



An Introduction to Neural Networks

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Why you should consider Neural Networks

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Why I don't need to convince you to use Neural Networks

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The short answer

- They're useful!



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- They're useful!
- They're fast!



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- They're useful!
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- They're (now) easy to implement!

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<https://twitter.com/gdb/status/1512521912064229377>

The short answer

- They're useful!
- They're fast!
- They're (now) easy to implement!
- They're cute!
- They're ***definitely*** not going to take over the world!



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OpenAI

The short answer

- They're useful!
- They're fast!
- They're (now) easy to implement!
- They're cute!
- They're ***definitely*** not going to take over the world!

The long answer

It's a bit more complicated than that...



<https://twitter.com/gdb/status/1512521912064229377>



OpenAI



Introduction to the introduction

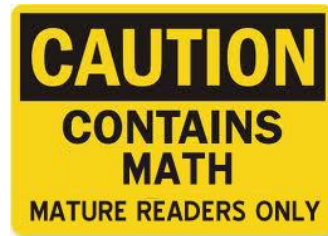
Goals of this lecture:

The whats, hows, whys, whichs and wheres

- Teach you what a neural network is and how it works
- Why you should use them, and why not
- Which neural networks are used today
- Where neural networks are headed next

Along with:

- A demo in a simulated environment
- A few tips on building and training your own networks



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Introduction to Supervised Machine Learning

Given: Input-output examples of the form:

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



Introduction to *Supervised* Machine Learning

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



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



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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 .

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



Aim: Learn a function with low “risk”

Risk: What we want to minimize

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



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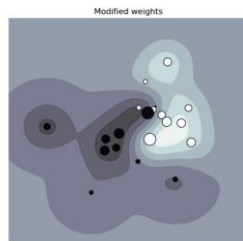
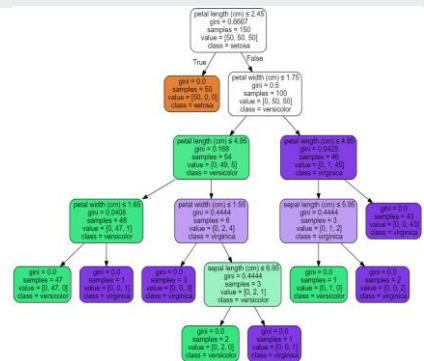
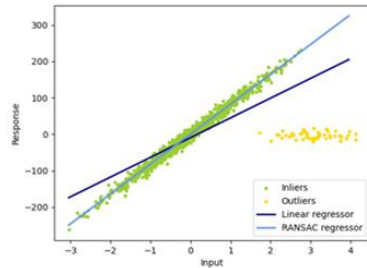
Empirical Risk: What we can actually calculate

(for a “candidate” model h , averaged over N training examples)

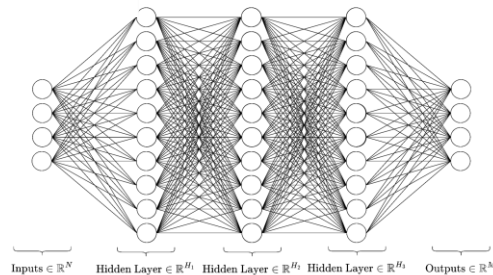
$$R^{\text{emp}}(h) = 1/N \sum_{i=1}^N L(h(\mathbf{x}_i), \mathbf{y}_i)$$

Common Approaches

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



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



you vs the guy she told you not to worry about:

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

McCulloch & Pitts (1943)

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

Rosenblatt (1958)

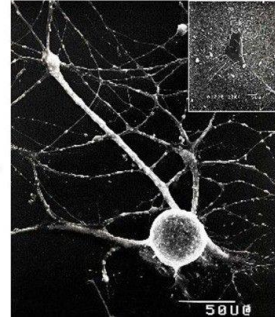
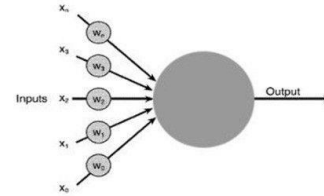
Description of the *perceptron*

Rumelhart, Hinton & Williams (1986)

Multi-layer perceptrons and error backpropagation (learning principle)

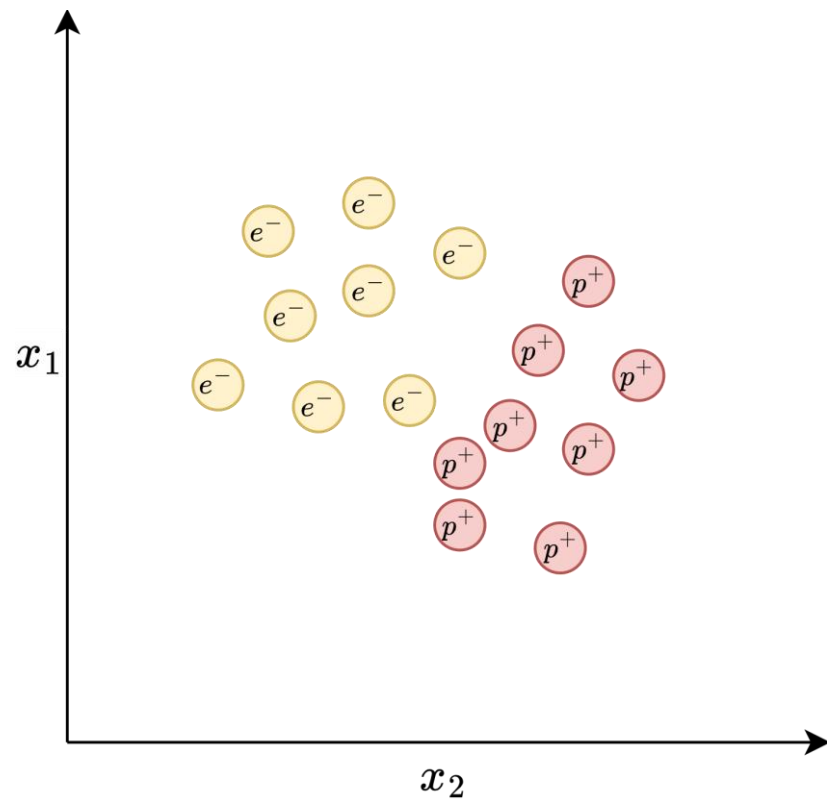
Modern:

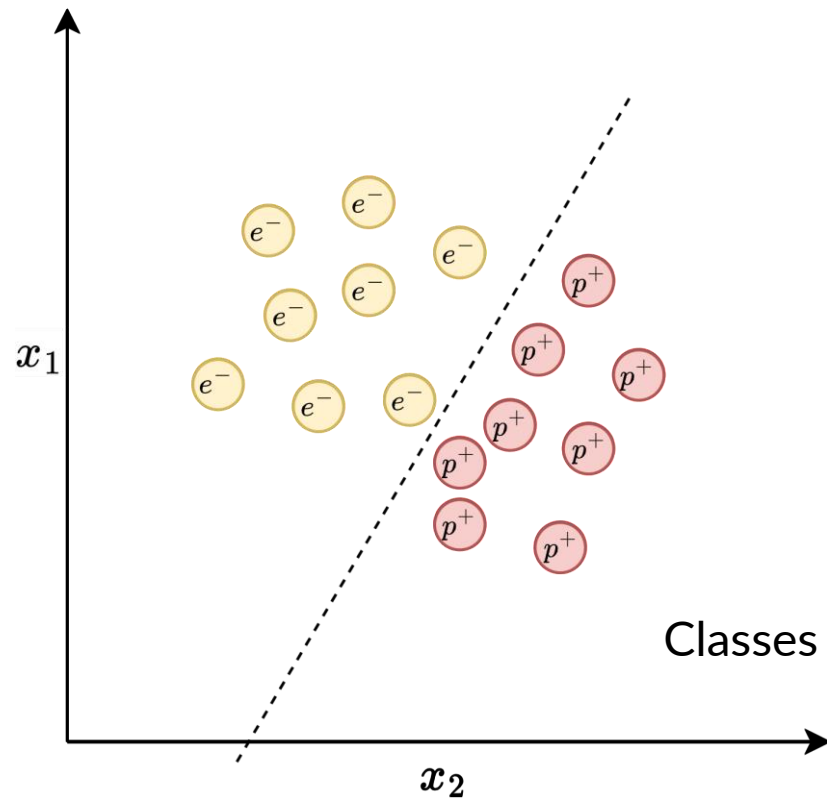
- ANNs used *everywhere for everything!*
- Simplified, abstracted version of “synaptically”-connected “neurons”
- Biologically implausible



Source: [linkedin.com/company/deeplearningai](https://www.linkedin.com/company/deeplearningai)

Building a Neural Network From Scratch (mathematically)





Classes are "linearly separable"

$$\hat{y} = w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n$$

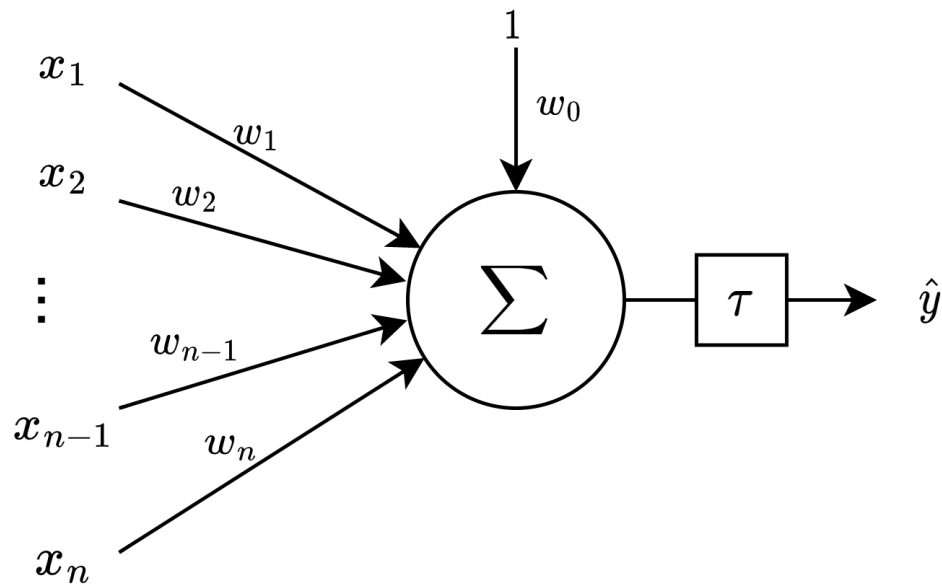
$w_i \leftarrow$ Coefficients

$x_i \leftarrow$ Variables

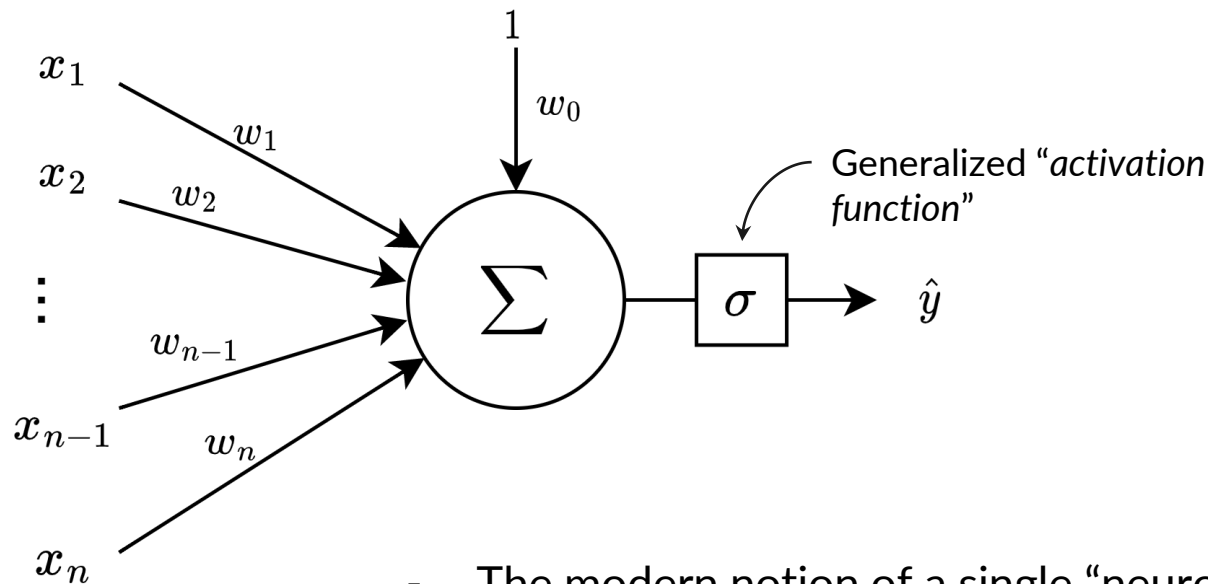
$$\hat{y} = \tau(w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n)$$

$$\tau(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases} \begin{matrix} \text{e}^- \\ \text{p}^+ \end{matrix}.$$

