^{(1)} = 1$$

$$z_k^{(2)} = \sum_{j=0}^{M} a_j^{(1)} w_{kj}^{(2)}, \quad k = 1 \cdots K$$

post-activation:

$$y_k = a_k^{(2)} = \sigma(z_k^{(2)}) = \sigma\left(\sum_{j=0}^{M} w_{kj}^{(2)} a_j^{(1)}\right)$$

$$= \sigma\left(\sum_{j=0}^{M} w_{kj}^{(2)} h(z_j^{(1)})\right)$$

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

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.
- $\mathbf{t}$ is the target variables of interest.

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:

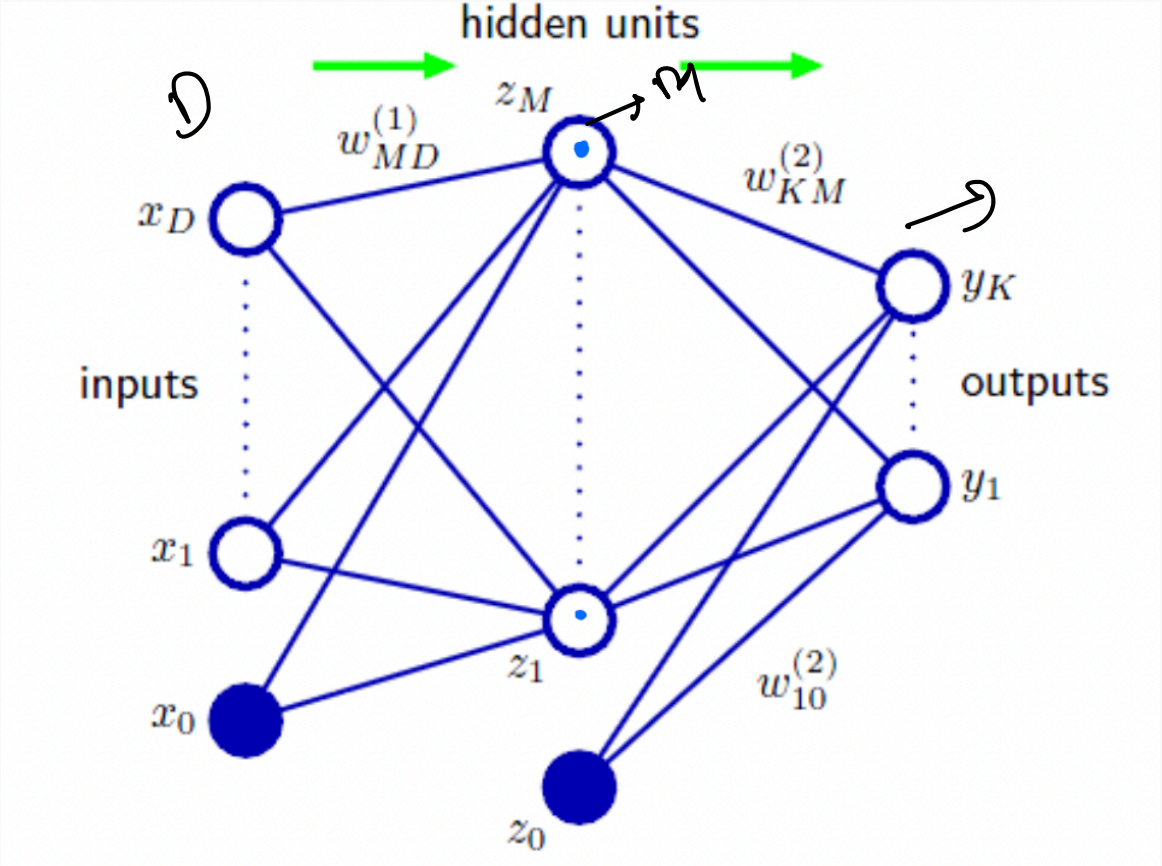
$$\mathbf{z}^{(l)} = \mathbf{W}^{(l)}\mathbf{a}^{(l-1)} + \mathbf{b}^{(l)}$$

  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)

