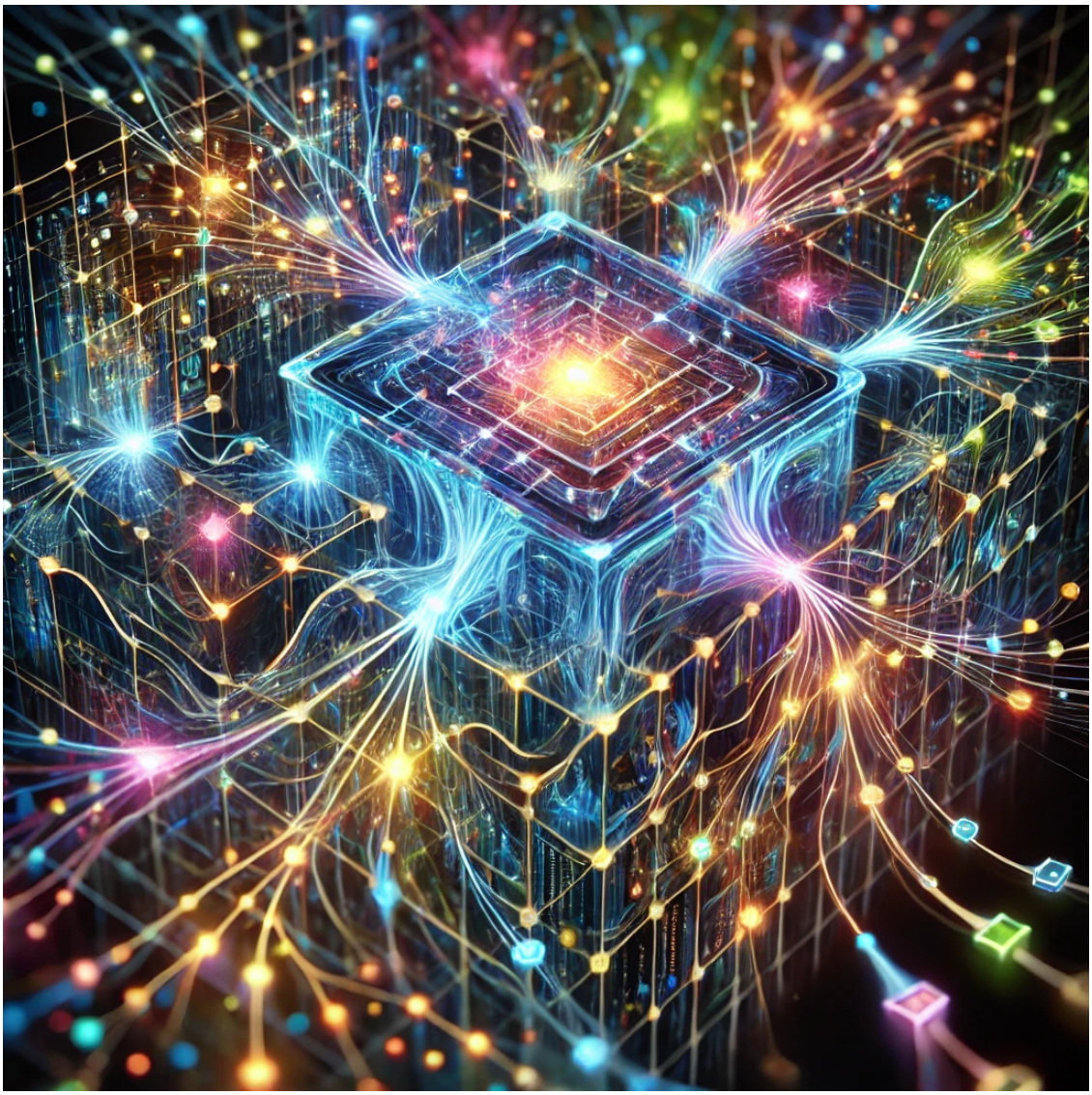
# Neural Networks

University at Illinois of Chicago



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# Contents

# 1 Lecture 1

**Why Study Neural Networks?**

- The human brain is very successful at certain tasks that prove to be difficult to accomplish on a classical computer, such as learning and pattern recognition. For example, consider the generic classification task: when you see a picture of an apple, you immediately recognize it as an apple. Similarly, you understand what someone says when they speak. Computers, however, often struggle with these tasks. For instance, even with modern technology, most commercial speech recognition systems cannot perfectly understand speech, especially with accents. This motivates us to study how the brain, or the human neural network, functions.

- Why is the human brain better at certain tasks compared to computers? Could it be about speed? No, because while a transistor can switch in nanoseconds, it takes a few milliseconds for your brain to process a stimulus, such as pricking your leg with a needle. Hence, the difference is not necessarily due to speed. What the brain lacks in speed, it compensates for in the number of processing elements and the massively interconnected and parallel nature of its operations, unlike the serial operations of classical computers. Additionally, the human brain is adaptive; its functionality evolves through learning, whereas the physical structure of a CPU in a computer is fixed and does not change over time.

**Summary:**

- **Classical computer:** Almost operates in serial (e.g., running a program while ignoring pipelining), but each operation can be performed extremely fast (less than nanoseconds per operation).

- **Neural network:** Operates massively in parallel, and may be more powerful than a classical computer, despite the fact that a given neuron is relatively "slow" (a neuron can fire at most hundreds of times per second, which translates to milliseconds per operation).

- **Motivation:** By imitating the brain's operation (through artificial neural networks), we may be able to solve complex tasks that classical computers struggle to perform. This is arguably the most important motivation for advancements in this field.

- **Other motivation:** To understand how the brain and nervous system function.

**Neural Networks Summary:**

1. Neural networks are massively parallel distributed processors composed of simple processing units (mathematical neurons) and the connections between them.

2. Neural networks can store and utilize experiential knowledge through a learning process.

An artificial neural network resembles the brain in two key respects:

- Knowledge is acquired by the network from its environment through a learning process.
- Inter-neuron connection strengths, known as synaptic weights, are used to store the acquired knowledge.

# 2 Lecture 2

Neural Networks are characterized by **non linearity** and by a **learning component**.

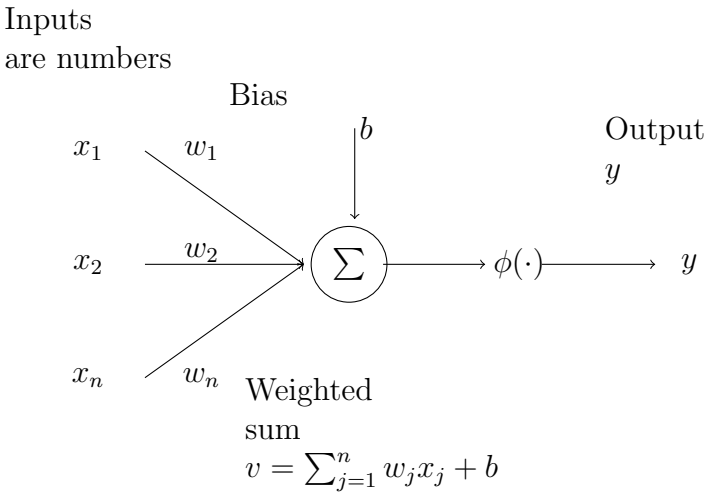
It is useful to understand what a **biological neuron** is, since Neural Networks get inspiration from them. To make it simple: some excitation comes in and the neuron may be activated, if there is enough excitation. The more it is used, the stronger it becomes (**Hebbian Algorithm**).

- n neurons in the brain: $10^{11}$
- n neurons in the whole nervous system: $10^{12}$
- n synapses: $10^{14}$

In our body there are different types of neurons: sensory, internal, motor... and there are special architectures that adapt to different tasks.

Ex. when we born our brain is not fine tuned yet, we must give input data to it $\rightarrow$ **language learning**

## 2.1 Mathematical Model of the Neuron




The inputs are pulses, chemical perturbations (in biology). In our context, they are basically numbers.

The inputs are going to be weighted. They don't have all the same importance. **Weights** represent the strength of the connection (synaptic weight).

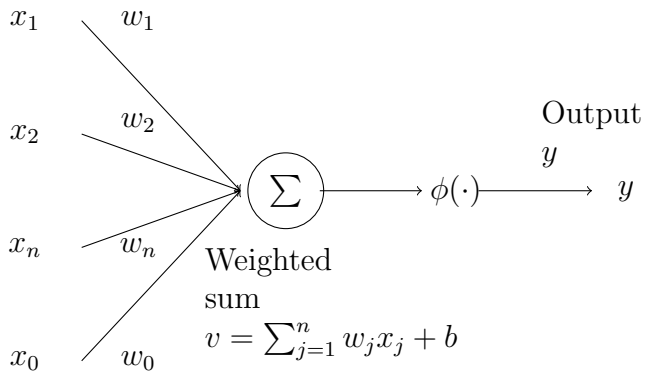
The **activation function** controls whether the input is strong enough.
The **Bias** is an internal excitation.

$$v = \sum_{j=1}^{n} w_j x_j + b$$

*This is an affine equation (linear + constant).*

*A lot of nature is linear. If the input is scaled, the output is also scaled. If I add inputs, the output gets added up. This is the essence of linearity.*

Inputs
are numbers




If we add an input $x_0$ we can remove the bias and have a linear equation, but usually, we keep the bias separated.