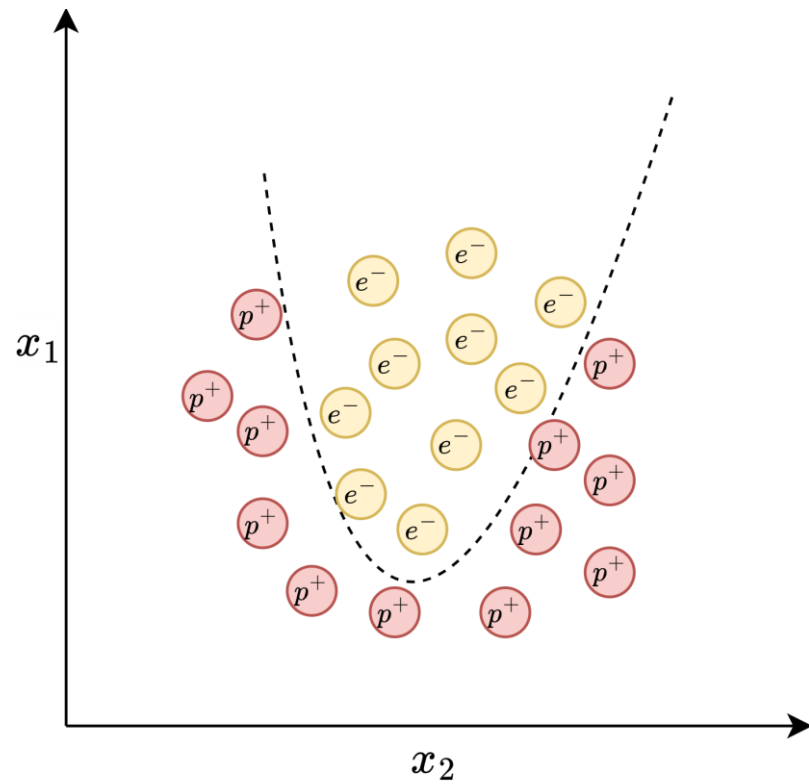
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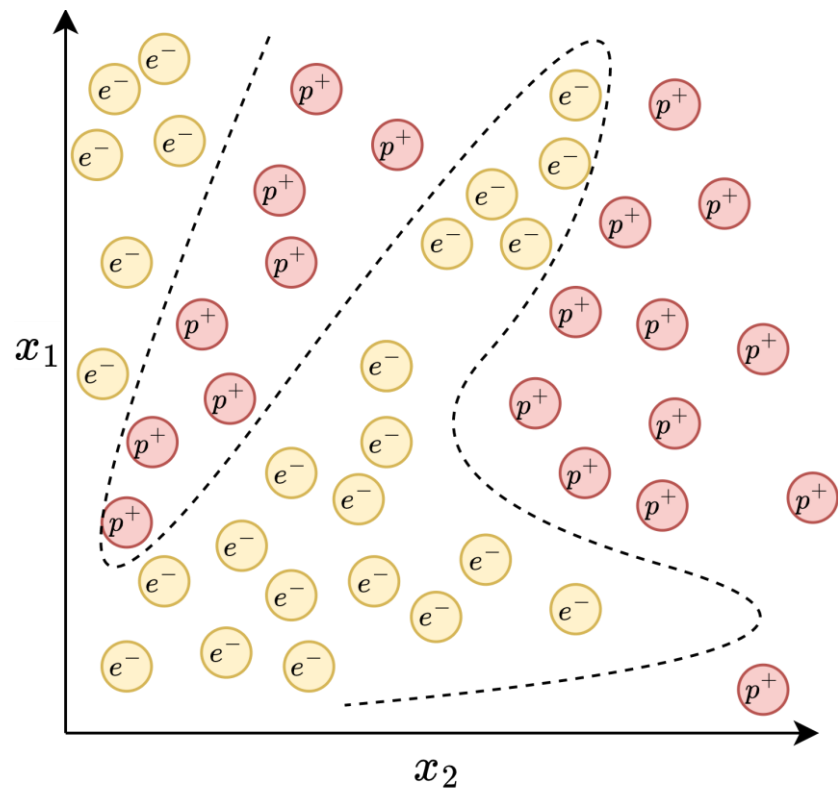


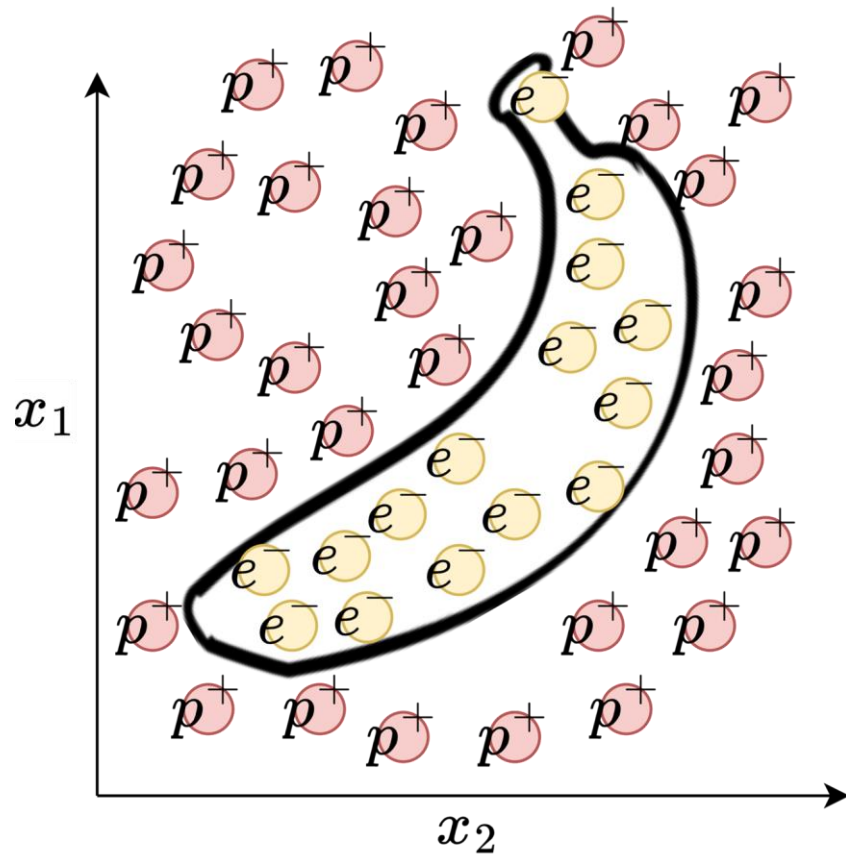
The “Perceptron”

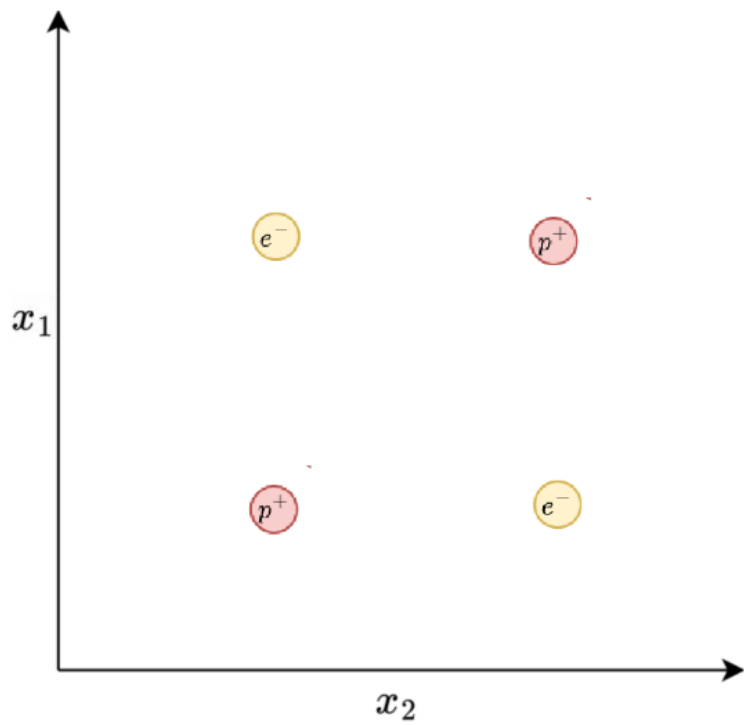


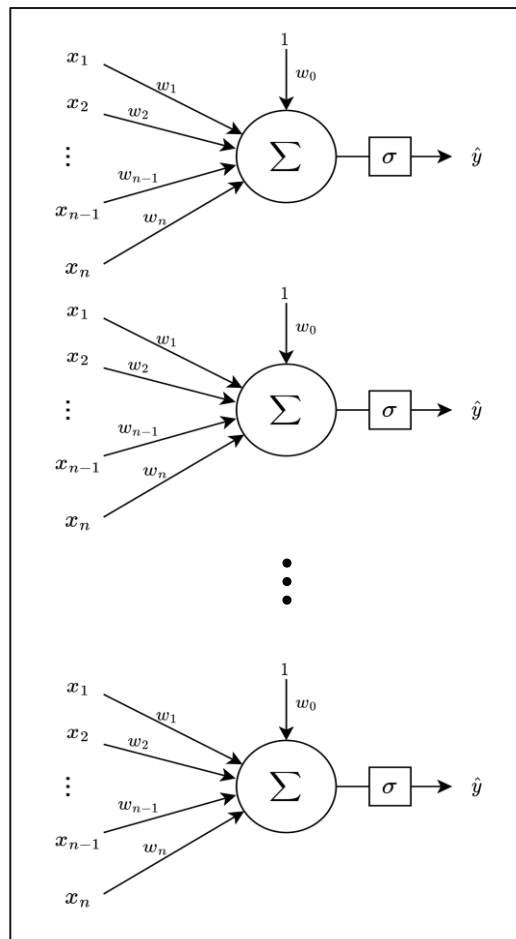
- The modern notion of a single “neuron”
- BUT: Only works on linearly separable classes

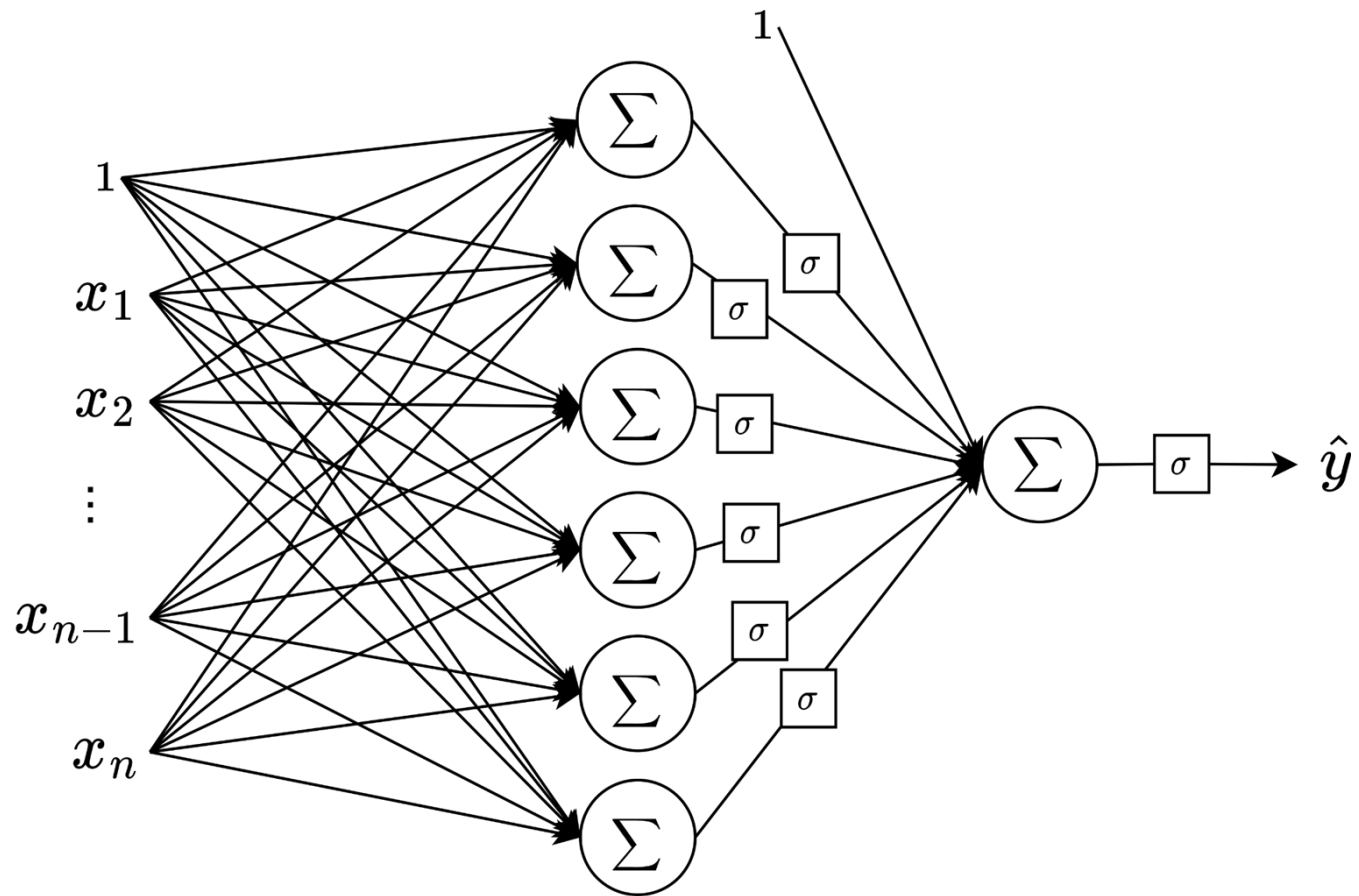




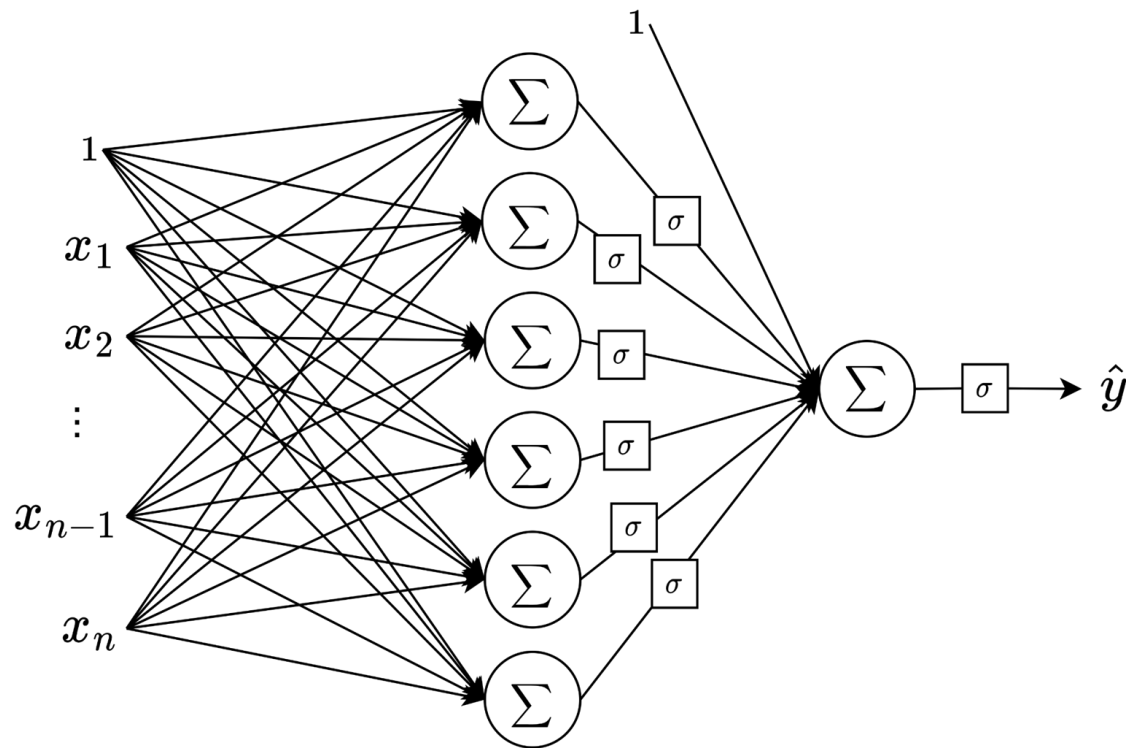








Multi-layer Perceptrons (MLPs)



$$\hat{y} = \sigma(w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n)$$

$$\begin{aligned}\hat{y} &= \sigma(w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n) \\ &= \sigma(\vec{w}^\top \vec{x})\end{aligned}$$

