Python for Data Science Lecture 5: Introduction to Machine Learning

Satchit Chatterji
satchit.chatterji@gmail.com

ML In Theory

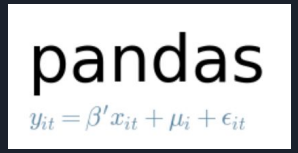
- Field comprised of:
  - Statistics
  - Linear Algebra
  - Probability Theory
  - Multivariable Calculus
  - …

ML In *Practice*

- Field comprised of:
  - Statistics
  - Linear Algebra
  - Probability Theory
  - Multivariable Calculus
  - …

ML In *Practice*

- Field comprised of:
  - Statistics
  - Linear Algebra
  - Probability Theory
  - Multivariable Calculus
  - …
- The good news:
  - People have done it for you!*



Itinerary for today

Goals of this lecture:

Explore different machine learning domains and algorithms

Itinerary for today

Goals of this lecture:

Explore different machine learning domains and algorithms
Get a brief feel for how they work

Itinerary for today

Goals of this lecture:

Explore different machine learning domains and algorithms
Get a brief feel for how they work
A high-level tour of the frontiers of ML

Itinerary for today

Goals of this lecture:

Explore different machine learning domains and algorithms
Get a brief feel for how they work
A high-level tour of the frontiers of ML
Hands-on practice

The Domains of ML

Domains of ML

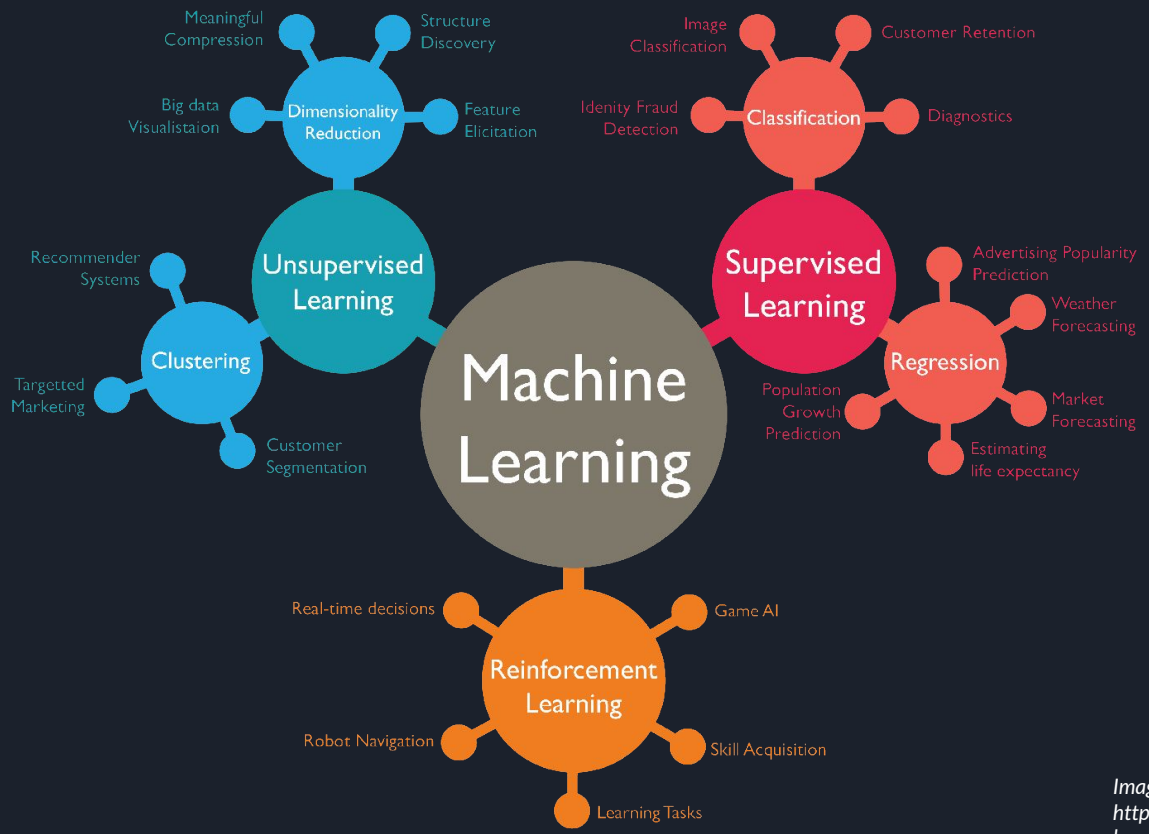


Image credit: https://zappy.ai/ai-blogs/reinforcement-learning-how-intelligent-bots-are-built

Domains of ML

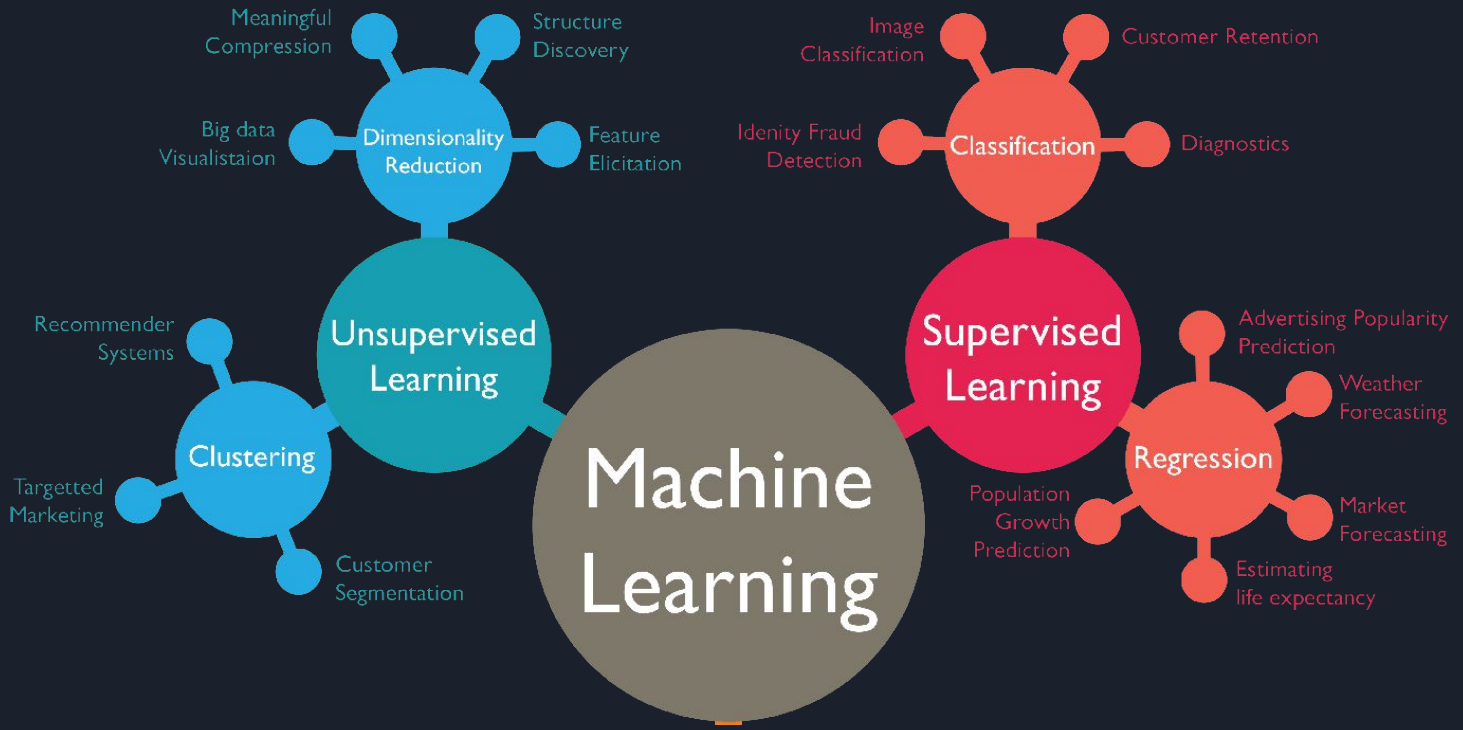
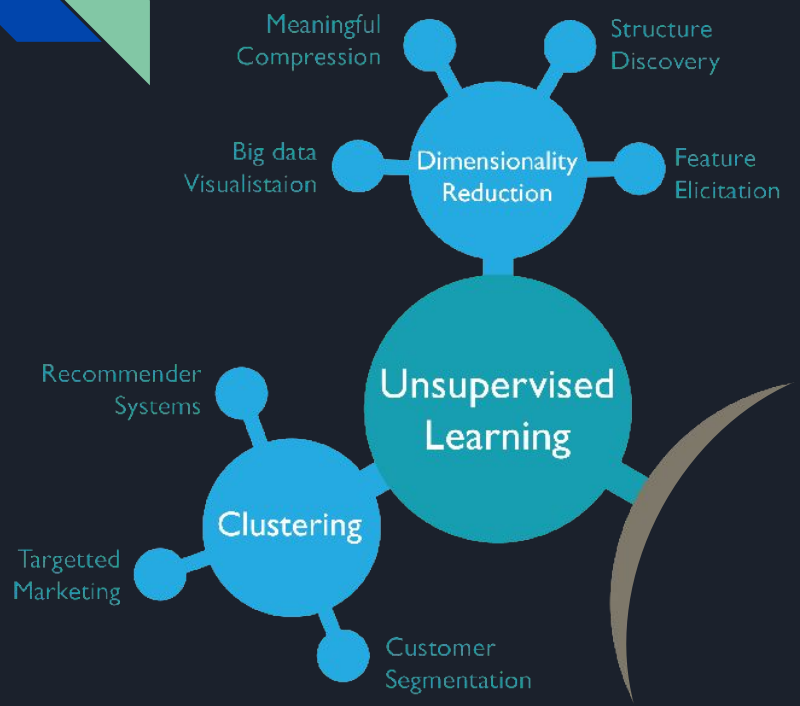


Image credit: https://zappy.ai/ai-blogs/reinforcement-learning-how-intelligent-bots-are-built

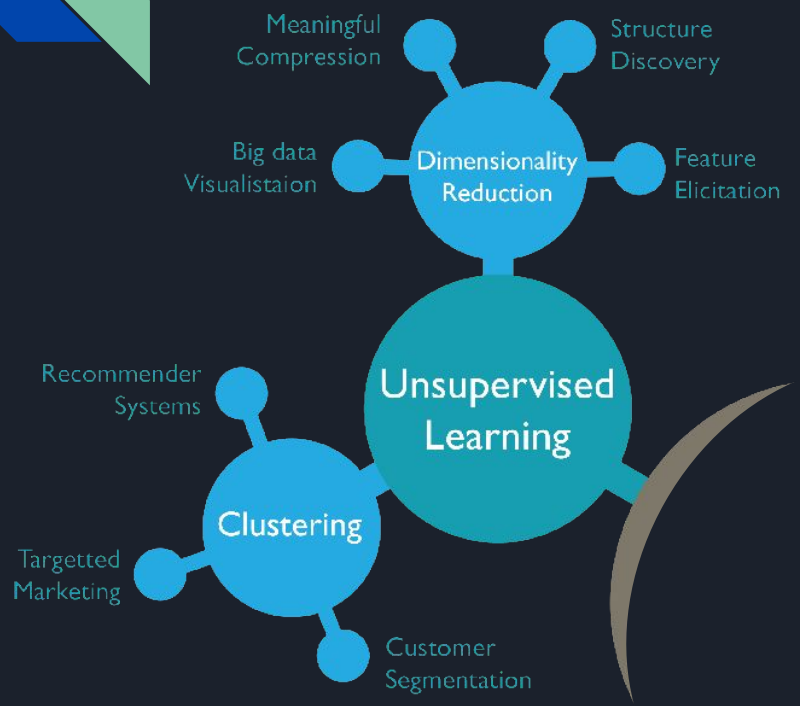
Unsupervised ML



- ***Given:*** Unlabelled, possibly unstructured data

$$x_i$$

Unsupervised ML

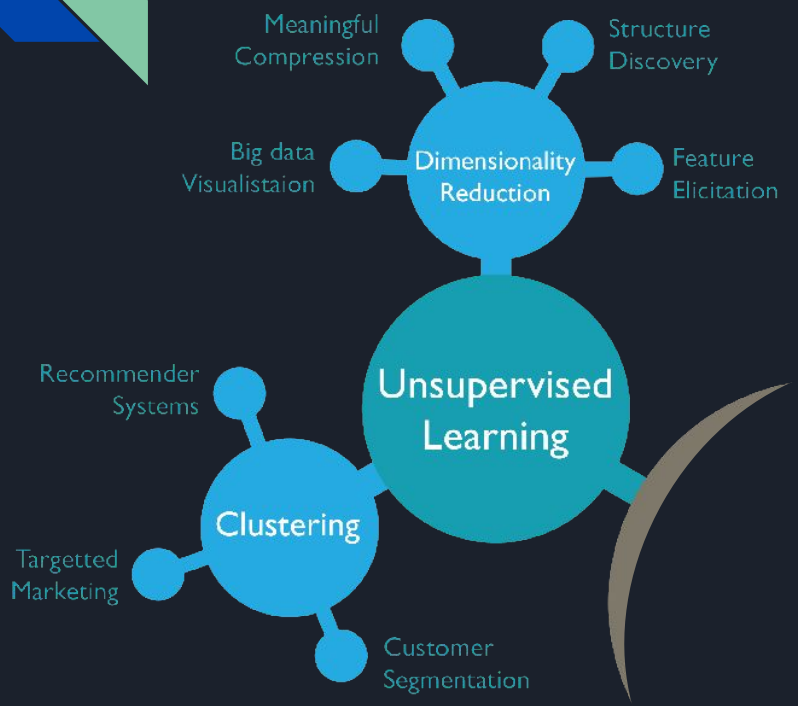


- ***Given:*** Unlabelled, possibly unstructured data

$$x_i$$

- ***Goal***: Several, including:
  - Dimensionality reduction
  - Model probability densities
  - Find patterns/structures/groups

Unsupervised ML



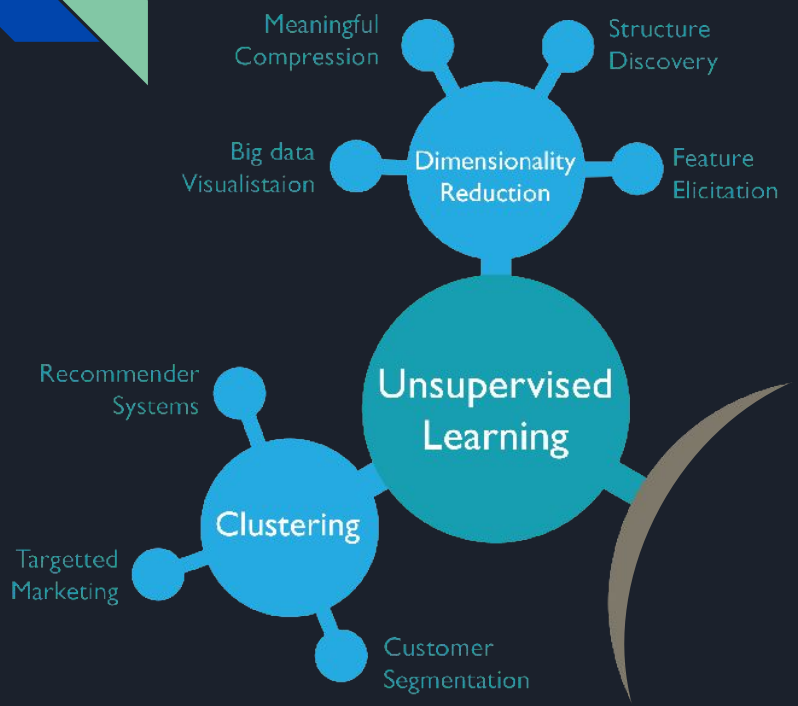
- ***Given:*** Unlabelled, possibly unstructured data

$$x_i$$

- ***Goal***: Several, including:
  - Dimensionality reduction
  - Model probability densities
  - Find patterns/structures/groups

- e.g. PCA, K-means clustering, autoencoders

Unsupervised ML



- ***Given:*** Unlabelled, possibly unstructured data

$$x_i$$

- ***Goal***: Several, including:
  - Dimensionality reduction
  - Model probability densities
  - Find patterns/structures/groups

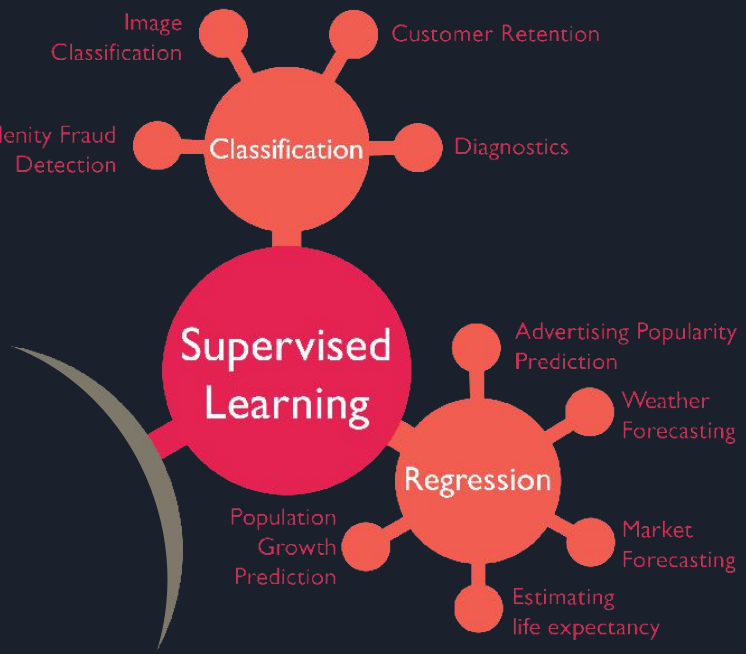
- e.g. PCA, K-means clustering, autoencoders

Lecture 4!