The output $y$ is the result of a final **activation function** ($y = \phi(v)$).

$$y = \phi(v) = \phi(\sum_{j=1}^{n} w_j x_j + b) \tag{1}$$

This is what is doing the whole neuron.

## 2.2 Types of activation functions

For the moment, we will focus on "squashing" type of function, i.e. It limits the amplitude range of the neuron output.

1. **Step function:** threshold function, Heaviside. As long as the input is negative, nothing happens, then something happens.

$$\phi(v) = \begin{cases} 1 & \text{if } v \geq 0, \\ 0 & \text{if } v < 0. \end{cases} \tag{2}$$

   We can have flexibility and change where the jump is happening. We do that with the bias: the threshold at which the bias occurs.

How do we define the weights? We should design them to create a specific behavior. The problem with the step function is that it becomes a discrete problem and finding the proper weights becomes a long process of trial and error → **optimization algorithms**, to gradually change the weights and see what happens. This is the motivation behind the **sigmoid function.**

2. **Sigmoid function:** "smoothed" threshold function

$$\phi(v) = \frac{1}{1 + e^{-aV}}, a > 0 \tag{3}$$

When a becomes larger, the function becomes sharper, while if a becomes closer to 0, we will have a smoother function.

Step and sigmoid function have outputs $\in [0, 1]$, but sometimes we may want to have outputs $\in [-1, 1]$ → we can change both the step and sigmoid function.

1. **Sign:**

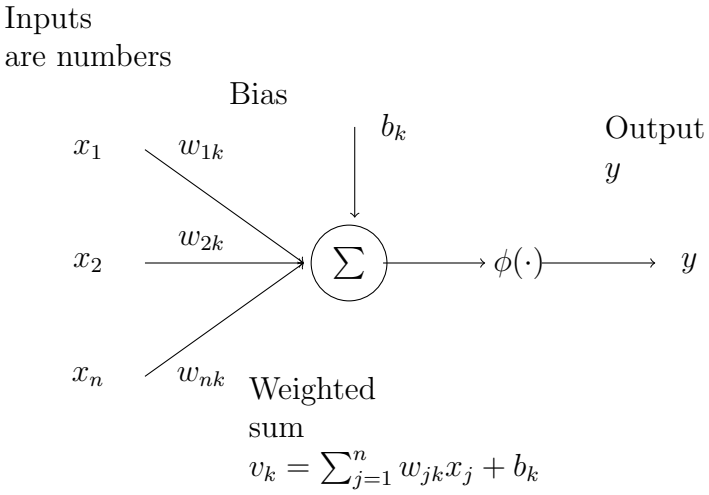
$$\phi(v) = \begin{cases} -1 & \text{if } v < 0, \\ 0 & \text{if } v = 0, \\ 1 & \text{if } v > 0 \end{cases} \tag{4}$$

2. **Hyperbolic Tangent:**

$$\phi(v) = \frac{e^{aV} - e^{-aV}}{e^{aV} + e^{-aV}} \tag{5}$$

## 2.3 Neural Network architectures

Up to now, we have talked about just one neuron, but we need to connect them. Let's name the first neuron, neuron K. We need to label all the neuron to book keep them




All the k's tell you that these units belong to that neuron.

# 3 Lecture 3

In the neural network, the **activation function** is what is creating the **non-linearity**

$$\phi(v) = \begin{cases} 1 & \text{if } v \geq 0, \\ 0 & \text{if } v < 0. \end{cases} \tag{6}$$

This is an idealization of what is happening inside the neuron, but it is quite rough, sometimes it is better to use a smoother function, like the sigmoid:

$$\phi(v) = \sigma(v) = \frac{1}{1 + e^{-aV}} \tag{7}$$

$a$ is a parameter that defines the sharpness of the transition.

There are also variants that bring the step and the sigmoid functions in the range [-1, 1], and they are the **sign** and the **hyperbolic tangent**.

**Also**, there are **non squashing** types of functions:

**Rectified Linear Unit (ReLu):**

$$\phi(v) = \begin{cases} v & \text{if } v \geq 0, \\ 0 & \text{if } v < 0. \end{cases} \tag{8}$$

## 3.1 Feed Forward Neural Network

K different neurons, each one with its weights and biases. We index the neurons and the inputs are the same for each neuron. Each neuron produces its output $y_k$.

$w_{ki}$ is the weight that connects neuron k to input i. All this bunch of neurons form a single layer. So this is a **single layer fully connected feed-forward neural network**, but we can have multiple layers.

The information flow is only over one direction, i.e. the input layer of source nodes projects directly onto the output layer of neurons. There is no feedback of the network's output to the network's input. We thus say that the network in Fig. 1 is of feed forward type.

If, for example, we have two layers, we no longer see the output of the first layer, so this becomes an **hidden layer**, while the second layer (in this case) is the output layer.

$$x = \begin{pmatrix} x1 \\ x2 \\ ... \\ x_n \end{pmatrix}$$

it is a vector

$$W = \begin{pmatrix} w_{11} & w_{12} & ... & w_{1n} \\ w_{21} & w_{22} & ... & w_{2n} \\ w_{31} & ... & & \\ ... & & & \\ w_{k1} & ...w_{kn} & & \end{pmatrix}$$

All the weights are inside a matrix, every row is associated to one neuron, while every column is associated with an input.

$$b = \begin{pmatrix} b_1 \\ b_2 \\ ... \\ b_k \end{pmatrix}$$

One bias for each neuron

$$U = \begin{pmatrix} u_{11} & ... & u_{1k} \\ u_{21} & ... & u_{2k} \end{pmatrix}$$

In this case, 2 neurons, k inputs.

$$c = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

All these vectors and matrices are parameters, i.e. everything needed to define the neural network.

## 3.2 Linear Algebraic Representation

Any linear operator can be written as **inner products**.

$$\sum_{i=1}^{n} w_{1i}x_i + b_1 = \begin{pmatrix} w_{11} & w_{12} & \dots & w_{1n} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} + b_1$$

Repeat per neuron 2 (second row of the matrix)

$$\sum_{i=1}^{n} w_{2i}x_i + b_2 = \begin{pmatrix} w_{21} & w_{22} & \dots & w_{2n} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} + b_2$$

...

Repeat per neuron k

$$\sum_{i=1}^{n} w_{ki}x_i + b_k = \begin{pmatrix} w_{k1} & w_{k2} & \dots & w_{kn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} + b_k$$

**Single Layer**

$$z = \phi(Wx + b)$$

**Two Layers**

The second layer does the same thing, not to $x$ , but to $z$

$$y = \phi(Uz + c) = \phi(U(\phi(Wx + b) + c)$$

It is extremely important to bookkeep dimensions:

$$x \in R^n \tag{9}$$
$$W \in R^{k \times n} \tag{10}$$
$$b \in R^k \tag{11}$$
$$z \in R^k \tag{12}$$
$$U \in R^{2 \times k} \tag{13}$$
$$c \in R^2 \tag{14}$$

In this case the **naming** is: n-k-2 fully connected feed forward neural network (each dash is a layer).

**N.b** A neural network is called fully-connected when we allow all weights; sometimes we can decide to force some of them to zero: in this care connections are removed and the network is not fully-connected anymore.

**Example:** Convolutional Neural Networks. If some outputs feed back (after some delay) as inputs, the network is not feed forward.

**Example:** LSTM (Long Short Term Memory)

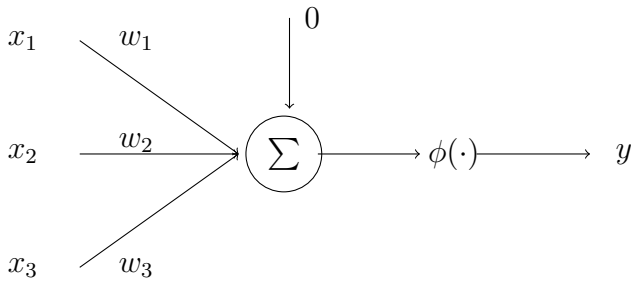
## 3.3 Examples:

a) **Majority Applications**

- n = 3 inputs $x \in \{-1, +1\}^3$
- Activation Function: sign: $\phi(v) = \begin{cases} +1 & \text{if } v > 0 \\ 0 & \text{if } v = 0 \\ -1 & \text{if } v < 0 \end{cases}$

- Goal: design a simple neuron that outputs the value that most appears in the input.

  E.g. $x = \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix} \rightarrow$ y = -1




$$y = \text{sign}(x_1 + x_2 + x_3) = \text{majority}(\{x1, x2, x3\}$$

This neural network has 100% accuracy. If there are more +1 the result is going to be positive, otherwise it is going to be negative.

b) **Logical Statements**

c) **Classification:** e.g. Image representing a 3, the neural network needs to provide 3 as output.

We need to break the image into sth that the NN can take as input → we need to **vectorize** it.