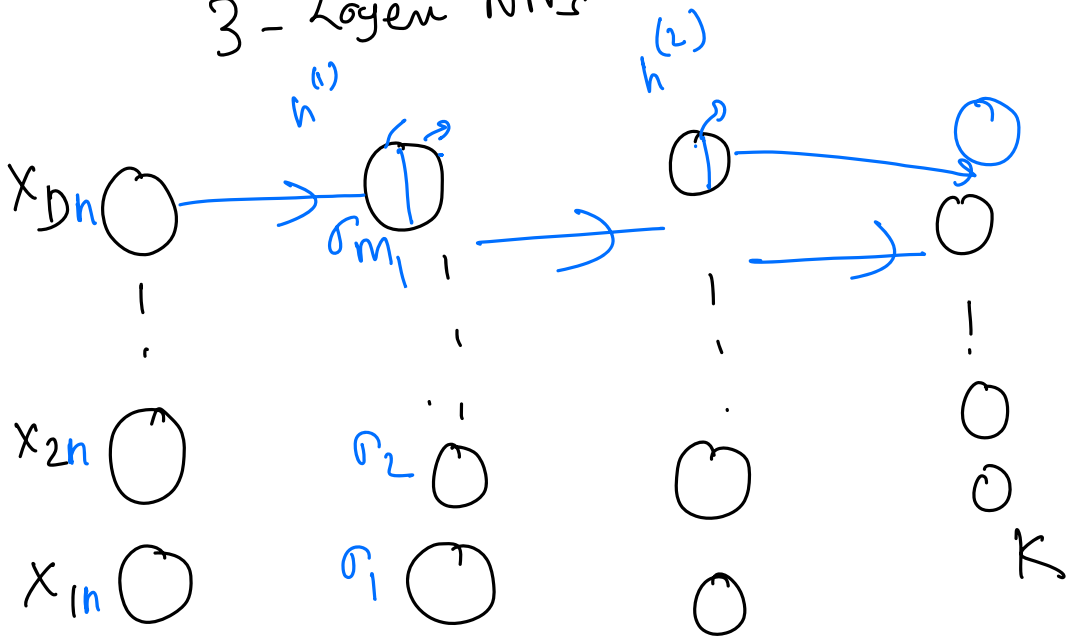
After substituting $y_k = \sigma(z_k^{(2)})$;

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

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

3 - Layer NNs



1000 images

$\rightarrow N = 1000$

$n = 1$

$$\downarrow \quad \begin{matrix} x_{11} \\ x_{21} \\ \vdots \\ x_{D1} \end{matrix} \begin{bmatrix} \quad \end{bmatrix} \rightarrow$$

M_1 $\quad$ M_2

$w^{(1)}, w^{(2)}, w^{(3)}$ $\rightarrow$

$n = 2 =$ $\begin{bmatrix} \quad \end{bmatrix}$ $w^{(1)}, w^{(2)}, w^{(3)}$

$w^{(1)}, w^{(2)}, w^{(3)}$

$n = N \rightarrow$ $\begin{bmatrix} \quad \end{bmatrix}$

Exercise: Three-Layer Neural Network (Forward Propagation)

Similar to two-layer neural network show that the network output for a three layer-neural network would be

$$\hat{y}_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{m=0}^{M_2} w_{km}^{(3)}\, h^{(2)}\left(\sum_{j=0}^{M_1} w_{mj}^{(2)}\, h^{(1)}\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right)\right)\right).$$

Here:

- $w_{ji}^{(1)}$ are weights from input components x_i to first hidden layer neuron j (with $i = 0$ representing bias and $x_0 = 1$).
- $h^{(1)}$ and $h^{(2)}$ are the activation functions for hidden layer 1 and hidden layer 2 respectively.
- $w_{mj}^{(2)}$ are weights from first hidden layer (j) to second hidden layer (m); $w_{km}^{(3)}$ are weights from second hidden layer (m) to output unit k (again $m = 0$ may be bias).
- D = input dimension, M_1 = number of units in first hidden layer, M_2 = number of units in second hidden layer.

Special cases (Think about these as well):

- If $h^{(1)}, h^{(2)}, \sigma$ are *identity*, the whole map reduces to a single affine function of $\mathbf{x}$ (linear regression).
- If σ is softmax and the hidden activations are non-linear, this is a multi-class classification model.

