



ÖAW

ÖSTERREICHISCHE
AKADEMIE DER
WISSENSCHAFTEN

AI

WinterSchool

January 20 - 24, 2025

Today's Program

Part I: Introduction lecture

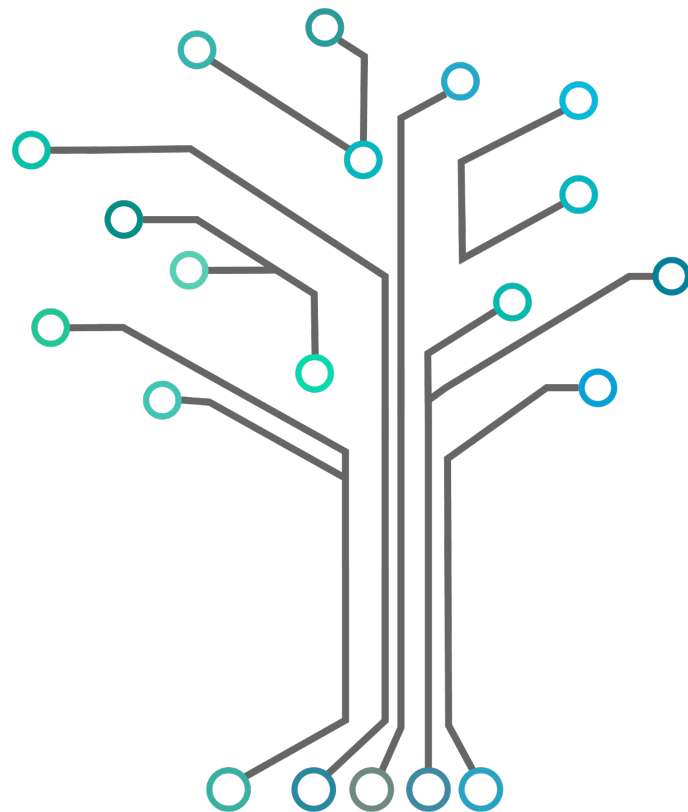
14:15 - 15:45

- Overview
- Theoretical Basics
- Data
- Training
- Evaluation
- Design and Techniques

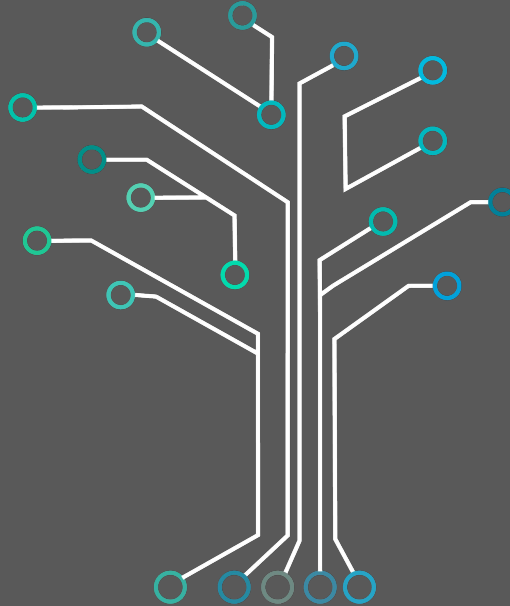
Part II: Hands-on

16:15 - 18:00

- Questions
- Setup
- Some coding

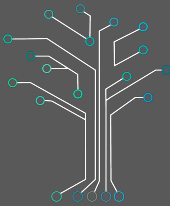


Introduction to Deep Learning



Jan 20, 2025

Overview



Machine Learning as Artificial Intelligence

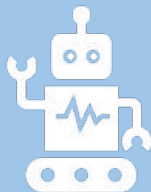
Artificial Intelligence

Any technique that enables computers to mimic human behaviour



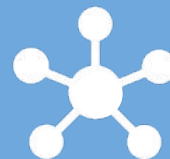
Machine Learning

Learn to perform tasks from data without being explicitly programmed



Deep Learning

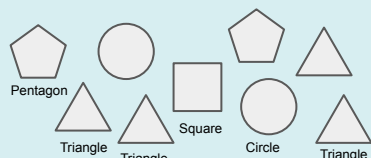
Extract patterns from data using deep neural networks



Disciplines of Machine Learning

Supervised Learning

Labeled Training Data



Learning  to label

New Data



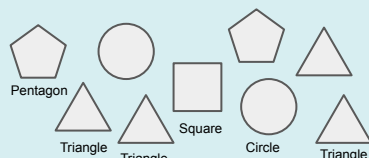
Model

Square!

Disciplines of Machine Learning

Supervised Learning

Labeled Training Data



Learning



to label

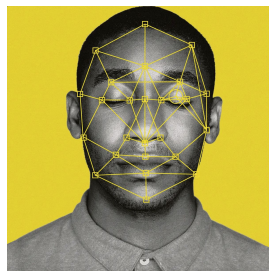
New Data



Model

Square!

Face recognition



<https://www.theguardian.com/technology/2019/jul/29/what-is-facial-recognition-and-how-sinister-is-it>

Handwritten transcription

so IN MY 2029 AND
WELL HEATED evening
since I feel a sea
of BALLPOINT pens
AND write IN MY
notebooks to record
THE EPHEMERA
OF MY LIFE

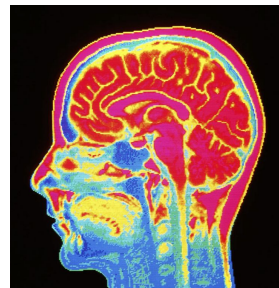
<https://www.behance.net/gallery/71324093/The-Handwritten-A>

Speech recognition



<https://support.apple.com/de-de/HT208336>

Medical diagnosis

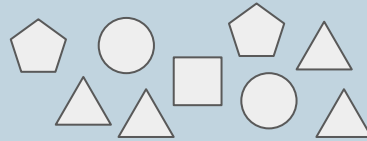


<https://www.wired.com/story/fmri-ai-suicide-ideation/>

Disciplines of Machine Learning

Unsupervised Learning

Unlabeled Training Data



Learning



meaningful representations

New Data

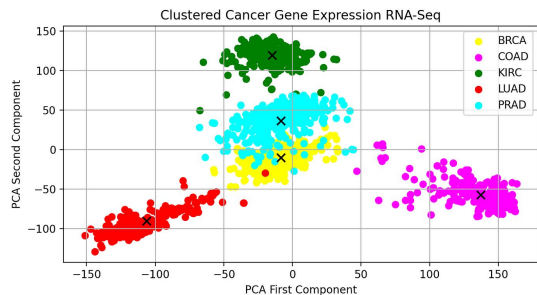


Model



Disciplines of Machine Learning

Gene clustering



<https://ernest-bonat.medium.com/building-machine-learning-clustering-models-for-gene-expression-rna-seq-data-d0e5af10416d>

Language processing



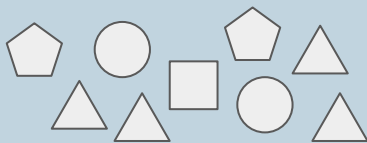
Despite the rapid advances in AI, computer vision (CV) is still challenged in matching the precision of human perception. The training data here is as important as algorithms. The more accurate the input data annotation, the more effective the model prediction.

How do we annotate data, though? There are multiple ways to go with this one, but it all depends on your use case. For the purposes of this article, we'll take a deeper dive into bounding

<https://www.superannotate.com/blog/what-is-natural-language-processing>

Unsupervised Learning

Unlabeled Training Data

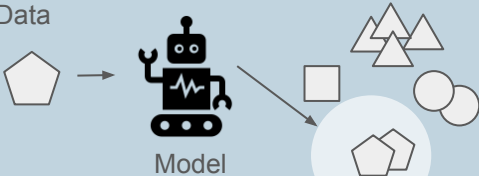


Learning



meaningful representations

New Data



Model

Image clustering



<https://neurohive.io/en/state-of-the-art/deep-clustering-approach/>

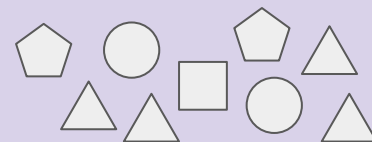
Generation tasks



Disciplines of Machine Learning

Reinforcement Learning

Unlabeled Training Data



Learning



to make decisions

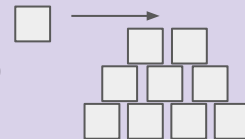
New Task:

“build a pyramid with suitable item”



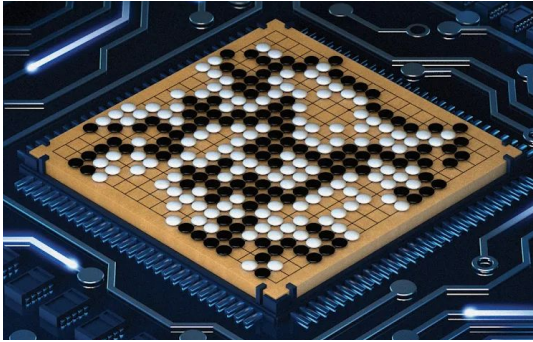
Model

best reward!



Disciplines of Machine Learning

Game playing



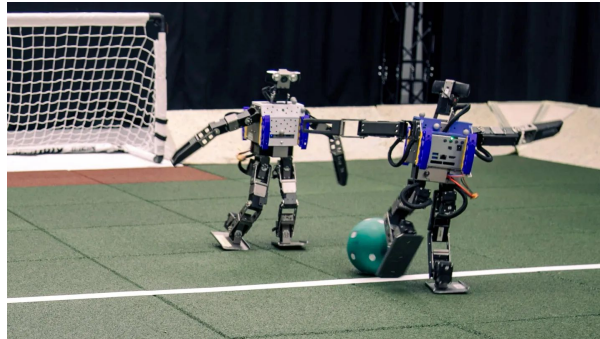
<https://deepmind.google/research/breakthroughs/alphago/>

Algorithmic trading



<https://www.mathworks.com/videos/reinforcement-learning-in-finance-1578033119150.html>

Robotics



<https://www.sciencenews.org/article/reinforcement-learn-ai-humanoid-robots>

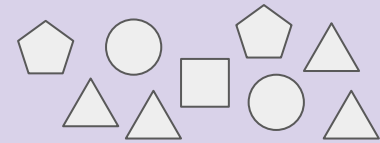
Goal-oriented chatbots



<https://towardsdatascience.com/training-a-goal-oriented-chatbot-with-deep-reinforcement-learning-part-i-introduction-and-dce3af21d383>

Reinforcement Learning

Unlabeled Training Data



Learning



to make decisions

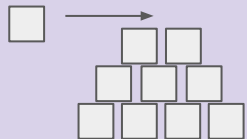
New Task:

“build a pyramid with suitable item”



Model

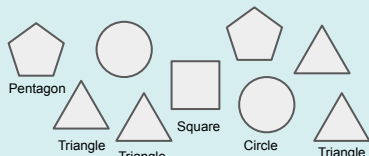
best reward!