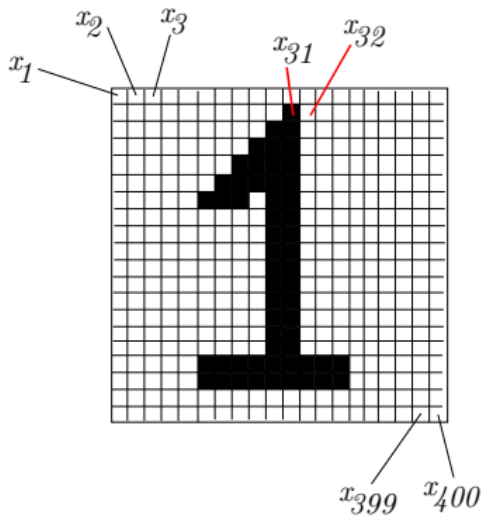



Figure 1: An image of a digit. Each pixel corresponds to one input node

One may design a feedforward neural network for digit classification. We are given 20 pixel by 20 pixel images of handwritten digits. Our job is to find, for each given

image, the actual digit corresponding to the image. Suppose that each pixel assumes binary values, i.e. the images are black and white only with no grayscale. We can then consider a feedforward neural network with 400 nodes in the input layer (labeled as $x_1, x_2, \ldots, x_{400}$), some large number of nodes (say 1000 nodes) in a hidden layer, and 10 nodes in the output layer giving outputs $y_0, \ldots, y_9$. Ignoring the biases, this fully-connected network has:

$$400 \times 1000 + 1000 \times 10 = 410000$$

parameters (synaptic weights) that we can optimize.

Neurons in a neural network can act as shape-detecting units, extracting **salient features** from the input. To represent this layer, we might need 1000 weights. For example, we could have one neuron specialized in detecting the digit '1', similar to how specialized areas in the brain work. While multiple neurons might be activated, the network can only predict one number at a time. To resolve this, at the end of the neural network, we can apply an operation called ARGMAX. This produces a one-hot representation, where the '1' indicates which neuron 'won' the prediction.

In other scenarios, using a SOFTMAX layer might be beneficial, which outputs a probability distribution. This helps determine the network's confidence in its prediction, offering insight into how wrong or uncertain the network might have been.

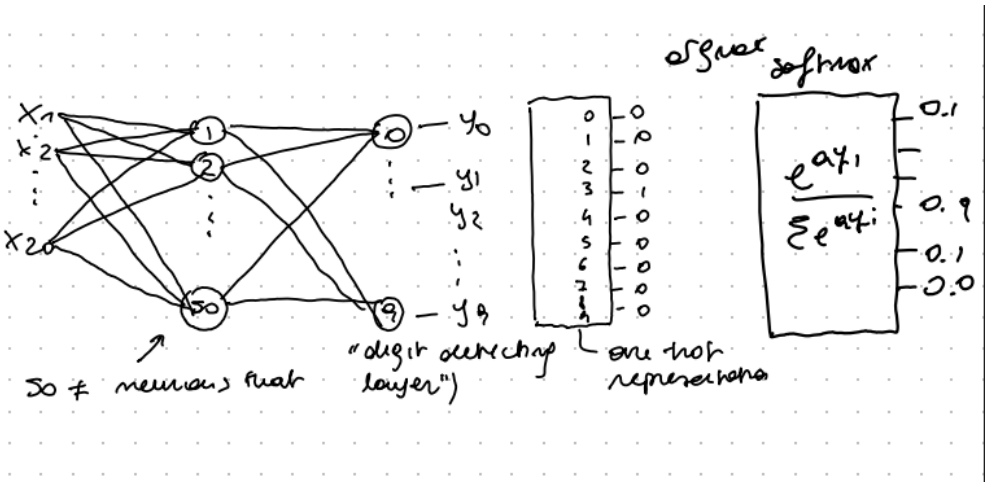



Figure 2: Graphical Representation of the neural network to perform digit classification

- Each node in the input layer will correspond to one pixel in the image, as illustrated in Fig. 2. For example, if the image in Fig. 2 is to be fed to the network as input, the inputs would be $x_0 = 0, x_1 = 0, \ldots, x_{30} = 0, x_{31} = 1, x_{32} = 0, \ldots, x_{399} = 0, x_{400} = 0$, i.e., we use 0 to represent a white pixel, and we use 1 to represent a black square.
- It is possible to design the network (choose the weights) such that when some image of digit 0 is fed to the network, the output will be $y_0 = 1, y_1 = \ldots, y_9 = 0$. Likewise,

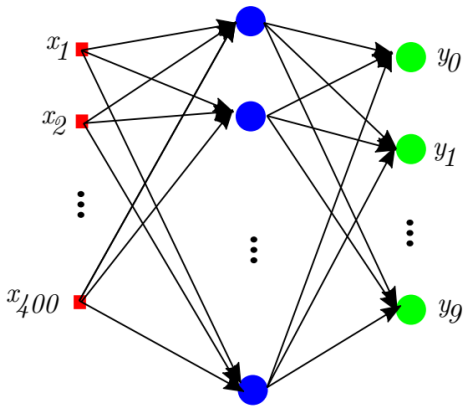



Figure 3: The 2-layer feedforward neural network for digit classification

for any $i \in \{0, \ldots, 9\}$, when some image of digit $i$ is fed to the network, the output will be $y_i = 1$ and $y_j = 0, \forall j \neq i$.

- This is usually done via supervised learning. We prepare (or usually acquire!) a large number of $20 \times 20$ training images, each of which looks like Fig. 2 but of course with different digits, and differently written versions of the same digit. See Fig. 4 for some sample portion of such a training set. Each training image has a label that specifies the actual digit corresponding to the image. For example, in Fig. 4, the images in the first row will be labeled as 0, the second row as 1, and so on.

# 4 Lecture 4

## 4.1 Approximation theorems and learning algorithms

- Can we always find weights and biases (parameters) to do what we want to do?
- Given enough neurons and layers, almost every function can be approximated (as accurately as we want)
- with logic (binary inputs/outputs) the **DNC/CNF** theorem shows that 2 layers are enough.

  The DNF/CNF theorem states that every Boolean formula can be transformed into either a **Disjunctive Normal Form (DNF)** or a **Conjunctive Normal Form (CNF)**. In DNF, the formula is expressed as a disjunction (OR) of conjunctions (AND) of literals, such as $(x_1 \wedge \neg x_2) \vee (x_3 \wedge x_4)$. Conversely, in CNF, the formula is expressed as a conjunction (AND) of disjunctions (OR) of literals, for example, $(x_1 \vee \neg x_2) \wedge (x_3 \vee x_4)$. This theorem is important because it guarantees that any Boolean function can be represented in one of these two canonical forms, which is useful in logic, computer science, and digital circuit design.

- But how do we set these parameters to achieve the desired behavior? Manual adjustment is impractical, except in simple cases. Instead, **learn using guidance from data**.

$$y_{\text{params}}(x) = \phi(U\phi(Wx + b) + c)$$

This output ideally is equal to our target $y$, but this is not always the case. **Goal:** Minimize the number of mistakes. Mathematically we have a mistake when $y_{\text{params}} \neq y$.

What we can do is to look at the whole dataset and count how many times mistakes are made.

$$\sum_{(x,y)\in\text{data}} \{y_{\text{params}} \neq y\}$$

**Typical algorithm:** Local search + gradual data.

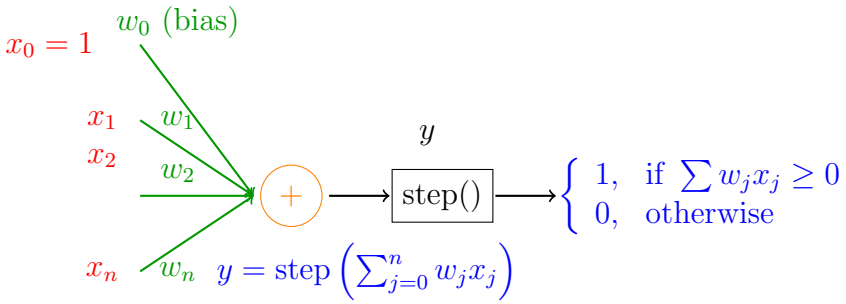
1. Initialize parameters **randomly**
2. for each (x,y) in the data
   - Feed x to NN and get $y_{\text{params}}(x)$
   - Look in the neighborhood of params to make $y_{\text{params}}(x)$ closer to y
3. Repeat 2. until parameters converge

Steps 2. and 3. represent an **epoch**, i.e. one full pass over the dataset.

## 4.2 Perceptrons

This is the simplest situation we are going to consider.

Consider the **McCullock-Pitt (1945)** neuron, with bias and weights.




What can it do?

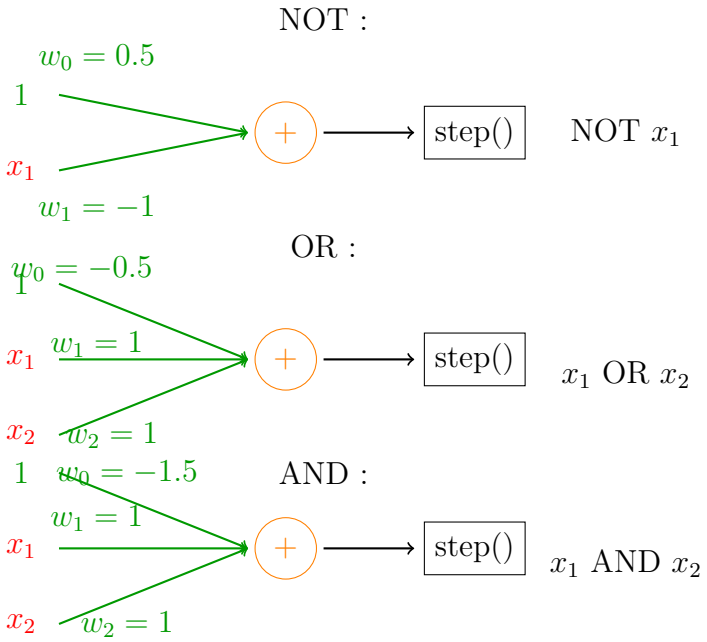
- **Recall:** $\begin{bmatrix} w_0 & w_1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = 0$ This is a line that passes through the origin.