$\underline{x}_n = (x_{1n}, x_{2n} \dots x_{Dn})$ ↓

$y_k(x_n, w) =$ ------ x_{in}

$y_k(x_1, w)$ — - - - x_{1n}

$y_k(x_2, w)$ → - - . x_{2n}

$y_k(x_N, w)$ — - x_{Nn}

↳ **Regression :-** → $K = 1$

$w = (w^{(1)}, w^{(2)}, w^{(3)})$

$\hat{y}(\underline{x}_1, w) \longrightarrow t_1$

$\hat{y}(\underline{x}_2, w) \longrightarrow t_2$

$\hat{y}(\underline{x}_3, w) \longrightarrow t_3$

$\hat{y}(\underline{x}_N, w) - - - t_N$

MSE

$$\mathcal{L}(w) = \frac{1}{2n} \sum_{n=1}^{N} \left(\hat{y}(x_n, w) - t_n \right)^2$$

for 2-layer NN

$$\mathcal{L}(w) = -\frac{1}{2n} \sum_{n=1}^{N} \left(\sigma\left(\sum_{j=0}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_{in} \right) \right) - t_n \right)^2$$

$w = (w^{(1)}, w^{(2)})$

↳ **Recall:**

→ gradient D

→ NR

→ Adam

→ Rmsprop

$\sigma(z_F^{(2)})$

NN

$$L(w) = -\frac{1}{2n} \sum_{n=1}^{N} \left(\sigma\left(\sum_{j=0}^{M} w_{kj}^{(2)}\, h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_{in} \right) \right) - t_n \right)^2$$

y_n

$w = (w^{(1)}, w^{(2)})$

↳ Adam

(i) momentum

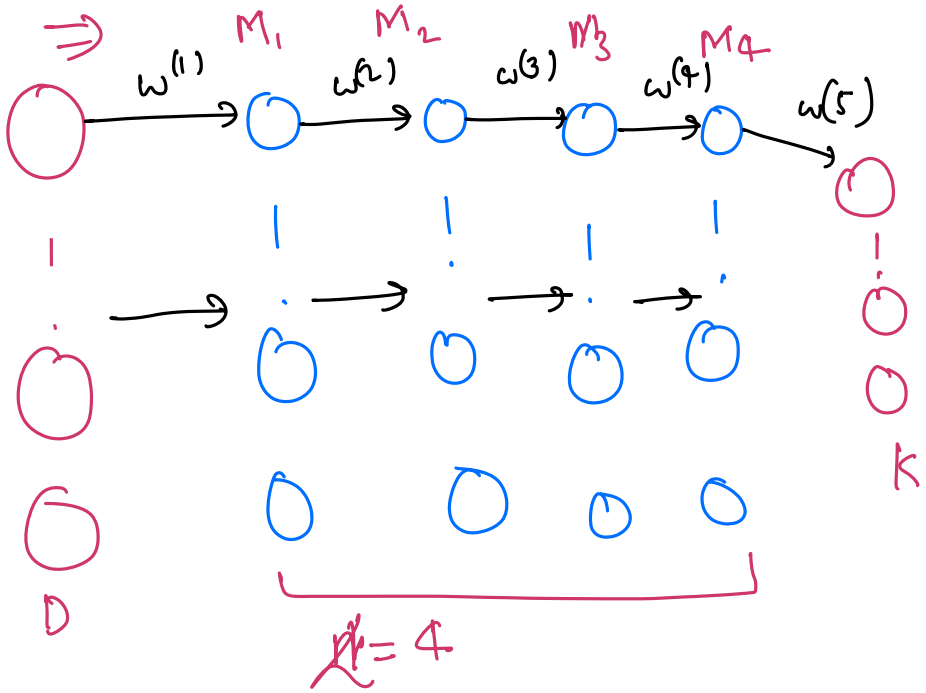
$$\frac{\partial L(w)}{\partial w^{(2)}} \rightarrow \frac{\partial L(w)}{\partial w^{(1)}}$$

$$\frac{\partial L(w)}{\partial w_{kj}^{(2)}} = \frac{\partial L}{\partial \sigma} \times \frac{\partial \sigma}{z_k^{(2)}} \times \frac{\partial z_k^{(2)}}{\partial w_{kj}^{(2)}} \quad ③$$