Supervised ML

***Given*:** Input-output examples of the form:

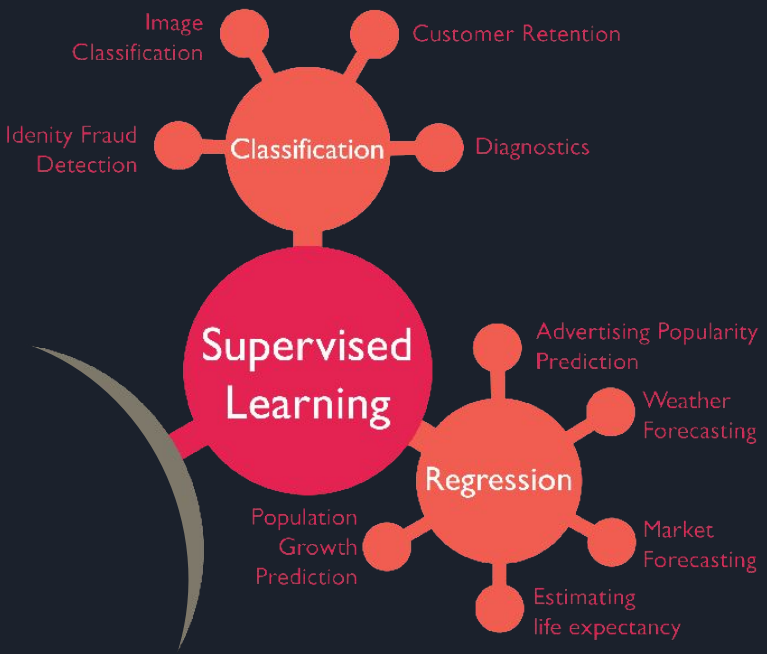
$$S = (\mathbf{x}_i, \mathbf{y}_i)_{i=1,\dots,T} \quad \mathbf{x}_i \in \mathbb{R}^N, \mathbf{y}_i \in \mathbb{R}^M$$



Supervised ML

***Given*:** Input-output examples of the form:

$$S = (\mathbf{x}_i, \mathbf{y}_i)_{i=1,\ldots,T} \quad \mathbf{x}_i \in \mathbb{R}^N, \mathbf{y}_i \in \mathbb{R}^M$$



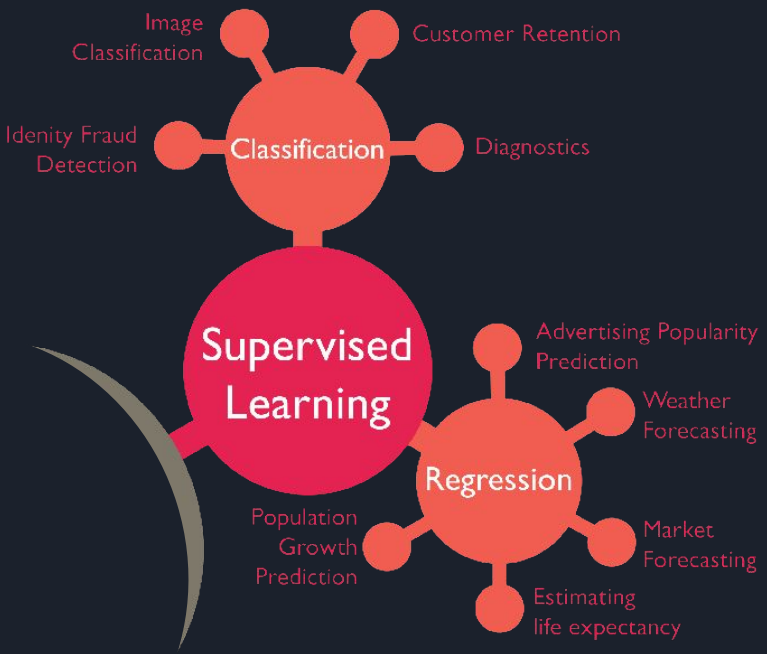
Supervised ML

***Given*:** Input-output examples of the form:

$$S = (\mathbf{x}_i, \mathbf{y}_i)_{i=1,\dots,T} \quad \mathbf{x}_i \in \mathbb{R}^N, \mathbf{y}_i \in \mathbb{R}^M$$

***Assumption*:** Data is generated by a “true ” function, with some added noise:

$$\mathbf{y}_i = f(\mathbf{x}_i) + v_i$$



Supervised ML

***Given*:** Input-output examples of the form:

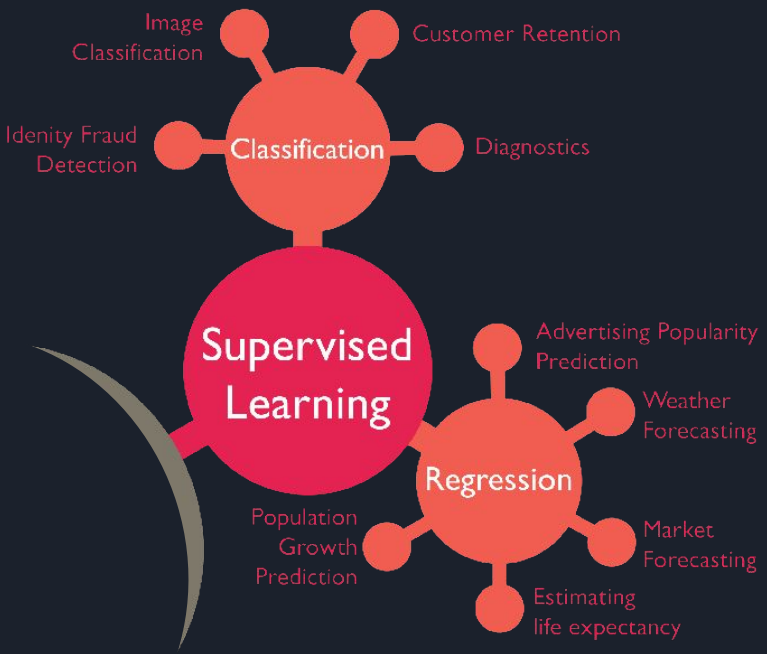
$$S = (\mathbf{x}_i, \mathbf{y}_i)_{i=1,\dots,T} \quad \mathbf{x}_i \in \mathbb{R}^N, \mathbf{y}_i \in \mathbb{R}^M$$

***Assumption*:** Data is generated by a "true " function, with some added noise:

$$\mathbf{y}_i = f(\mathbf{x}_i) + v_i$$

***Goal*:** Learn an approximation $\hat{f}(\mathbf{x})$ of the function:

$$\hat{f}(\mathbf{x}) \approx f(\mathbf{x})$$



Supervised ML

***Given*:** Input-output examples of the form:

$$S = (\mathbf{x}_i, \mathbf{y}_i)_{i=1,\dots,T} \quad \mathbf{x}_i \in \mathbb{R}^N, \mathbf{y}_i \in \mathbb{R}^M$$

***Assumption*:** Data is generated by a "true " function, with some added noise:

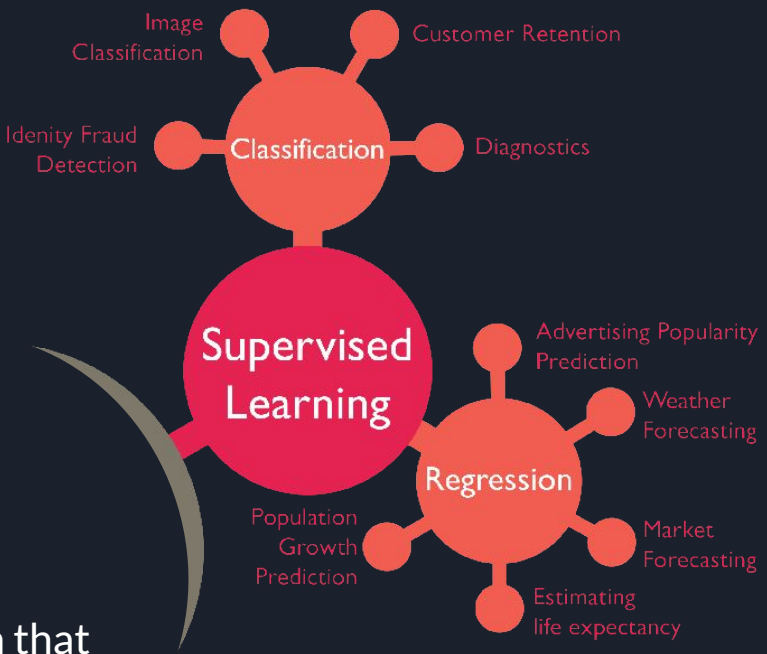
$$\mathbf{y}_i = f(\mathbf{x}_i) + v_i$$

***Goal*:** Learn an approximation $\hat{f}(\mathbf{x})$ of the function:

$$\hat{f}(\mathbf{x}) \approx f(\mathbf{x})$$

***Loss function*:** A distance between $\hat{f}(\mathbf{x})$ and $f(\mathbf{x})$ such that we can say $\hat{f}(\mathbf{x})$ is "good" if *L* is low across many given instances of *S*.

$$L : \mathbb{R}^M \times \mathbb{R}^M \rightarrow \mathbb{R}^{\geq 0}$$



SML: Learn a function with low “risk”

***Risk*:** What we want to minimize over the population

$$R(\hat{f}) = E[L(\hat{f}(X), Y)]$$

Slide adapted from Jaeger, H. (2022) *Neural Networks* Lecture Notes, https://www.ai.rug.nl/minds/uploads/LN_NN_RUG.pdf

SML: Learn a function with low “risk”

***Risk*:** What we want to minimize over the population

$$R(\hat{f}) = E[L(\hat{f}(X), Y)]$$

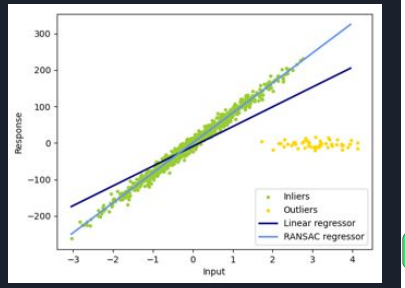
***Empirical Risk*:** What we can actually calculate
(for a “candidate” model ***h***, averaged over ***N*** training examples)

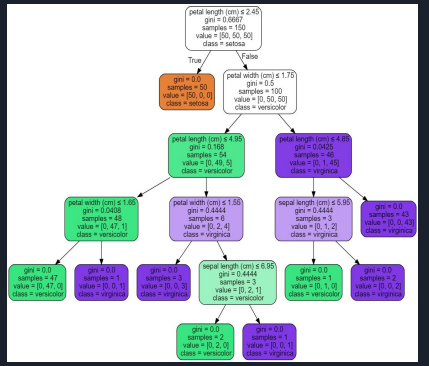
$$R^{\text{emp}}(h) = 1/N \sum_{i=1}^{N} L(h(\mathbf{x}_i), \mathbf{y}_i)$$

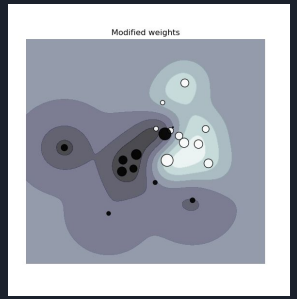
Slide adapted from Jaeger, H. (2022) *Neural Networks* Lecture Notes, https://www.ai.rug.nl/minds/uploads/LN_NN_RUG.pdf

Common Approaches

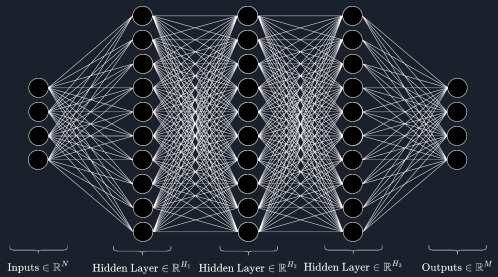
- Linear/Polynomial/Logistic Regression
- (Boosted) Decision trees
- Support Vector Machines
- Naive Bayes
- Neural Networks
- …







$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

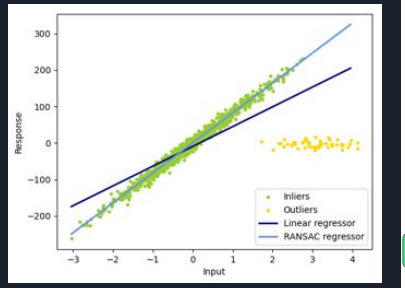


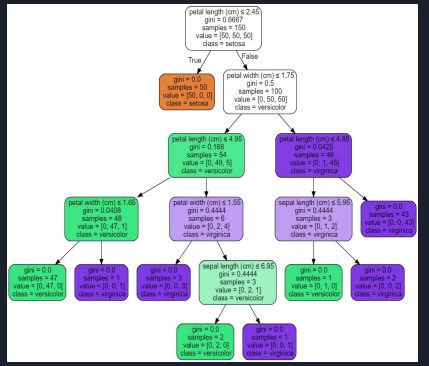
Images of regressions, decision tree, and SVM from scikit-learn.org

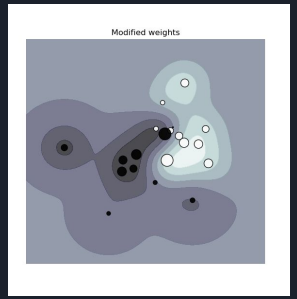
Common Approaches

Lecture 3/4

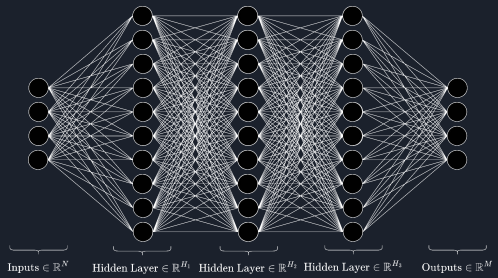
- *Linear/Polynomial/Logistic Regression*
- (Boosted) Decision trees
- Support Vector Machines
- Naive Bayes
- Neural Networks
- …







$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

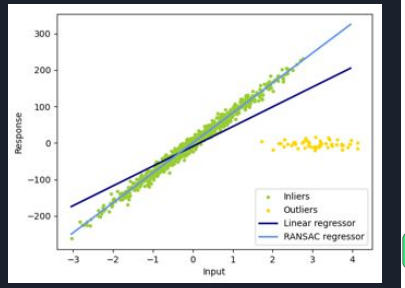


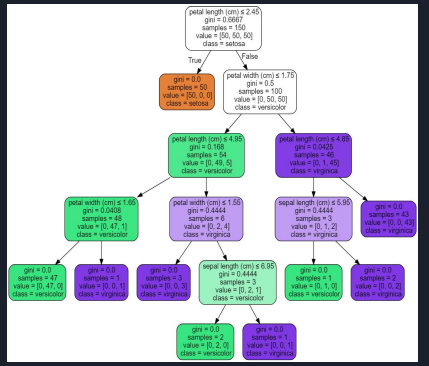
Images of regressions, decision tree, and SVM from scikit-learn.org

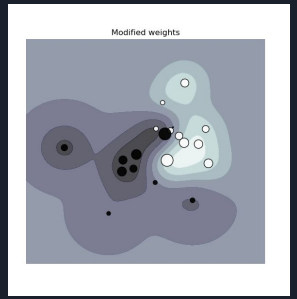
Common Approaches

Lecture 3/4

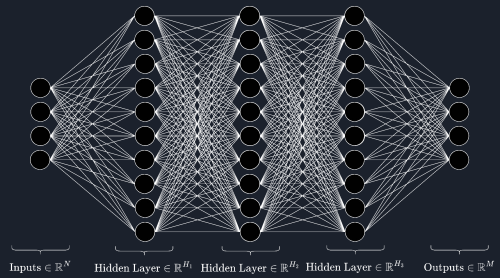
- *Linear/Polynomial/Logistic Regression*
- (Boosted) Decision trees
- Support Vector Machines
- Naive Bayes
- **Neural Networks**
- …







$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$



Images of regressions, decision tree, and SVM from scikit-learn.org

Bonus domains!