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

“Activation
”

“Bias”

$$\hat{y} = \sigma(w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n)$$
$$= \sigma(\vec{w}^T \vec{x})$$

“Activation function”

$$\vec{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

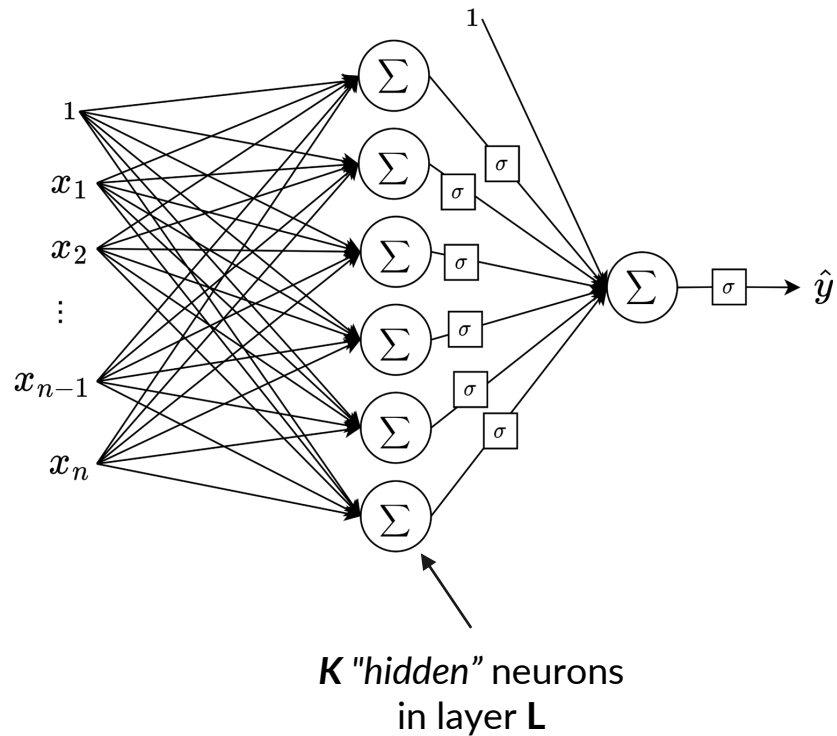
“Weight vector”

$$\vec{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

“Feature vector”

Activation/
output
of neuron k

$$o^k = [w_0^k \ w_1^k \ \dots \ w_n^k] \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$



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

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

$$\begin{array}{c}
 o^1 = [w_0^1 \quad w_1^1 \quad \cdots \quad w_n^1] \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \\
 \\
 o^2 = [w_0^2 \quad w_1^2 \quad \cdots \quad w_n^2] \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \\
 \\
 \vdots \\
 \\
 o^k = [w_0^k \quad w_1^k \quad \cdots \quad w_n^k] \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}
 \end{array}$$

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

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

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

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

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

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$$\hat{y} = \sigma(w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n)$$

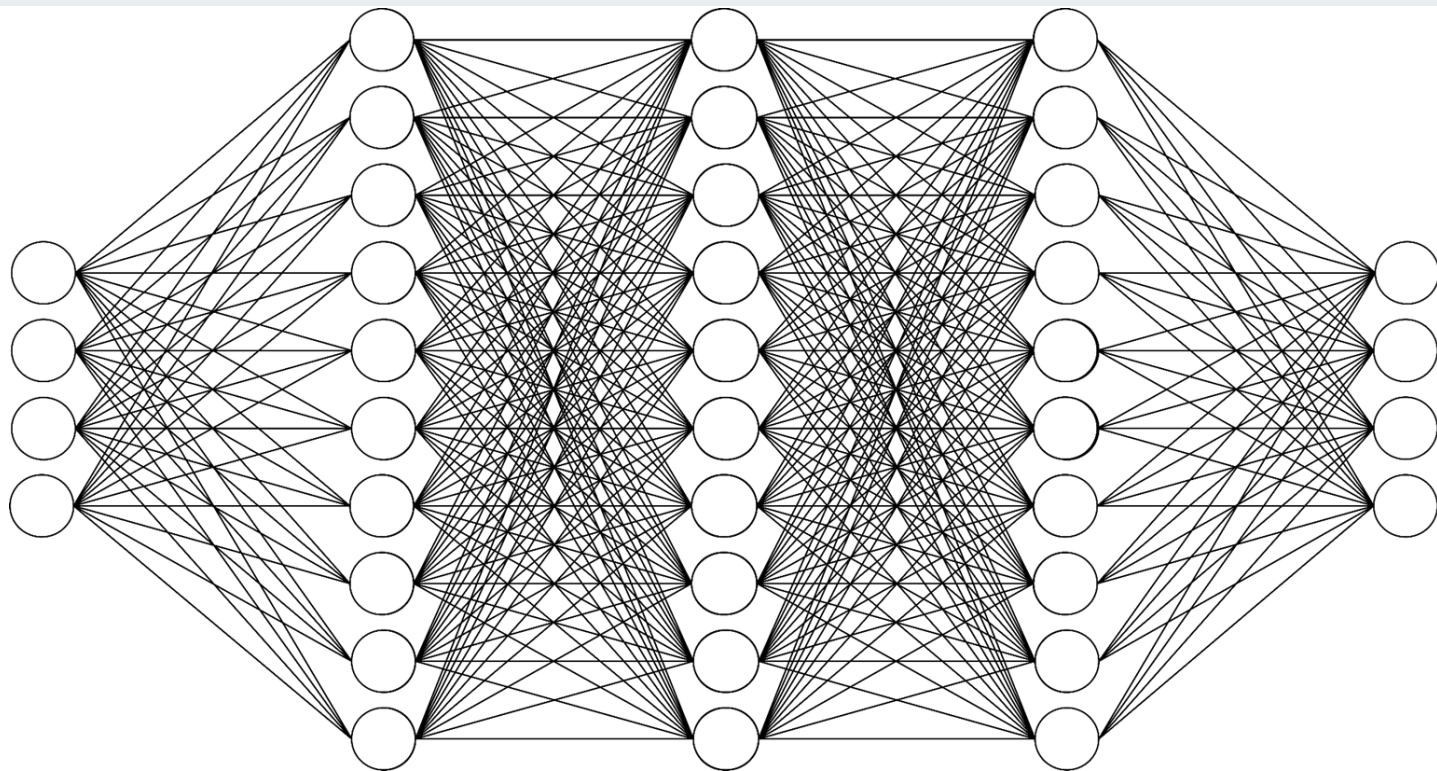
$$o^L = W\vec{x} + \vec{b}$$

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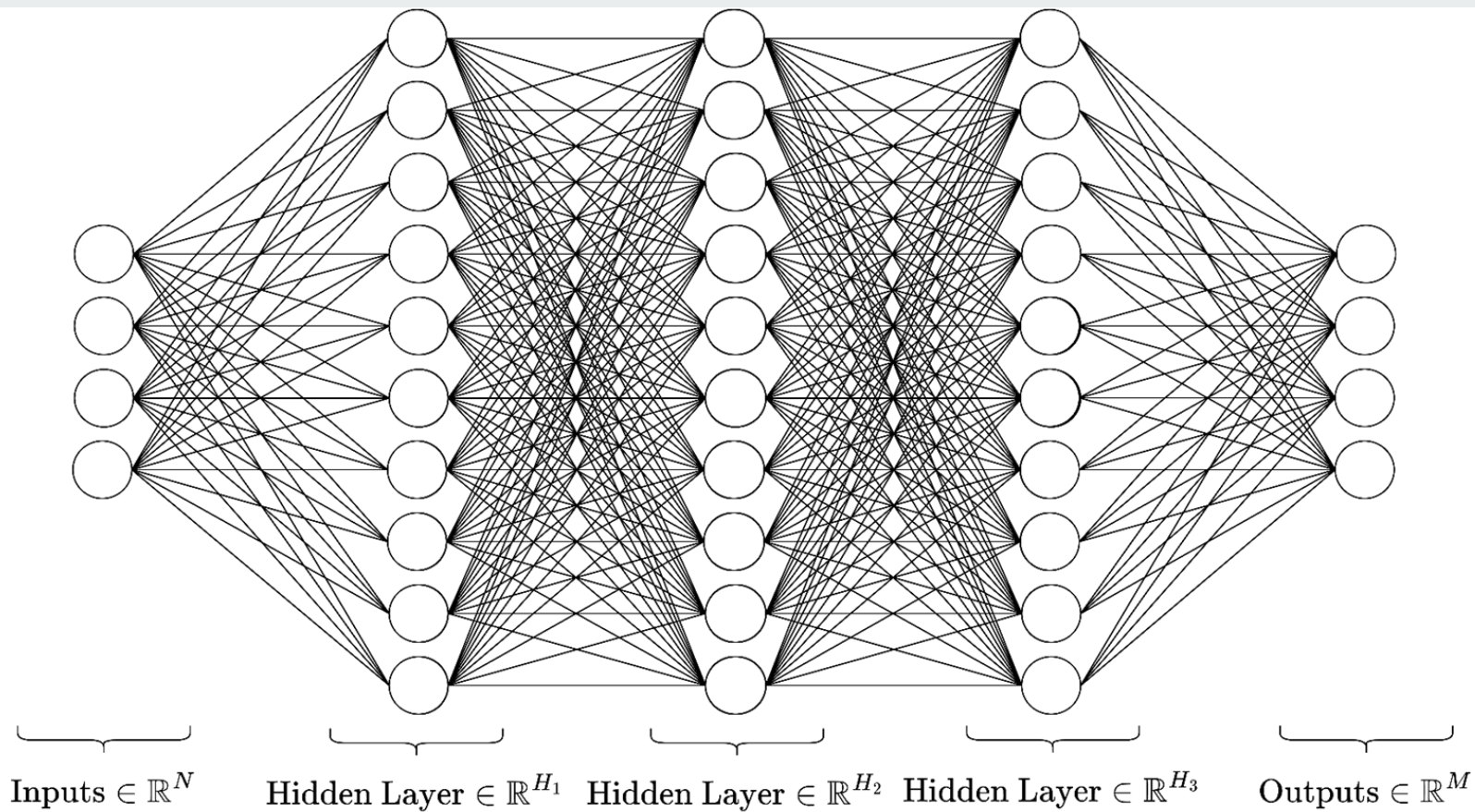
$$o = \sigma(Wx^{in} + b)$$

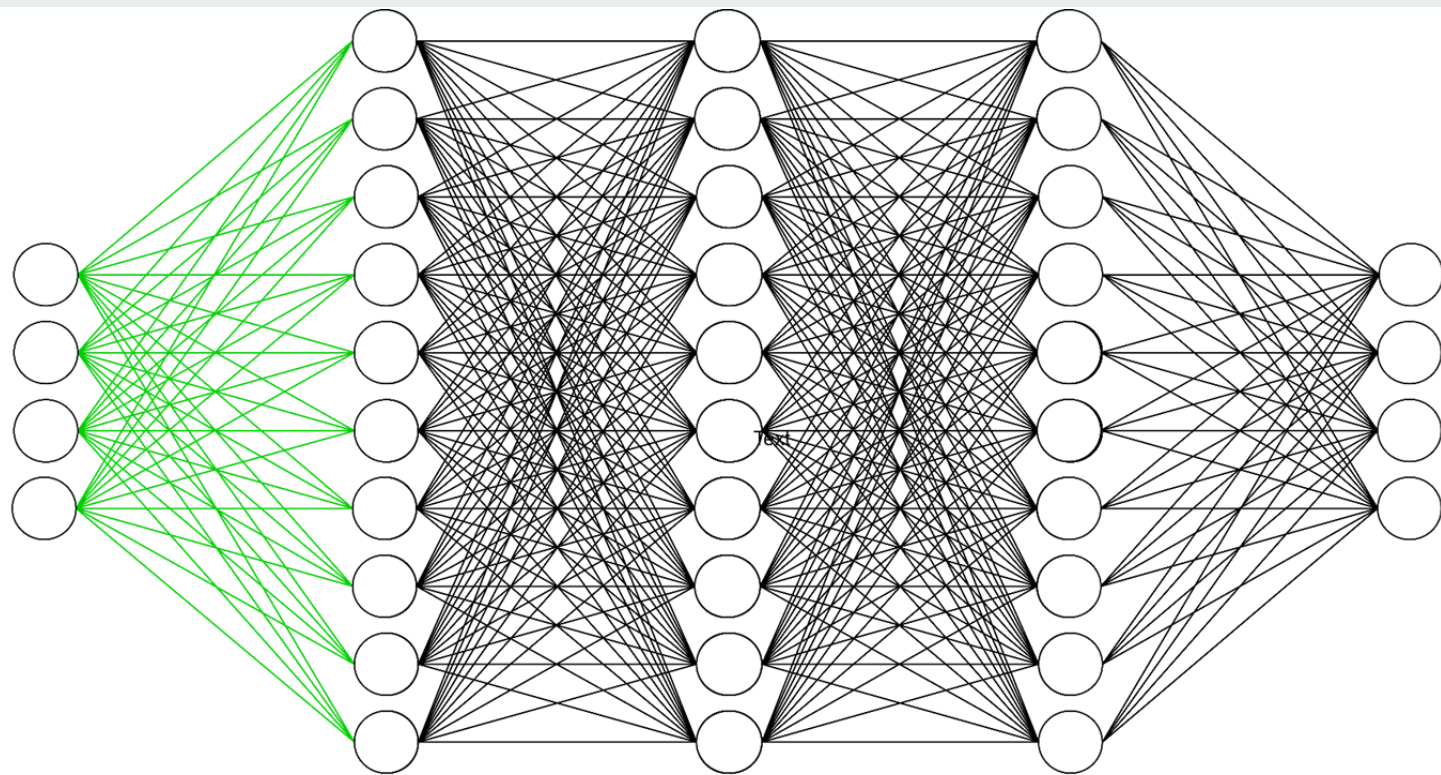
The **output** of each layer is the product of its **weight matrix** and the **input vector** plus its **bias vector**, all wrapped in a **non-linear activation function**.