1st Layer

$$= 2\,(\sigma(\;) - t_n)\; \sigma'(z_F^{(2)})\; h\left(z_j^{(1)}\right)$$

$$\frac{\partial L(w)}{\partial w_{ji}^{(1)}} = \leftrightarrow \quad ④ \quad (\;)\,(1-x)\,(\;) \rightarrow 100$$



(1) forward propagation

$$\hat{y}(x_n, w)$$

$$L(w) = -\frac{1}{2N} \sum_{n=1}^{N} \left(\hat{y}(x_n, w) - t_n \right)^2$$

(2) → calculate gradient

$$\frac{\partial L}{\partial w^{(5)}} \rightarrow \frac{\partial L}{\partial w^{(4)}} \rightarrow \frac{\partial L}{\partial w^{(3)}} \rightarrow \frac{\partial L}{\partial w^{(2)}} \rightarrow \frac{\partial L}{\partial w^{(1)}}$$

↳ update parameter using → Adam

(A1.) $w_0 = \underbrace{w_0^{(1)}, w_0^{(2)}, w_0^{(3)}, w_0^{(4)}, w_0^{(5)}}_{N}$

↳ $L(w_0) = \frac{1}{2} \sum_{n=1} \left(y(x_n, w_0) - t_n \right)$

↳ forward

↳ gradient

$$\frac{\partial L(w_0)}{\partial w_0^{(5)}} \longrightarrow \frac{\partial L(w_0)}{\partial w_0^{(1)}}$$

↳ update parameters

↳ $w_1^{(1)} = w_0^{(1)} - \eta \frac{\partial L(w_0)}{\partial w_0^{(1)}}$

$$w_1^{(5)} = w_0^{(5)} - \eta \frac{\partial L(w_0)}{\partial w_0^{(5)}}$$

↳ Forward propagation → $L(w_1)$

Back-prop ← → gradient

$w_2^{(1)} =$ ⟷

$w_2^{(5)} =$ →

↳ forward → $L(w_2)$ ↳ 1000, 2000

$y \to x_i^2$ ⟷ MLR ⟷ SLR

Agenda

Recall: Error (Loss) Function

Training a neural network involves estimating the weights and biases by optimizing a loss function.

- Multi-class classification: Neural networks with a softmax output layer use the Cross-entropy loss:

$$\mathcal{L}(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \log y_k(\mathbf{x}_n, \mathbf{w}),$$

  where:
  - K = number of classes,
  - $t_{nk} = 1$ if sample n belongs to class k, else 0,
  - $y_k(\mathbf{x}_n, \mathbf{w})$ = softmax probability for class k.

- Regression: Sum of squared

$$\mathcal{L}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N} \{y(\boldsymbol{x}_n, \boldsymbol{w}) - t_n\}^2,$$

  where $t_n, n = 1, \ldots, N$ is the observed response. N is the total number of training samples (examples).

Training a Neural Network: Forward and Backward Pass

- **Goal**: Minimize the error/loss function $\mathcal{L}(\boldsymbol{w})$
- **Recall:** We will be using gradient based algorithm for minimizing the loss function which require calculation of gradient of loss function.
- **Each training step has two key phases:**
  - **Forward Pass**: Compute output predictions from input through the layers. (We covered this part previously)
  - **Backward Pass (Backpropagation)**: Compute gradients of loss w.r.t. weights using the chain rule.
- Then update weights using gradient descent (or a variant).

Backpropagation: overview

- **Goal:** compute $\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{y}(\mathbf{x}, \mathbf{w}), \mathbf{t})$ efficiently for all weights in the network.
- Use chain rule to propagate "errors" from the output layer to backward through layers.
- For example, for a two-layer NNs (input $\rightarrow$ 1-hidden layer $\rightarrow$ output) we compute:

$$\frac{\partial \mathcal{L}}{\partial w_{kj}^{(2)}}, \qquad \frac{\partial \mathcal{L}}{\partial w_{ji}^{(1)}}$$

where indices follow the earlier slides in case of forward propagation:

$$z_j^{(1)} = \sum_{i=0}^{D} w_{ji}^{(1)} x_i, \quad x_0 = 1, \qquad a_j^{(1)} = h(z_j^{(1)}), \quad j = 1, \ldots, M$$

$$z_k^{(2)} = \sum_{j=0}^{M} w_{kj}^{(2)} a_j^{(1)}, \quad a_0^{(1)} = 1, \qquad y_k = \sigma(z_k^{(2)}), \quad k = 1, \ldots, K.$$