- Self-supervised learning
  - Learn input-output pairs from unlabelled data

Bonus domains!

- Self-supervised learning
  - Learn input-output pairs from unlabelled data
- Reinforcement learning
  - Learning by trial and error

AlphaGo

Bonus domains!

- Self-supervised learning
  - Learn input-output pairs from unlabelled data
- Reinforcement learning
  - Learning by trial and error
- Evolution/Genetic Algorithms
  - Learn by Darwinian evolution
  - Using data or trial and error

AlphaGo

Intro to Neural Networks

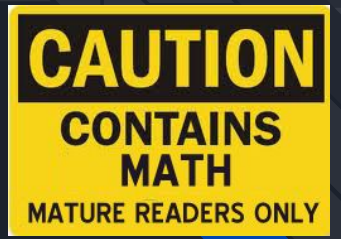
Intro to Neural Networks

Warning: Light mode oncoming

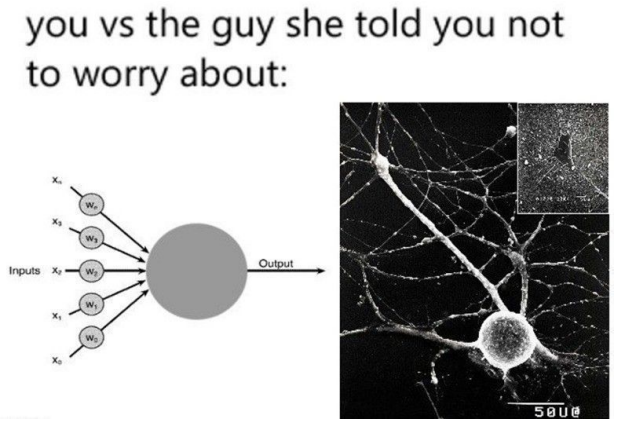
Slides stolen from ISOTDAQ 2022

Intro to Neural Networks

Warning: Light mode oncoming



Slides stolen from ISOTDAQ 2022



Source: linkedin.com/company/deeplearningai

Artificial vs Biological NNs

ANNs initially inspired by the brain:

Alexander Bain (1873), William James (1890)

Electrical connections/flow of neurons result in thought and movement

McColloch & Pitts (1943)

Modern mathematical “artificial” NN models (not the only neural network model!)

Rosenblatt (1958)

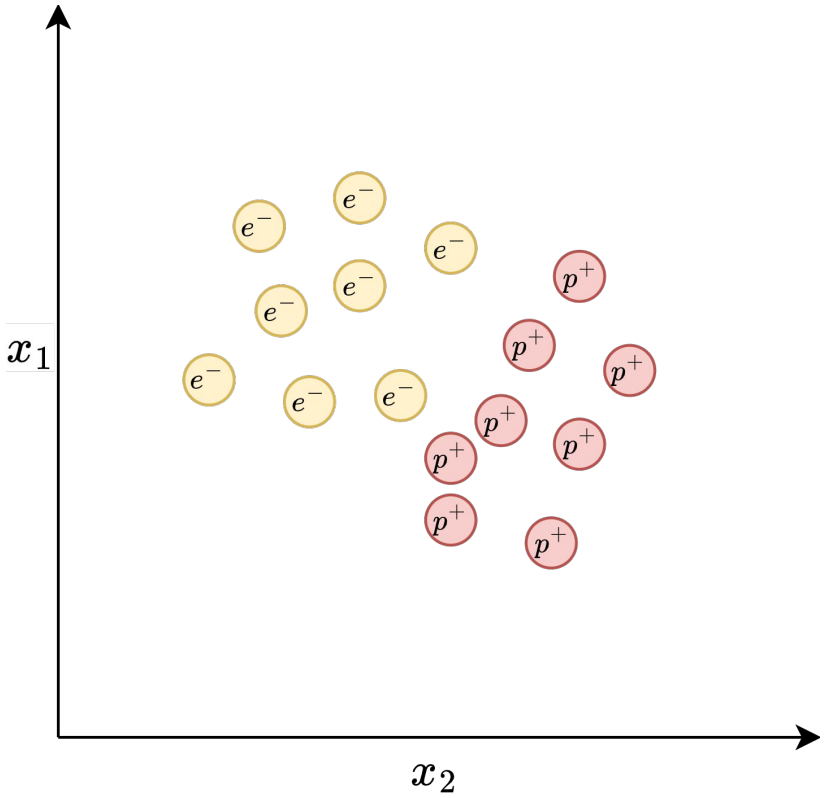
Description of the *perceptron*

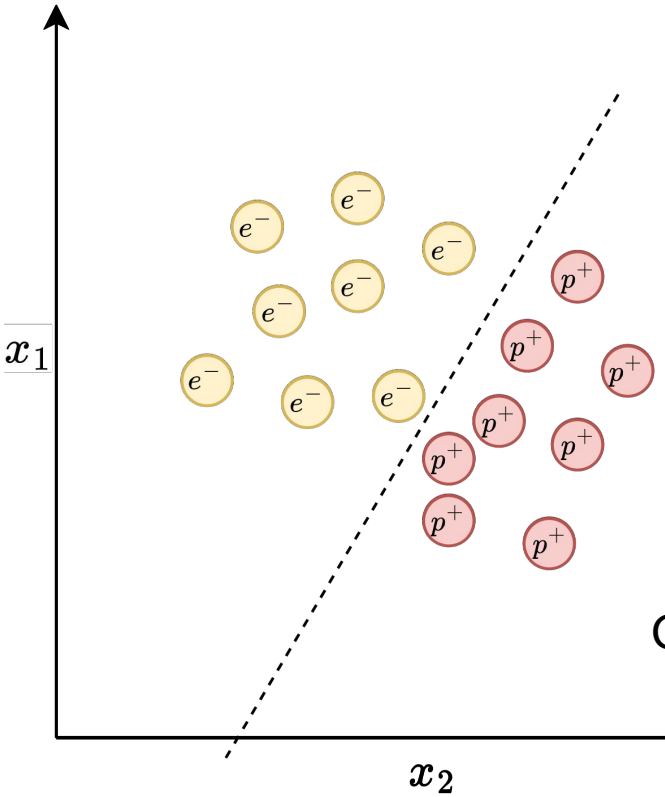
Rumelhart, Hinton & Williams (1986)

Multi-layer perceptrons and error backpropagation (learning principle)

Modern:

- ANNs used *everywhere* for *everything!*
- Simplified, abstracted version of “synaptically”-connected “neurons”
- Biologically implausible


x_1
x_2
e^-
e^-
e^-
e^-
e^-
e^-
e^-
e^-
p^+
p^+
p^+
p^+
p^+
p^+
p^+



Classes are *“linearly separable”*

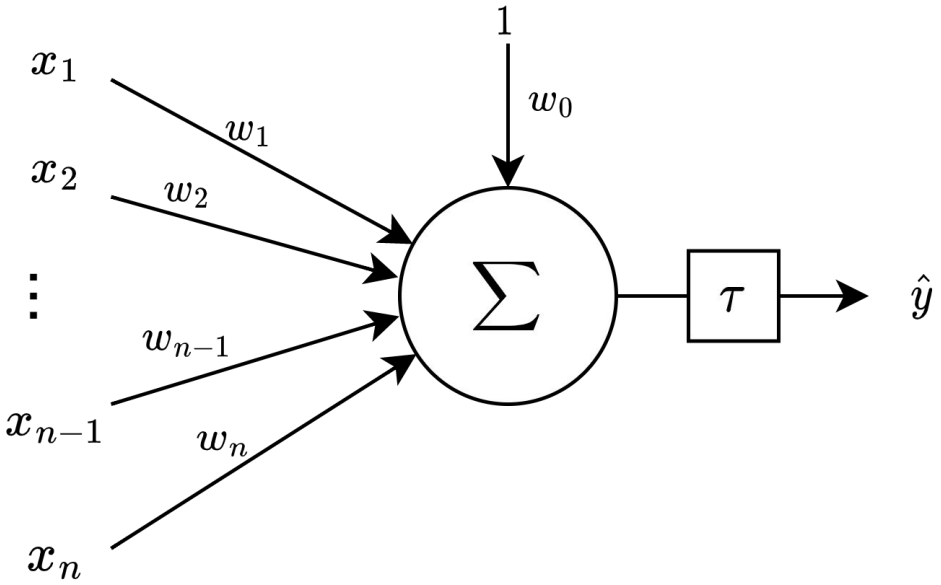
$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2 + ... + w_n x_n$$

$w_i \leftarrow$ Coefficients
$x_i \leftarrow$ Variables

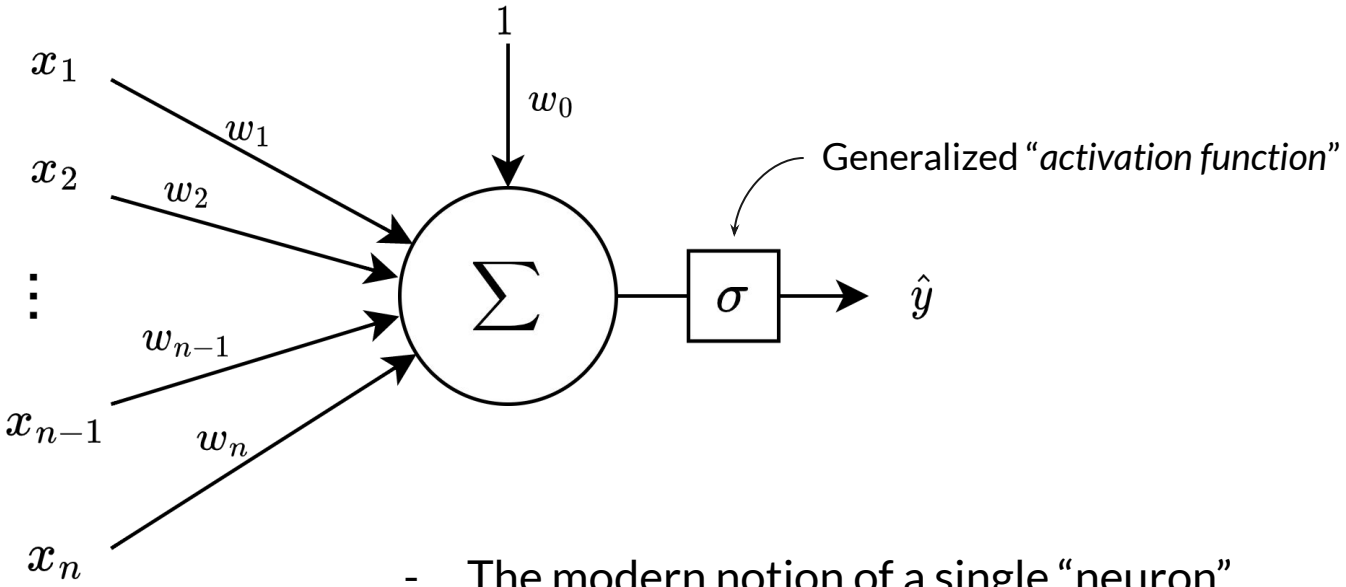
$$\hat{y} = \tau(w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n)$$

$$\tau(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

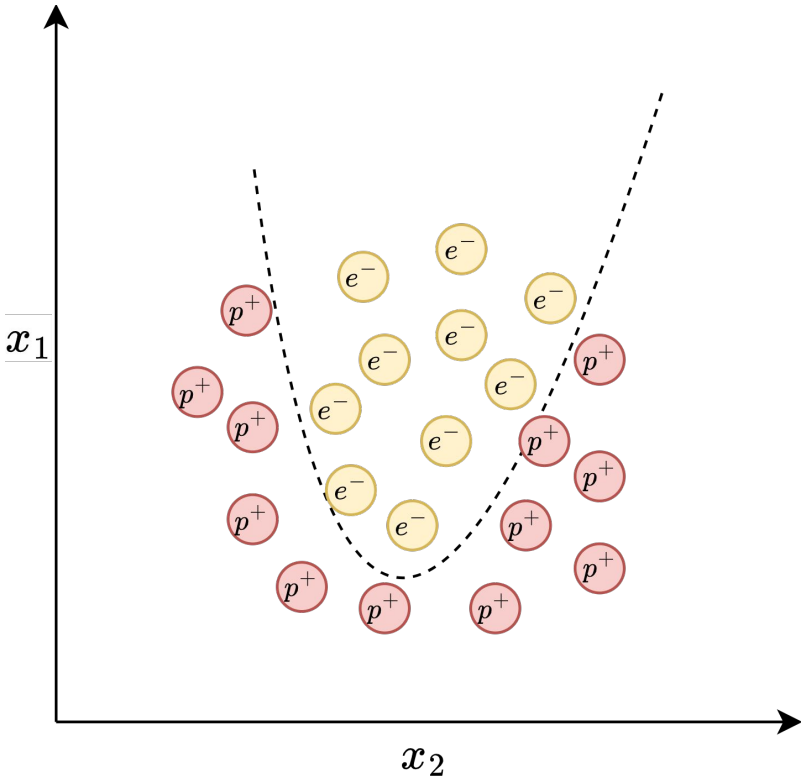
$$\hat{y} = \tau(w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n)$$