⇒
Inputs

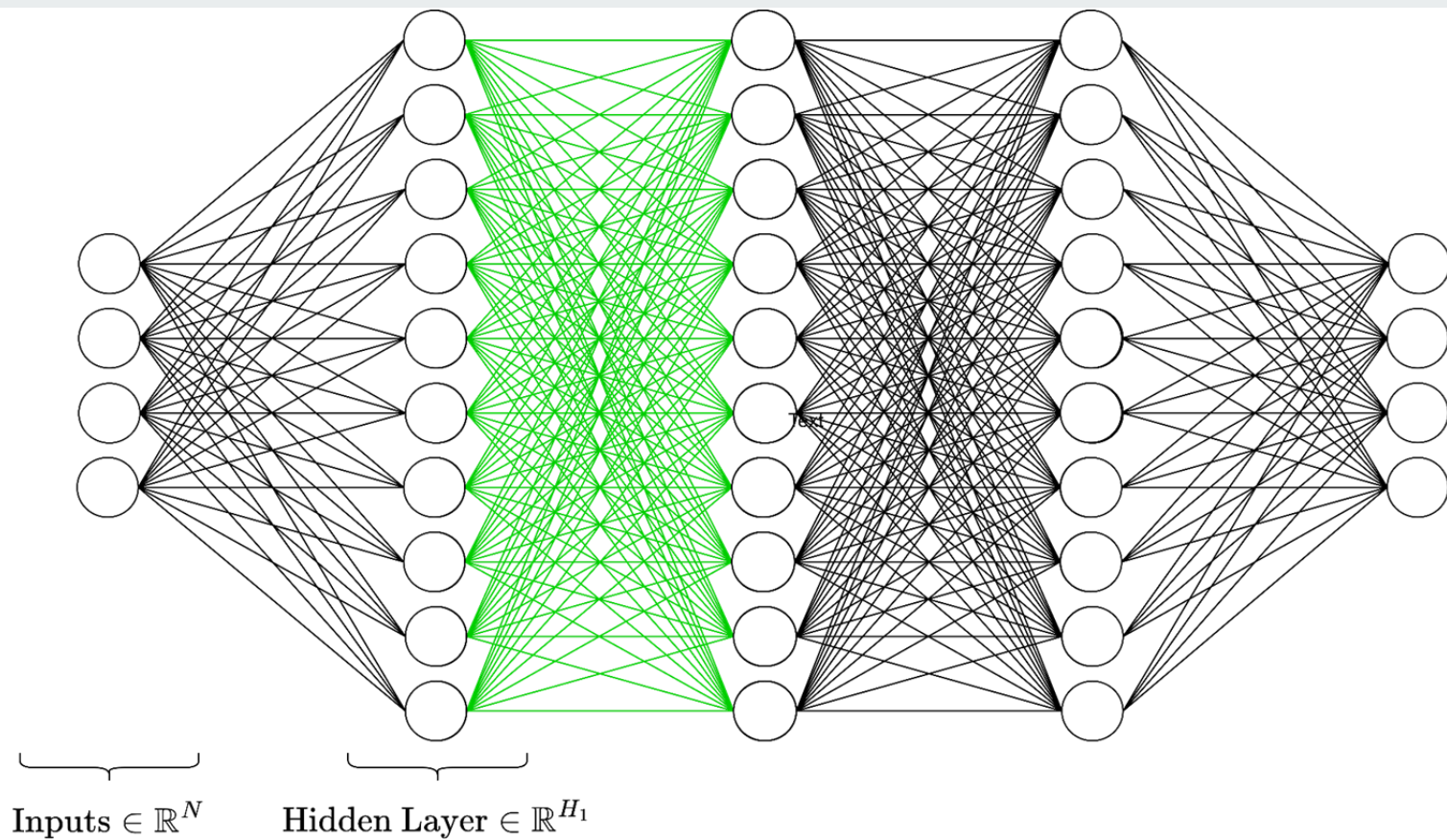


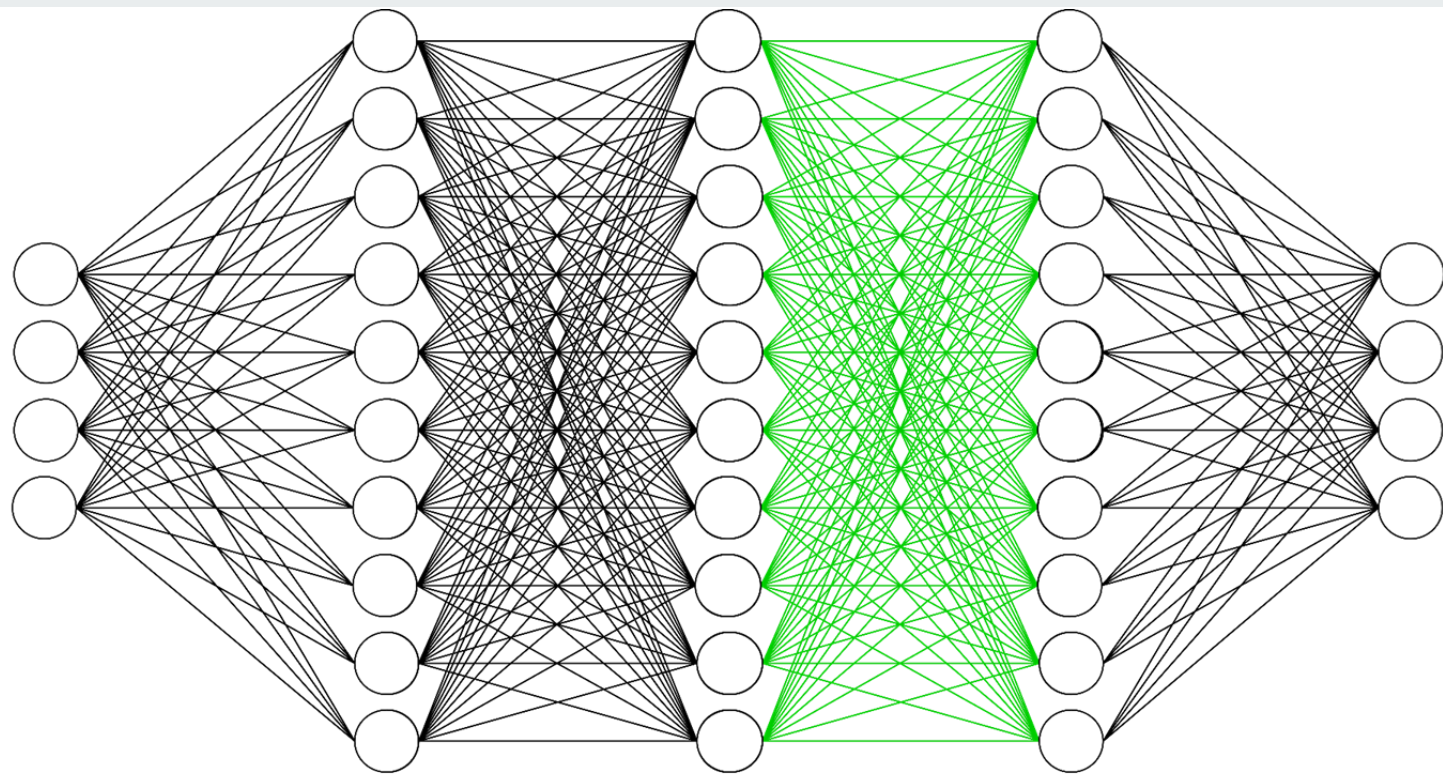
⇒
Outputs





$\underbrace{\hspace{1.5cm}}$
Inputs $\in \mathbb{R}^N$

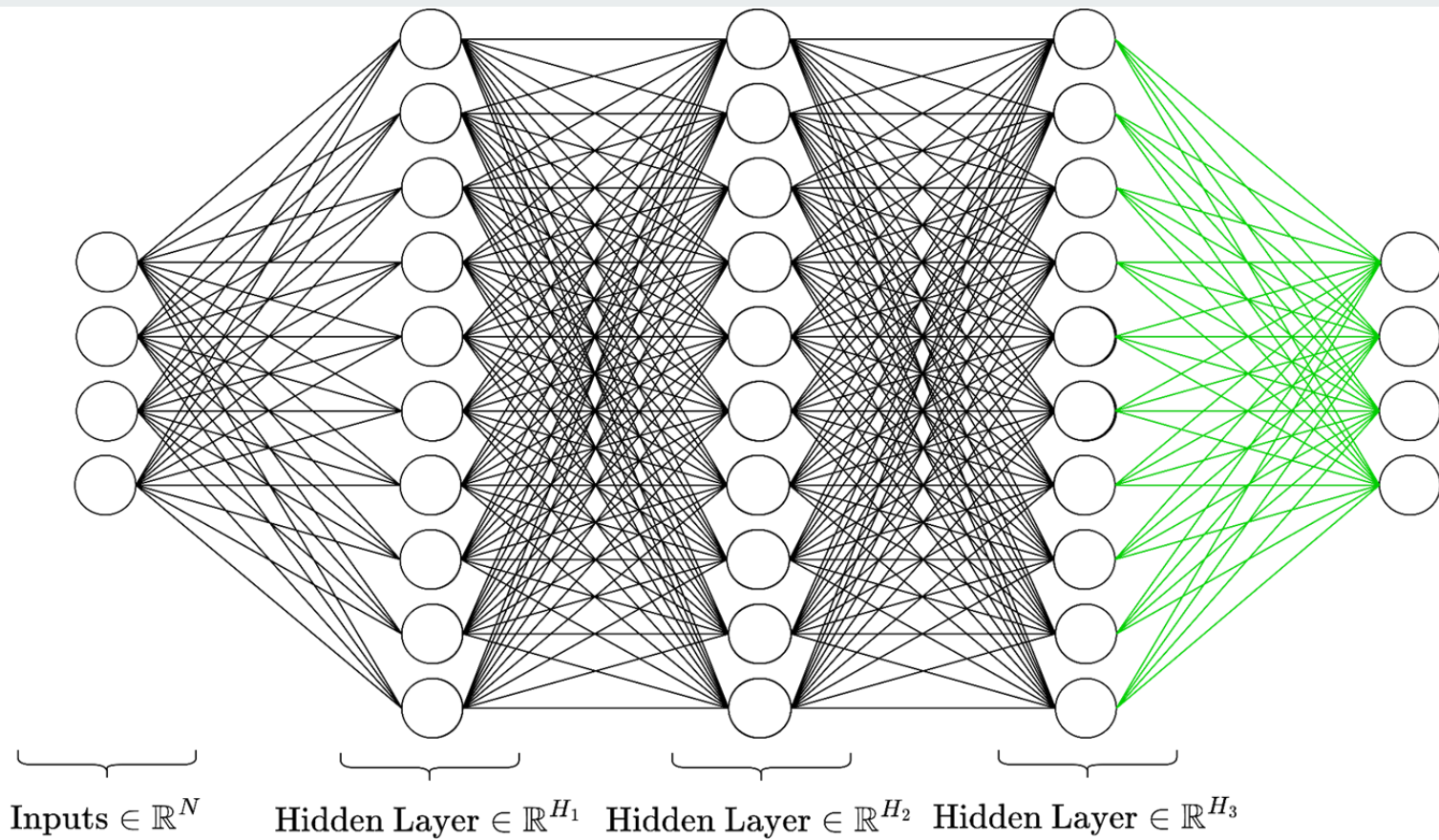


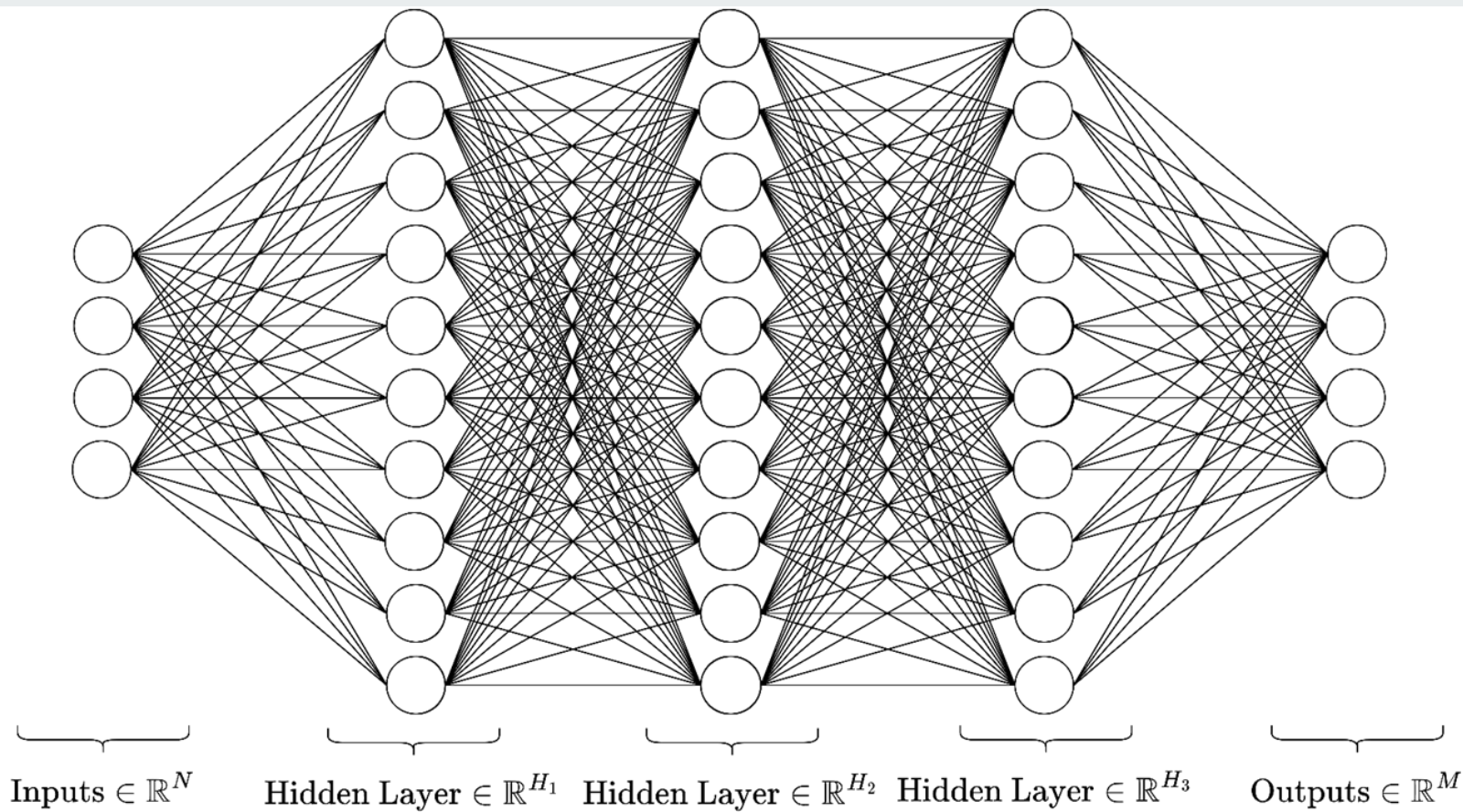


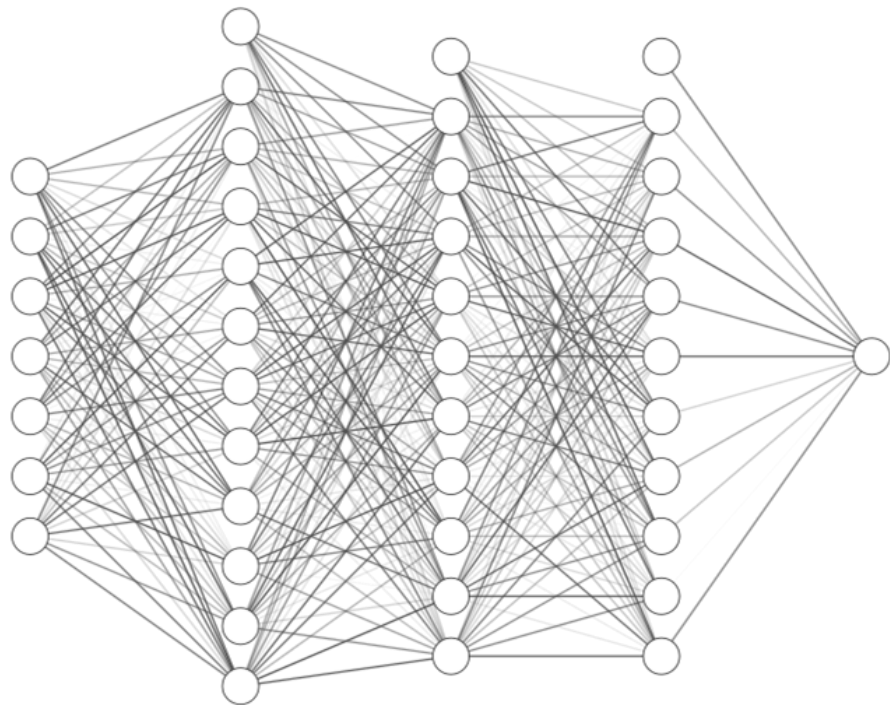
$\text{Inputs} \in \mathbb{R}^N$

$\text{Hidden Layer} \in \mathbb{R}^{H_1}$

$\text{Hidden Layer} \in \mathbb{R}^{H_2}$







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!