  $\begin{bmatrix} w_0 & w_1 & w_2 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = 0$ This is a plane that passes through the origin

- In higher dimensions, this is called **hyperplane**: $\begin{bmatrix} . & . & w & . & . \end{bmatrix} \begin{bmatrix} . \\ . \\ x \\ . \\ . \end{bmatrix} = 0.$

  $\begin{bmatrix} . & . & w & . & . \end{bmatrix} \begin{bmatrix} . \\ . \\ x \\ . \\ . \end{bmatrix} \geq 0$ is a **halfspace**

- It can model **logic gate**




- It can classify using an hyperplane as **decision boundary**, which is the boundary with which we decide to switch from 0 to 1. This classifier is a linear separator

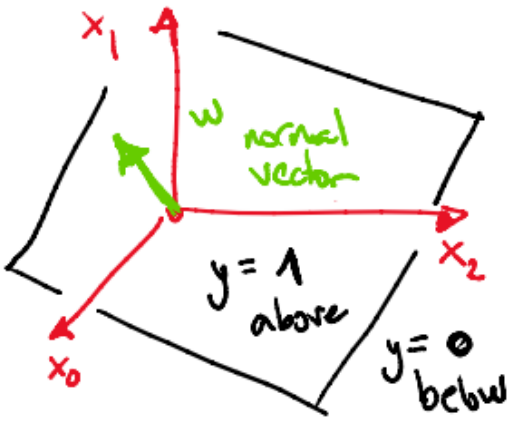



Figure 4: The image illustrates the decision boundary of a hyperplane in a 3D space. The axes $x_0$, $x_1$, and $x_2$ represent input features, and the green vector $w$ is the normal vector to the plane, representing the weight vector of a binary classifier (e.g., a perceptron). Points above the plane are classified as $y = 1$, while points below it are classified as $y = 0$. The plane itself serves as the decision boundary between these two classes.

# 5 Lecture 5

**Last time:** Approximation theories and learning theories. Percpetrons → one of the simplest algorithms

## 5.1 Example

$$\neg x_1 \wedge \neg x_2 ... \wedge \neg x_n \wedge x_{n+1} \wedge x_{n+2} ... \wedge x_{n+m}$$

This is a logic description, but we can move towards an arithmetic description:

$$(1 - x_1) + (1 - x_2) + ... + (1 - x_n) + (x_{n+1}) + ... + (x_{n+m})$$

If I add these guys, depending on their values, I can obtain a different range of results: the smallest one is zero, while the biggest is n+m.

Now we want to **threshold** it (i.e. **adjust the bias**), to build an AND operator.

$$(1 - x_1) + (1 - x_2) + ... + (1 - x_n) + (x_{n+1}) + ... + (x_{n+m}) \geq n + m - \frac{1}{2}$$

If it is an AND the output should be 1 only when they are all 1, so when the sum is equal to n+m:

$$\underbrace{-(m + \frac{1}{2})}_{w_0} \cdot x_0 + \underbrace{(-x_1)}_{w_1} + \underbrace{(-x_2)}_{w_2} + \cdots + \underbrace{(-x_n)}_{w_n} + \underbrace{x_{n+1}}_{w_{n+1}} + \cdots + \underbrace{x_{n+m}}_{w_{n+m}}$$

Because NOT and either AND or OR together are **weighted gates**, **multiplayer perceptron** can represent **any** logical operator. How many layers are sufficient to implement

any operator? **We need 2 layers**, thanks to the **DNF/CNF** formula. May it not be the most efficient way, to implement a table, that's why the concept of **depth** is then introduced.

If we make a **truth table**, we need many entries, while with depth, fewer neurons are needed.

Is 1 layer sufficient? Answer: NO.

## 5.2 Perceptron Learning Algorithm

Given a description of the desired behavior, $y = f(x)$, how do we find parameters such that $y_{params}(x) \cong f(x)$? (In this case, params = w). Manually find this pattern is out of question, we aim for an automatic way.

We assume that exists w such that the perception can do the job exactly:

$$y_w(x) = \text{step}(w^T x) = y$$

**Jargon:** we define **classes**, which are y=0 and y=1 regions; they represent higher-level concepts of what we should do.

In **supervised learning**, the description takes the form of **data**.

**Algorithm:** **Input:** Data $= \{(x, y), ...\}$ $x \in R^n, y \in \{0, 1\}$
**Output:** weight vector $w \in R^{n+1}$.
**n.b.** we have $w_{n+1}$ weights because we also have $w_0$.

1. Initialize w randomly. In general there are errors
2. While errors: $\exists (x, y) \in$ data such that $y_w(x) \neq y$
3. For each $(x, y) \in$ Data:

$$\text{If } y_w(x) = y: \text{ do nothing}$$

$$\text{Else if } y_w(x) = 0 \text{ and } y = 1: \quad \mathbf{w} \leftarrow \mathbf{w} + \eta \mathbf{x}$$

$$\text{Else if } y_w(x) = 1 \text{ and } y = 0: \quad \mathbf{w} \leftarrow \mathbf{w} - \eta \mathbf{x}$$

$$\begin{cases} \mathbf{w} \leftarrow \mathbf{w} + \eta \mathbf{x} & \text{if } y_w(x) = 0 \text{ and } y = 1 \\ \mathbf{w} \leftarrow \mathbf{w} - \eta \mathbf{x} & \text{if } y_w(x) = 1 \text{ and } y = 0 \end{cases}$$

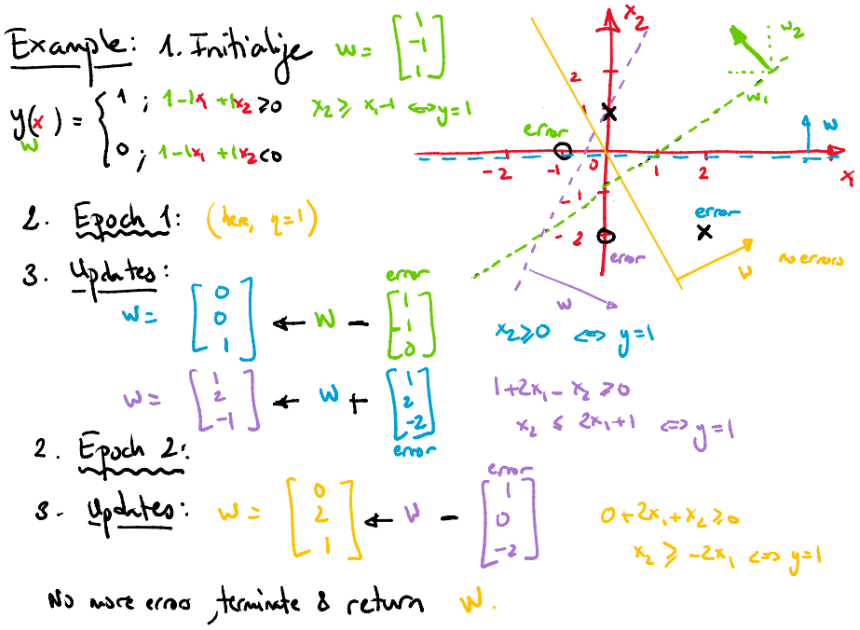
Simplifies to: $\mathbf{w} \leftarrow \mathbf{w} + \eta \mathbf{x}(y - y_w(x))$We move the weights toward the example.

$\eta$ represents the speed at which we update. Controls how smoothly/roughly we converge

**Epoch:** one full pass over data
**Theorem:** If classes are linearly separable, the algorithm will converge

# 6 Lecture 6

## 6.1 Example




In this example, weights are initialized to

$$\begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$$

In this case, the weight vector is pointing in the negative direction for $x_1$ and in the positive direction for $x_2$ and $x_0$ controls the shift from the origin.
This separator is making errors, so we have to change the weights every time we notice an error.
**Epoch 1:** weights are updated using the error point: the first error point considered is $(-1, 0)$, which has been classified as 1 but should have been classified as 0, so we subtract

that point from the weight vector. We obtain

$$\begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} - \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 2 \\ -1 \\ 0 \end{bmatrix}$$

We obtain a vector that is still making errors. The point $(2, -2)$ is classified as 0 but should be classified as 1, so we add this point to the weight vector:

$$\begin{bmatrix} 2 \\ -1 \\ 0 \end{bmatrix} + \begin{bmatrix} 2 \\ -2 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ -3 \\ 1 \end{bmatrix}$$

## 6.2 Supervised Learning

In **supervised learning** we are dealing with data $(x, y)$, where y is a sort of supervision. There is not a specific task, but it is defined according to how x behaves.