Disciplines of Machine Learning

Supervised Learning

Labeled Training Data



New Data

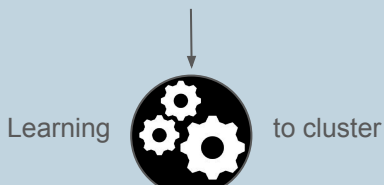
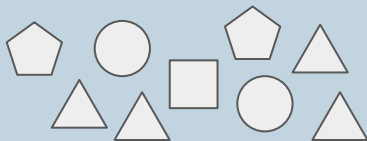


Model

Square!

Unsupervised Learning

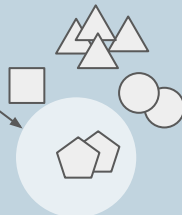
Unlabeled Training Data



New Data

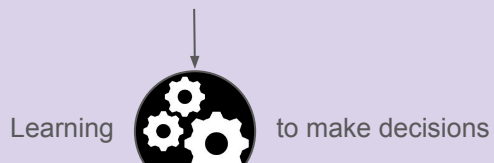
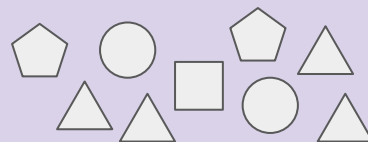


Model



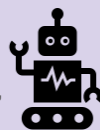
Reinforcement Learning

Unlabeled Training Data



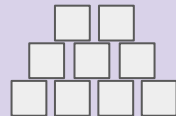
New Task:

"build a pyramid with suitable item"



Model

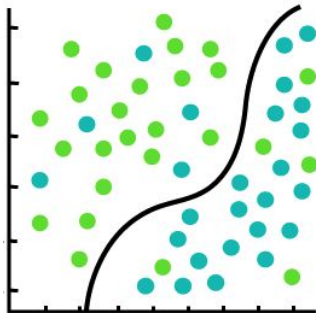
best reward!



Supervised Learning Tasks

Classification

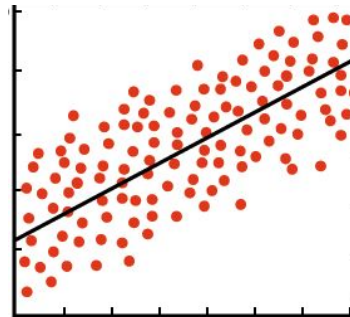
Training: learn to predict a label out of a discrete set



Testing: accuracy as # of correctly predicted

Regression

Training: predict a label as a continuous value directly

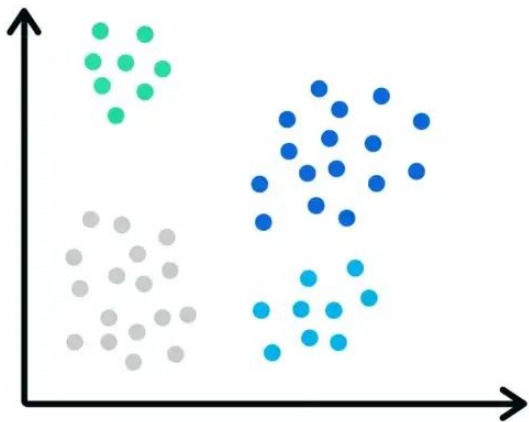


Testing: distance/similarity to actual outcomes

Unsupervised Learning Tasks

Clustering

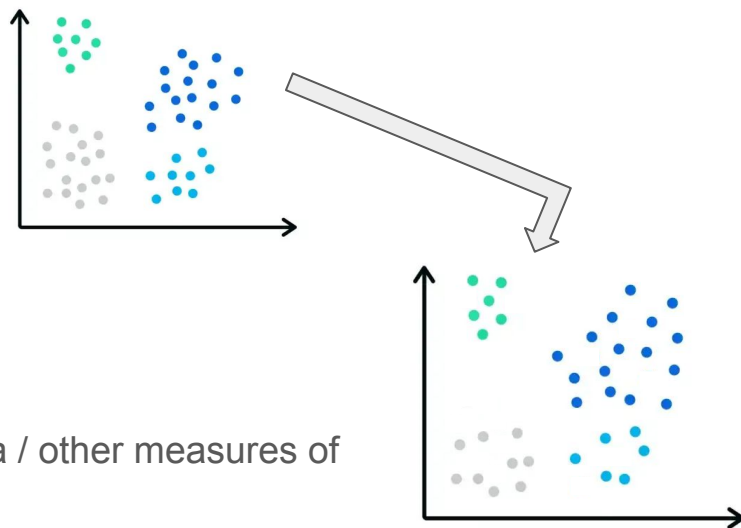
Training: learn to identify groups



Testing? Depends on the availability of ground truth data / other measures of performance...

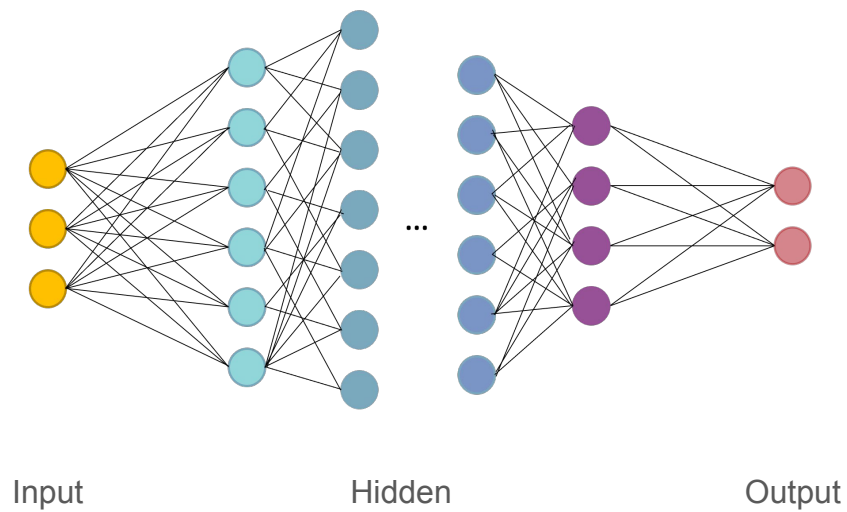
Generation

Training: create representations to sample realistic outputs



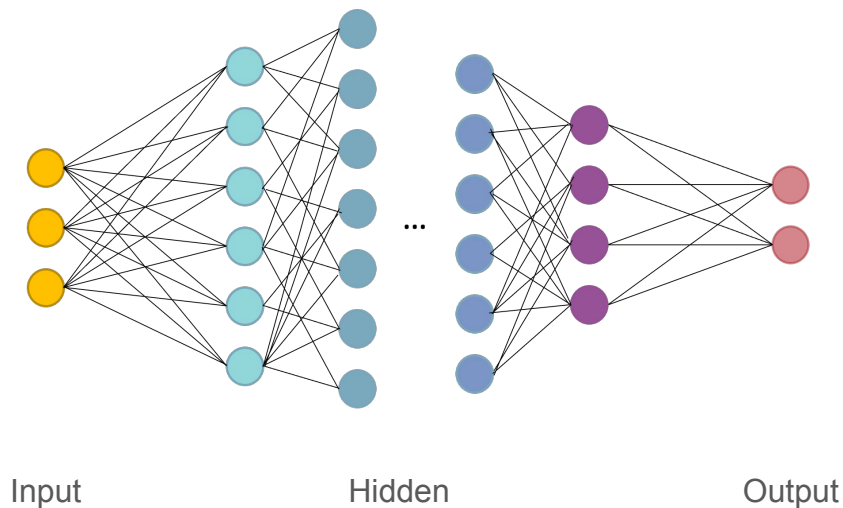
Deep Learning

Deep Neural Networks



Deep Learning

Deep Neural Networks

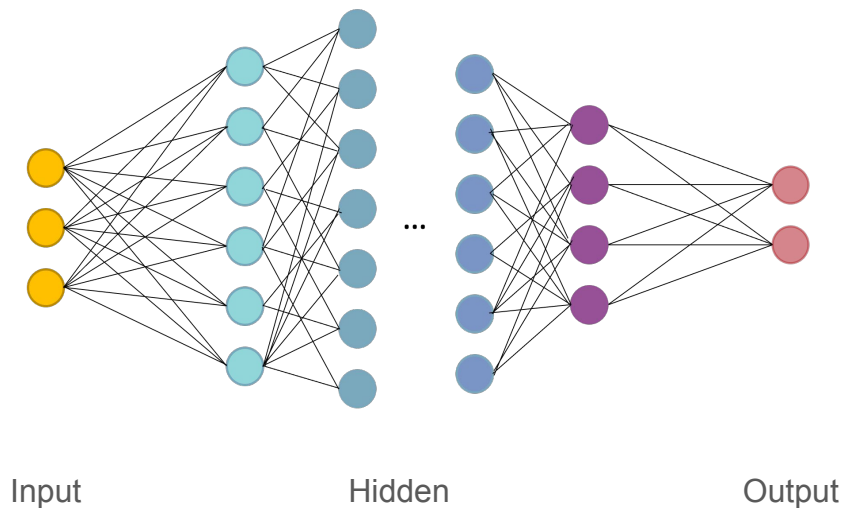


Why this?

- Hierarchical processing: several levels
- All-in-one model: human out of the loop (?!)
- Extremely expressive: can learn “anything”

Deep Learning

Deep Neural Networks



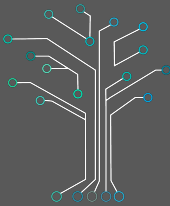
Why this?

- Hierarchical processing: several levels
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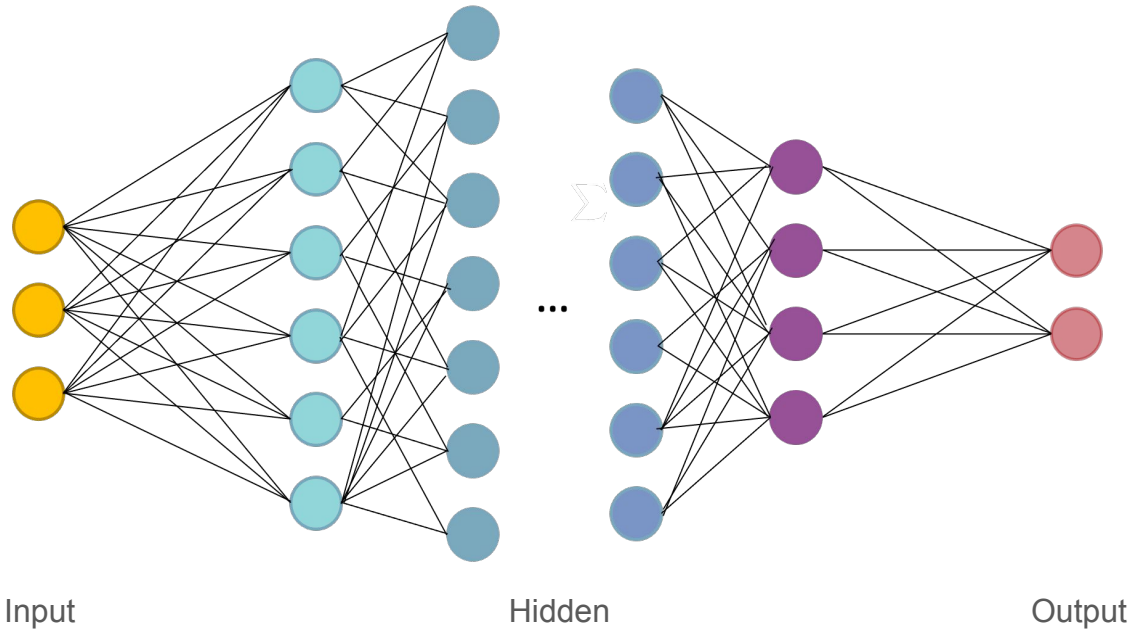
Why now?