Loss functions

Depends on the task!

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

Mean Squared Error

Used for e.g. regression tasks

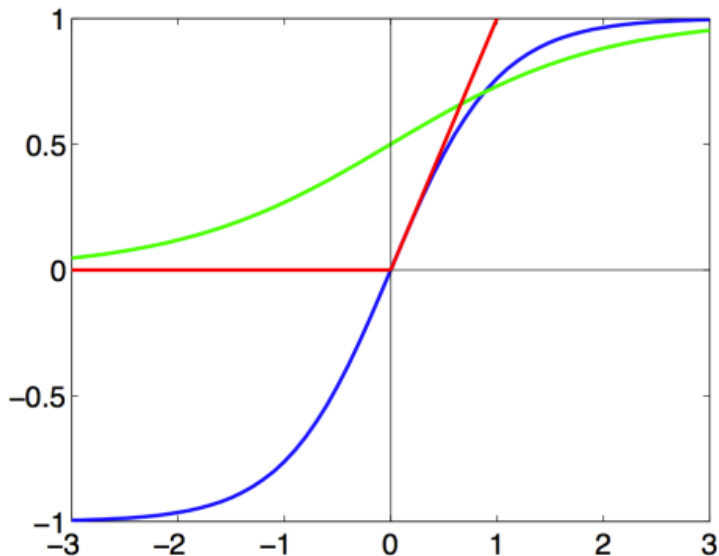
Cross Entropy

Used for e.g. classification tasks

Define your own!

Note: Must be differentiable for gradient descent based methods

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: Gradient Descent

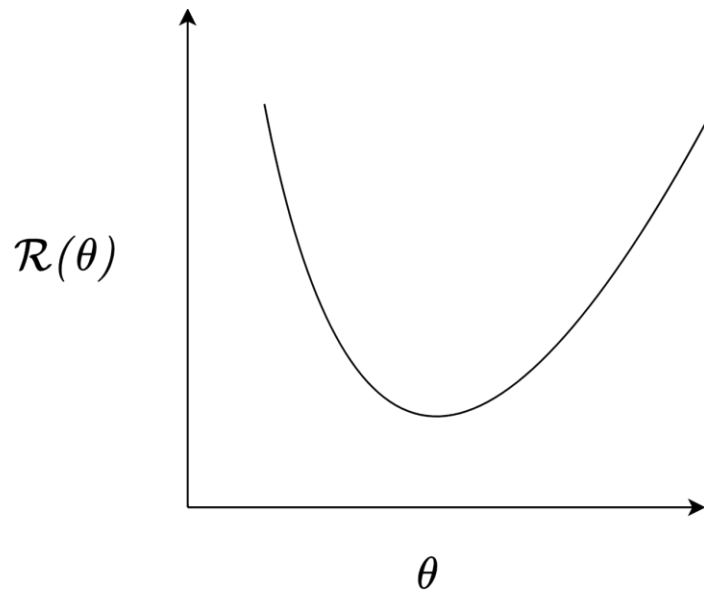
Given:

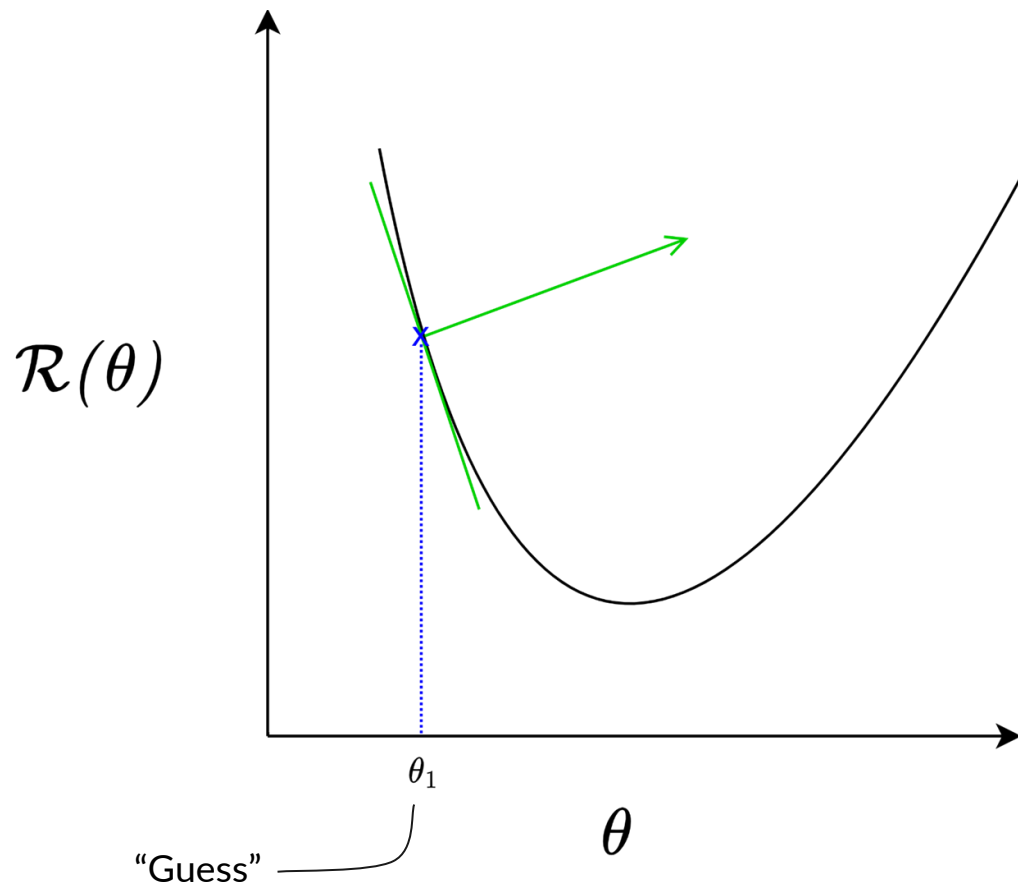
- Family of parameters Θ (e.g. possible weights of a NN)
- Differentiable risk function $\mathcal{R}(\theta)$

Goal:

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

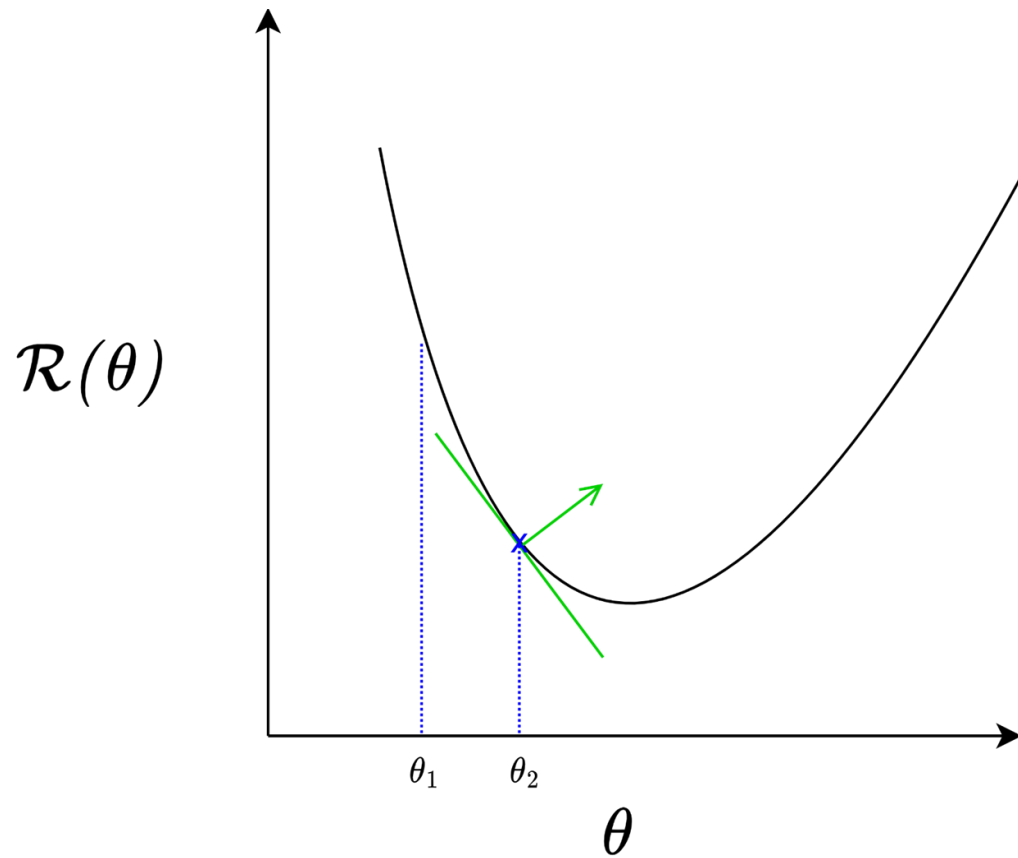
Backprop: Gradient descent



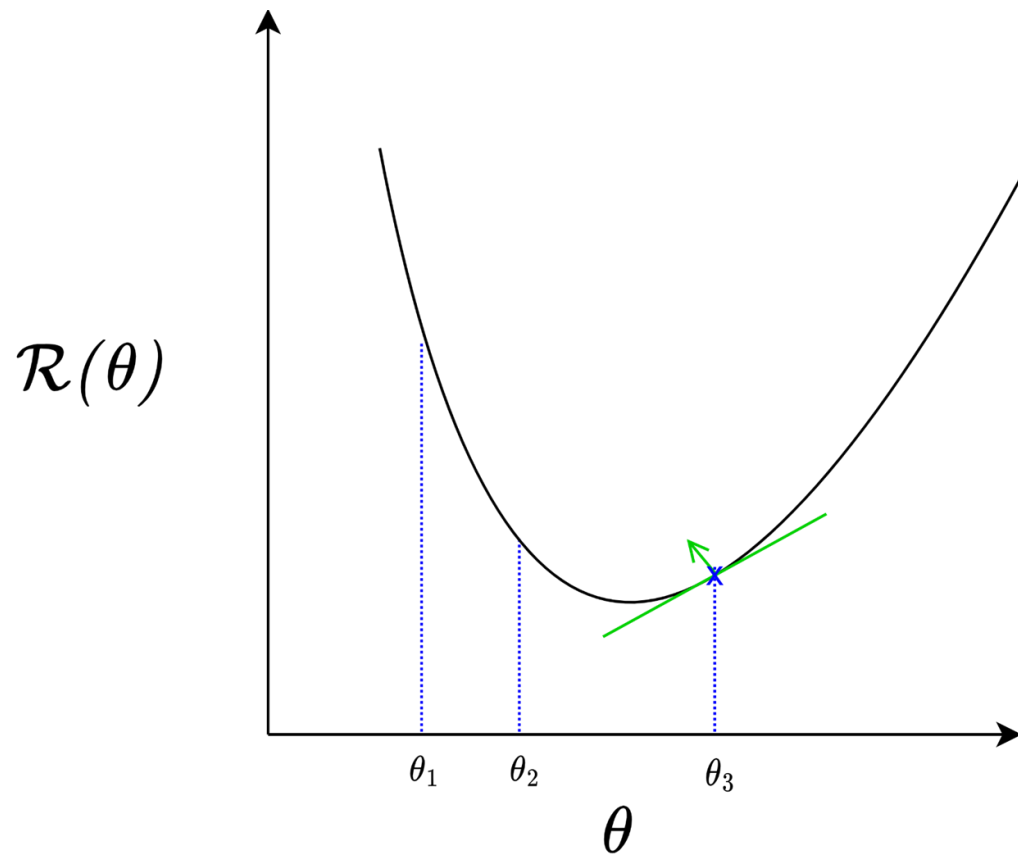


"Learning rate"