$$x \in \chi \text{ (\textbf{feature space:} context where we perform the task)}$$

$$y \in Y \textbf{ (label space:} \text{ target)}$$

- y can be **discrete** and in this case we talk about **classification**, but it can also be **continuous** and in this case we talk about **regression**.
- **Task:** predict/imitate y using only x.
- **How?** Use a neural network: $y_w(x) = f(x, w)$ (function of x, with parameter w). This gives us a predictor, which is a function of x parametrized by w.
- **Loss:** measures how far y and f(x,w) are:
  - **0-1 loss:** $l(y, f) = 1\{y \neq f\}$
  - **squared loss:** $l(f, y) = ||y - f||^2 \rightarrow$ euclidean distance between them
- **Risk:** Average loss over a dataset

$$\text{Data} = \{(x, y), ...\}$$

$$\text{Risk: } \frac{1}{\text{Data}} \sum_{(x,y)\in \text{Data}} l(y, f(x, w))$$

  The risk is a property of the data and of the weights. The risk for the perception is the rate of mistakes and it represents the probability of making a mistake.
- **Goal:** Minimize (empirical) risk. Make as few mistakes as possible, remaining as close to y as possible $\rightarrow$ search the space fo w, to find the one that gives the smallest R(w).
- **Types of algorithms:**

- **Online:** We use these algorithms when data streams in. Weights are updated **along the way**. (usually) don't revisit data points. If we forgo epoch and get new data, the perceptron will be online.
- **Batch:** data is available in whole, so we don't have to look at each point singularly, but we can have a global perspective. (Usually) pass over data multiple times (epochs).
- **Mini batch:** Process data gradually in small batches.

# 7 Lecture 7

## 7.1 Linear Regression with Squared Loss

- Data: $\{(x, y), ...\}$, $x \in R^n, y \in R^m$ (x is an n-dimensional vector to predict an m-dimensional vector).
- **Predictor:** $f(x, W) = Wx$, $W \in R^{nxm}$ (this is a single neuron with $\phi(v) = v$, identity activation).

- **Goal:** Minimize $R(w) = \sum_{(x,y)\in \text{Data}} ||y - Wx||^2$

How do we solve a problem like this? Analytic solution: Optimality condition, because we are unconstrained, we want:

$$\nabla_w R = 0$$

This is not an equation, but $n \cdot m$ equations.

Let's consider a single data point to start:

$$l = (\sum_{k=1}^{m} y_{k'} - \sum_{j'=1}^{n} w_{kj'} x_{j'})^2$$

This is the loss of a single point, on m neurons

$$\frac{\partial l}{\partial w_{kj}} = -2y_k x_j + 2\sum_{j=1}^{n} w_{kj} x_j x_j$$

We are making the derivative with respect to a particular j

in terms of vectorial operation is an **outer product**, so it takes two vectors as input and gives a matrix as output.

This matrix is multiplied by matrix W. For every w we find the gradient and put it in a matrix.

$$\nabla_w l = -2 \cdot y \cdot x^T$$

$$\begin{bmatrix} ... \\ y \\ ... \end{bmatrix} \begin{bmatrix} ... & x^T & ... \end{bmatrix}$$

The rank of this matrix is 1

$$\nabla_w l = -2 \cdot y \cdot x^T + 2 \cdot W \cdot x \cdot x^T$$

This is the gradient of the loss for a single data point.

The risk is the sum of the losses of the data points. We want to find the derivative of that. But since the derivative is a linear operator, the derivative of the sum is the sum of the derivatives $\rightarrow$ the gradient of the sum is the sum of the gradients.

$$R(w) = \sum_{(x,y)\in \text{Data}} l(y, Wx) \rightarrow \nabla_w R = \sum_{(x,y} \nabla_w l$$

$$\nabla_w R = \sum_{(x,y} -2 \cdot y \cdot x^T + 2 \cdot W \cdot x \cdot x^T$$

$$-2 \cdot \begin{bmatrix} ... & .... & ... \\ y & y & y \\ ... & .... & ... \end{bmatrix} \cdot \begin{bmatrix} ... & x^T & ... \\ ... & x^T & ... \\ ... & x^T & ... \end{bmatrix} + 2 \begin{bmatrix} W \end{bmatrix} \cdot \begin{bmatrix} ... & ... & .... \\ x & x & x \\ ... & ... & ... \end{bmatrix} \cdot \begin{bmatrix} ... & x^T & ... \\ ... & x^T & ... \\ ... & x^T & ... \end{bmatrix}$$

$$(m \cdot \text{Data}) \cdot (\text{Data} \cdot n) + 2 \cdot (m \cdot n) \cdot (n \cdot \text{Data}) \cdot (Data \cdot n)$$

In terms of data matrices:

$$\nabla_w R = 0 \iff -2 \cdot y \cdot x^T + 2 \cdot w \cdot x \cdot x^T = 0$$

$$-2 \cdot y \cdot x^T + 2 \cdot w \cdot x \cdot x^T = 0 \Rightarrow W = y \cdot x^T \cdot (x \cdot x^T)^{-1}$$

We are trying to solve $W \cdot x \sim y$, but the problem is that we can't always invert X, because it isn't always a square matrix. We can almost invert it with $X^T \cdot (X \cdot X^T)^{-1}$, which is the **Moon-Penrose Pseude-Inverse**.

# 8 Lecture 8

## 8.1 Gradient Descend

- **Goal:** minimize over w $R(w) = \sum_{(x,y)\in \text{data}} l((x,y),w) = l(y, f(x,W))$
- **Idea:** in general the optimal condition is to set the derivative to 0. In multivariate case we should change the notion of derivative to the notion of **gradient**, which is a collection of derivatives. However, we are not going to find a good solution by setting it to 0! We are going to reduce it step by step to 0.

Let's call the amount of change **delta**. At each step we change the weights by an amount $\Delta w$.

$$w' = w + \Delta w$$

$$R(w') = R(w + \Delta w) = R(w) + \nabla R(w)^T \Delta w + O(||\Delta w||^2)$$

We want to move in such a way to make this function as negative as possible. How should we choose $\Delta w$ to get the best reduction?

$O(||\Delta w||^2)$ represents other terms that are smaller than the norm squared of $\Delta w$

To minimize $a^T v$, $v = \frac{-a}{||a||_2} \rightarrow ||v||_2 \leq 1$.

Let $\Delta w \propto -\nabla R(w)$

$$w' = w - \eta \nabla R(w)$$

It's like rolling down the hill, but without momentum

### 8.1.1 1-D example

$R(w)w^4$ The minimum of this function is 0.

$$\frac{dR}{dw} = 4w^3, \eta = \frac{1}{8}$$

$$w(0) = 1$$

,

$$w(1) = w(0) - \nabla R(w(0)) \cdot \eta = \frac{1}{2}$$

$$w(2) = w(1) - \nabla R(w(1)) \cdot \eta = \frac{1}{2} - 4 \cdot \frac{1}{2}^3 \cdot \frac{1}{8} = \frac{7}{16}$$

Now us smaller than $\frac{1}{2}$, but the algorithm has slowed down. What happens if we continue? The algorithm at each step is slowing down more and more, but this does not work for all *eta*. If $\eta < 0$, there will be oscillations, and the algorithm may not converge. If $\eta$ is small enough, always diminishes since bounded from below (by 0). Will it converge to 0? Yes, think about it.

It is extremely important **to have $\eta$ small enough**.

## 8.2 Widrow-Hoff LMS Algorithm

Let's apply gradient descend to linear regression.

The update now becomes:

$$w = w + \eta \cdot \sum_{(x,y)} (y - w^T \cdot x) \cdot x$$

This is one pass across the data, so it is a big **batch**.
Now we change the batch algorithm into an online algorithm (one data point at a time).

For each (x, y) ∈ Data: $w = w + \eta \cdot (y - w^T \cdot x) \cdot x$

This algorithm looks like the perceptron, which is in some sense a gradient descend algorithm.

What would neurons satisfy to implement the gradient descend? The activation function must be **differentiable**.

## 8.3 Delta Rule

We have to make sure our loss is **differentiable**, otherwise we can't apply the **gradient descend algorithm**.

**Squared Loss for Simple neuron with differentiable** $\phi(.)$

$$R(w) = \sum_{(x,y)} (y - \phi(W^T x))^2$$

Apply GD to it

$$\nabla R(w) = \sum_{(x,y)} 2 \cdot (y - \phi(w^t \cdot x)) \cdot (-\phi'(W^T \cdot x) \cdot x)$$

$$w' \leftarrow w - \eta \nabla R(w) w' \leftarrow w + \eta \sum_{(x,y)} 2 \cdot (y - \phi(w^t \cdot x)) \cdot \phi'(W^T \cdot x) \cdot x$$

One data point at a time

$$\phi(v) = \frac{1}{1 + e^{[} - av]} \tag{15}$$

$$\phi'(v)) \frac{-e^{-av}}{1 + e^{-av}} = \phi(v)(1 - \phi(v)) \tag{16}$$

# 9 Lecture 9

Last time: Gradient Descent
Minimize$_w$ R(w) = $\sum_{(x,y) \in \text{Data}} l(y, f(x, w))$

$$w' \leftrightarrow w - \eta \nabla R(W)$$

The minus sign is because we are moving towards the direction where the gradient is decreasing.

$$f(x, w) = Wx \tag{17}$$

$$l(y, f(x, w)) = ||y - f(x, w)||^2 \tag{18}$$

$$w' \leftarrow w - \eta \nabla R(w) = w - 2 \cdot \eta (y - \sum_{(x,y)\in \text{data}} (y - wx) \cdot (-x)) \tag{19}$$

$$w' \leftarrow w + 2 \cdot \eta (y - \sum_{(x,y)\in \text{data}} (y - Wx) x^T \tag{20}$$

The delta method allows to put in an activation function.
How do we update weights in a computationally efficient way?