- Unprecedented amount of available data
- Parallelization of computations by GPUs
- Many available toolkits

Theoretical Basics

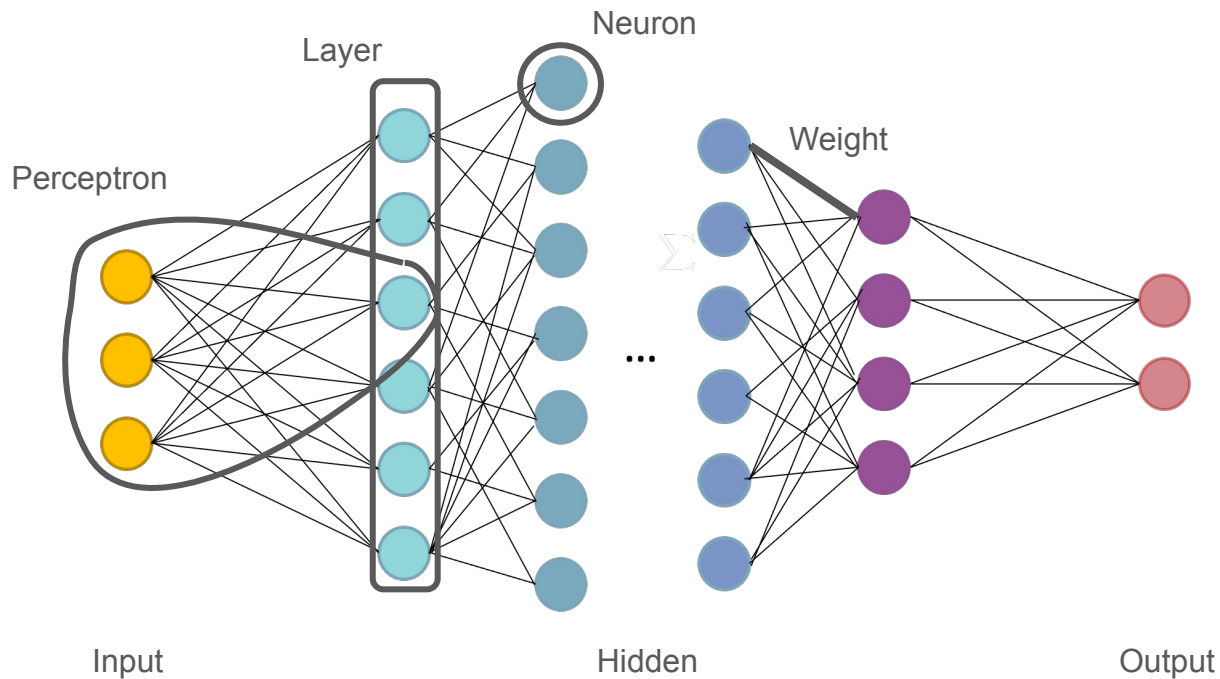


A Neural Network



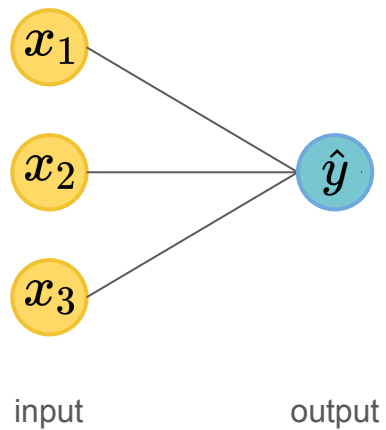
A Neural Network

“Multi-layer Perceptron”



A Neural Network

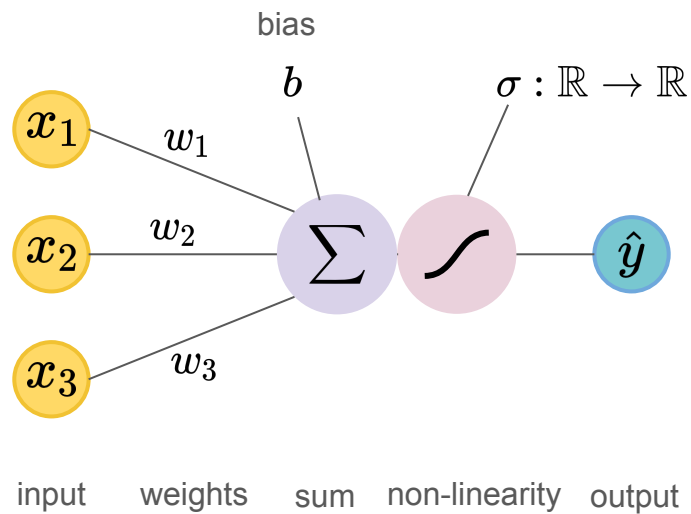
Perceptron



Σ

A Neural Network

Perceptron

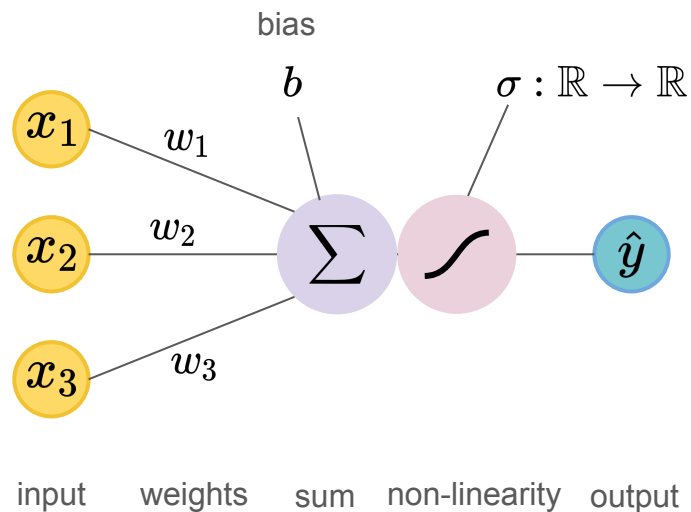


The math

$$\hat{y} = \sigma \left(\sum_{i=1}^3 w_i \cdot x_i + b \right)$$

A Neural Network

Perceptron



Σ

The math...

$$\hat{y} = \sigma \left(\sum_{i=1}^3 w_i \cdot x_i + b \right)$$

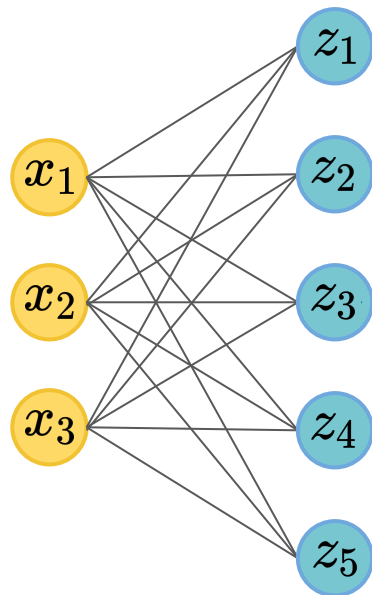
linear combination of input activation bias

$$[w_1 \quad w_2 \quad w_3] \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = w^T x$$

$$\hat{y} = \sigma(w^T x + b)$$

A Neural Network

Single Layer Network



input

layer

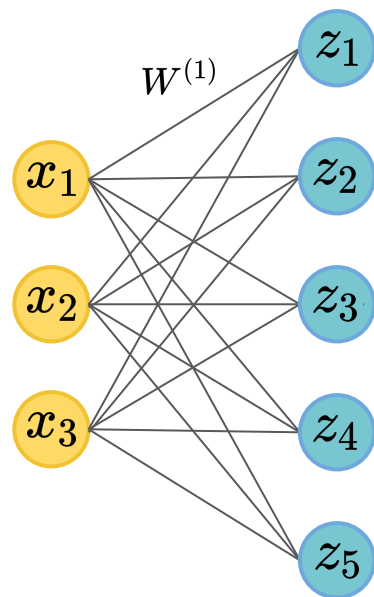
The math...

$$z_j = \sigma \left(\sum_{i=1}^3 w_{j,i}^{(1)} \cdot x_i + b_j^{(1)} \right), j = 1, \dots, 5$$

Σ

A Neural Network

Single Layer Network



input

layer

The math...

Σ

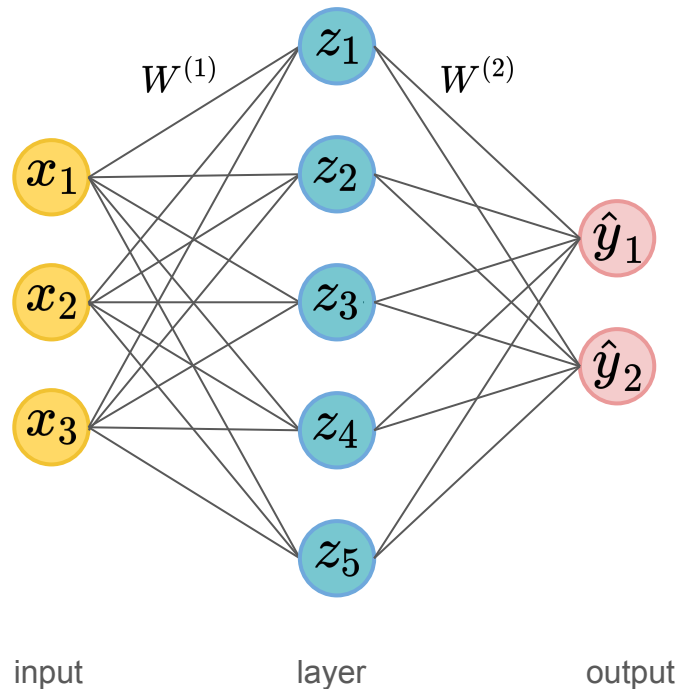
$$\begin{bmatrix} w_{1,1}^{(1)} & w_{1,2}^{(1)} & w_{1,3}^{(1)} \\ w_{2,1}^{(1)} & w_{2,2}^{(1)} & w_{2,3}^{(1)} \\ w_{3,1}^{(1)} & w_{3,2}^{(1)} & w_{3,3}^{(1)} \\ w_{4,1}^{(1)} & w_{4,2}^{(1)} & w_{4,3}^{(1)} \\ w_{5,1}^{(1)} & w_{5,2}^{(1)} & w_{5,3}^{(1)} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix} = W^{(1)}x + b^{(1)}$$

$$z_j = \sigma \left(\sum_{i=1}^3 w_{j,i}^{(1)} \cdot x_i + b_j^{(1)} \right), \quad j = 1, \dots, 5$$

$$z = \sigma \left(W^{(1)}x + b^{(1)} \right)$$

A Neural Network

Single Layer Network



The math...