Fist-Step: Calculate Output-layer gradients

Let $\mathcal{L}$ be loss. Define

$$\delta_k^{(2)} \equiv \frac{\partial \mathcal{L}}{\partial z_k^{(2)}}.$$

By chain rule,

$$\frac{\partial \mathcal{L}}{\partial w_{kj}^{(2)}} = \frac{\partial \mathcal{L}}{\partial z_k^{(2)}} \frac{\partial z_k^{(2)}}{\partial w_{kj}^{(2)}} = \delta_k^{(2)} \, a_j^{(1)}.$$

Bias gradient:

$$\frac{\partial \mathcal{L}}{\partial w_{k0}^{(2)}} = \delta_k^{(2)}.$$

Key: $\delta_k^{(2)} = \frac{\partial \mathcal{L}}{\partial y_k} \sigma'(z_k^{(2)})$.

Output-layer $\delta_k^{(2)}$ — examples

(1) MSE + output activation σ:

$$\mathcal{L} = \tfrac{1}{2}\sum_k (y_k - t_k)^2 \Rightarrow \frac{\partial \mathcal{L}}{\partial y_k} = y_k - t_k,$$

$$\delta_k^{(2)} = (y_k - t_k)\,\sigma'(z_k^{(2)}).$$

(2) Softmax + CE:

$$\delta_k^{(2)} = y_k - t_k.$$

(Simplifies: no σ' term — standard for classification.)

Hidden-layer gradients: backpropagate deltas

We now propagate to **hidden units**. Define

$$\delta_j^{(1)} \equiv \frac{\partial \mathcal{L}}{\partial z_j^{(1)}}.$$

Using **chain rule** (sum over contributions of hidden unit to all outputs):

$$\delta_j^{(1)} = \sum_{k=1}^{K} \frac{\partial \mathcal{L}}{\partial z_k^{(2)}} \frac{\partial z_k^{(2)}}{\partial a_j^{(1)}} \frac{\partial a_j^{(1)}}{\partial z_j^{(1)}} = h'(z_j^{(1)}) \sum_{k=1}^{K} w_{kj}^{(2)} \delta_k^{(2)}.$$

Then **gradients for layer-1 weights**:

$$\frac{\partial \mathcal{L}}{\partial w_{ji}^{(1)}} = \delta_j^{(1)} x_i, \qquad \frac{\partial \mathcal{L}}{\partial w_{j0}^{(1)}} = \delta_j^{(1)}.$$

Vectorized backpropagation (single example)

Using **column-vector** notation:

$$\mathbf{z}^{(1)} = W^{(1)}\mathbf{x}, \quad \mathbf{a}^{(1)} = h(\mathbf{z}^{(1)}), \quad \mathbf{z}^{(2)} = W^{(2)}\mathbf{a}^{(1)}, \quad \mathbf{y} = \sigma(\mathbf{z}^{(2)}).$$

Define **error vectors**:

$$\boldsymbol{\delta}^{(2)} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(2)}} \in \mathbb{R}^K, \qquad \boldsymbol{\delta}^{(1)} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(1)}} \in \mathbb{R}^M.$$

Then **matrix gradients**:

$$\nabla_{W^{(2)}} \mathcal{L} = \boldsymbol{\delta}^{(2)} \, (\mathbf{a}^{(1)})^\top, \qquad \nabla_{W^{(1)}} \mathcal{L} = \boldsymbol{\delta}^{(1)} \, \mathbf{x}^\top.$$

Backprop relation:

$$\delta^{(1)} = \left((W^{(2)})^\top \boldsymbol{\delta}^{(2)} \right) \odot h'(\mathbf{z}^{(1)}),$$

where $\odot$ = **elementwise** product.