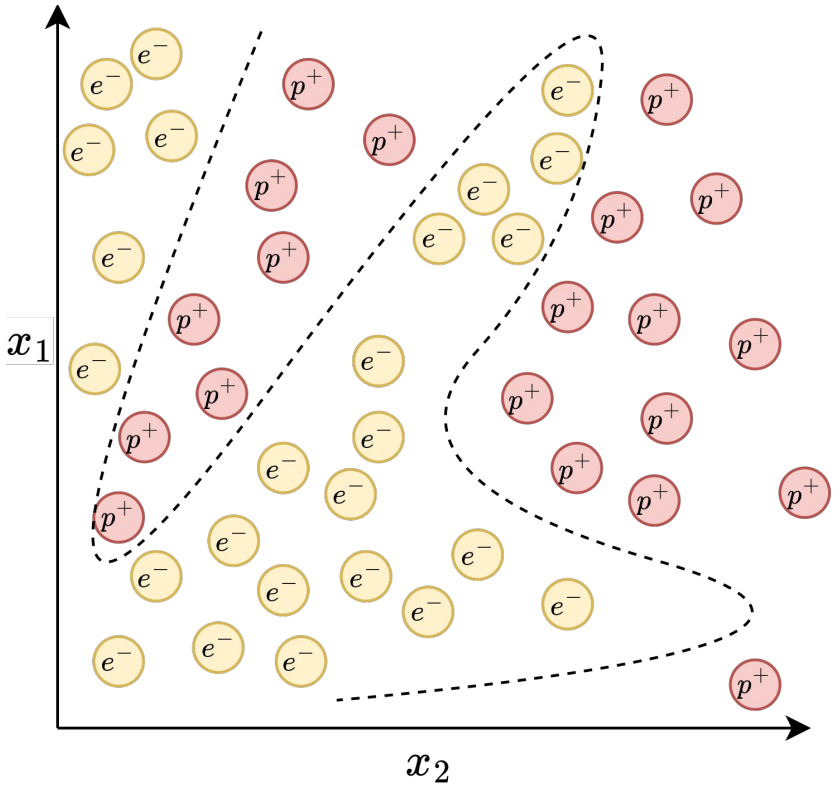


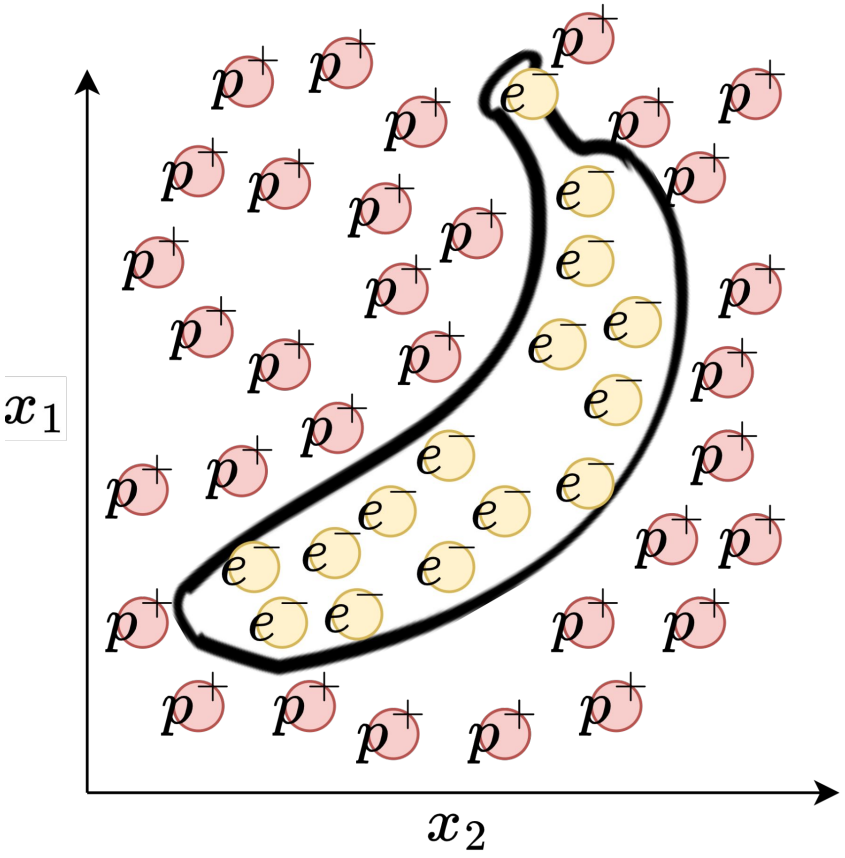
The “Perceptron”

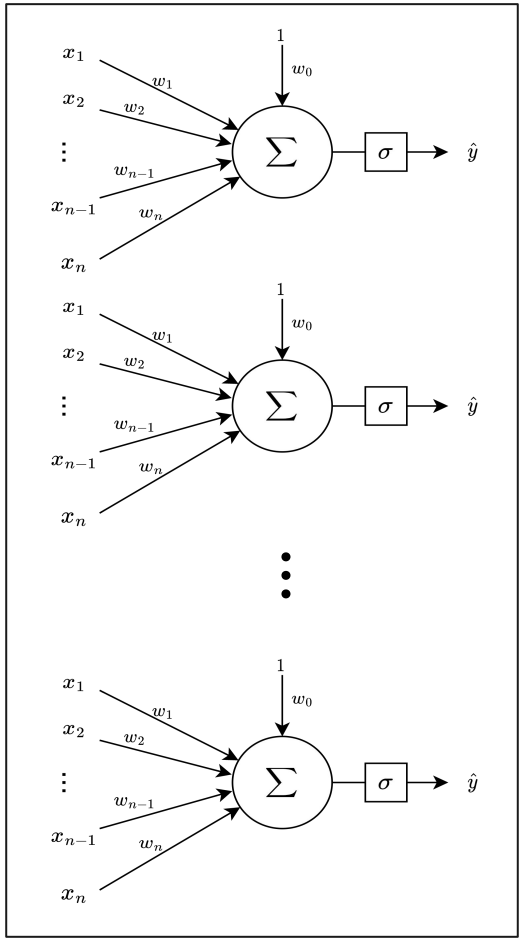


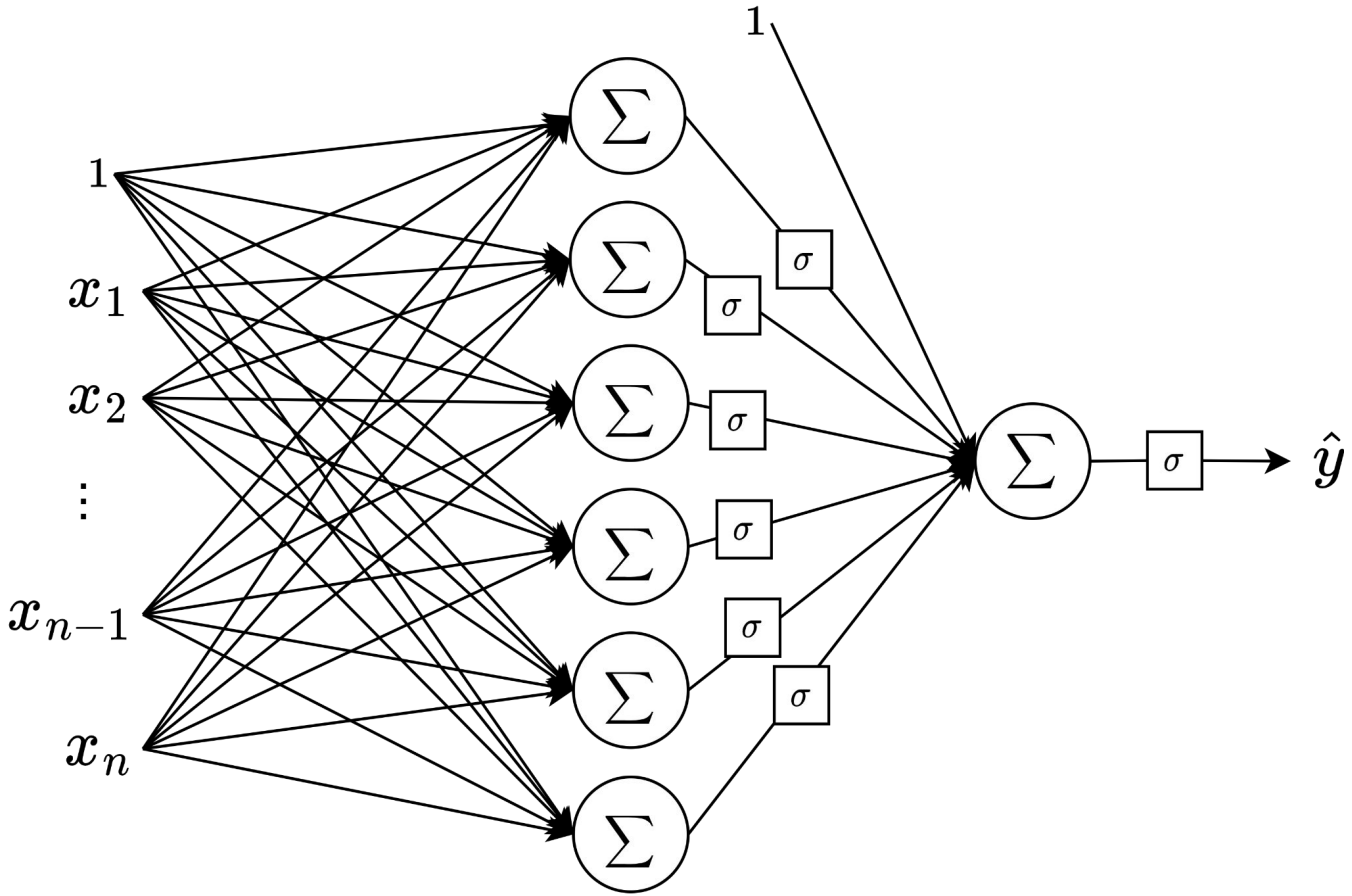
- The modern notion of a single “neuron”
- BUT: Only works on linearly separable classes


x_1
x_2
e^-
p^+

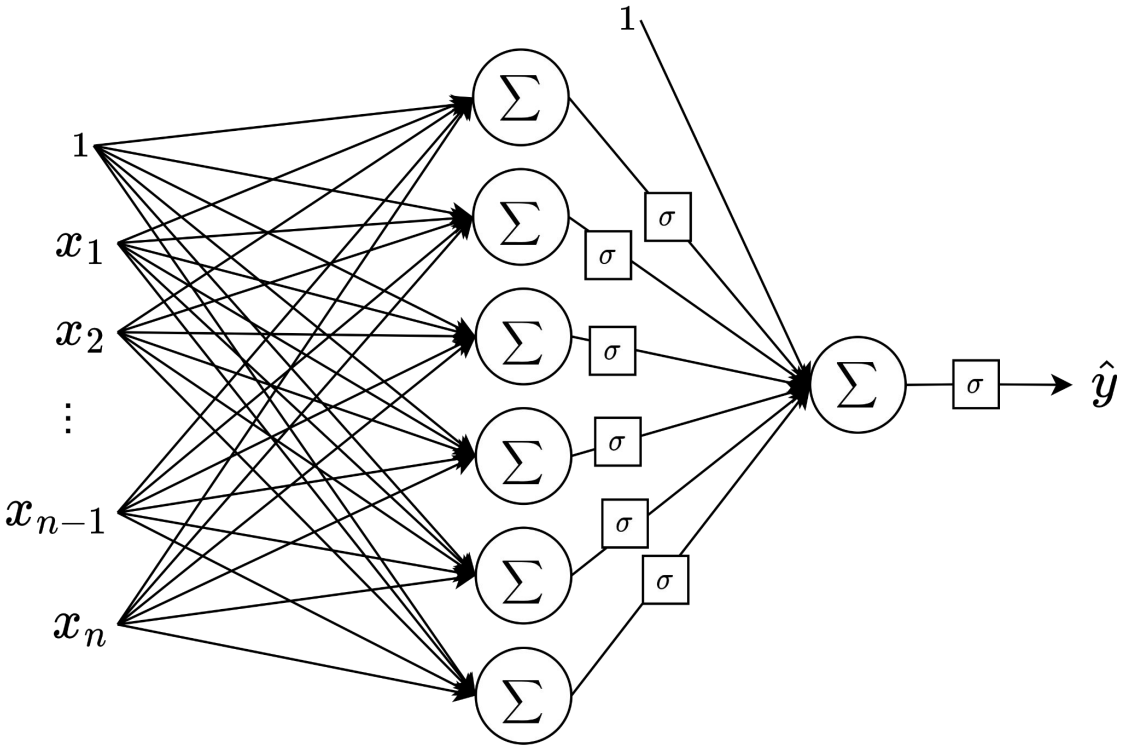

x_1
x_2


x_1
x_2


1
w_0
x_1
w_1
x_2
w_2
w_{n-1}
x_{n-1}
w_n
x_n
$\sum$
σ
$\hat{y}$


1
x_1
x_2
$\vdots$
x_{n-1}
x_n
Σ
σ
1
$\hat{y}$

Multi-layer Perceptrons (MLPs)



$$\hat{y} = \sigma(w_0 + w_1 x_1 + w_2 x_2 + ... + w_n x_n)$$

$$\begin{aligned}\hat{y} &= \sigma(w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n) \\ &= \sigma(\vec{w}^{\mathsf{T}} \vec{x})\end{aligned}$$

$$\vec{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} \qquad \vec{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

"Activation" "Bias"

$$\hat{y} = \sigma(w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n)$$
$$= \sigma(\vec{w}^\mathsf{T} \vec{x})$$

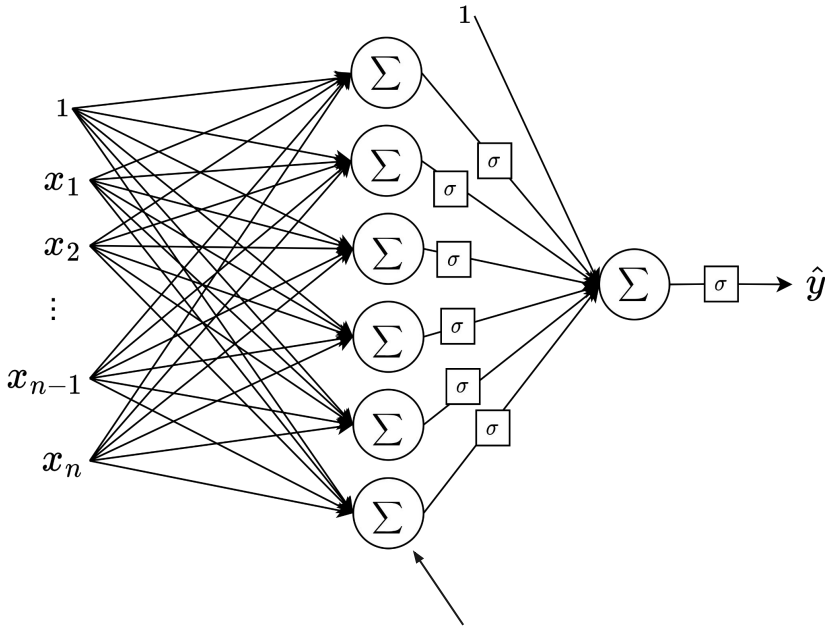
"Activation function"

$$\vec{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} \qquad \vec{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

"Weight vector" "Feature vector"

Activation/
output
of neuron *k*

$$o^k = \begin{bmatrix} w_0^k & w_1^k & \cdots & w_n^k \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$



K *"hidden"* neurons
in layer **L**

$$o^1 = \begin{bmatrix} w_0^1 & w_1^1 & \cdots & w_n^1 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$o^1 = \begin{bmatrix} w_0^1 & w_1^1 & \cdots & w_n^1 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$o^2 = \begin{bmatrix} w_0^2 & w_1^2 & \cdots & w_n^2 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$o^1 = \begin{bmatrix} w_0^1 & w_1^1 & \cdots & w_n^1 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