$$\begin{bmatrix} w_{1,1}^{(1)} & w_{1,2}^{(1)} & w_{1,3}^{(1)} \\ w_{2,1}^{(1)} & w_{2,2}^{(1)} & w_{2,3}^{(1)} \\ w_{3,1}^{(1)} & w_{3,2}^{(1)} & w_{3,3}^{(1)} \\ w_{4,1}^{(1)} & w_{4,2}^{(1)} & w_{4,3}^{(1)} \\ w_{5,1}^{(1)} & w_{5,2}^{(1)} & w_{5,3}^{(1)} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix} = W^{(1)}x + b^{(1)}$$

$$z_j = \sigma \left(\sum_{i=1}^3 w_{j,i}^{(1)} \cdot x_i + b_j^{(1)} \right), j = 1, \dots, 5$$

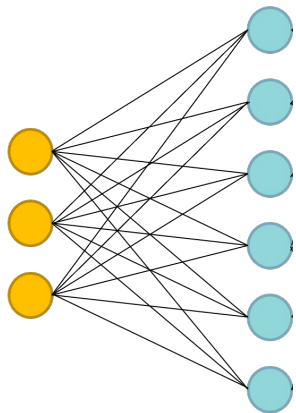
$$z = \sigma \left(W^{(1)}x + b^{(1)} \right)$$

$$\hat{y}_j = \sigma \left(\sum_{i=1}^5 w_{j,i}^{(2)} \cdot z_i + b_j^{(2)} \right), j = 1, 2$$

$$\hat{y} = \sigma \left(W^{(2)}z + b^{(2)} \right)$$

A Neural Network

Multi-layer Network

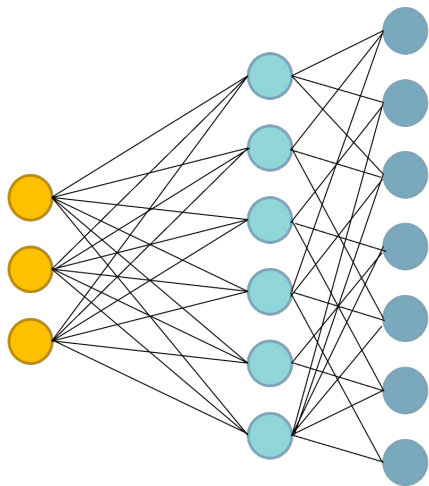


$$\hat{y} =$$

$$\sigma\left(W^{(1)}x + b^{(1)}\right)$$

A Neural Network

Multi-layer Network

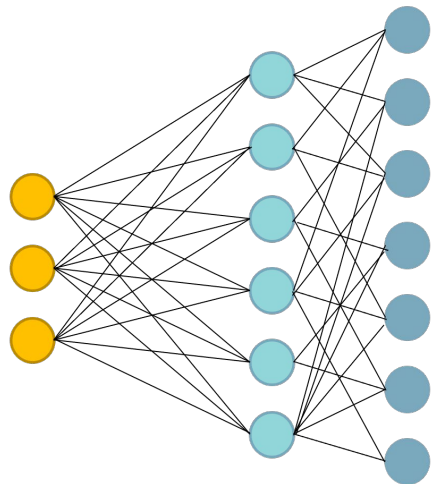


$\hat{y} =$

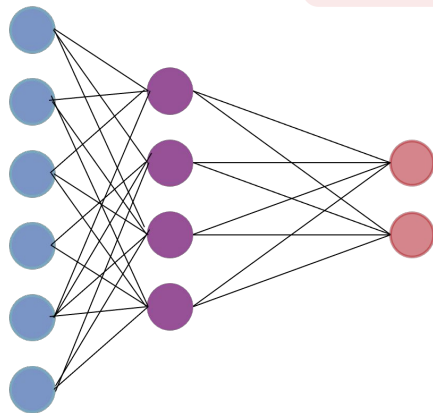
$$\sigma\left(W^{(2)}\sigma\left(W^{(1)}x + b^{(1)}\right) + b^{(2)}\right)$$

A Neural Network

Multi-layer Network



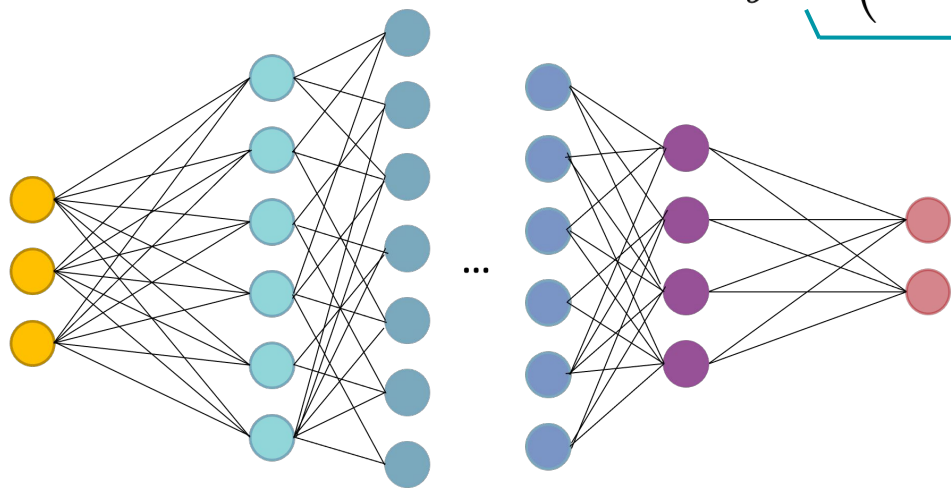
...



$$\hat{y} = \sigma\left(W^{(k)} \dots \sigma\left(W^{(2)} \sigma\left(W^{(1)}x + b^{(1)}\right) + b^{(2)}\right) \dots + b^{(k)}\right)$$

A Neural Network

Multi-layer Network



network output ("prediction")

$$\hat{y} = \sigma\left(W^{(k)} \dots \sigma\left(W^{(2)} \sigma\left(W^{(1)}x + b^{(1)}\right) + b^{(2)}\right) \dots + b^{(k)}\right)$$

$$=: \Phi(x; \theta)$$

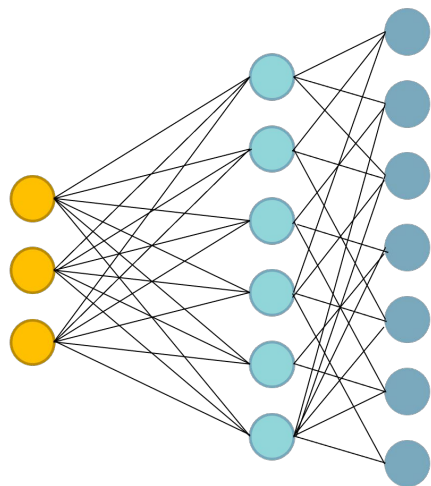
input

network parameters
= weights

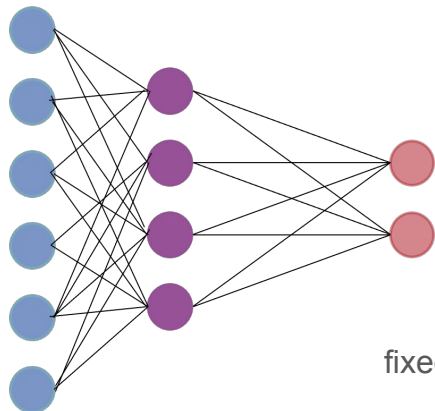
$$\theta = \{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \dots, W^{(k)}, b^{(k)}\}$$

A Neural Network

Multi-layer Network



...



network output ("prediction")

$$\hat{y} = \sigma\left(W^{(k)} \dots \sigma\left(W^{(2)} \sigma\left(W^{(1)}x + b^{(1)}\right) + b^{(2)}\right) \dots + b^{(k)}\right)$$

$$=: \Phi(x; \theta)$$

input

network parameters
= weights

$$\theta = \{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \dots, W^{(k)}, b^{(k)}\}$$

fixed θ

Φ has two faces

fixed x

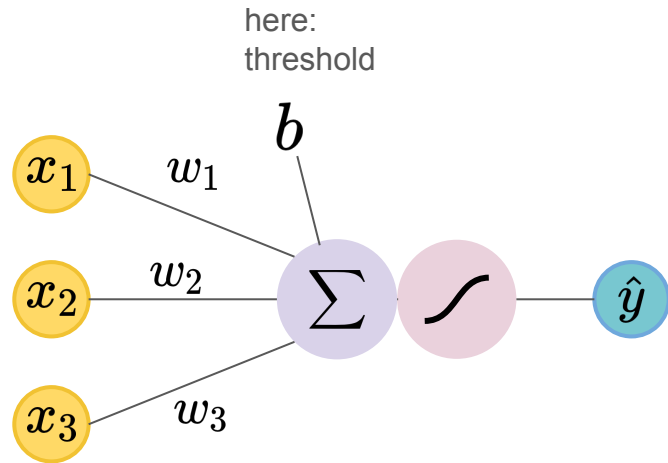
Evaluation function

$$\Phi_x : \mathbb{R}^d \rightarrow \mathbb{R}^n$$

Training function

$$\Phi_\theta : \mathbb{R}^{|\theta|} \rightarrow \mathbb{R}^n$$

Non-Linearities: Activation Functions

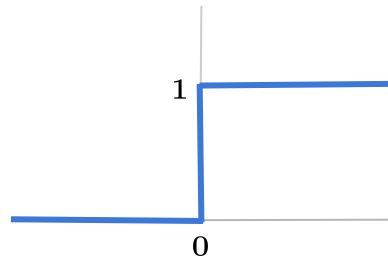


Biological motivation:

activate neuron if threshold b is exceeded

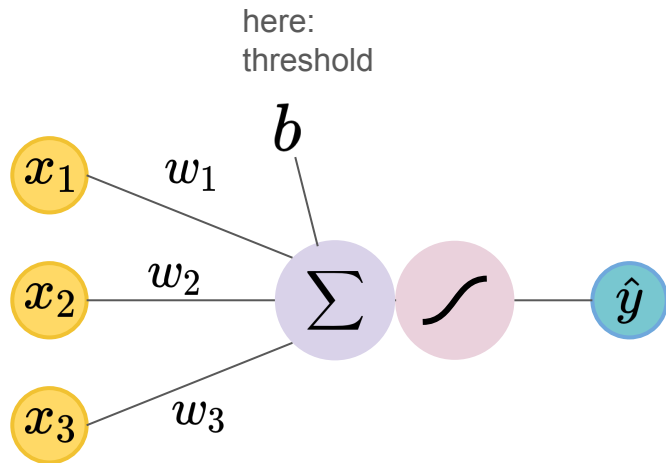
$$\sum_{i=1}^3 w_i \cdot x_i > b \longrightarrow 1 \quad \text{activate!}$$

$$\sum_{i=1}^3 w_i \cdot x_i \leq b \longrightarrow 0 \quad \text{discard!}$$

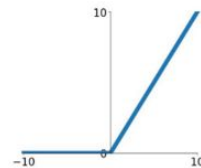


Heaviside (step) function

Non-Linearities: Activation Functions

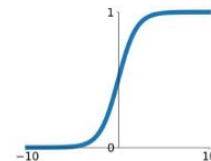


ReLU
 $\max(0, x)$



the “default”