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



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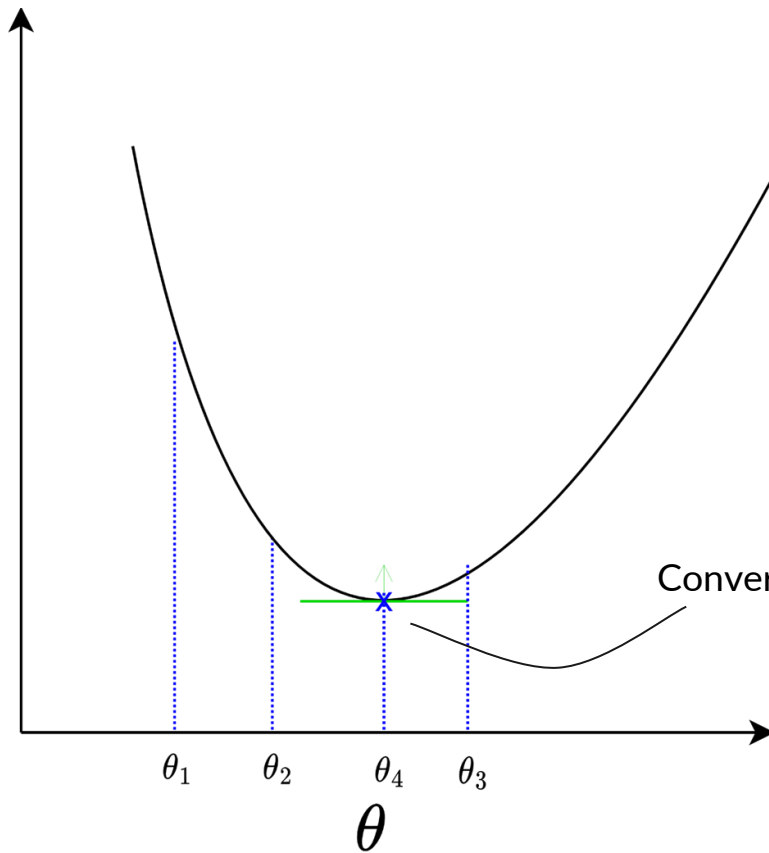


$$\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} \mathcal{R}(\theta_i)$$

$\mathcal{R}(\theta)$

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

Converges to local minima





Backprop: Efficient NN GD

- Goal: change $\mathcal{O}(|\theta|^2)$ to $\mathcal{O}(|\theta|)$

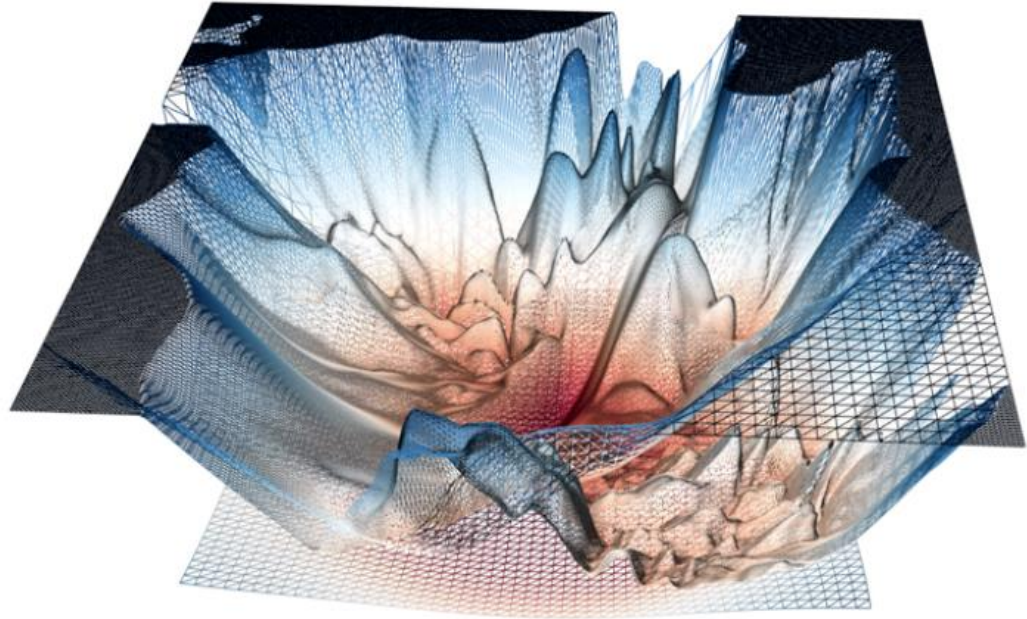
- Recall a NN:

$$\mathcal{N}(x) = a^\ell \circ h^\ell \circ a^{\ell-1} \circ h^{\ell-1} \circ \dots \circ a^1 \circ h^1 x$$

- Use the chain rule to compute the derivatives from output to input
“Backpropagation of errors”

A “real” loss landscape:

- Many (many many) local minima
- Saddle points



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



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



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ML Training paradigms (a selection)

- **Supervised**
 - Train a model with explicit input-output pairs
- **Unsupervised**
 - Learns “patterns” from unlabelled data
- **Semi-supervised learning**
 - Learn a few things with input-output pairs, relate them to patterns learnt unsupervised
- **Reinforcement Learning**
 - Learn an optimal “policy” that gives you the best action to take at any given state space by taking random actions and learning through positive or negative reinforcement.
- **Evolution**
 - Optimize parameters through (Darwinian) evolution; e.g. genetic algorithms.

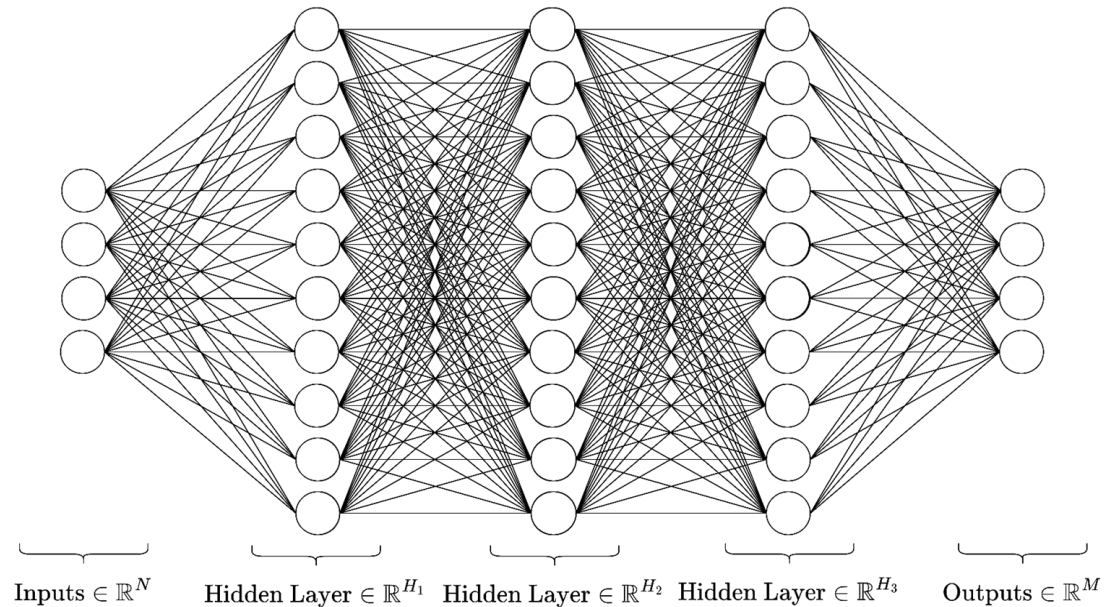
Types of Neural Networks

Multi-layer Perceptrons

Useful for **static** input-output relations

More hidden layers ~ better approximation of more complicated functions

Quick to design and implement

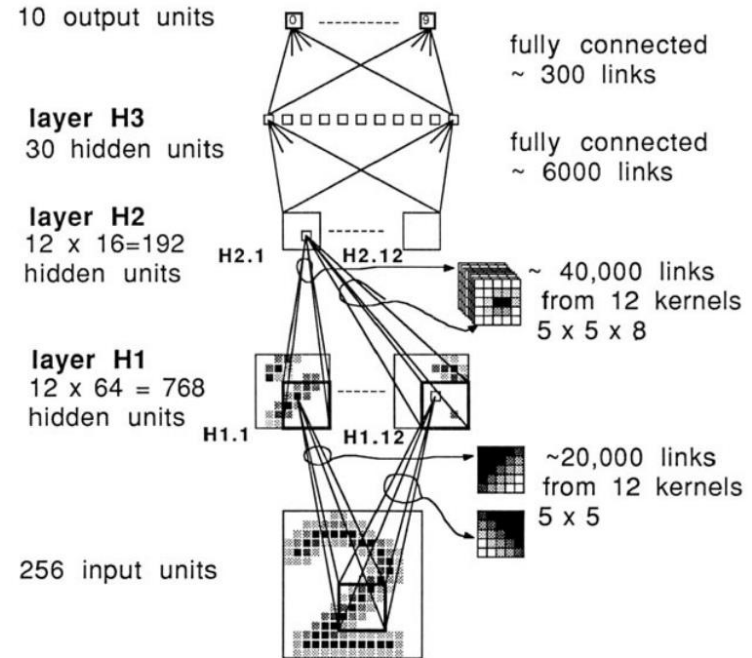


Convolutional Neural Networks

Learn “**kernels**”, i.e. matrices that convolve over n -dimensional data to extract abstract, lower-dimensional features.

Used often in **image and signal processing tasks** such as object detection and segmentation.

Accounts for translational variance: the object can be anywhere in the image and still be found



Recurrent Neural Networks

Outputs go back and forth between neurons (loops exist in the graphs)

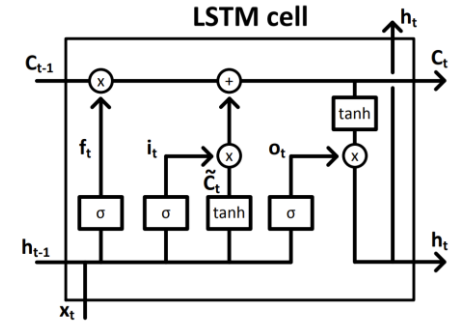
Approximates dynamical systems

- Any time-based function
- Any data that can be modelled as being

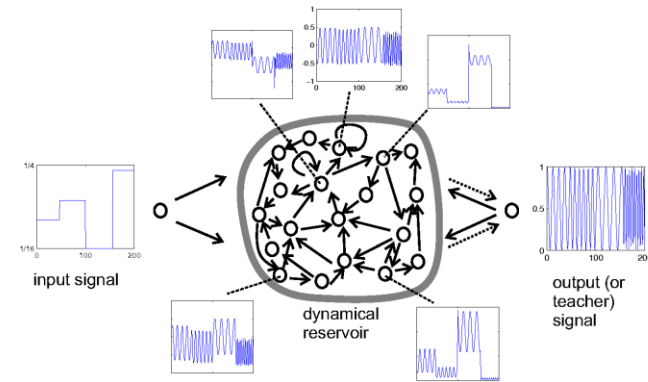
“ordered”

Used often in **time-series tasks** like signal processing, natural language processing

Several types: Fully-connected, LSTMs, GRUs, reservoirs



An LSTM cell schematic. Adapted from: doi.org/10.4233/uuid:dc73e1ff-0496-459a-986f-de37f7f250c9



Echo state network schematic. Adapted from www.scholarpedia.org/article/Echo_state_network

Graph Neural Networks

Models any system that can be modelled as a graph

Learns relations between nodes, edges, global properties

Used in e.g. image segmentation, chemistry and pharmacy models, NLP, hierarchically-related data

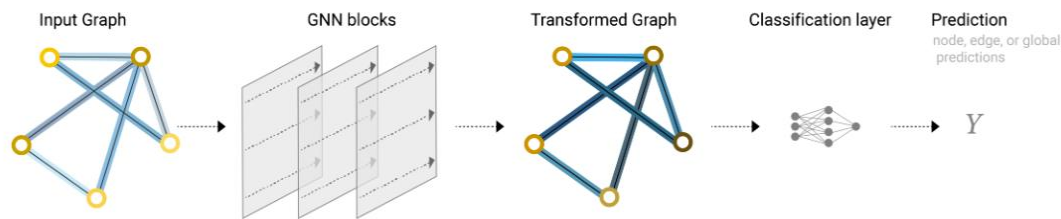


Image adapted from this excellent intro to GNNs: <https://distill.pub/2021/gnn-intro/>

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



Universal Approximation Theorem

***Theorem (schematic).** Let \mathcal{F} be a certain class of functions $f : \mathbb{R}^K \rightarrow \mathbb{R}^M$. 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

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

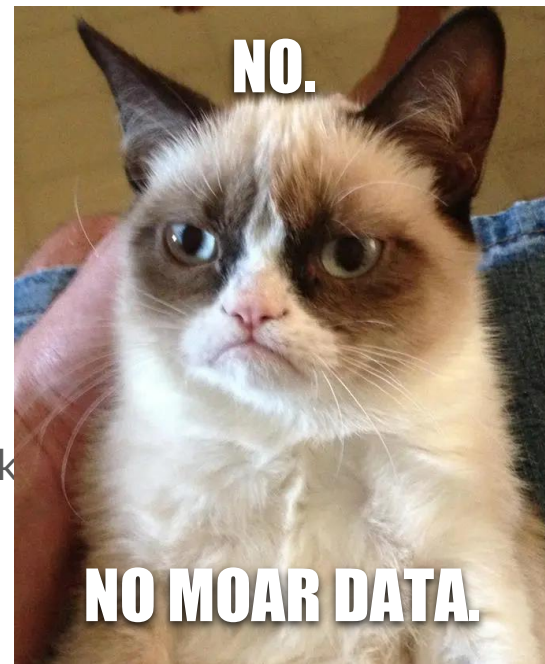


<https://lasp.colorado.edu/home/minxss/2016/07/12/minimum-mission-success-criteria-met/>

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>

In practice

Frameworks

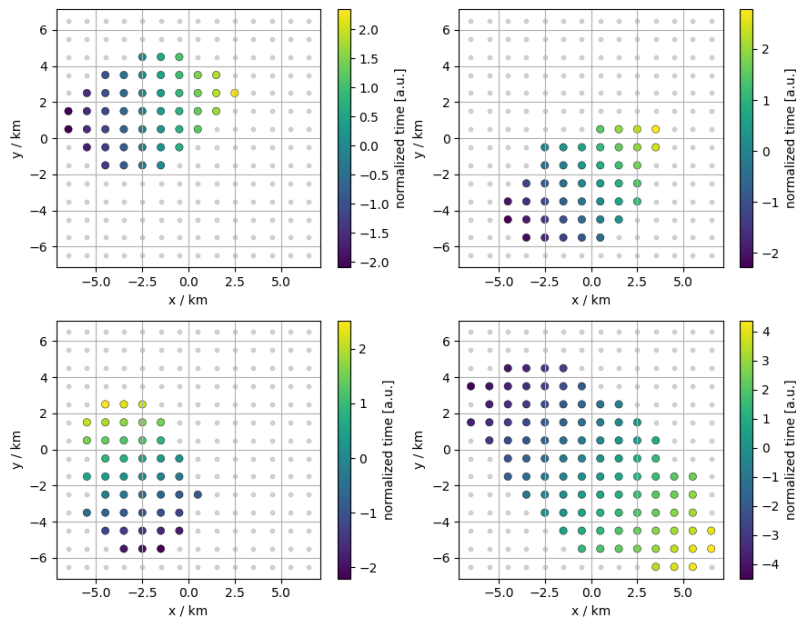
You don't need any maths or programming skills (but hopefully you do!)