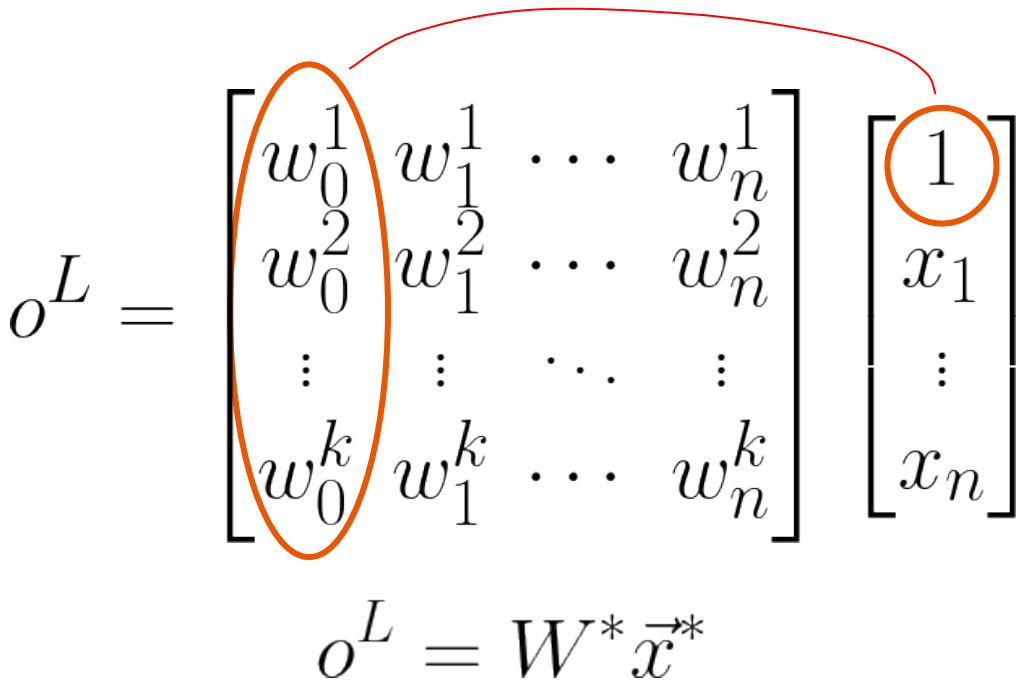
$$o^2 = \begin{bmatrix} w_0^2 & w_1^2 & \cdots & w_n^2 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$\vdots$$

$$o^k = \begin{bmatrix} w_0^k & w_1^k & \cdots & w_n^k \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$o^L = \begin{bmatrix} w_0^1 & w_1^1 & \cdots & w_n^1 \\ w_0^2 & w_1^2 & \cdots & w_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ w_0^k & w_1^k & \cdots & w_n^k \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$o^L = W^* \vec{x}^*$$


$o^L = \begin{bmatrix} w_0^1 & w_1^1 & \cdots & w_n^1 \\ w_0^2 & w_1^2 & \cdots & w_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ w_0^k & w_1^k & \cdots & w_n^k \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$
$o^L = W^* \vec{x}^*$

$$o^L = \begin{bmatrix} w_1^1 & w_2^1 & \cdots & w_n^1 \\ w_1^2 & w_2^2 & \cdots & w_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ w_1^k & w_2^k & \cdots & w_n^k \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} w_0^1 \\ w_0^2 \\ \vdots \\ w_0^k \end{bmatrix}$$

$$o^L = W\vec{x} + \vec{b}$$

Most common way of writing out the activation of a layer of an MLP

$$o^L = W\vec{x} + \vec{b}$$

$$o^L = W\vec{x} + \vec{b}$$

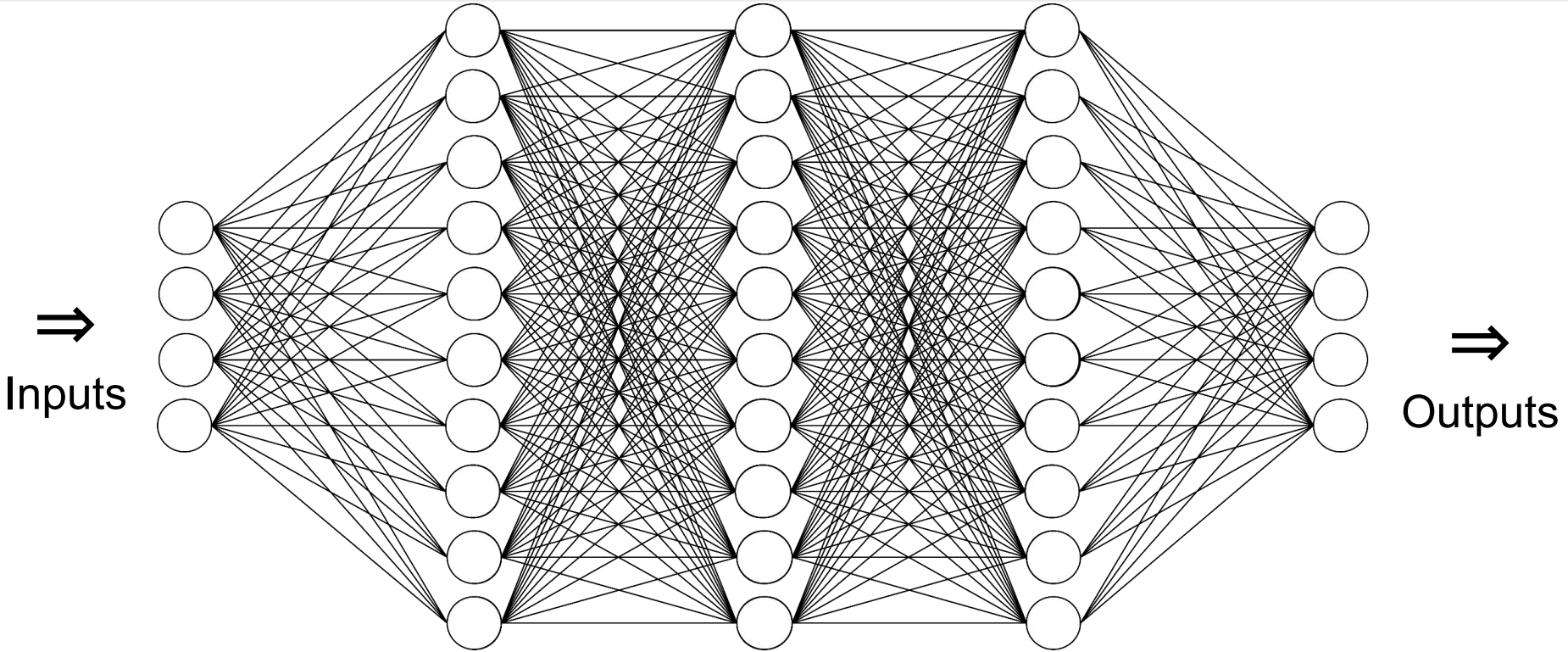
$$\hat{y} = \sigma(w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n)$$

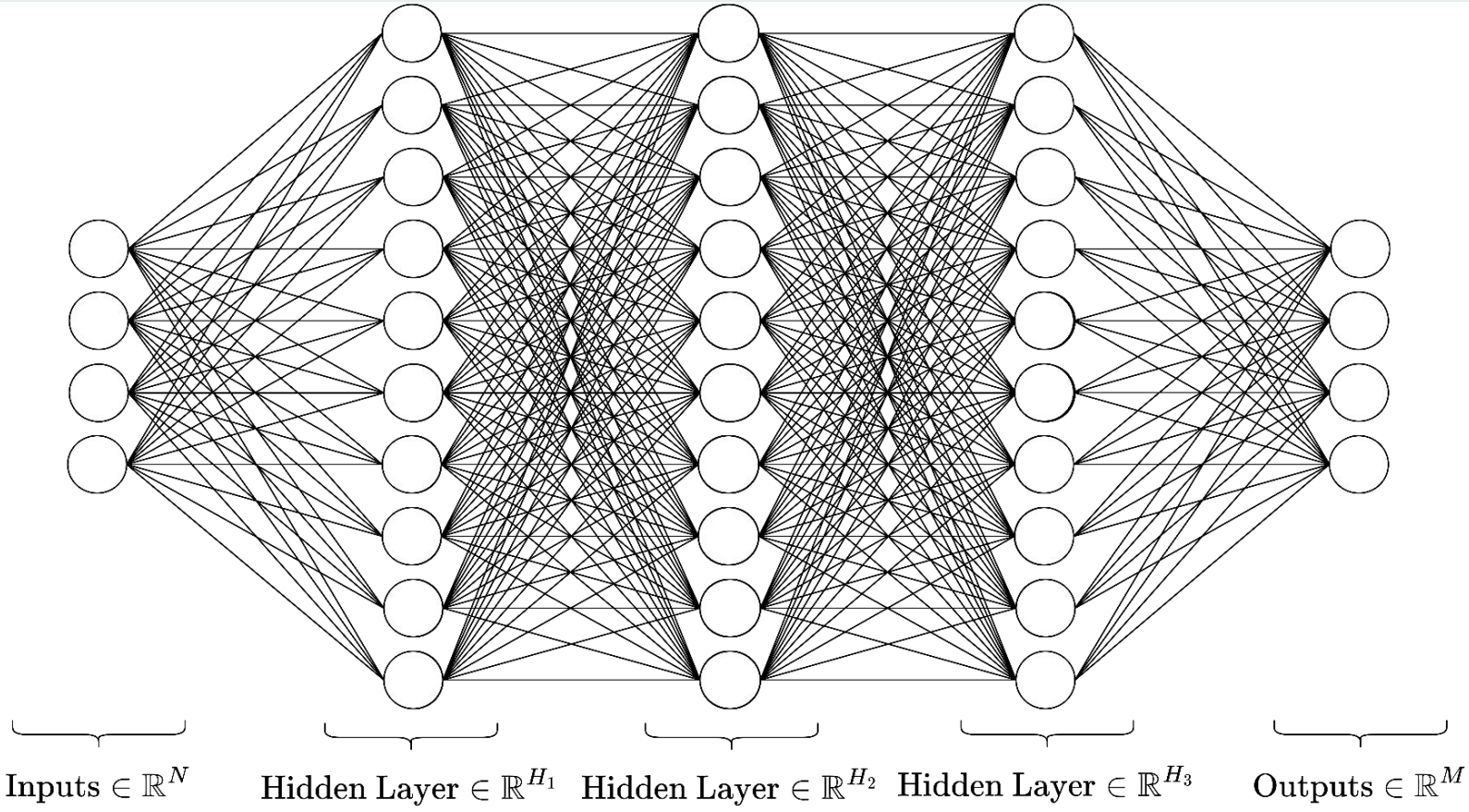
$$o^L = W\vec{x} + \vec{b}$$

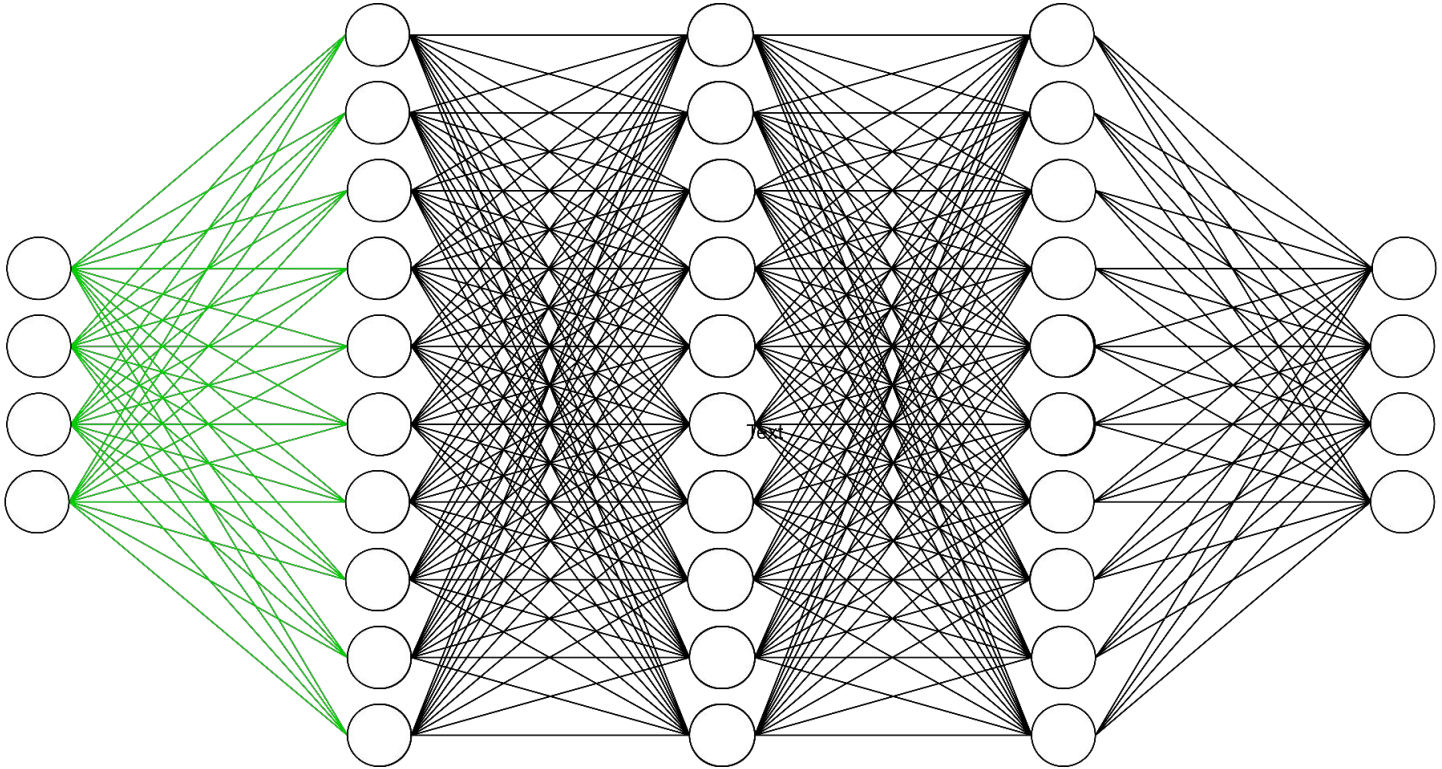
$$\hat{y} = \sigma(w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n)$$

$$o = \sigma(W x^{in} + b)$$

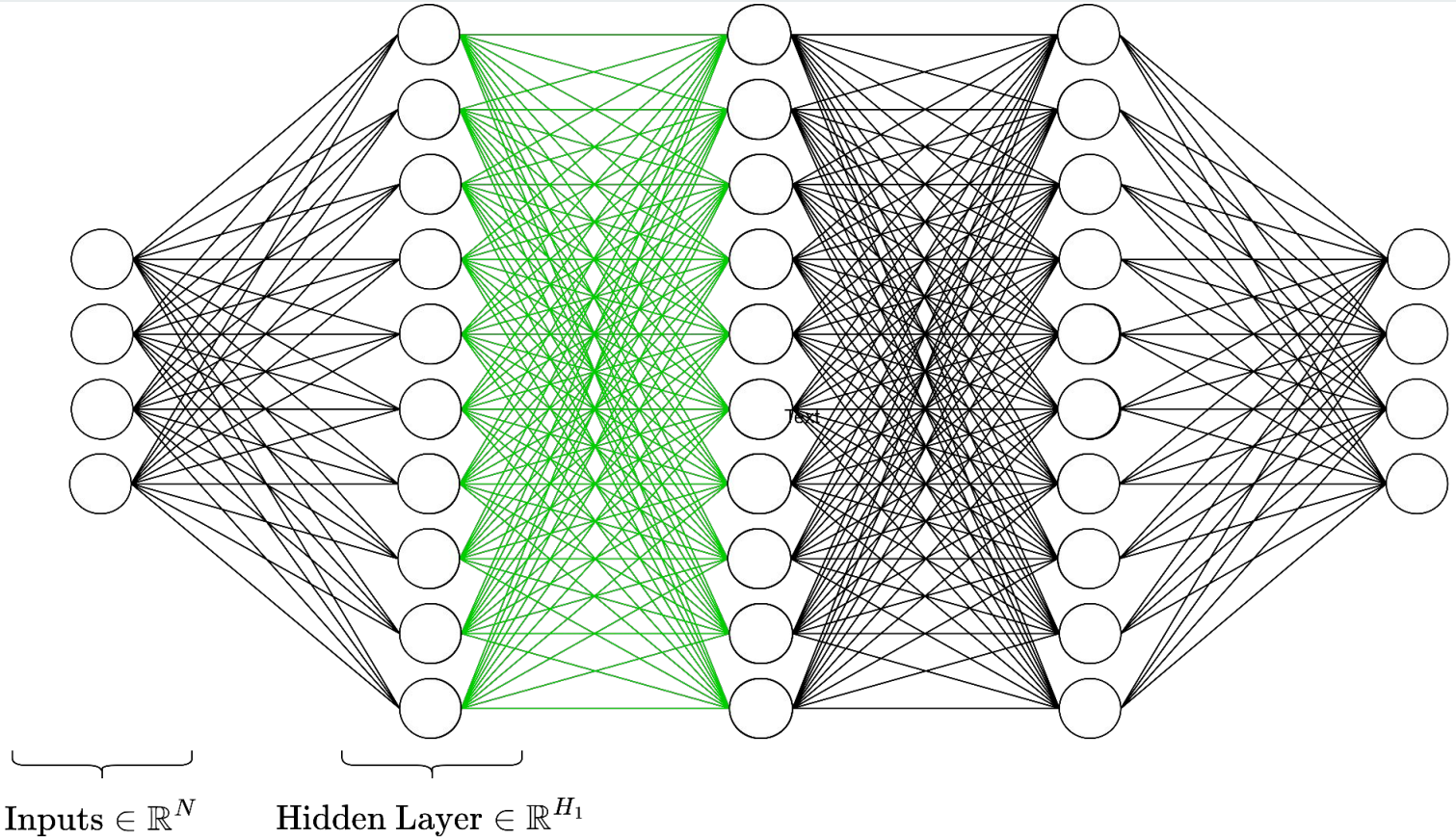
The **output** of each layer is the product of its **weight matrix** and the **input vector** plus its **bias vector**, all wrapped in a **non-linear activation function**.