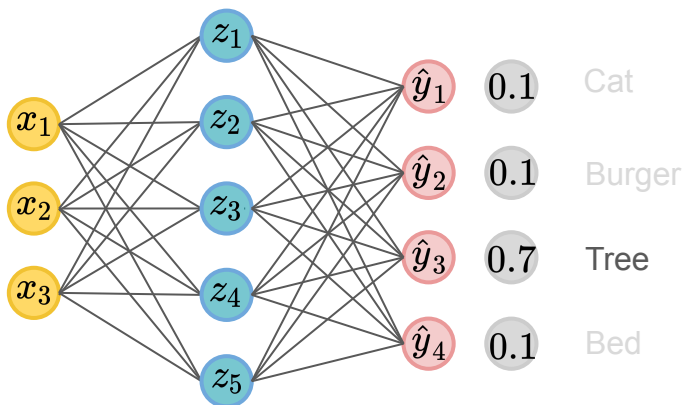
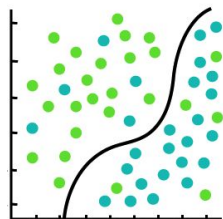
Sigmoid
 $\sigma(x) = \frac{1}{1+e^{-x}}$



output within $[0, 1]$

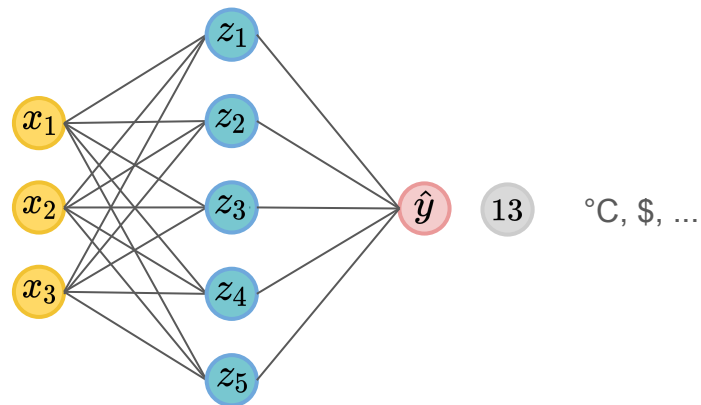
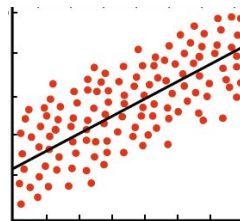
Supervised Learning Tasks

Classification



$\hat{y}_i \in [0, 1] \rightarrow$ probability distribution (soft-max)

Regression



predict the value directly

“Expressive Power”

What can a neural network learn?

“Expressive Power”

What can a neural network learn?

anything

“Expressive Power”

What can a neural network learn?

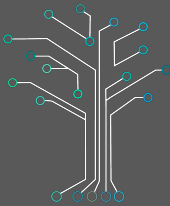
“anything”

Universal Approximation Theorem

“Neural networks with a non-polynomial activation function can approximate any continuous function arbitrary well”

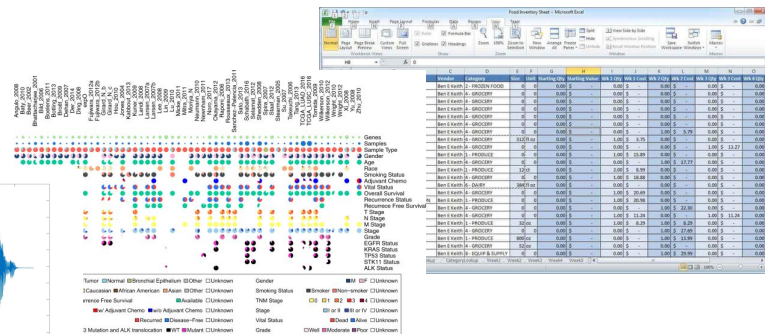
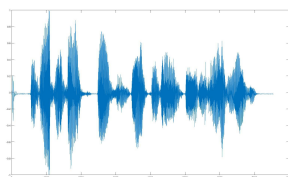
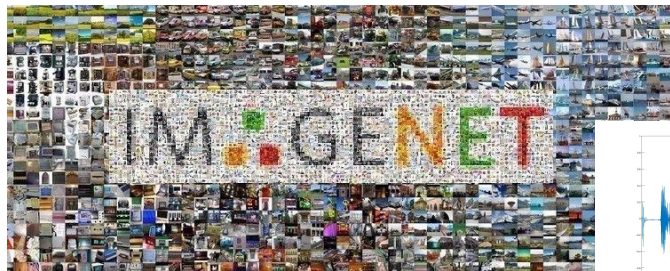
For any continuous f there is $\theta^\#$ st. $\|\Phi(x; \theta^\#) - f(x)\| < \varepsilon$

Data



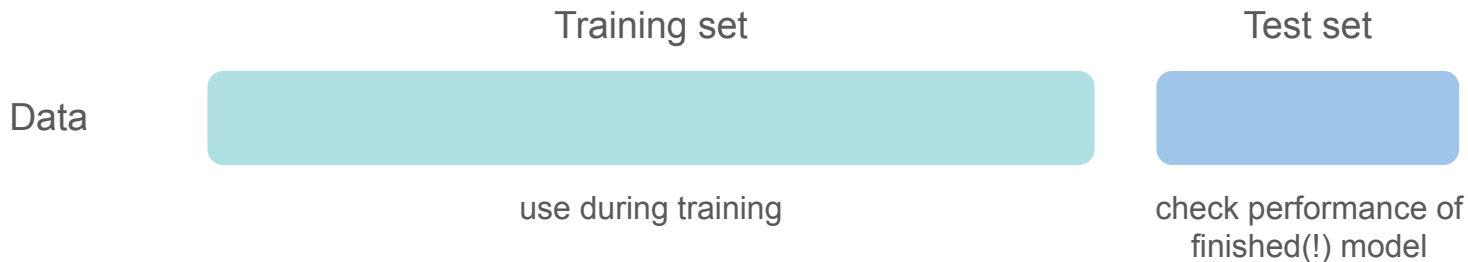
What is a dataset?

- An organized collection of data
 - One “unit” of data = an instance / data point
 - Information about a data point = *Features*
 - Labels or other annotations often included
 - Required for supervised tasks but not (necessarily) for unsupervised
 - Normalize it: $[0, 1]$, $[-1, 1]$, $[0, 256]$, $(x(k) - \mu) / \sigma$

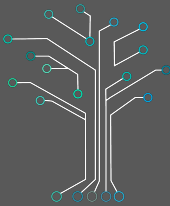


Properties of a (good) dataset

- What about dataset size...?
 - Defined entirely by the task (from dozens/hundreds to millions)
 - Only certainty is that “the more the merrier”, but also “the more representative the merrier”
- Do not forget: the **data split** (~80/20%)



Training



Training

Supervised learning:

Given samples of training data with corresponding labels (x, y)



camel



cat



Pikachu

input x (matrix with values)

label y (binary vector with a 1 at the correct class)

0 camel

0 cat

1 Pikachu

Goal: Optimize the weights such that

$\Phi(\text{cat image}) = \text{cat}$ for all of the samples in the training data.

but also

$\Phi(\text{cat image}) = \text{cat}$ for samples outside!

Training

How to achieve this goal?


Loss function (*error, cost*) $\mathcal{L}(\hat{y}, y)$: how good is prediction \hat{y} compared to the true label y

- Zero-one loss: $\mathcal{L}_{0-1}(\hat{y}, y) = 1$ if $\hat{y} \neq y$ and 0 else - *Is it exactly the same or not?*
- Square loss (L2): $\mathcal{L}_{sq}(\hat{y}, y) = \|\hat{y} - y\|^2$ - *Euclidean distance*
- Cross entropy loss: $\mathcal{L}_{ce}(\hat{y}, y) = -(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}))$ - *maximize likelihood*

→ **minimizing the loss function will improve the prediction!**

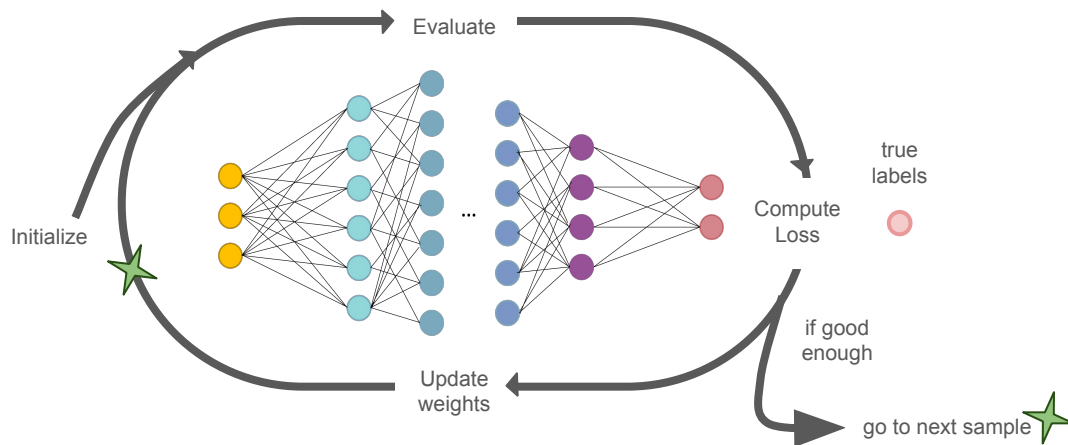
Training

Idea: Start with random weights

- 1) Take a sample  and measure good bad the prediction is: $\Phi(\text{cat}) = \text{Pikachu}$
- 2) Update the weights to improve the prediction (i.e., loss decreases): $\Phi(\text{cat}) = \text{cat}$



Repeat the process for every sample in the training data set.



Training

GOAL: find a weight update rule that produces a sequence that gradually decreases the loss.

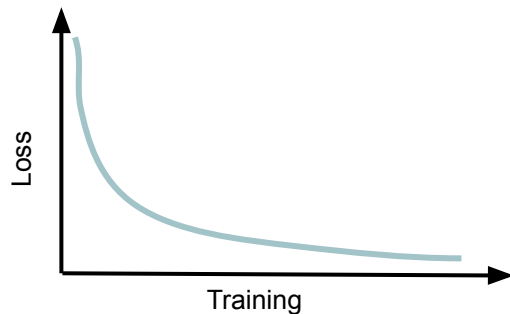
$(\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \dots, \theta^{(k)})$ such that $\mathcal{L}(\Phi(x; \theta^{(0)}), y) \geq \mathcal{L}(\Phi(x; \theta^{(1)}), y) \geq \mathcal{L}(\Phi(x; \theta^{(2)}), y) \geq \dots \geq \mathcal{L}(\Phi(x; \theta^{(k)}), y)$

As training progresses, later weights should result in smaller losses.