Mini-batch and averaging

For a **mini-batch** of size N with examples $(\mathbf{x}^{(n)}, \mathbf{t}^{(n)})$ compute per-example deltas and **average**:

$$\nabla_{W^{(2)}} \mathcal{L}_{\text{batch}} = \frac{1}{N} \sum_{n=1}^{N} \boldsymbol{\delta}^{(2),(n)} (\mathbf{a}^{(1),(n)})^{\top}.$$

Same for $W^{(1)}$. In practice use **vectorized** matrix operations: stack activations by columns/rows and compute **matrix products** to get all gradients in one call.

Common activation derivatives

- **Sigmoid** $\sigma(u) = \frac{1}{1+e^{-u}}$: $\sigma'(u) = \sigma(u)(1-\sigma(u))$.
- **Tanh**: $h(u) = \tanh(u)$: $h'(u) = 1 - \tanh^2(u)$.
- **ReLU**: $h(u) = \max(0, u)$: $h'(u) = \begin{cases} 1 & u > 0 \\ 0 & u < 0 \end{cases}$ (undefined at 0, set 0 or 1 in practice).
- **Leaky ReLU**: $h'(u) = 1$ if $u > 0$, else α.

Note: compute derivatives using **pre-activation values** z (numerically stable).

Softmax+Cross-Entropy: derivation (brief)

Softmax $y_k = \frac{e^{s_k}}{\sum_\ell e^{s_\ell}}$, **CE loss**: $\mathcal{L} = -\sum_k t_k \log y_k$. Compute $\frac{\partial \mathcal{L}}{\partial s_j}$:

$$\frac{\partial \mathcal{L}}{\partial s_j} = \sum_k -t_k \frac{1}{y_k} \frac{\partial y_k}{\partial s_j}.$$

Using $\frac{\partial y_k}{\partial s_j} = y_k(\delta_{kj} - y_j)$ leads to:

$$\frac{\partial \mathcal{L}}{\partial s_j} = y_j - t_j.$$

Thus **output delta:** $\boldsymbol{\delta}^{(2)} = \mathbf{y} - \mathbf{t}$ (key simplification!)

Add L2 regularization (weight decay)

If the training objective is:

$$\mathcal{J}(\mathbf{w}) = \mathcal{L}(\mathbf{w}) + \frac{\lambda}{2} \sum_{\ell} \| W^{(\ell)} \|_F^2,$$

then gradients get an **extra term**:

$$\nabla_{W^{(\ell)}} \mathcal{J} = \nabla_{W^{(\ell)}} \mathcal{L} + \lambda W^{(\ell)}.$$

Biases are not regularized.

Backpropagation algorithm (single minibatch) — pseudocode

1. **Forward pass**: compute $\mathbf{z}^{(1)}$, $\mathbf{a}^{(1)}$, $\mathbf{z}^{(2)}$, $\mathbf{y}$.
2. **Output error**: set $\boldsymbol{\delta}^{(2)} = \partial \mathcal{L} / \partial \mathbf{z}^{(2)}$ (e.g. $\mathbf{y} - \mathbf{t}$).
3. Compute **output weight** gradient:

$$G^{(2)} = \frac{1}{N} \sum_n \boldsymbol{\delta}^{(2),(n)} (\mathbf{a}^{(1),(n)})^\top$$

4. **Backpropagate** to hidden:

$$\boldsymbol{\delta}^{(1),(n)} = ((W^{(2)})^\top \boldsymbol{\delta}^{(2),(n)}) \odot h'(\mathbf{z}^{(1),(n)})$$

5. Compute **input weight** gradient:

$$G^{(1)} = \frac{1}{N} \sum_n \boldsymbol{\delta}^{(1),(n)} (\mathbf{x}^{(n)})^\top$$

6. If **L2 regularization**:

$$G^{(\ell)} \leftarrow G^{(\ell)} + \lambda W^{(\ell)}$$

7. **Update weights** (SGD, Adam, etc.)