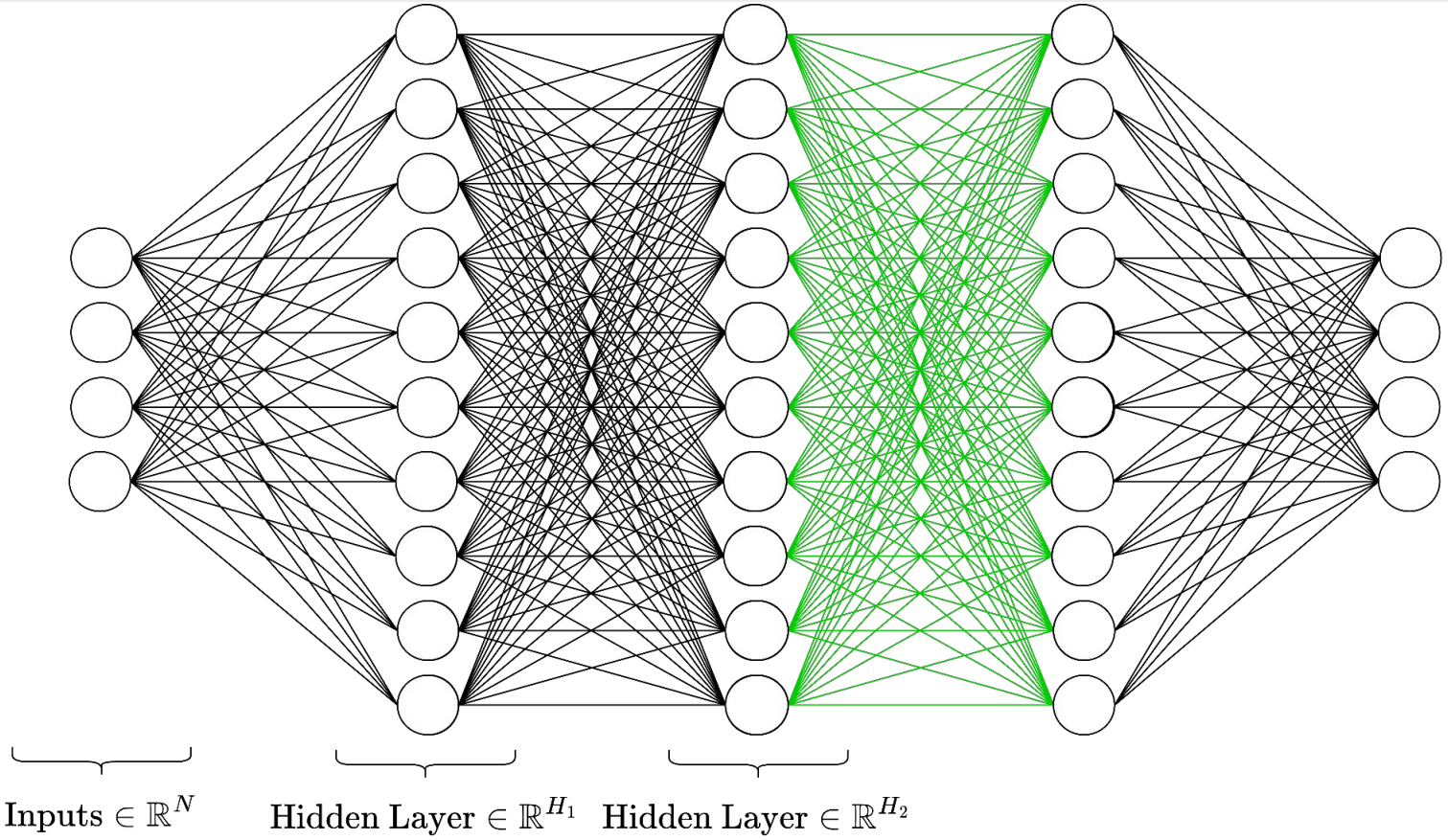

⇒
Inputs
⇒
Outputs

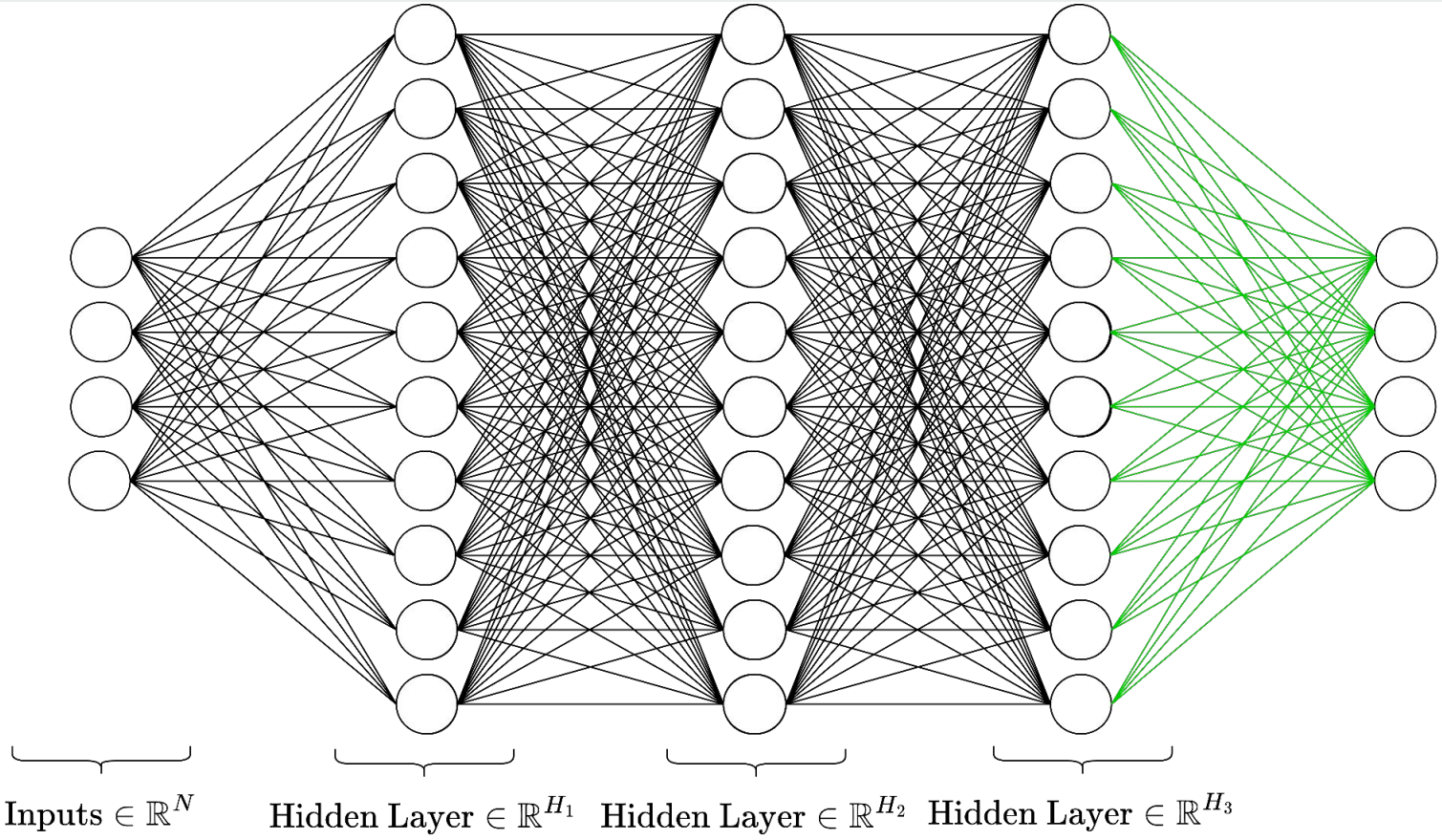

Inputs $\in \mathbb{R}^N$
Hidden Layer $\in \mathbb{R}^{H_1}$
Hidden Layer $\in \mathbb{R}^{H_2}$
Hidden Layer $\in \mathbb{R}^{H_3}$
Outputs $\in \mathbb{R}^M$

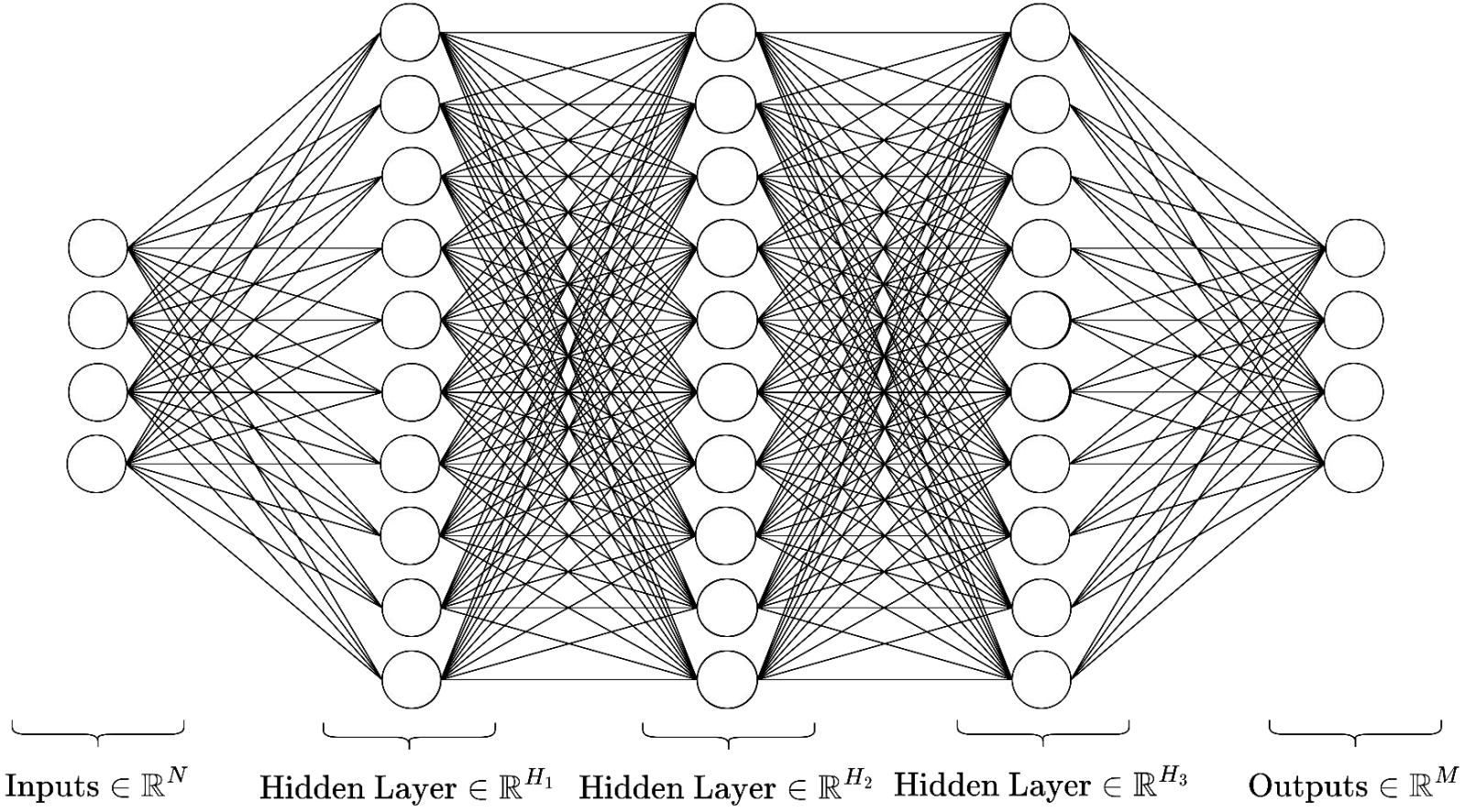


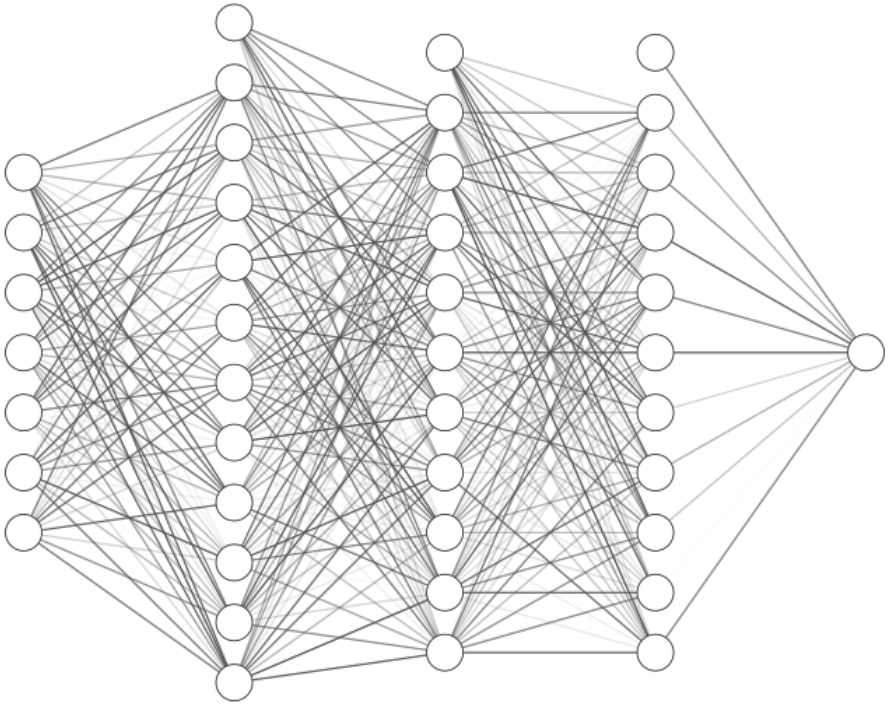
$\underbrace{\qquad\qquad}_{\textbf{Inputs} \in \mathbb{R}^N}$


Inputs $\in \mathbb{R}^N$
Hidden Layer $\in \mathbb{R}^{H_1}$


Inputs $\in \mathbb{R}^N$
Hidden Layer $\in \mathbb{R}^{H_1}$
Hidden Layer $\in \mathbb{R}^{H_2}$


Inputs $\in \mathbb{R}^N$
Hidden Layer $\in \mathbb{R}^{H_1}$
Hidden Layer $\in \mathbb{R}^{H_2}$
Hidden Layer $\in \mathbb{R}^{H_3}$


Inputs $\in \mathbb{R}^N$
Hidden Layer $\in \mathbb{R}^{H_1}$
Hidden Layer $\in \mathbb{R}^{H_2}$
Hidden Layer $\in \mathbb{R}^{H_3}$
Outputs $\in \mathbb{R}^M$



A multi-layer perceptron is a series of affine transformations of an input vector, each of which is wrapped in a non-linear activation function.

$$\mathcal{N} : \mathbb{R}^N \rightarrow \mathbb{R}^M$$
$$N, M \in \mathbb{N}$$

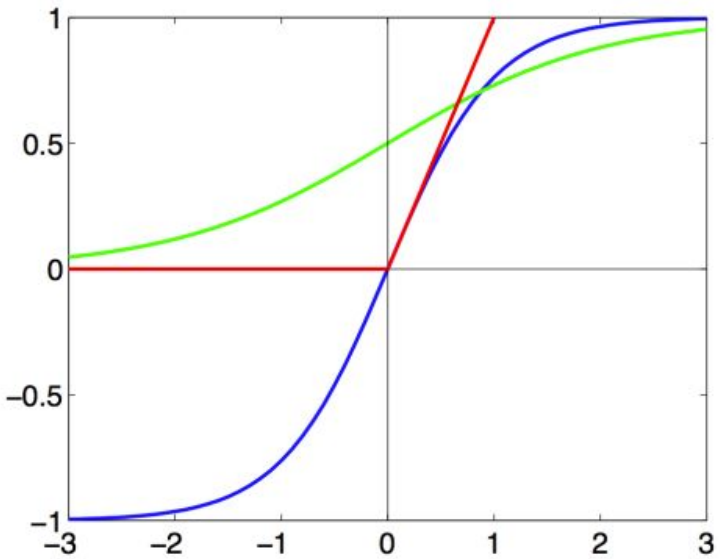
(*Translation:* an MLP is a fancy function)

A Note on Nonlinearity

Without a non-linear activation function, a series of linear transformations would result in just a linear transformation of the input to the output.