And do it over the whole training set:

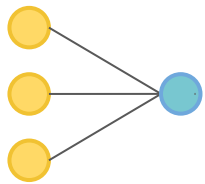
$$\theta^\# := \arg \min_{\theta} \frac{1}{K} \sum_{k=1}^K \mathcal{L}(\Phi(x_{(k)}; \theta), y_{(k)})$$

Find the weights which result in minimal loss over the whole training set.



→ **non-linear, non-convex optimization problem!**

Special Case: Linear Perceptron

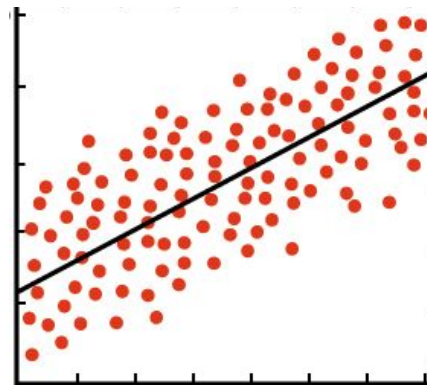


$$\hat{y} = \Phi(x) = w^T x = w_1 x_1 + w_2 x_2 + \dots + w_n x_n$$

Loss $\mathcal{L}_{sq}(\hat{y}, y) = \|\hat{y} - y\|^2$

Least squares problem!

→ Linear Regression!



Weight Updates: A simple optimization technique

Gradient Descent

Gradient of the loss: “how does the loss change, if a weight changes?”

$$\nabla L(w_1, \dots, w_n) = \begin{bmatrix} \frac{\partial L}{\partial w_1} \\ \vdots \\ \frac{\partial L}{\partial w_n} \end{bmatrix}$$

→ points to **steepest ascent** (i.e., the direction to change the weights, so that there is maximal change in the loss)

Weight Updates: A simple optimization technique

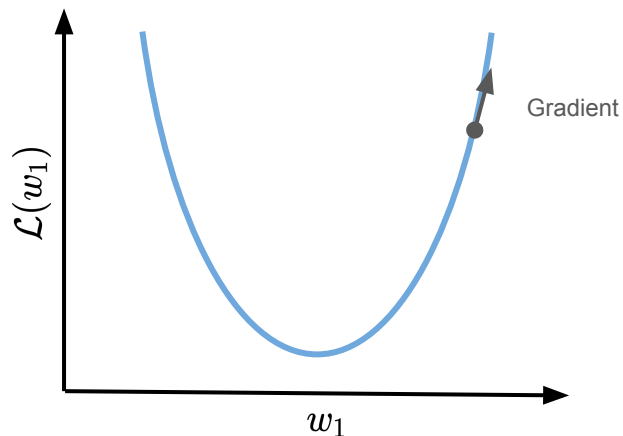
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$n = 1$



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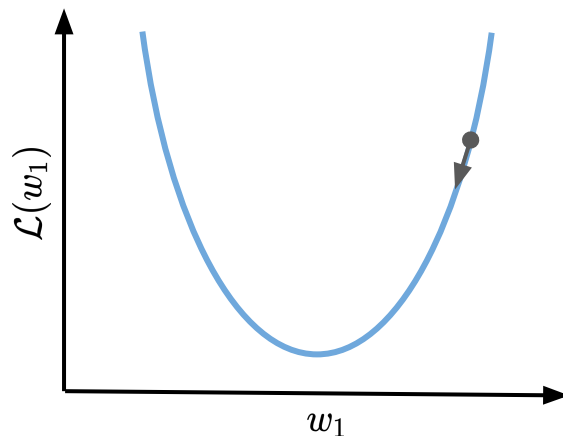
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go opposite direction of steepest ascent

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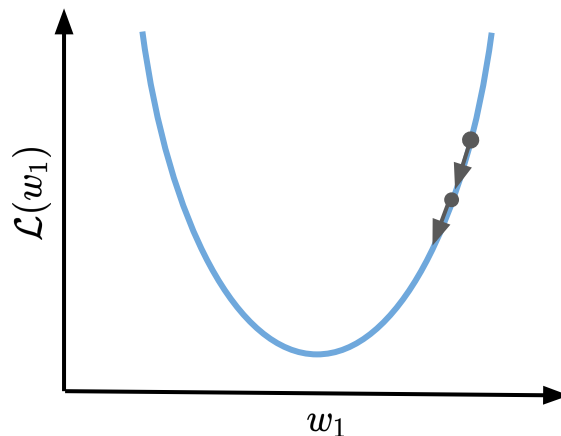
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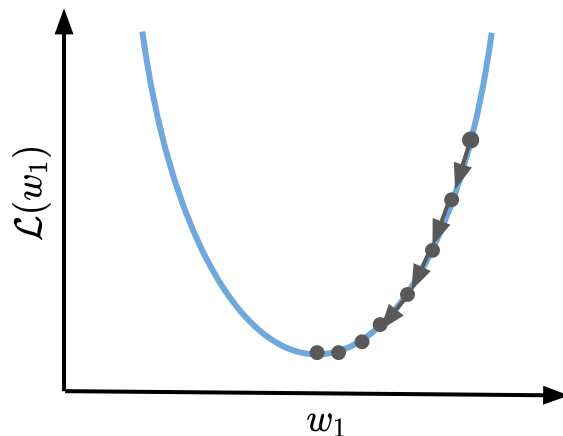
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$$w_1^{new} \leftarrow w_1^{old} - \eta \cdot \nabla \mathcal{L}(w_1^{old})$$

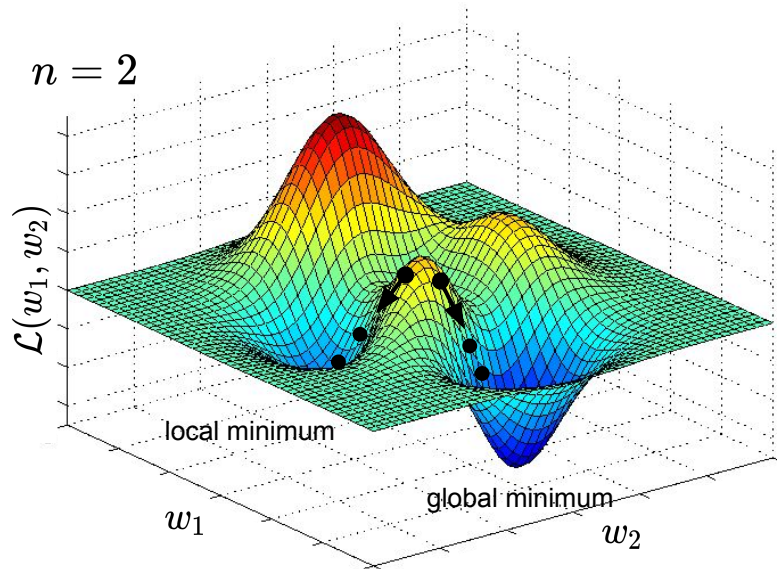
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→ points to **steepest ascent**



go opposite direction of steepest ascent

$$w_1^{new} \leftarrow w_1^{old} - \eta \cdot \nabla \mathcal{L}(w_1^{old}, w_2^{old})$$

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Weight Updates: A simple optimization technique

Gradient Descent

Gradient of the loss:

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→ points to **steepest ascent**

Algorithm

Initialize $\theta^{(0)}, \eta > 0$

Until convergence:

Compute gradient $\nabla \mathcal{L}(\theta^{(n)})$

Update weights $\theta^{n+1} \leftarrow \theta^n - \eta \cdot \nabla \mathcal{L}(\theta^{(n)})$

Return weights

“learning rate”

Training on Batches

Gradient descent is very expensive...

Example: A single step of gradient descent for AlexNet (neural network $\sim 160\text{M}$ parameters) on ImageNet (dataset $\sim 1.2\text{M}$ images) requires $\sim 2 \cdot 10^{14}$ flops!

Training on Batches

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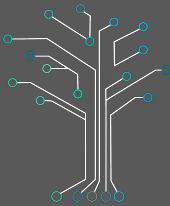
Example: A single step of gradient descent for AlexNet (neural network ~160M parameters) on ImageNet (dataset ~1.2M images) requires $\sim 2 \cdot 10^{14}$ flops!

Train on small batches of the dataset!

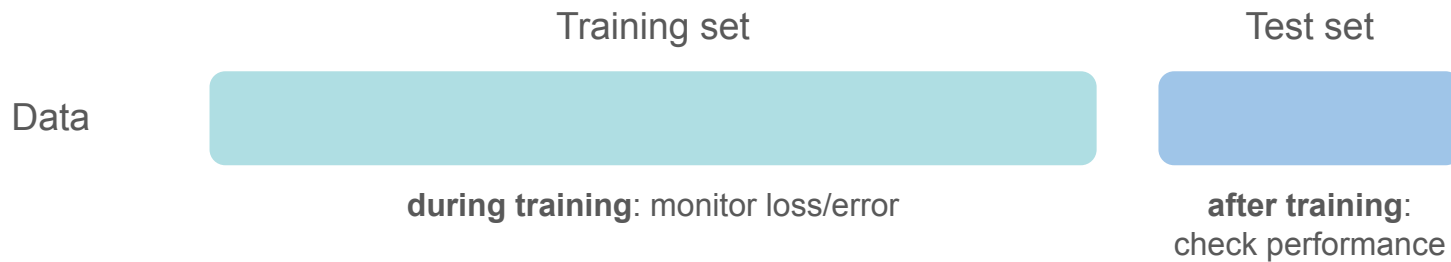
“Training with large minibatches is bad for your health. More importantly, it’s bad for your test error. Friends don’t let friends use minibatches larger than 32.”