Worked scalar example (1 hidden neuron)

Network: $z^{(1)} = w^{(1)}x + b^{(1)}$, $a^{(1)} = h(z^{(1)})$, $s = z^{(2)} = w^{(2)}a^{(1)} + b^{(2)}$, $y = \sigma(s)$, loss $\mathcal{L} = \frac{1}{2}(y - t)^2$.

$$\delta^{(2)} = (y - t)\sigma'(s)$$

$$\frac{\partial \mathcal{L}}{\partial w^{(2)}} = \delta^{(2)} a^{(1)}, \qquad \frac{\partial \mathcal{L}}{\partial b^{(2)}} = \delta^{(2)}$$

$$\delta^{(1)} = h'(z^{(1)})\, w^{(2)}\, \delta^{(2)}$$

$$\frac{\partial \mathcal{L}}{\partial w^{(1)}} = \delta^{(1)} x, \qquad \frac{\partial \mathcal{L}}{\partial b^{(1)}} = \delta^{(1)}.$$

Forward Propagation Through L Hidden Layers

Input Layer

$$a^{(0)} = \mathbf{x}$$

Hidden Layers:

$$z^{(l)} = W^{(l)}\, a^{(l-1)} + b^{(l)}, \qquad l = 1, 2, \ldots, L$$

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

Output Layer:

$$z^{(L+1)} = W^{(L+1)}\, a^{(L)} + b^{(L+1)}$$

$$\hat{y} = \sigma\left(z^{(L+1)}\right)$$

Loss:

$$\mathcal{L} = \mathcal{L}(\hat{y}, y)$$

General Backpropagation in Deep Networks

Given: A network with L hidden layers

$$a^{(0)} = x, \quad z^{(l)} = W^{(l)}\, a^{(l-1)} + b^{(l)}, \quad a^{(l)} = \sigma(z^{(l)}), \quad l = 1, 2, ..., L$$

Output Layer (layer $L+1$):

$$z^{(L+1)} = W^{(L+1)} a^{(L)} + b^{(L+1)}, \quad \hat{y} = a^{(L+1)}$$

Loss Function:

$$\mathcal{L}(y, \hat{y})$$

Goal: $\dfrac{\partial \mathcal{L}}{\partial W^{(l)}}, \quad \dfrac{\partial \mathcal{L}}{\partial b^{(l)}} \quad \forall\, l = 1, \ldots, L+1$

Backprop Through L Hidden Layers

Step 1: Error at Output Layer

$$\delta^{(L+1)} = \frac{\partial \mathcal{L}}{\partial z^{(L+1)}} = (\hat{y} - y) \odot \sigma'(z^{(L+1)})$$

Step 2: Error Propagation Backwards

$$\delta^{(l)} = \left(W^{(l+1)}\right)^{\top} \delta^{(l+1)} \odot \sigma'(z^{(l)}) \quad (\textit{ChainRule})$$

$$\text{for } l = L, L-1, \ldots, 1$$

Step 3: Gradients for Each Layer

$$\frac{\partial \mathcal{L}}{\partial W^{(l)}} = \delta^{(l)} \left(a^{(l-1)}\right)^{\top}$$

$$\frac{\partial \mathcal{L}}{\partial b^{(l)}} = \delta^{(l)}$$

$$\textit{Update } W^{(l)} \leftarrow W^{(l)} - \eta \frac{\partial \mathcal{L}}{\partial W^{(l)}}, \quad b^{(l)} \leftarrow b^{(l)} - \eta \frac{\partial \mathcal{L}}{\partial b^{(l)}}$$

Practical notes & numerical stability

- For **softmax**: use log-sum-exp trick $\rightarrow s' = s - \max_k s_k$
- Sigmoid: avoid saturation $\rightarrow$ proper **initialization** (Xavier/He)
- ReLU: **subgradient** at 0
- **Use GPUs + batching** $\rightarrow$ matrix ops
- Combine **softmax + CE** as single operation $\rightarrow$ stable and efficient $(y - t)$

Summary (what to take away)

- **Backprop = chain rule**: compute δ, then gradients layer-wise
- **Key identities:**

$$\nabla_{W^{(2)}} = \delta^{(2)}(\mathbf{a}^{(1)})^\top, \quad \delta^{(1)} = ((W^{(2)})^\top \delta^{(2)}) \odot h'(\mathbf{z}^{(1)})$$

- **Softmax + CE**: $\delta^{(2)} = \mathbf{y} - \mathbf{t}$
- **Regularization** adds λW