## 9.1 Back Propagation

The **backpropagation** is an algorithm to compute the gradient. So far we have been computing gradients with 1 layer of neurons. What if we have a network of interconnected neurons? **We are going to apply the chain rule multiple times.**

$$\frac{\partial R}{\partial w_k} = \sum_{(x,y)} \frac{\partial l}{\partial w_k} = \sum_{(x,y)} \frac{\partial l}{\partial f} \cdot \frac{\partial f}{\partial w_k} \tag{21}$$

since it is a linear operator, we can bring the gradient inside the sum. Equation 21 works if we have just one output. If we have multiple outputs, we have to repeat the same things for all the i outputs.

$$\frac{\partial R}{\partial w_k} = \sum_{(x,y)} \cdot \frac{\partial l}{\partial w_k} = \frac{\partial l}{\partial f_i} \cdot \frac{\partial f_i}{\partial w_k} \tag{22}$$

To solve the equation we need $\frac{\partial \mathbf{f_i}}{\partial \mathbf{w_k}}$.
This f is a function of $t_k$, which is a function of $v_k$, which is a function of $w_k \rightarrow$ **proof by induction**.

$$\frac{\partial f}{\partial w_k} = \frac{\partial}{\partial w_k} f(k_1, t_k, \ldots) \tag{23}$$

con $t_k = \phi(v_k)$ e $v_k = w_k x + \ldots$

$$= \left[ \frac{\partial f}{\partial t_k}\bigg|_{t_k = \phi(v_k)} \right] \cdot \phi'(v_k) \cdot x \tag{24}$$

dove $\delta_k = \frac{\partial f}{\partial t_k}$

$$\frac{\partial f}{\partial \xi}\bigg|_{\xi = \phi(u)} = \frac{\partial f}{\partial \xi} f(x, t_{k_1}, \ldots, t_{k_m}, \ldots) \tag{25}$$

where,

$$t_{k_1} = \phi(w_1 x + \dots) \tag{26}$$

$$t_{k_2} = \phi(w_2 \xi + \dots) \tag{27}$$

$$t_{k_m} = \phi(w_m \xi + \dots) \tag{28}$$

$$t_{k_n} = \phi(w_n \xi + \dots) \tag{29}$$

To calculate $\frac{\partial \mathbf{f_i}}{\partial \mathbf{w_k}}$, we first perform a **forward pass**, to get all the outputs ($u$, $\xi$, $v$, $t$), then we perform a **backward pass**.

$\xi$ feed into w in the forward pass, while $\delta$ feeds into w in the backward pass- To find all the gradients we need to compute the forward signal with the backward signal.

$$\textbf{Gradient of W = forward signal} \cdot \textbf{backward signal}$$

If we have multiple neurons, each one with its $\xi$ we just have to index each $\xi$.

# 10 Lecture 10: Backpropagation Algorithm

With the gradients computed via backpropagation, we can perform **gradient descent** to find the optimal weights $\mathbf{w}$ that minimize the risk (loss) function. In this lecture, we will delve deeper into the backpropagation algorithm, elucidating the mathematical foundations and providing a step-by-step explanation of the gradient computations.

## 10.1 Overview of Gradient Descent

Gradient descent is an optimization algorithm used to minimize the loss function $R(\mathbf{w})$. The core idea is to iteratively update the weights in the opposite direction of the gradient of the loss function with respect to the weights.

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} R(\mathbf{w})$$

where:

- $\eta$ is the learning rate.
- $\nabla_{\mathbf{w}} R(\mathbf{w})$ is the gradient of the loss function with respect to the weights.

## 10.2 Computing Gradients with Backpropagation

Backpropagation efficiently computes the gradients of the loss function with respect to each weight by applying the chain rule of calculus. Let's explore the mathematical formulation in detail.

### 10.2.1 Basic Gradient Computation

Consider a neuron with input $\xi$, weight $w_k$, bias $b$, activation function $\phi$, and output $t_k$:

$$t_k = \phi(w_k \xi + b)$$

The loss function $\ell$ depends on the output $t_k$, the input $x_i$, and possibly other parameters. To perform gradient descent, we need to compute the partial derivative of the loss with respect to each weight $w_k$.

$$\frac{\partial \ell}{\partial w_k} = \frac{\partial \ell}{\partial t_k} \cdot \frac{\partial t_k}{\partial w_k}$$

Applying the chain rule:

$$\frac{\partial \ell}{\partial w_k} = \left[ \left. \frac{\partial \ell}{\partial t_k} \right|_{t_k = \phi(w_k \xi + b)} \right] \cdot \phi'(w_k \xi + b) \cdot \xi$$

Introducing the notation $\delta_{t_k}$:

$$\delta_{t_k} = \frac{\partial \ell}{\partial t_k}$$

Thus, the gradient becomes:

$$\frac{\partial \ell}{\partial w_k} = \delta_{t_k} \cdot \phi'(w_k \xi + b) \cdot \xi$$

### 10.2.2 Aggregating Gradients for the Risk

When considering the entire dataset, the risk $R(\mathbf{w})$ is typically the average loss over all training examples. The gradient of the risk with respect to a weight $w_k$ is the sum of the gradients of the individual losses:

$$\frac{\partial R}{\partial w_k} = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial \ell_i}{\partial w_k}$$

For simplicity, we often omit the scaling factor $\frac{1}{N}$ in gradient descent updates, as it can be absorbed into the learning rate $\eta$.

## 10.3 Backpropagation Through Layers

In neural networks with multiple layers, backpropagation propagates the error gradients from the output layer back through the hidden layers. Here's a detailed breakdown of this process.

### 10.3.1 Forward Pass

During the forward pass, we compute the activations of each neuron in the network:

$$\mathbf{t} = \phi(\mathbf{W}\xi + \mathbf{b})$$

where:

- $\mathbf{W}$ is the weight matrix.
- $\xi$ is the input vector.
- $\mathbf{b}$ is the bias vector.
- $\phi$ is the activation function applied element-wise.

### 10.3.2 Backward Pass

After computing the forward pass, we perform the backward pass to calculate the gradients.

**Gradient with Respect to Weights** For a weight matrix $\mathbf{W}$, the gradient of the loss with respect to $\mathbf{W}$ is:

$$\nabla_{\mathbf{W}}\ell = [\phi'(\mathbf{W}\xi + \mathbf{b})] \circ (\nabla_{\mathbf{t}}\ell) \cdot \xi^T$$

Breaking it down:

- $\phi'(\mathbf{W}\xi + \mathbf{b})$ is the element-wise derivative of the activation function.
- $\nabla_{\mathbf{t}}\ell$ is the gradient of the loss with respect to the output $\mathbf{t}$.
- $\circ$ denotes the Hadamard (element-wise) product.
- $\xi^T$ is the transpose of the input vector.

**Gradient with Respect to Inputs** To propagate the gradient to the previous layer, we compute the gradient of the loss with respect to the input $\xi$:

$$\nabla_{\xi}\ell = \mathbf{W}^T \cdot (\phi'(\mathbf{W}\xi + \mathbf{b}) \circ \nabla_{\mathbf{t}}\ell)$$

Simplifying the notation with $\delta$:

$$\delta = \phi'(\mathbf{W}\xi + \mathbf{b}) \circ \nabla_{\mathbf{t}}\ell$$

Thus,

$$\nabla_{\xi}\ell = \mathbf{W}^T \cdot \delta$$

This $\delta$ is then used to compute gradients for the preceding layers, enabling the backward propagation of errors.

## 10.4 Handling Biases in Backpropagation

Bias terms are treated similarly to weights but do not have an associated input $\xi$. Instead, their input is always 1.

### 10.4.1 Gradient with Respect to Bias

Given the neuron activation:

$$t = \phi(\mathbf{w}^T \xi + b)$$

The gradient of the loss with respect to the bias $b$ is:

$$\frac{\partial \ell}{\partial b} = \frac{\partial \ell}{\partial t} \cdot \frac{\partial t}{\partial b} = \frac{\partial \ell}{\partial t} \cdot \phi'(\mathbf{w}^T \xi + b)$$

Using the $\delta$ notation:

$$\frac{\partial \ell}{\partial b} = \delta_t \cdot \phi'(\mathbf{w}^T \xi + b)$$

## 10.5 Linear Algebraic Expressions in Backpropagation

Expressing backpropagation in matrix form allows for efficient computation, especially with modern hardware optimizations.

### 10.5.1 Neuron Activation in Matrix Form

$$\mathbf{t} = \phi(\mathbf{W}\xi + \mathbf{b})$$

where:

- $\mathbf{W} \in R^{m \times n}$ is the weight matrix connecting $n$ inputs to $m$ neurons.
- $\xi \in R^n$ is the input vector.
- $\mathbf{b} \in R^m$ is the bias vector.
- $\mathbf{t} \in R^m$ is the output vector after activation.