Use other people's code! libraries, frameworks, modules



Image of logos adapted from S. Summers, ISOTDAQ
Lecture on Machine Learning (2020) – Slide 8

A demonstration in Keras



Adapted from:
Erdmann, M., Glombitza, J.,
Kasieczka, G., & Klemradt, U.
(2021).
Deep Learning for Physics Research.

Training tips



Overfitting & Underfitting

The real troublemakers in ML in general!

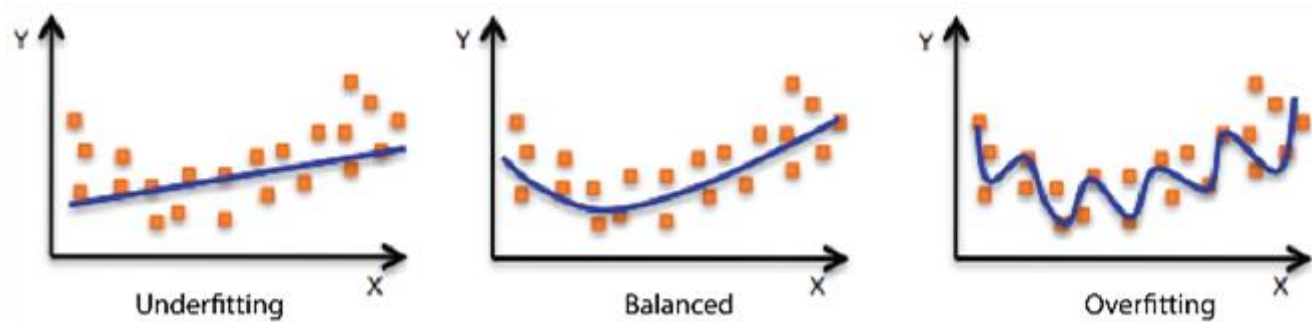
Underfitting: When the model fits the training data not well enough

- 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



Validation

Split your training set into two!

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

Train Set

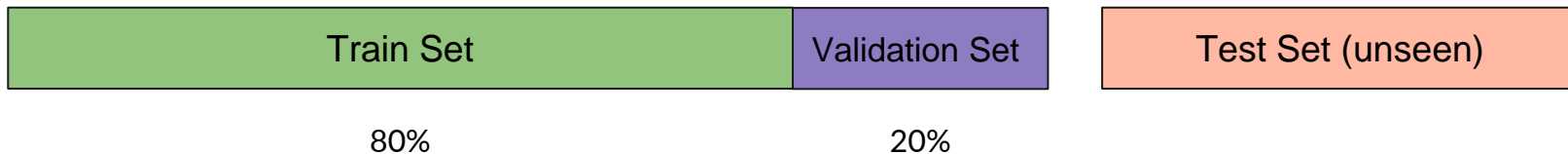
Test Set (unseen)



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)





***k*-fold Cross-validation**

Split training set into k -segments, iteratively train and validate with each segment.

- Accounts for irregularities in training set
- “Gold standard” for evaluating generality of neural network models



Train Set



***k*-fold Cross-validation**

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e.g. $k=5$ (5-fold cross-validation)

Train Set	Train Set	Train Set	Train Set	Train Set
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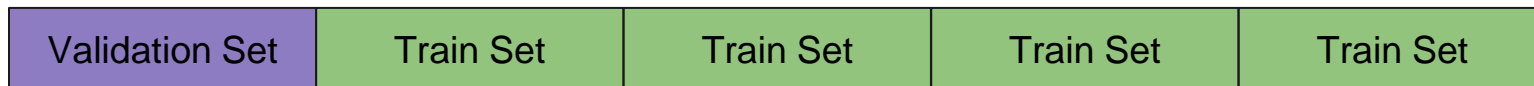


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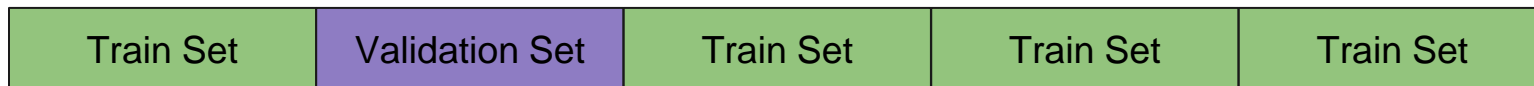


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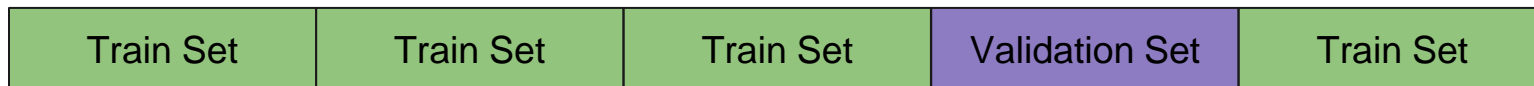


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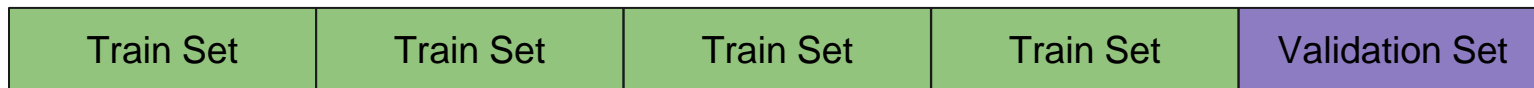


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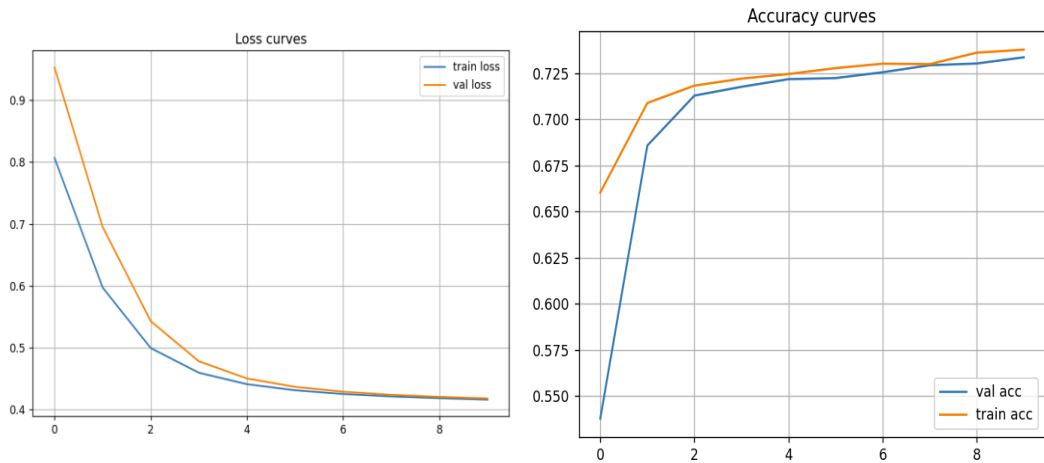
e.g. $k=5$ (5-fold cross-validation)



Result = average over all validation passes

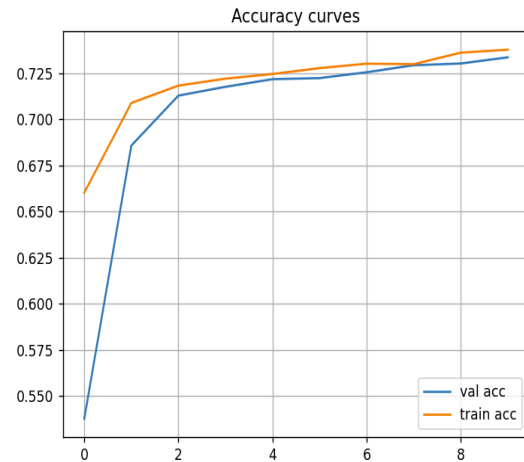
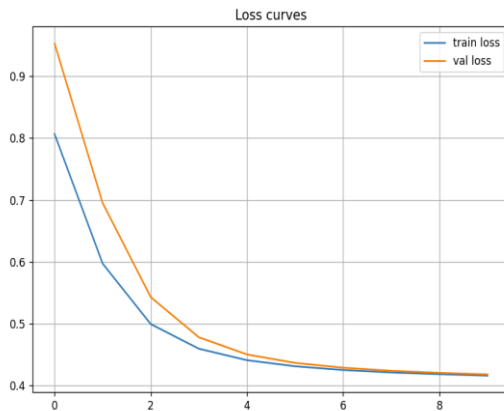
Training curves

Important to plot!



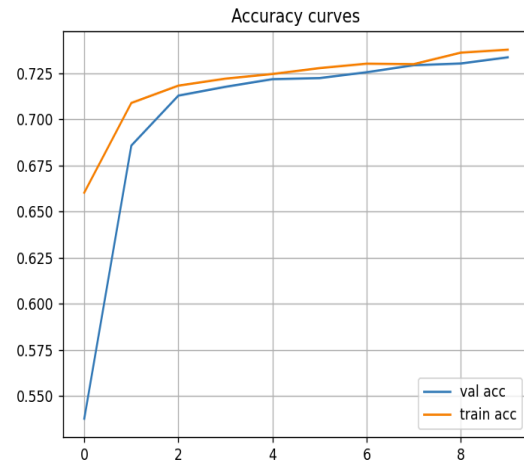
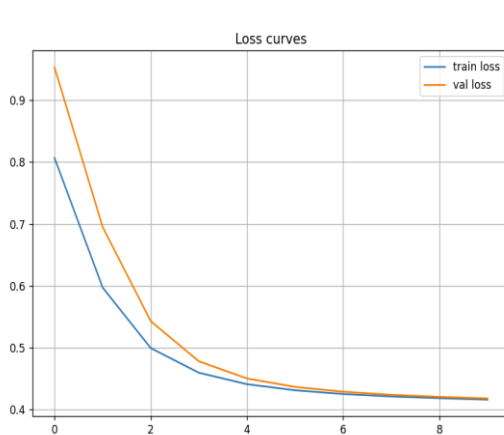
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Training curves

Important to plot!(!!!!)

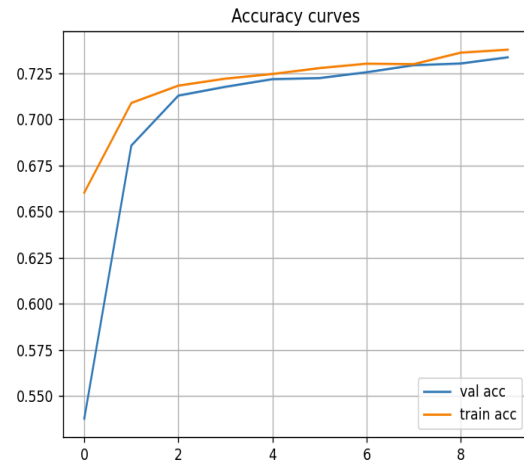
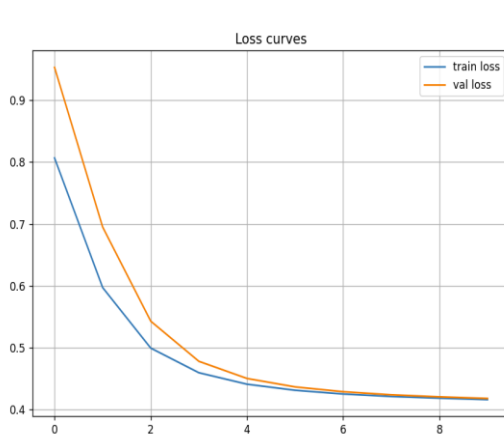


Shows if and how fast your model is learning on task-relevant metrics

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

Training curves

Important to plot!!!!



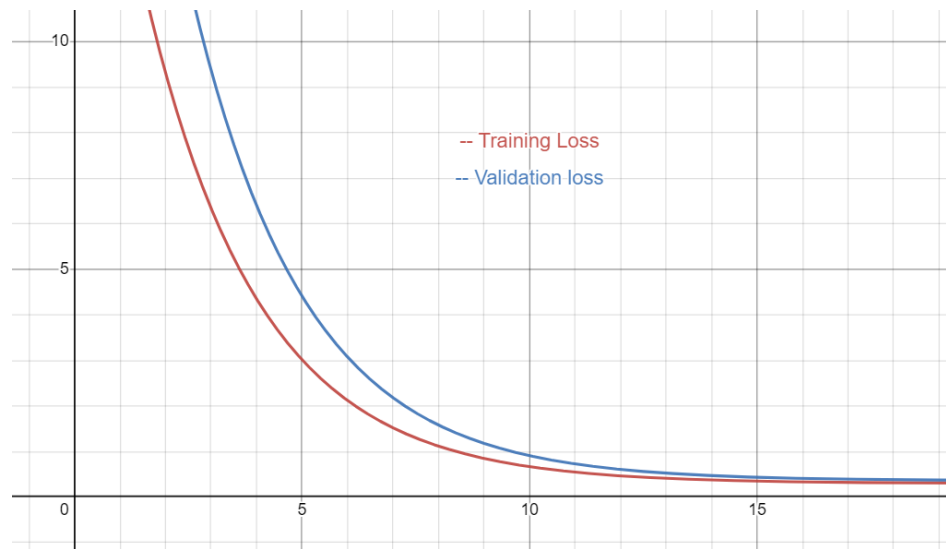
Shows if and how fast your model is learning on task-relevant metrics