We would still be stuck in the land of linear separability!

Common nonlinear functions



$$\text{Sigmoid: } \sigma(x) = \frac{1}{1+e^{-x}}$$

$$\text{Hyperbolic tangent: } \tanh(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$$

Rectified Linear Unit:

$$\text{ReLU}(x) = max(0, x)$$

Implementing learning: Backpropagation

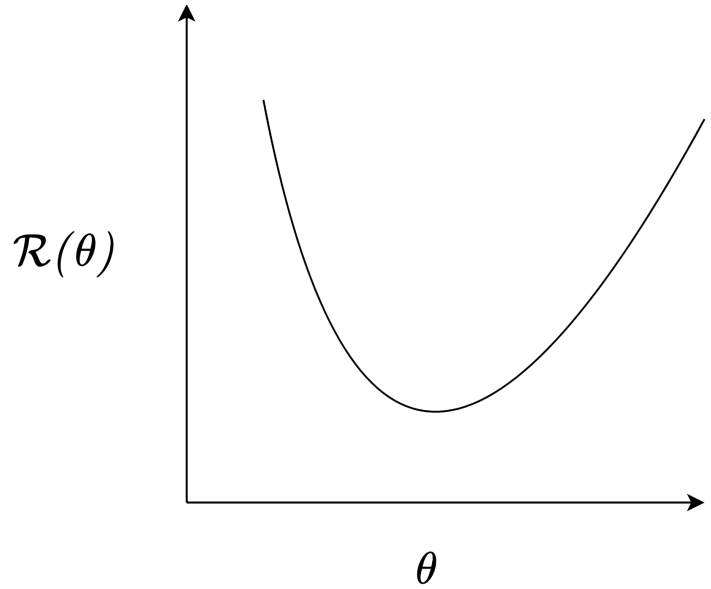
Given:

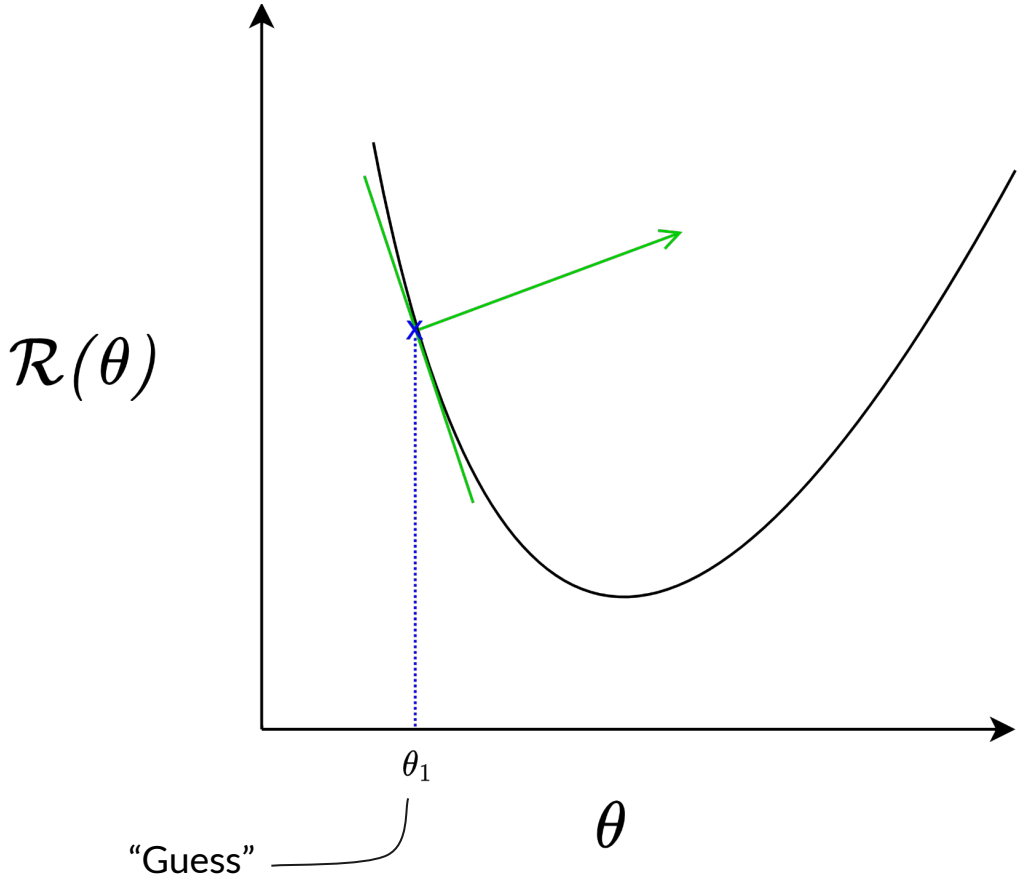
- Family of parameters Θ (e.g. possible weights of a NN)
- Differentiable risk function $\mathcal{R}(\theta)$

Goal:

$$\theta_{opt} = \underset{\theta \in \Theta}{\operatorname{argmin}}\ \mathcal{R}(\theta)$$

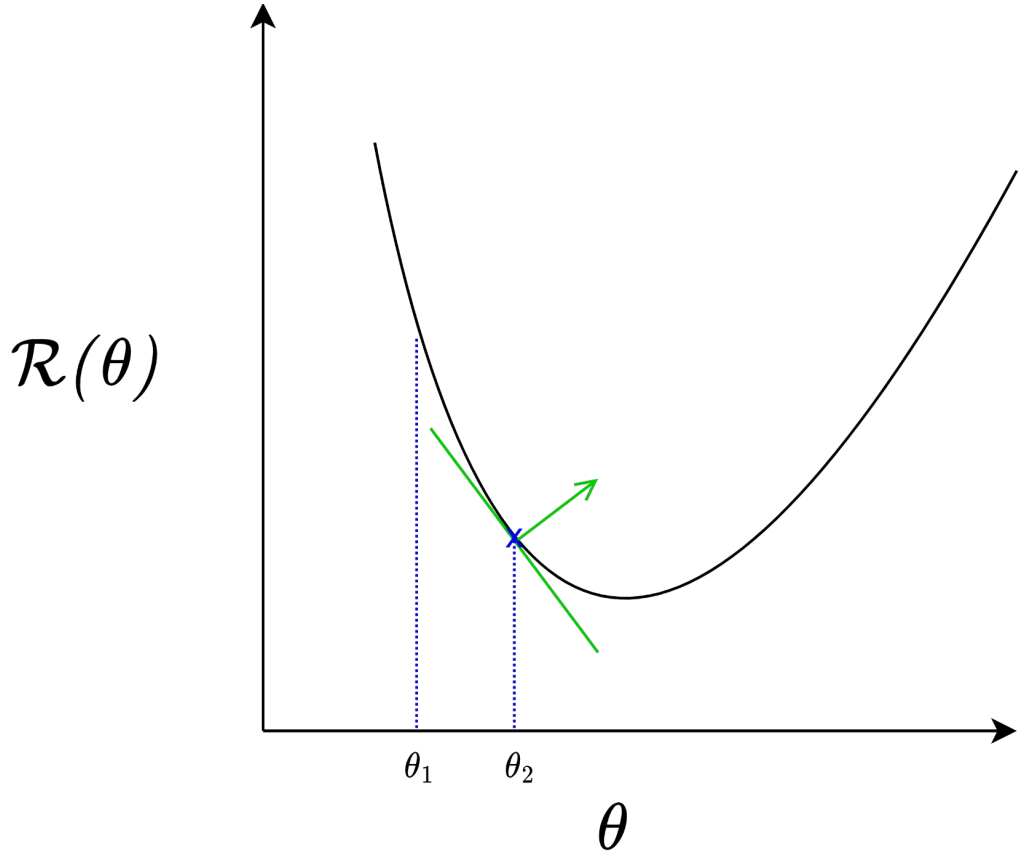
Backprop: Gradient descent



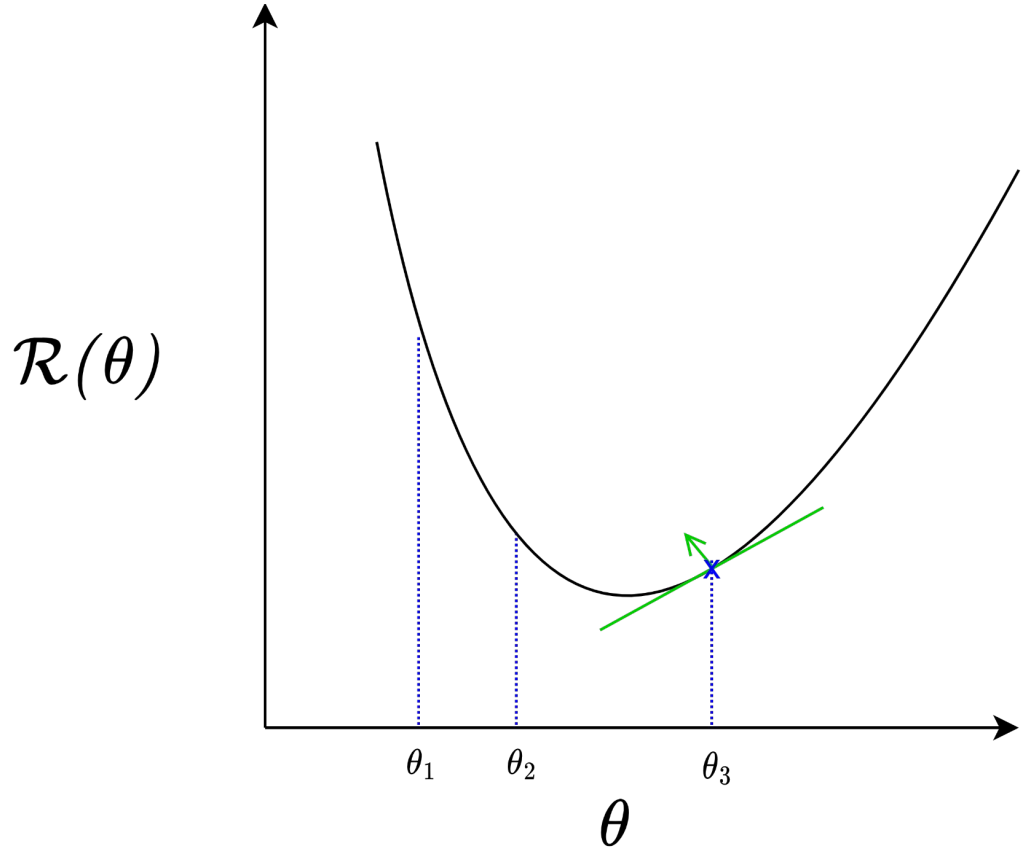


"Learning rate"

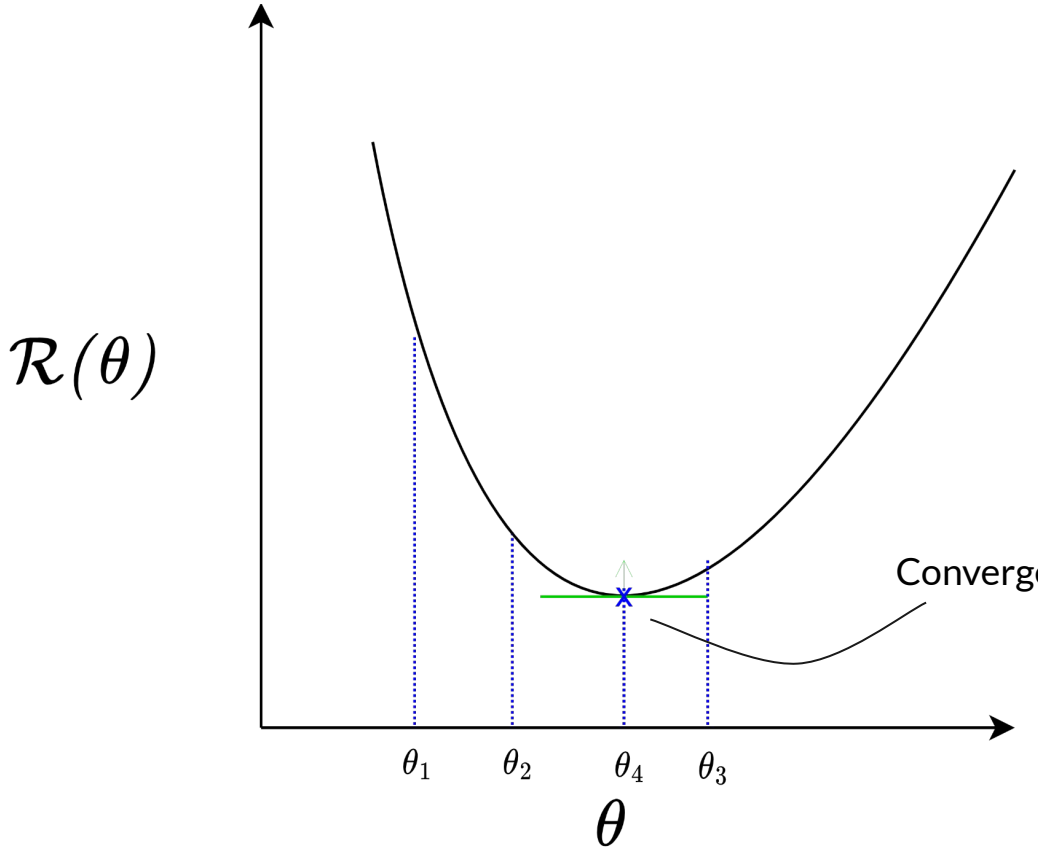
$$\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} \mathcal{R}(\theta_i)$$



$$\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} \mathcal{R}(\theta_i)$$



$$\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} \mathcal{R}(\theta_i)$$



$$\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} \mathcal{R}(\theta_i)$$

Converges to local minima

Optimizers

Stochastic/Mini-batch GD: *Speed improvement*!