-Yann LeCun

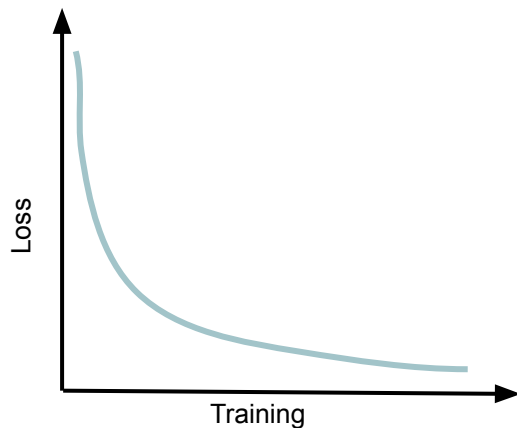
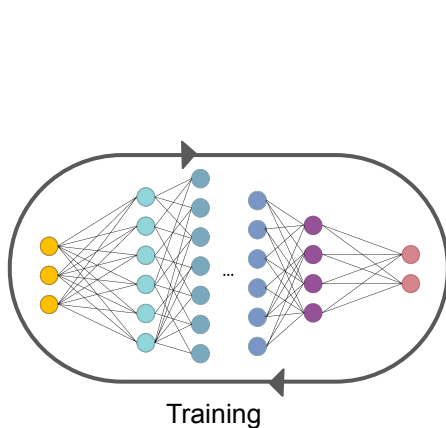
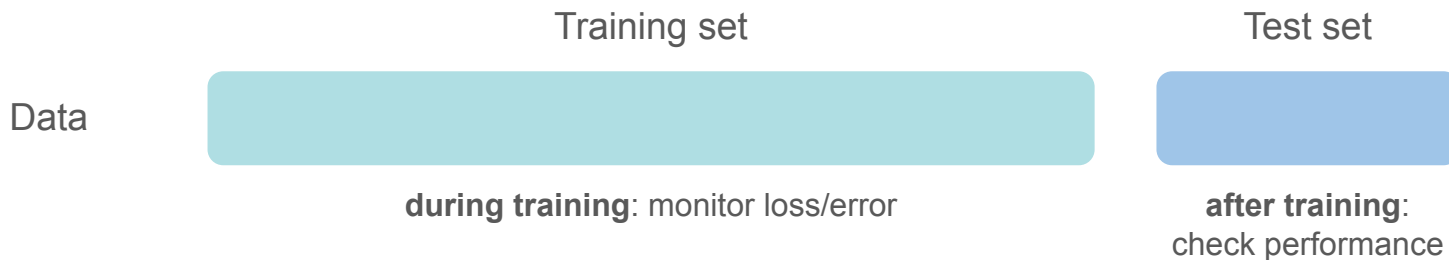
Evaluation



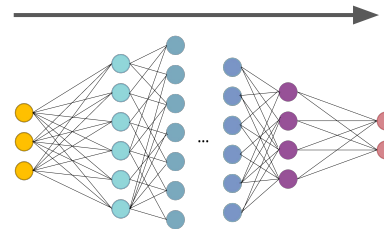
Training-Test



Training-Test



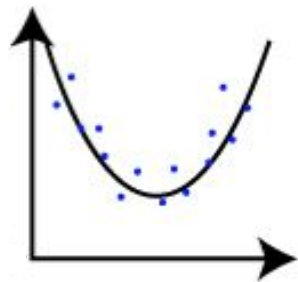
Evaluate on unseen data



Bias-Variance Tradeoff

Over- and underfitting

Example:
Learn a second-degree
polynomial from noisy
observations

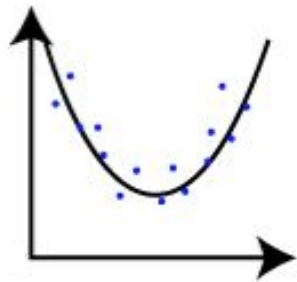


ground truth
deg = 2

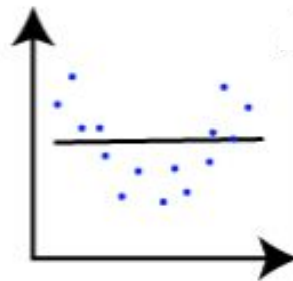
Bias-Variance Tradeoff

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underfitting
deg too low

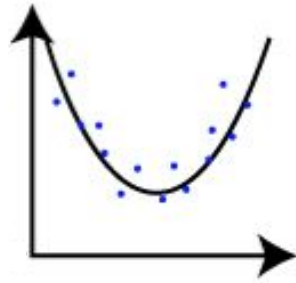
Simple model:

high bias,
good capturing of essentials,
bad fit

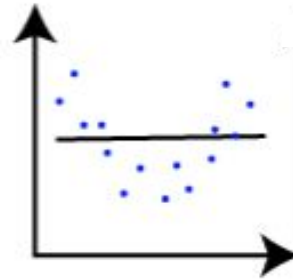
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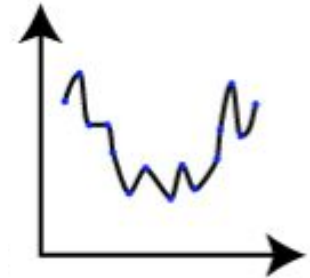
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ground truth
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underfitting
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overfitting
deg too high

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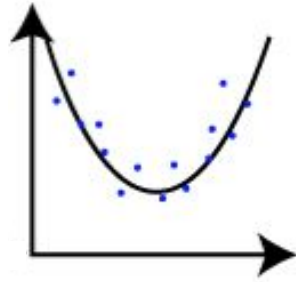
Complex model:

high variance,
good fit to data,
too specific

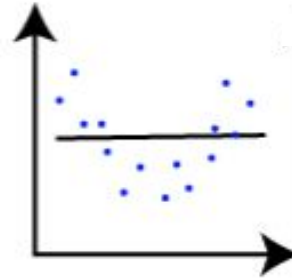
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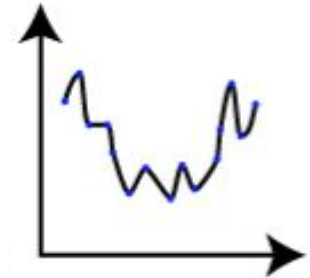
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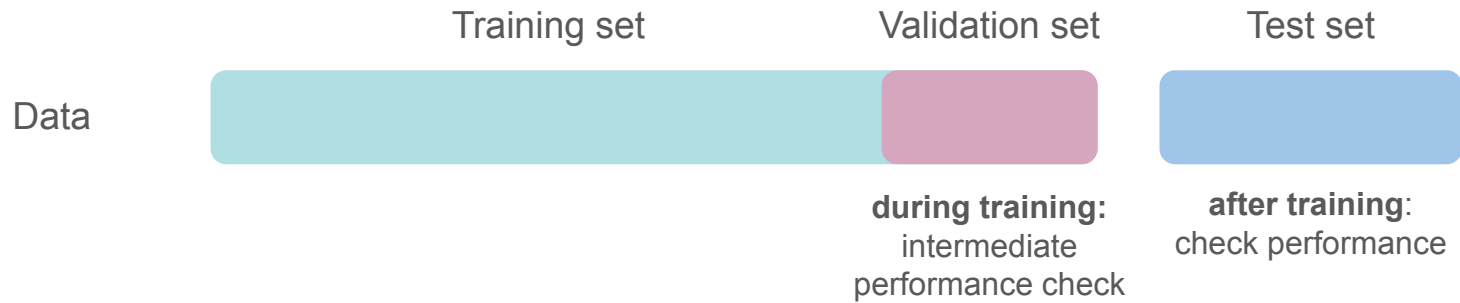
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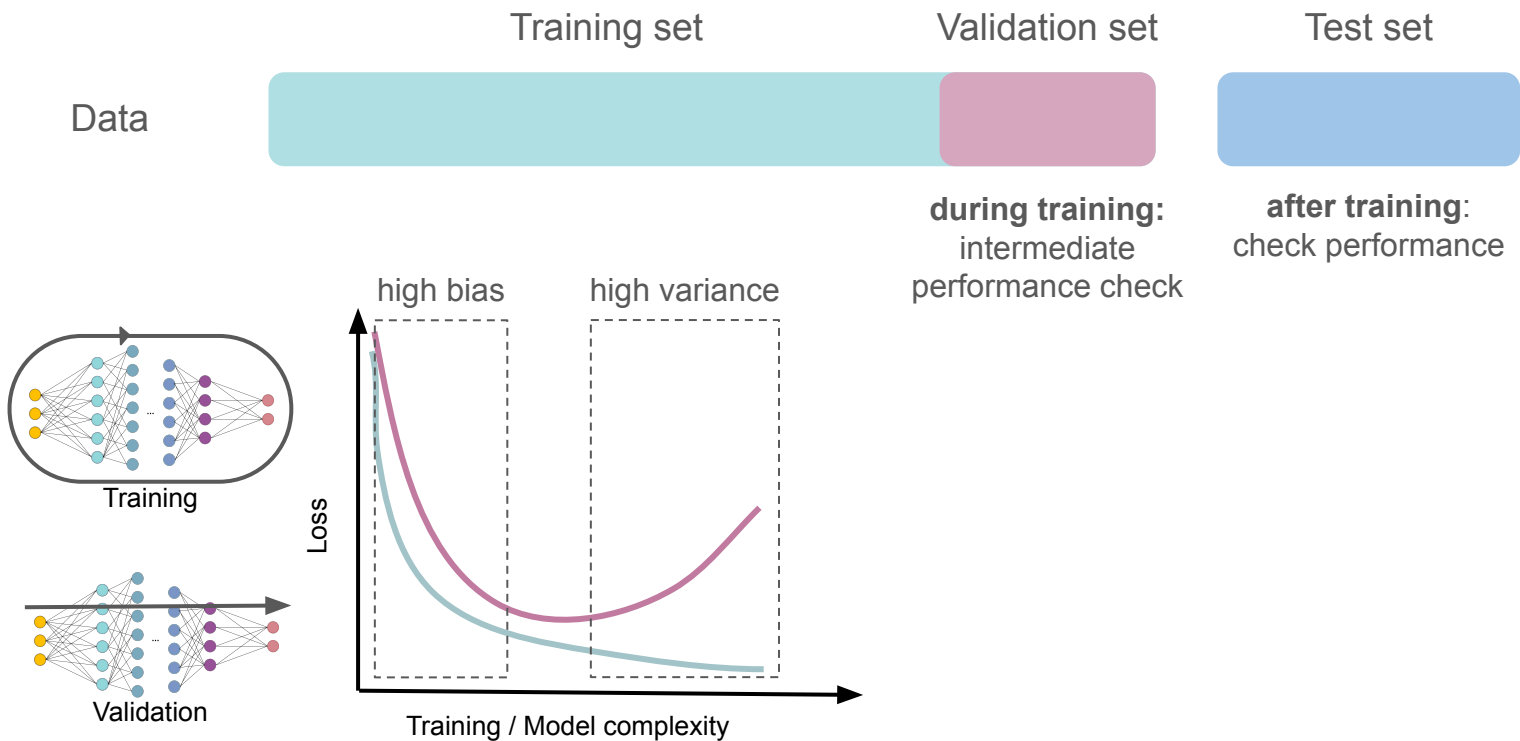


Trade-off between
model assumptions (bias) and
model complexity (variance)