### 10.5.2 Loss Function

$$\ell(\mathbf{t}) = \ell(\phi(\mathbf{W}\xi + \mathbf{b}))$$

### 10.5.3 Gradient with Respect to Weight Matrix

$$\nabla_{\mathbf{W}} \ell = [\phi'(\mathbf{W}\xi + \mathbf{b})] \circ (\nabla_{\mathbf{t}} \ell) \cdot \xi^T$$

where $\circ$ denotes element-wise multiplication.

### 10.5.4 Gradient with Respect to Input Vector

$$\nabla_{\xi}\ell = \mathbf{W}^T \cdot (\phi'(\mathbf{W}\xi + \mathbf{b}) \circ \nabla_{\mathbf{t}}\ell)$$

### 10.5.5 Delta Rule Representation

Using the delta rule, we represent the error term $\delta$ for each neuron:

$$\delta = \phi'(\mathbf{W}\xi + \mathbf{b}) \circ \nabla_{\mathbf{t}}\ell$$

Thus, the gradient update for the weights becomes:

$$\mathbf{W} \leftarrow \mathbf{W} - \eta \cdot (\delta \cdot \xi^T)$$

## 10.6 Weight Update Equations

After computing the gradients, we update the weights and biases using gradient descent.

### 10.6.1 Weight Update

$$\mathbf{W} \leftarrow \mathbf{W} - \eta\nabla_{\mathbf{W}}\ell$$

### 10.6.2 Bias Update

$$\mathbf{b} \leftarrow \mathbf{b} - \eta\nabla_{\mathbf{b}}\ell$$

## 10.7 Gradient Update: Rank-1 Nature

The gradient update for the weight matrix $\mathbf{W}$ is a rank-1 matrix:

$$\nabla_{\mathbf{W}}\ell = \delta \cdot \xi^T$$

This indicates that each weight update is influenced by the outer product of the error term $\delta$ and the input vector $\xi$.

## 10.8 Illustrative Example

To solidify understanding, consider a simple neural network with one input layer, one hidden layer, and one output neuron.

### 10.8.1 Network Structure

- **Input vector**: $\xi = \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix}$
- **Hidden layer weights**: $\mathbf{W}_1 \in R^{2\times 2}$
- **Hidden layer biases**: $\mathbf{b}_1 \in R^2$

- **Output layer weights**: $\mathbf{W}_2 \in R^{1\times 2}$
- **Output layer bias**: $b_2 \in R$
- **Activation functions**: $\phi$ for hidden layer, linear activation for output.

### 10.8.2 Forward Pass

$$\mathbf{h} = \phi(\mathbf{W}_1\xi + \mathbf{b}_1)$$
$$t = \mathbf{W}_2\mathbf{h} + b_2$$

### 10.8.3 Loss Function

Assume squared loss:

$$\ell = \frac{1}{2}(y-t)^2$$

### 10.8.4 Backward Pass

**Output Layer Gradients**

$$\frac{\partial \ell}{\partial t} = t - y$$
$$\delta_t = \frac{\partial \ell}{\partial t}\cdot\frac{\partial t}{\partial \mathbf{W}_2} = (t-y)\cdot\mathbf{h}$$
$$\frac{\partial \ell}{\partial \mathbf{W}_2} = (t-y)\cdot\mathbf{h}$$
$$\frac{\partial \ell}{\partial b_2} = t - y$$

**Hidden Layer Gradients**

$$\delta_h = \mathbf{W}_2^T\cdot(t-y)\cdot\phi'(\mathbf{W}_1\xi + \mathbf{b}_1)$$
$$\frac{\partial \ell}{\partial \mathbf{W}_1} = \delta_h\cdot\xi^T$$
$$\frac{\partial \ell}{\partial \mathbf{b}_1} = \delta_h$$

### 10.8.5 Weight Updates

$$\mathbf{W}_2 \leftarrow \mathbf{W}_2 - \eta\cdot(t-y)\cdot\mathbf{h}$$
$$b_2 \leftarrow b_2 - \eta\cdot(t-y)$$
$$\mathbf{W}_1 \leftarrow \mathbf{W}_1 - \eta\cdot(\delta_h\cdot\xi^T)$$
$$\mathbf{b}_1 \leftarrow \mathbf{b}_1 - \eta\cdot\delta_h$$

## 10.9 Implementation Considerations

### 10.9.1 Initialization of Weights

Proper initialization of weights is crucial for effective training. Common strategies include:

- **Random Initialization**: Weights are initialized randomly, often using a Gaussian or uniform distribution.
- **Xavier/Glorot Initialization**: Designed to keep the scale of the gradients roughly the same in all layers.
- **He Initialization**: Specifically for layers with ReLU activations.

### 10.9.2 Choosing the Learning Rate

The learning rate $\eta$ controls the size of the weight updates:

- **Too Small**: Training can be very slow.
- **Too Large**: May cause the algorithm to overshoot minima or diverge.

Techniques like learning rate scheduling, adaptive learning rates (e.g., Adam, RMSprop), and learning rate decay are often employed to address these issues.

### 10.9.3 Batch vs. Stochastic vs. Mini-batch Gradient Descent

- **Batch Gradient Descent**: Uses the entire dataset to compute gradients.
- **Stochastic Gradient Descent (SGD)**: Uses a single training example to compute gradients.
- **Mini-batch Gradient Descent**: Uses a subset (mini-batch) of the dataset to compute gradients.

Mini-batch gradient descent is commonly used as it balances the efficiency and convergence stability of batch and stochastic methods.

### 10.9.4 Handling Non-differentiable Points

Activation functions like ReLU have non-differentiable points. In practice, subgradients are used:

$$\phi'(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases}$$

This allows backpropagation to proceed despite the non-differentiability at certain points.

## 10.10 Summary of Backpropagation Steps

1. **Forward Pass**:
   - Compute activations for each layer.
   - Compute the output of the network.
   - Calculate the loss using the loss function.
2. **Backward Pass**:
   - Compute the gradient of the loss with respect to the output.
   - Propagate the gradients back through the network using the chain rule.
   - Compute gradients with respect to weights and biases at each layer.
3. **Update Weights and Biases**:
   - Adjust the weights and biases using the computed gradients and the learning rate.
4. **Iterate**:
   - Repeat the forward and backward passes for multiple epochs until convergence.

## 10.11 Visual Illustration

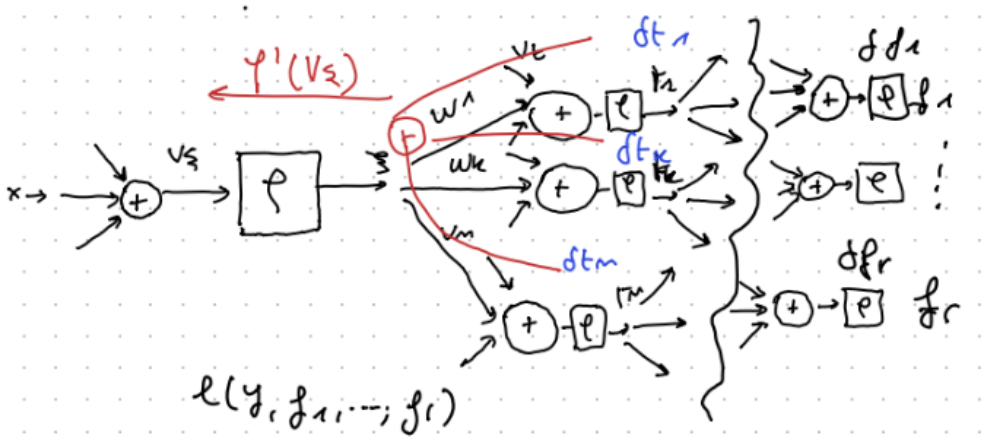


Figure 5: Illustration of the Backpropagation Process

**Figure 5** shows the flow of information during the forward and backward passes. During the forward pass, activations are computed layer by layer. In the backward pass, error gradients are propagated from the output layer back to the input layer, updating weights and biases accordingly.

## 10.12 Advanced Topics (Optional Extensions)

For a comprehensive understanding, consider exploring the following advanced topics related to backpropagation:

### 10.12.1 Vanishing and Exploding Gradients

- **Vanishing Gradients**: Gradients become very small, effectively preventing weights from updating, particularly in deep networks.
- **Exploding Gradients**: Gradients become excessively large, causing numerical instability.

Techniques to mitigate these issues include:

- Proper weight initialization.
- Using activation functions like ReLU.
- Gradient clipping.

### 10.12.2 Regularization in Backpropagation

Regularization techniques such as L1 and L2 regularization, dropout, and data augmentation can be integrated into the backpropagation process to prevent overfitting and enhance generalization.

### 10.12.3 Optimizers Beyond Basic Gradient Descent

Advanced optimization algorithms like Adam, RMSprop, and AdaGrad adapt the learning rate during training, often leading to faster convergence and better performance.

## 10.13 Conclusion

Backpropagation is a cornerstone algorithm in training neural networks, enabling efficient computation of gradients necessary for optimization. Understanding its mathematical foundations and implementation details is crucial for designing and training effective machine learning models.