Perform backprop on errors of *batches* of training samples instead of all at once

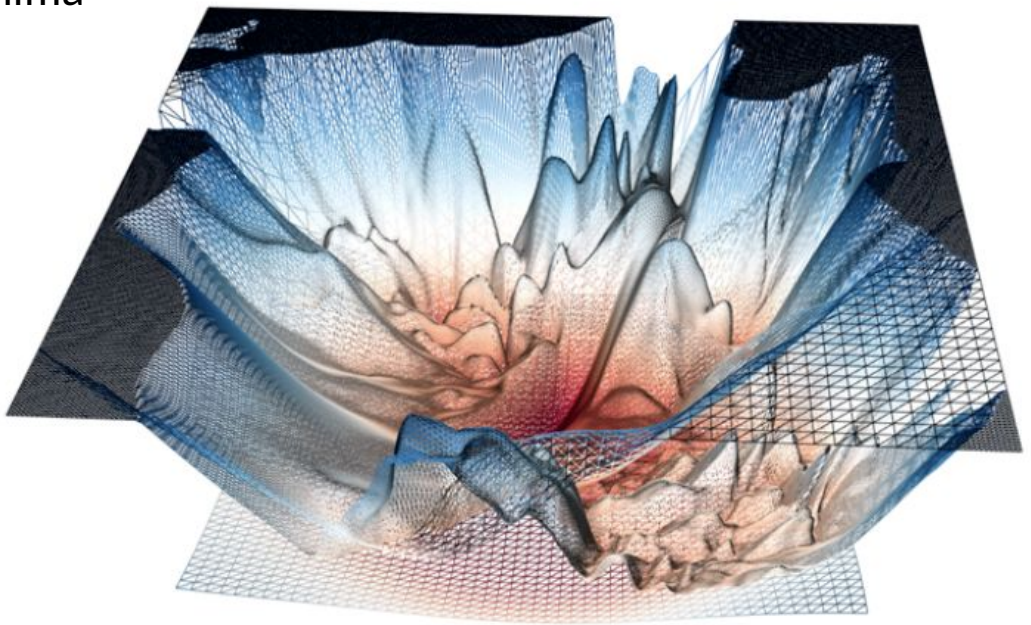
- Reduces the number of expensive backward passes

Optimizers determine exactly how backpropagation is implemented

- Stochastic Gradient Descent (most common)
- Adam
- RMSProp

A “real” loss landscape:

- Many (many many) local minima
- Saddle points



http://www.telesens.co/2019/01/16/neural-network-loss-visualization/

Loss functions

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

Depends on the task!

Mean Squared Error

Used for e.g. regression tasks

Cross Entropy

Used for e.g. classification tasks

Define your own!

Note: Must be differentiable for gradient descent based methods

What NNs *can* and *can't* do

Universal Approximation Theorem

Theorem (schematic). *Let $\mathcal{F}$ be a certain class of functions $f : \mathbb{R}^K \to \mathbb{R}^M$. Then for any $f \in \mathcal{F}$ and any $\varepsilon > 0$ there exists an multilayer perceptron $\mathcal{N}$ with one hidden layer such that $\|f - \mathcal{N}\| < \varepsilon$.*

⇒ We can approximate *any* function we want with a *one*-layer MLP!

More effective with more layers than just one (“deeper” networks)

Easier said than done in practice

Schematic borrowed from Jaeger, H. (2022) *Neural Networks* Lecture Notes, https://www.ai.rug.nl/minds/uploads/LN_NN_RUG.pdf

Collection of proofs: https://ai.stackexchange.com/questions/13317/where-can-i-find-the-proof-of-the-universal-approximation-theorem

Where NNs thrive

> **Statistical/correlation inference** needed

> There exists **a lot of good quality (labelled) training data**

> **Parallelizable** training and deployment

> Tasks **without expansion** (input-output fixed)

> **Specialized tasks**

> Good **in-range performance** IRL

https://lasp.colorado.edu/home/minxss/2016/07/12/minimum-mission-success-criteria-met/

Limits of NNs

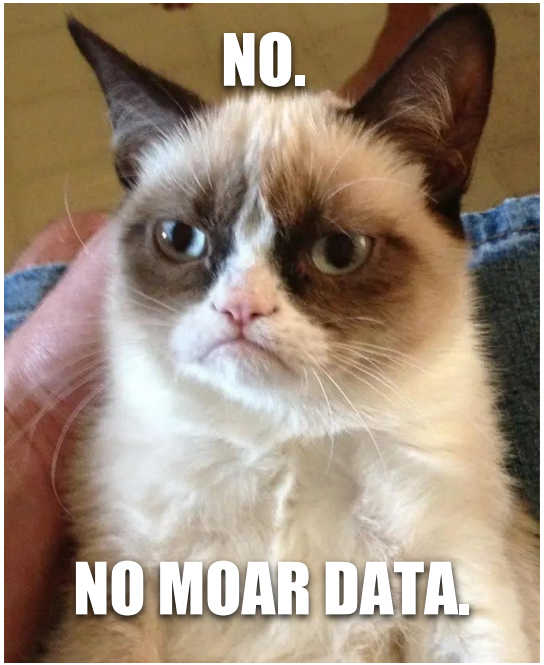
> **No causal relations** possible (yet)

> **Very data hungry** - "*Garbage in, garbage out*"

> **Often expensive to train**

> **Nonextensible** and **specialized** to a range and task

- Add one more neuron → retrain the entire network
- Undefined behaviour on out-of-domain test examples



https://knowyourmeme.com/memes/grumpy-cat

Demonstrations/Frontiers

The “AI Economist”: *https://www.youtube.com/watch?v=Sr2ga3BBMTc*

Dall-E 2: *https://labs.openai.com/*

This Person Does Not Exist: *https://thispersondoesnotexist.com/*

Tensorflow playground: *https://playground.tensorflow.org*

Github Copilot

Hands on NNs!

Overfitting & Underfitting

The real troublemakers in ML in general!

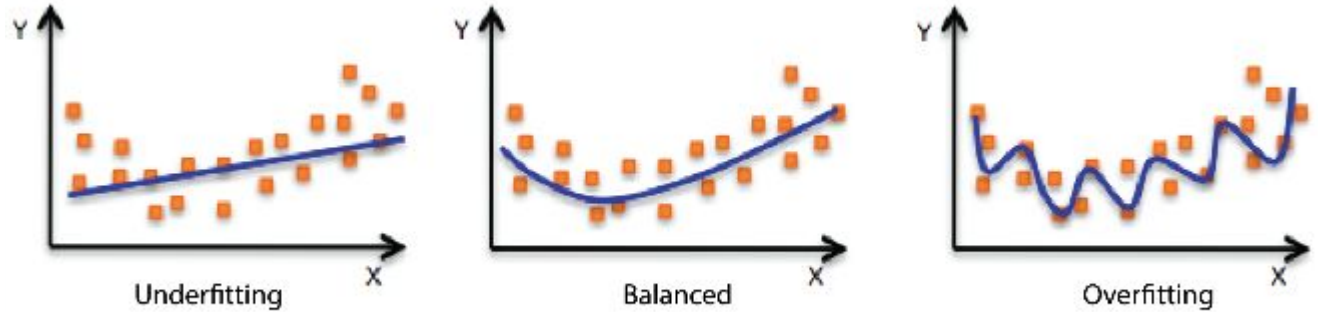
Underfitting: When the model fits the training data not well enough

- Empirical risk is high, actual risk is high
- Training loss is high, testing loss is not optimal

Overfitting: When the model fits the training data *too* closely (incl. noise)

- Empirical risk is low, actual risk is high
- Training loss is low, testing loss is not optimal
- e.g. An *D*-degree polynomial can fit *D-1* training points with *zero* error

Overfitting & Underfitting



More complex models (e.g. more layers, neurons per layer) -> higher likelihood of overfitting

Image source: https://docs.aws.amazon.com/machine-learning/latest/dg/model-fit-underfitting-vs-overfitting.html

Validation

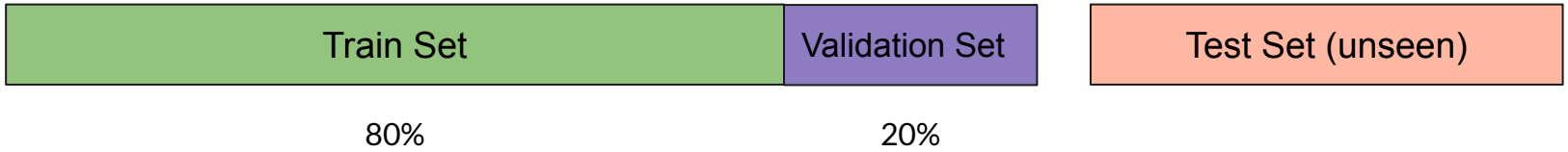
Split your training set into two!

- New train set
- Unseen-by-the-model “validation”set

Validation

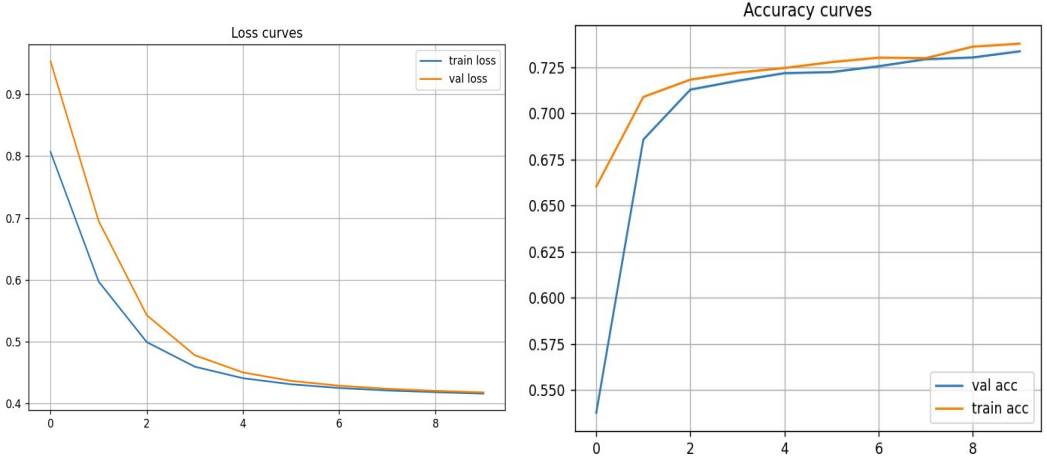
Split your training set into two!

- New train set
- Unseen-by-the-model “validation”set
- e.g. 80-20 split (Note: split ratio depends on the model, task and data)



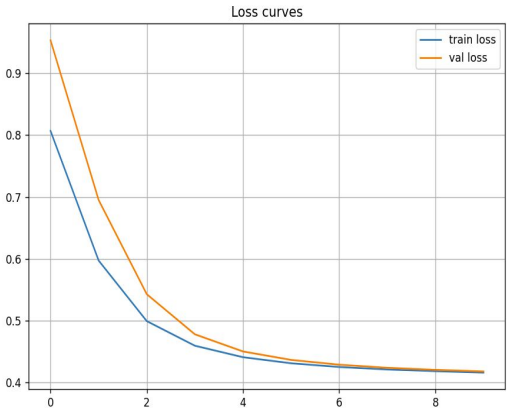
Training curves

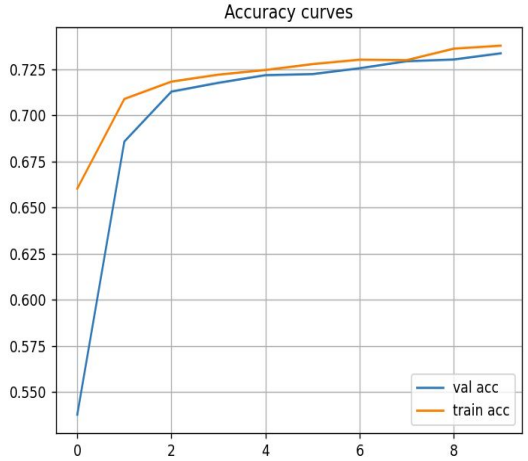
Important to plot!



Training curves

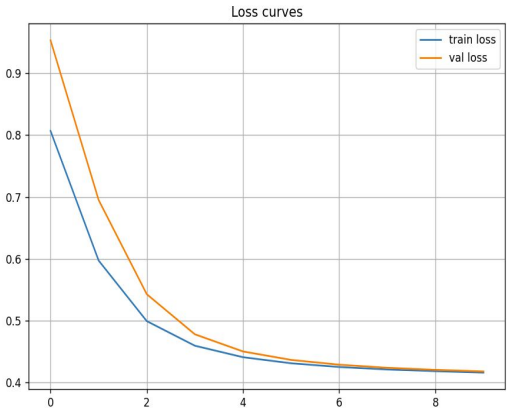
Important to plot!(!!!!)

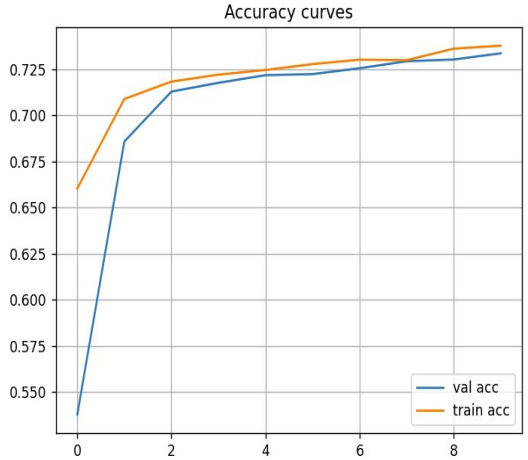




Training curves

Important to plot!(!!!!)



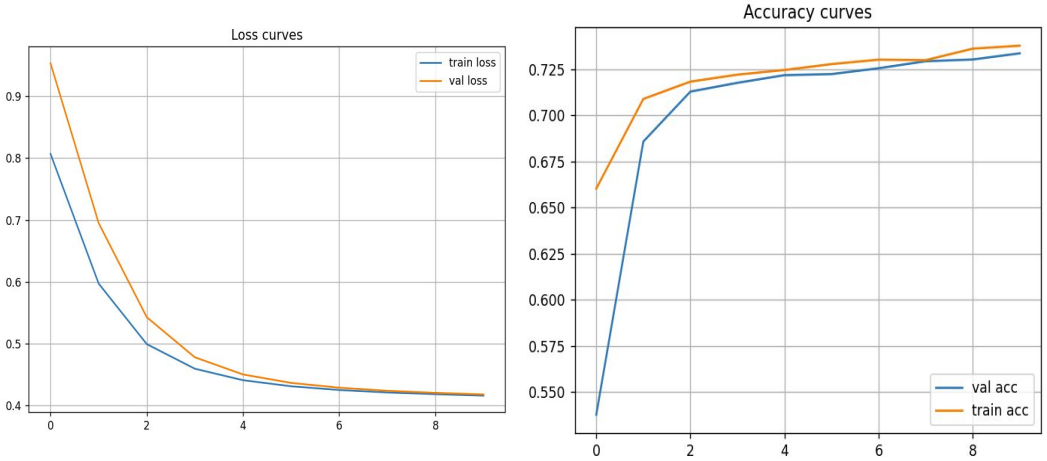


Shows if and how fast your model is learning on task-relevant metrics

- e.g. loss, accuracy, AUC, F1 score
- Plot scores over training epochs

Training curves

Important to plot!(!!!!)



Shows if and how fast your model is learning on task-relevant metrics

- e.g. loss, accuracy, AUC, F1 score
- Plot scores over training epochs

May indicate potential over and underfitting

Demonstrations/Frontiers

The “AI Economist”: *https://www.youtube.com/watch?v=Sr2ga3BBMTc*

Dall-E 2: *https://labs.openai.com/*

This Person Does Not Exist: *https://thispersondoesnotexist.com/*

Tensorflow playground: *https://playground.tensorflow.org*

Github Copilot