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

May indicate potential over and underfitting

Reading training curves

If



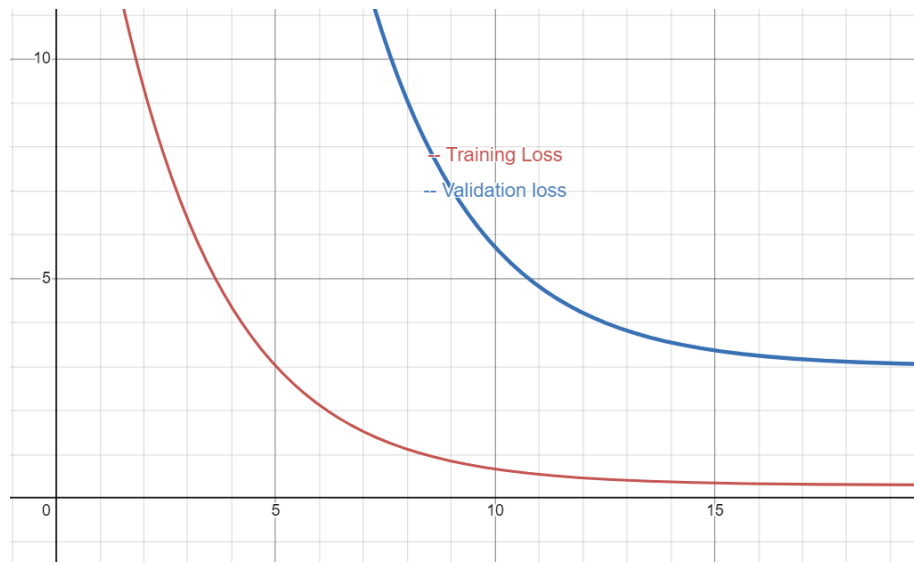
validation loss > training loss

then often the model is *good!*

Low loss ==
Better

Reading training curves

If



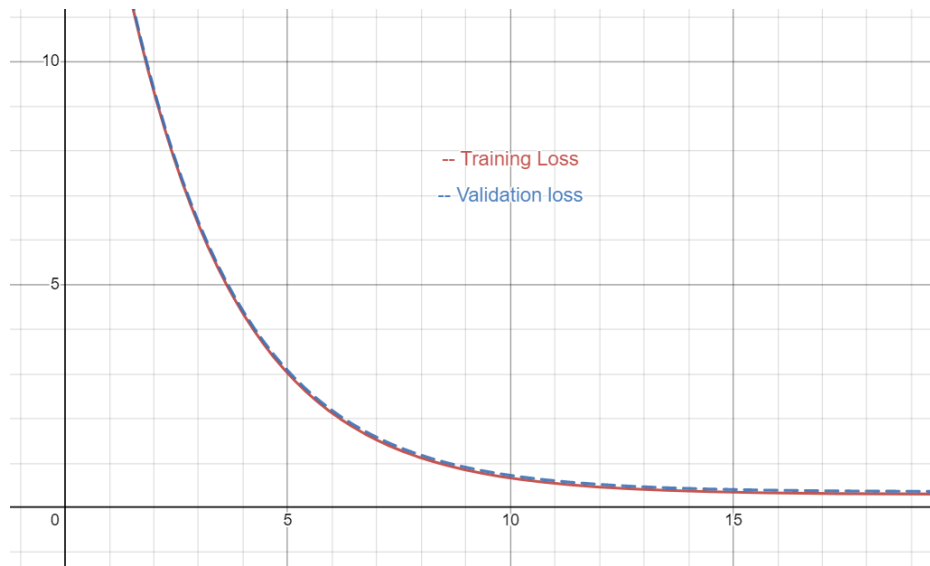
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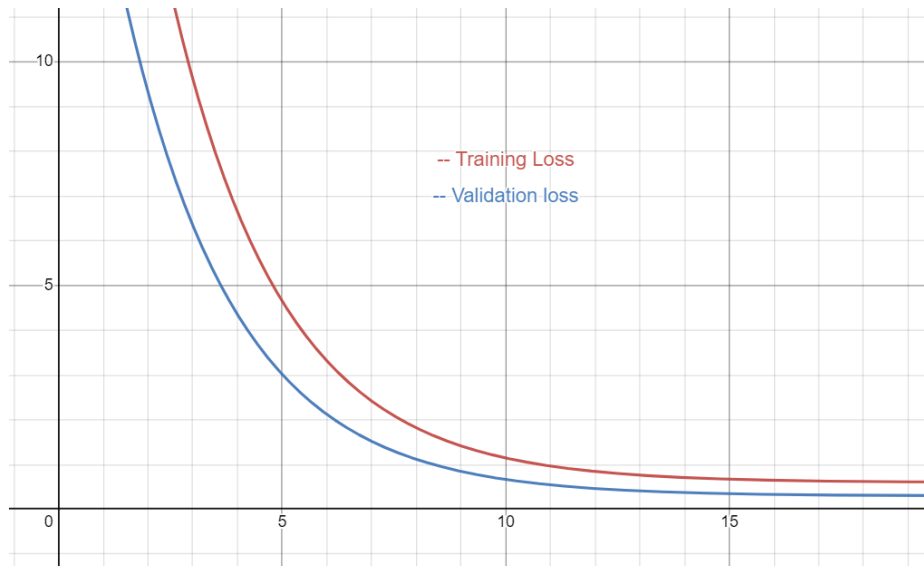
validation loss \sim training loss

then often the model is *underfitting*

Low loss ==
Better

Reading training curves

If



validation loss < training loss

then something is *very* wrong, or *totally expected*!

Low loss ==
Better



Regularization

- L1/L2 Regularization

Added losses:

$$\lambda \cdot \sum_{i=1}^d |w_i| \qquad \lambda \cdot \sum_{i=1}^d w_i^2$$

- Dropout (on when training, off when testing/deploying)
- Early stopping

Parallelization: Speeding up NNs

Main math operation in NNs:

- Matrix-vector multiplications
- Element-wise nonlinear activation functions

Parallelization can be used to **massively speed up** learning and deployment!

- Multi-core CPUs
- Graphics processing units (GPUs)
- Tensor processing units (TPUs)
- FPGAs

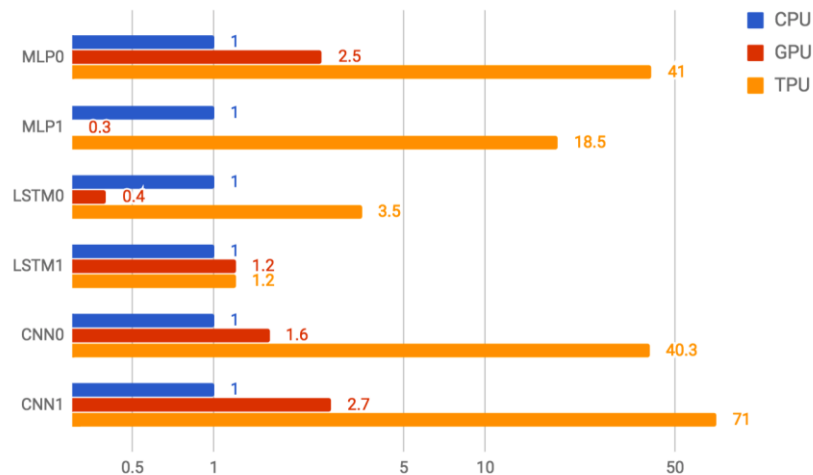
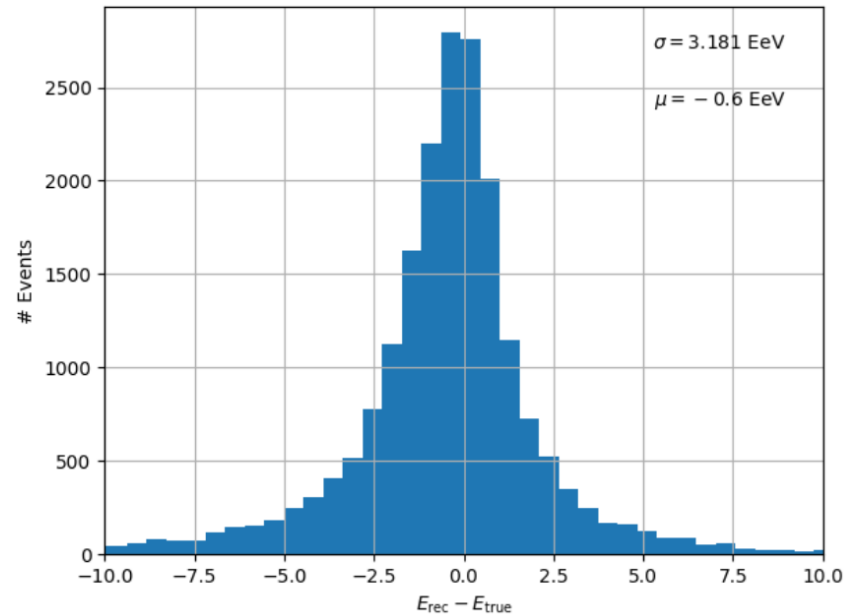
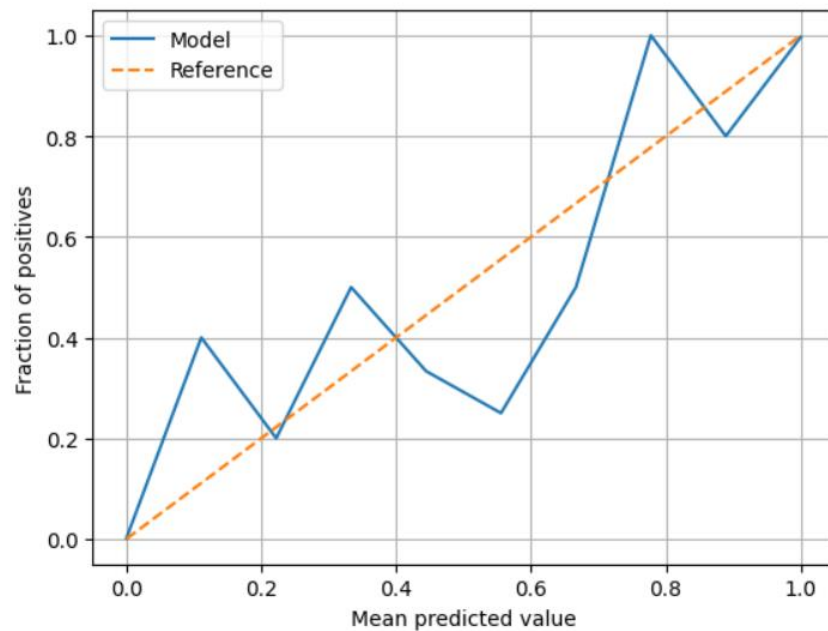


Image from <https://cloud.google.com/blog/products/ai-machine-learning/an-in-depth-look-at-googles-first-tensor-processing-unit-tpu>

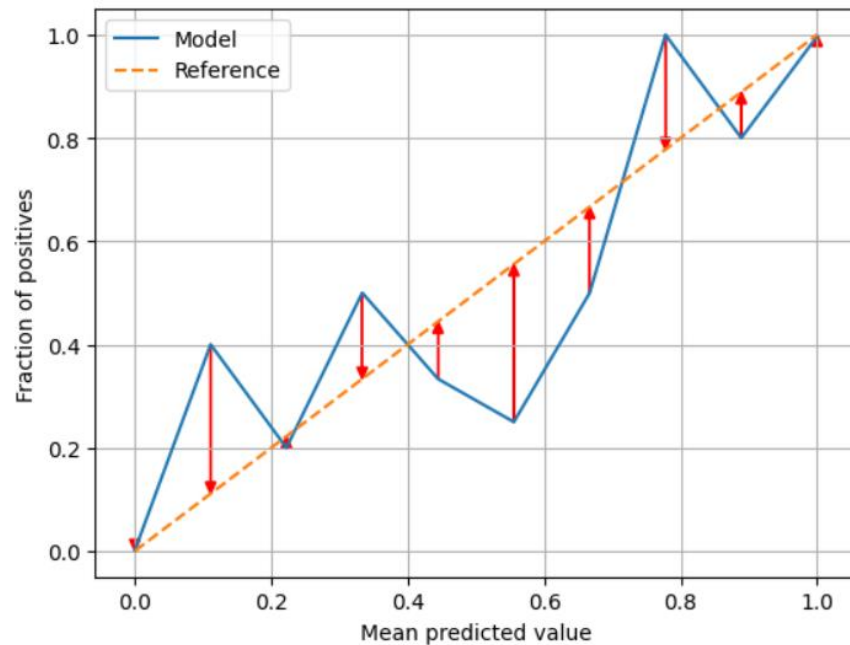
UQ 1: Bias-Variance Decomposition



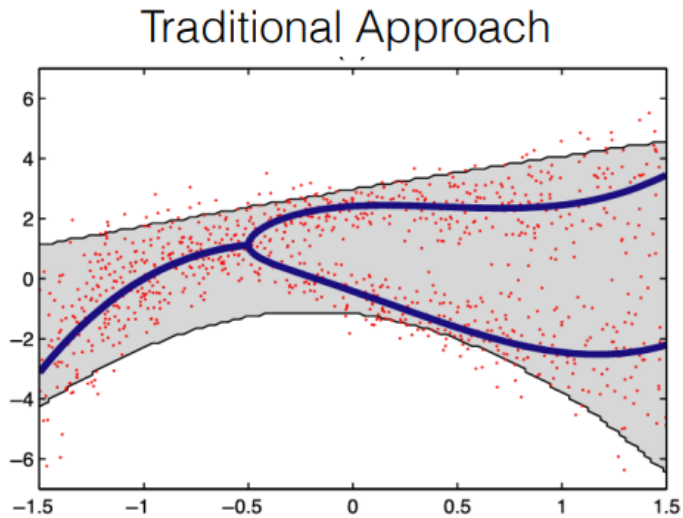
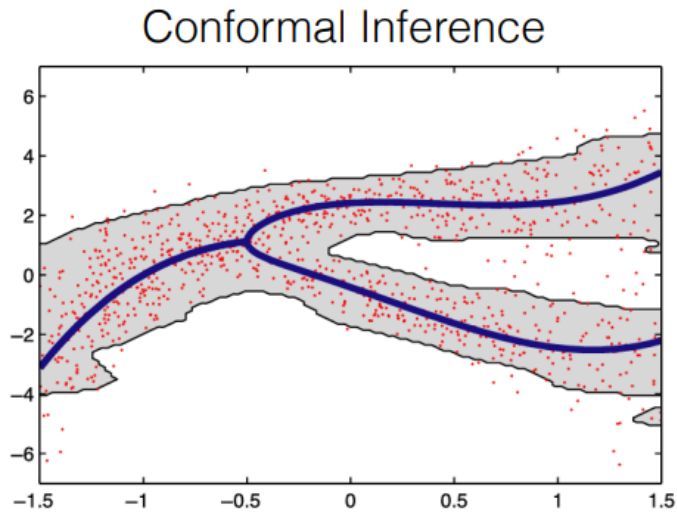
UQ2: Calibration



UQ2: Calibration



UQ3:



Winzler, E. A., Shoemaker, D. D., Astromoff, A., Liang, H., Anderson, K., Andre, B., ... & Davis, R. W. (1999). Functional characterization of the *S. cerevisiae* genome by gene deletion and parallel analysis. *science*, 285(5429), 901-906.



UQ Others

- Markov-chain Monte Carlo (and variations: HMC, Langevin Dynamics, etc)
- Neural linear models
- Deep Ensembles
- Variational Inference
- Monte Carlo Dropout
- ...



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- ...
- ...
- ...
- ...



Frontiers

Deep learning

- Models with hundreds of layers, billions of weights
- Transformers, generative adversarial networks, autoencoders
- AutoMLs: a tool to automatically generate good ML models for a task

Explainable AI (XAI)

- Explainable+interpretable models
- Human-like and human-understandable reasoning

Reservoir computing

- Echo state networks
- Conceptors

Others: Physics Informed NNs
Neural ODEs, PDEs
Group equivariant DL