# 11 Lecture 11

Last time: backpropagation

**Forward:**

$$\ell(_l) = l(\phi(w_l \xi_{l-1} + b_l)) \tag{30}$$

$$\phi(w_l \xi_{l-1} + b_l = xi_l \tag{31}$$

$$w_l \xi_{l-1} + b_l = v_l \tag{32}$$

**Backward:**

$$\nabla \xi_{l-1} \ell = w_l(\phi'(vl)\nabla \xi_l \ell) = w_l^T \delta_l \tag{33}$$

**Gradients:**

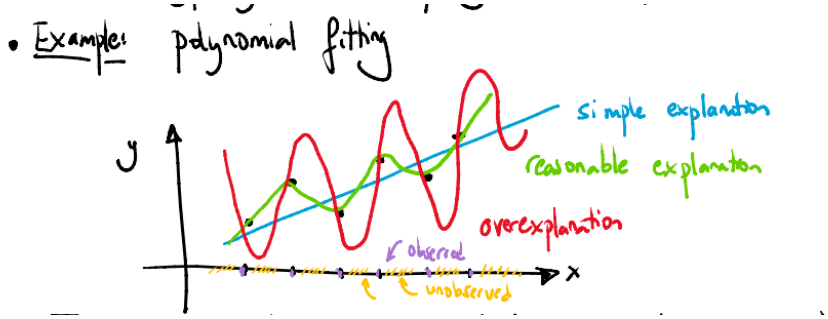
$$\nabla_w \ell = (\phi'(v_l)\nabla \xi_l \ell)\xi_l^t = \delta_l \xi_{l-1}^T \tag{34}$$

$$\nabla_b \ell = \delta_l \tag{35}$$

## 11.1 Overfitting

It is the tendency to **overexplain** the training data. Overexplaining means adding too much complicated and useless details.

Example: polynomial fitting




The opposite of overfitting is **underfitting**, when your model is to simple and it is not able to fit your data; on the other hand, when overfitting occurs, your model is perfectly capable of fitting your data, but lacks of generalization.

If you use a simple explanation you have a small variance, but high bias. With more complicated explanations, you lower the bias because you are able to catch the complexity of your data, but you increase the variance.

Typical problem to this: high sensitivity to changes in data. When learning, we have been focusing on observed contexts, but we mostly care about performance on new **unobserved contexts**. Performing well in unobserved contexts is called **generalization** and overfitting usually prevent it.

How do we quantify it?

Training Data = $\{(x, y), \dots\}$ → use this to build the model

Testing Data = $\{(x', y'), \dots\}$ → use this to assess generalization, **but** we must be very careful! We can't reuse test data, otherwise we'll overfit them too.

The train risk is not a good indicator of the model generalization capability; we must also look at the test risk; when it starts to increase, that's when overfitting occurs. Generally, if we have more data available, we can afford trying to overexplain it, but at a certain point overfitting will start again.

### 11.1.1 Observations

- stopping earlier can alleviate overfitting. Why? The neural network won't fit the noise.
- How? By staying close to its initialization. **Inductive bias** → preferring simple explanations.
- More data tends to help, but often it is not an option.
- **early stopping**, but we don't want to look at the date data

## 11.2 Cross-validation

Since training risk is not a good **proxy** tp test the risk, we could hold out some of the training data for **validation**.

**Training Data:** use it to train the model (often.
**Validation Data:** use it to check if okay (sometimes)
**Test Data:** test on this (once).

What is validation good for? You can choose what epoch to stop at, and it allows you to choose among possingle architectures, learning rates... (you choose the combination that provides the lowest validation risk). These choices are **coarser** than choosing weights and biases: they are called **hyperparameters**. Validation is used to adjust these parameters.

A common way to perform cross validation is the **k-fold cross-validation**: data are divided into k blocks. The model is trained on k-1 blocks and validated on block k. The process is repeated k times. The obtained values are averaged, to obtain a more accurate loss and a less noisy proxy. The extreme case for this is **leave-one-out cross-validation (LOOCV)**

# 12 Lecture 12

## 12.1 Regularization

Cross-validation helps to **monitor** overfitting, while regularization helps to **prevent** it. It is a concept that comes from physics, from **inverse problems**.

Regularization: collapse the possible explanations in fewer explanations. We need to be able to favor some of the solutions over the others. Ideally, we would like to favour 1. In physics we tend to favour simpler ones → **Occam's Razor** (choosing simple explanations). For example, in physics we prefer low energy because it is more likely for a system to go to a lower energy state. For polynomials and nueral networks we would favour **smaller weights** ("low energy" weights).

$$\min_w R(w), \text{ for } ||w||_2^2 \leq C \tag{36}$$

We want the **euclidean norm** to be smaller than a threshold.T This condition is the regularization part.

In a polynomial, when weights are smaller, we obtain a **smoother curve**. This is a version of multiple objective minimization and usually we see another version of the problem.

$$\min_w R(w), \text{ for } ||w||_2^2 \leq C \longleftrightarrow \min_w R(w) + \lambda||w||_2^2 \tag{37}$$

This is a **regularized empirical risk minimization**: a penalty term is added to penalize too large weights. This is called **weight decay**. The smoothness prevents overfitting the noise, so the empirical risk and regularization become better representatives of the test set. Together, they better track the empirical risk.

## How does this affect backpropagartion?

$$\nabla_w(R(w) + \lambda||w||_2^2) = \nabla_w R + \lambda 2 \cdot w \tag{38}$$

$$w \leftarrow w - \eta(\nabla_w R + 2\lambda w) \tag{39}$$

$$w \leftarrow (1 - 2\eta \cdot \lambda) \cdot w - \eta \nabla_w R \tag{40}$$

$$1 - 2\eta \cdot \lambda = \epsilon \tag{41}$$

Usually, $\epsilon$ is smaller than $1 \rightarrow$ in front of $w$ we have something smaller than 1 and this term in ML is called weight decay.

$$w = (w_1, w_2, w_3 \tag{42}$$

$$||w||_2 = (w_1^2 + w_2^2 + w_3^2)^{\frac{1}{2}} \tag{43}$$

$$||w||_p = (w_1^p + w_2^p + w_3^p)^{\frac{1}{p}} \tag{44}$$

$$||w||_1 = |w_1| + |w_2| + |w_3| \tag{45}$$

If we change the L2 norm with the L1 norm, we obtain:

$$\min_w R(w) + \lambda||w||_1 \tag{46}$$

$$\nabla_w(R(w) + \lambda||w||_1) = \nabla_w R + \lambda \cdot \text{sign}(w) \tag{47}$$

The L1 norm for w1 to be sparse $\rightarrow$ it is going to produce a sparse solution.

**L1 Norm**:

- Encourages sparsity in the weight vector
- Leads to many weights being exactly zero, effectively performing feature selection.
- The gradient involves the sign of each weight, promoting weights to either stay zero or become non-zero.

**L2 Norm**:

- Encourages smaller, but generally non-zero, weights.
- Does not inherently promote sparsity.
- The gradient is proportional to the weight value, leading to a smooth decay of weights.

**Why L1 Norm Introduces Sparsity**: The L1 norm creates a geometry with sharp corners (like a diamond shape in two dimensions). When minimizing the loss, the optimization process is more likely to hit these corners where one or more weights are exactly zero. This results in sparse solutions where only a subset of features contribute to the model, enhancing interpretability and reducing overfitting by eliminating irrelevant features.

In contrast, the L2 norm has a spherical geometry, promoting solutions where all weights are small but typically non-zero, distributing the penalty more evenly across all parameters.

## 12.2 Other types of regularizations

- Regularization can be viewed as incorporating prior beliefs about the model parameters. For example, in L2 regularization, we assume that smaller weights are a priori more likely, reflecting a preference for simpler models.
- **Invariance in Vision**:
  - **Concept of Invariance**: In computer vision, certain transformations of an image (such as rotation, translation, or scaling) do not alter the fundamental content. For instance, rotating a picture of a cat still results in a cat. This property is known as **invariance**.
  - **Equivalence Classes**: Due to invariance, a single data point can represent an entire class of equivalent points transformed by invariant operations. For example, an image and its rotated versions belong to the same equivalence class.
  - **Data Augmentation as Regularization**: Instead of modifying the model to be invariant (e.g., using convolutional neural networks that are inherently translation-invariant), another approach is to **augment the data**. This involves generating synthetic data points by applying invariant transformations to existing data. By training on these augmented datasets, the model learns to generalize better, effectively acting as a form of regularization by exposing the model to a wider variety of inputs.
  - **Benefits of Data Augmentation**:
    * Enhances model robustness to variations in input data.
    * Increases the effective size of the training dataset, reducing overfitting.
    * Encourages the model to focus on invariant features rather than spurious details.
- **Resilience in Neural Networks**:

- **Biological Inspiration**: Just as the human brain remains functional even if some neurons are damaged or removed, artificial neural networks can benefit from resilience to ensure reliability and robustness.
- **Dropout Regularization**: A popular technique to introduce resilience involves **dropout**, where during training, each neuron (or weight) is randomly "dropped out" with a probability $p$. This means setting the neuron's output to zero for that iteration.
  - **Mechanism**:
    - At each training step, independently flip a biased coin with probability $p$ for each neuron.
    - If the coin is heads, set the neuron's output to zero for that forward and backward pass.
    - During testing, use all neurons but scale their outputs by $(1 - p)$ to account for the dropped neurons during training.
  - **Effects**:
    - Prevents the network from becoming overly reliant on specific neurons.
    - Encourages the network to develop redundant representations, enhancing generalization.
    - Acts as a form of ensemble learning, where multiple subnetworks are implicitly trained and averaged.