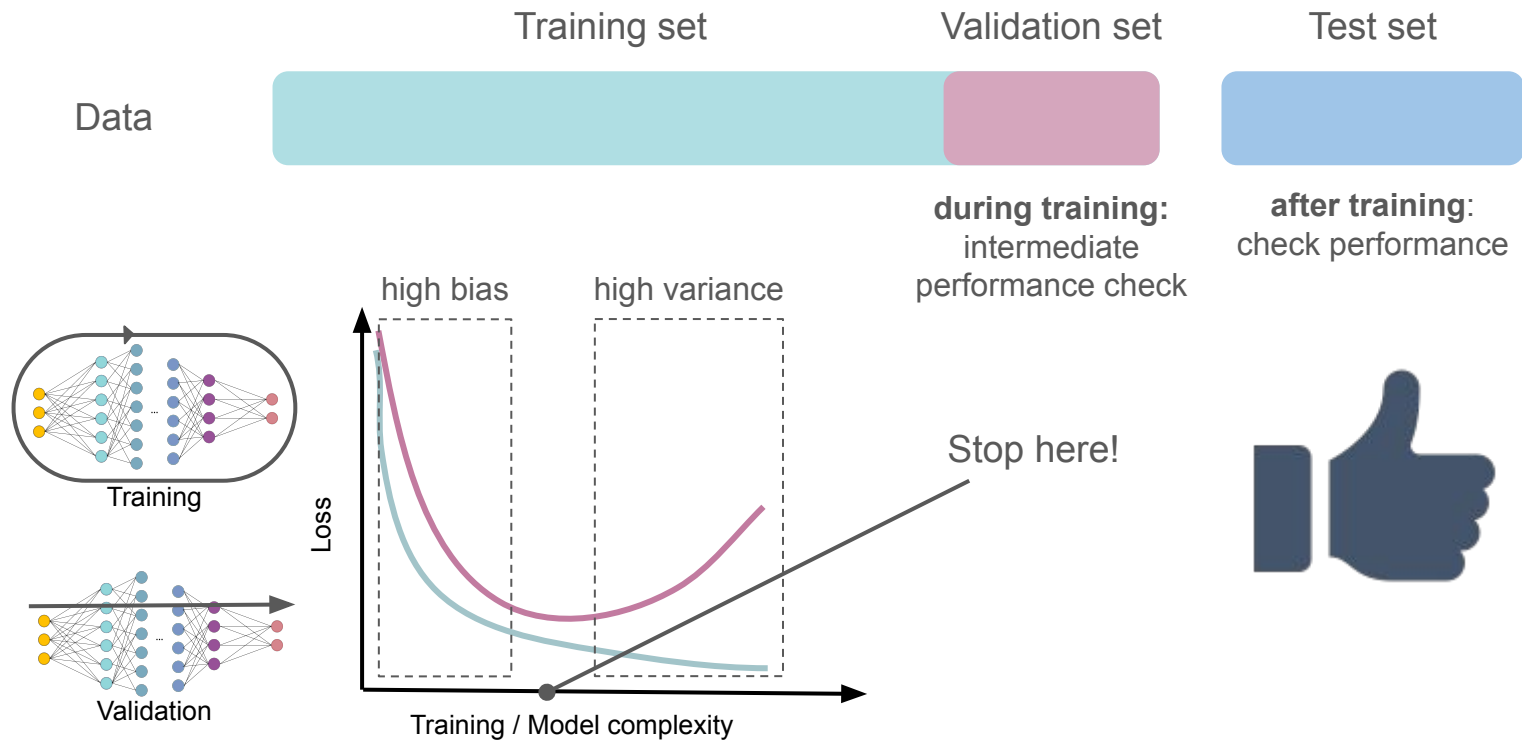
Training-Validation-Test



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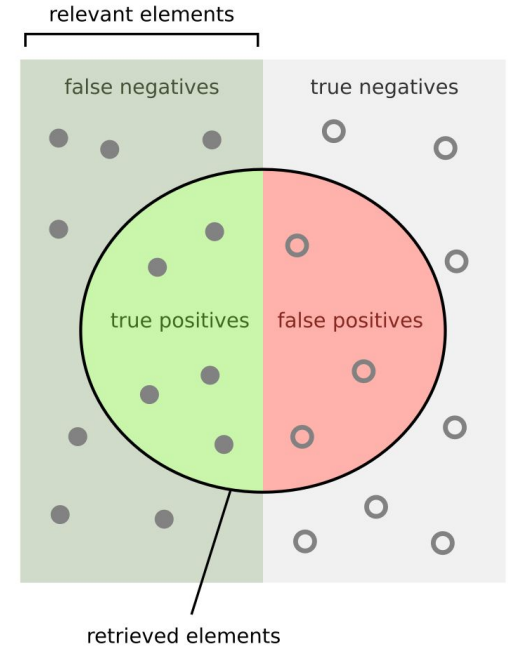
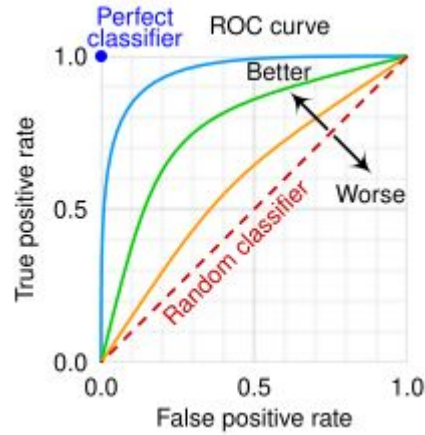
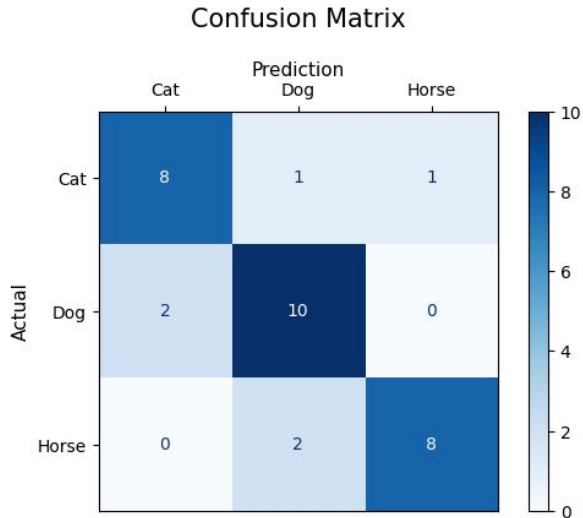


Metrics of performance


- Defined by the task: MSE, accuracy, mAP, etc...

$$\text{accuracy} = \frac{\text{number of correct predictions}}{\text{total number of predictions}}$$


- In case of **classification**:



How many retrieved items are relevant?

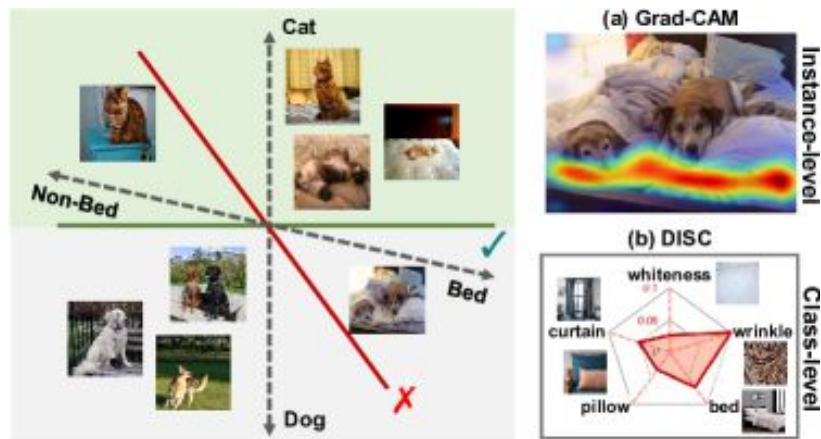
$$\text{Precision} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$


How many relevant items are retrieved?

$$\text{Recall} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$


Interpretability

- XAI: steering away from the black box
- Crucial in high-responsibility decision making, e.g. medicine
- **TOOLS:** explainable architecture, post-hoc analysis, etc.

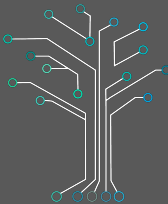


Bias

- Mitigating bias
 - Especially important in decision making with a social effect (e.g., granting parole [1])
- **TOOLS:** metrics to assess group fairness (demographic parity, equalized odds, etc.), transparency about biases in the data collection process...

| | WHITE | AFRICAN AMERICAN |
|---|-------|------------------|
| Labeled Higher Risk, But Didn't Re-Offend | 23.5% | 44.9% |
| Labeled Lower Risk, Yet Did Re-Offend | 47.7% | 28.0% |

Design and Techniques



Common Techniques

Regularizing:

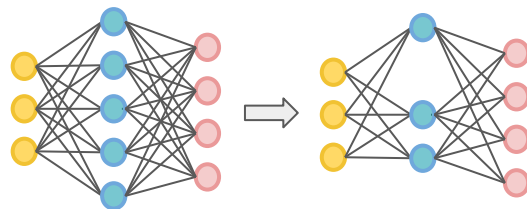
$$\min_{\theta} \mathcal{L}(\theta) + \lambda \cdot r(\theta)$$

regularization
term of the
network weights

...often $r(\theta) = \|\theta\|^p$

Dropout:

set weights to zero at random



Stochastic Gradient Descent (SGD):

use the gradient of a randomly selected subset

Batch normalization:

normalize the samples w.r.t. to the other samples in the batch

Popular architectures

Convolutional neural networks: apply “filters” to extract spatial features, textures, patterns, etc.

- Popular choice in image processing.
- Examples: VGG-16, VGG-19, AlexNet, etc.

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Transformers: capture relationships in sequential data by considering the whole context.

- Useful in applications with sequential data (e.g., text), but also otherwise (vision transformers).
- Examples: GPTs, BERT, ViT, DINOv2

Today's Program

Part I: Introduction lecture

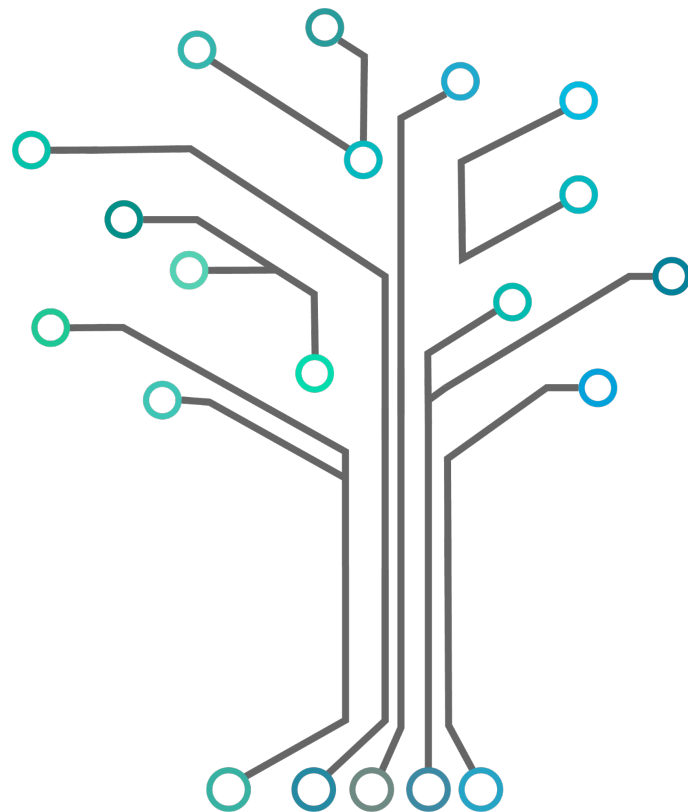
14:15 - 15:45

- Overview
- Theoretical Basics
- Data
- Training
- Evaluation
- Design and Techniques

Part II: Hands-on

16:15 - 18:00

- Questions
- Setup
- Some coding





ÖAW

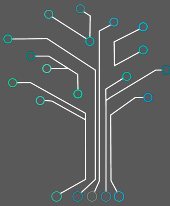
ÖSTERREICHISCHE
AKADEMIE DER
WISSENSCHAFTEN

AI

WinterSchool

January 20 - 24, 2025

Exercises



Exercises

Using Google Colab and PyTorch.

Open the notebook **Intro_WS_2025.ipynb**.

Follow the instructions in the notebook.

