Deep learning

Lecture 1

Marleen Balvert

The course - content

- Theoretical understanding of deep neural networks
- Build and use your own networks in Tensorflow
- Applications

The course - setup

- Seven lectures
- One tutorial (week 3)
- Two assignments (25% each)
  - Assignment 1: start week 3, deadline week 5
  - Assignment 2: start week 5, deadline week 7
- One final exam (50%)

Literature

- Intuitive explanation to deep learning:

http://neuralnetworksanddeeplearning.com

- Technical explanation to deep learning:

https://www.deeplearningbook.org/

Your background

Today

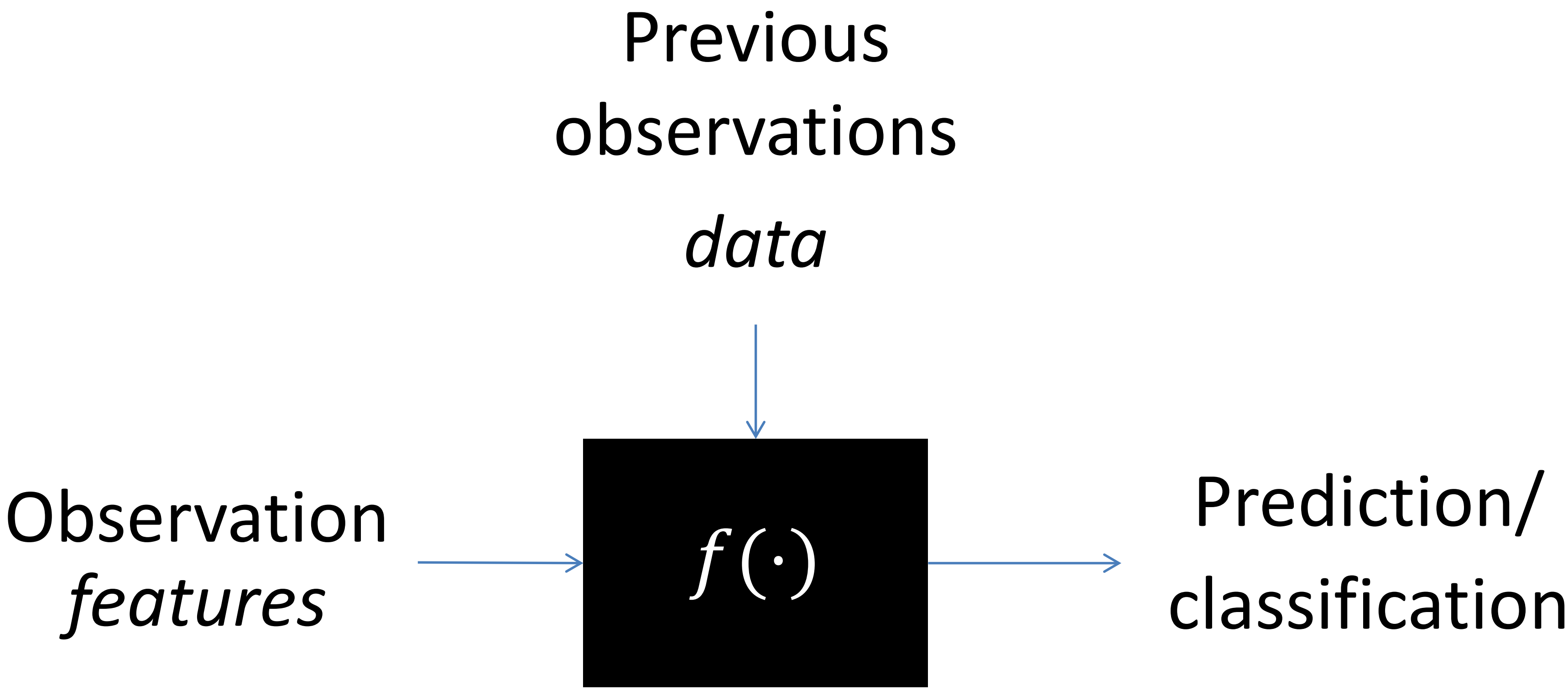
- What is machine learning?
- What is a perceptron?
- What is a (deep) neural network?
- Why use deep neural networks, and when not to use them?
- What is underfitting, overfitting and capacity?
- How to train your model and optimize hyperparameters?
- How to use regularization to prevent overfitting?

What is machine learning?

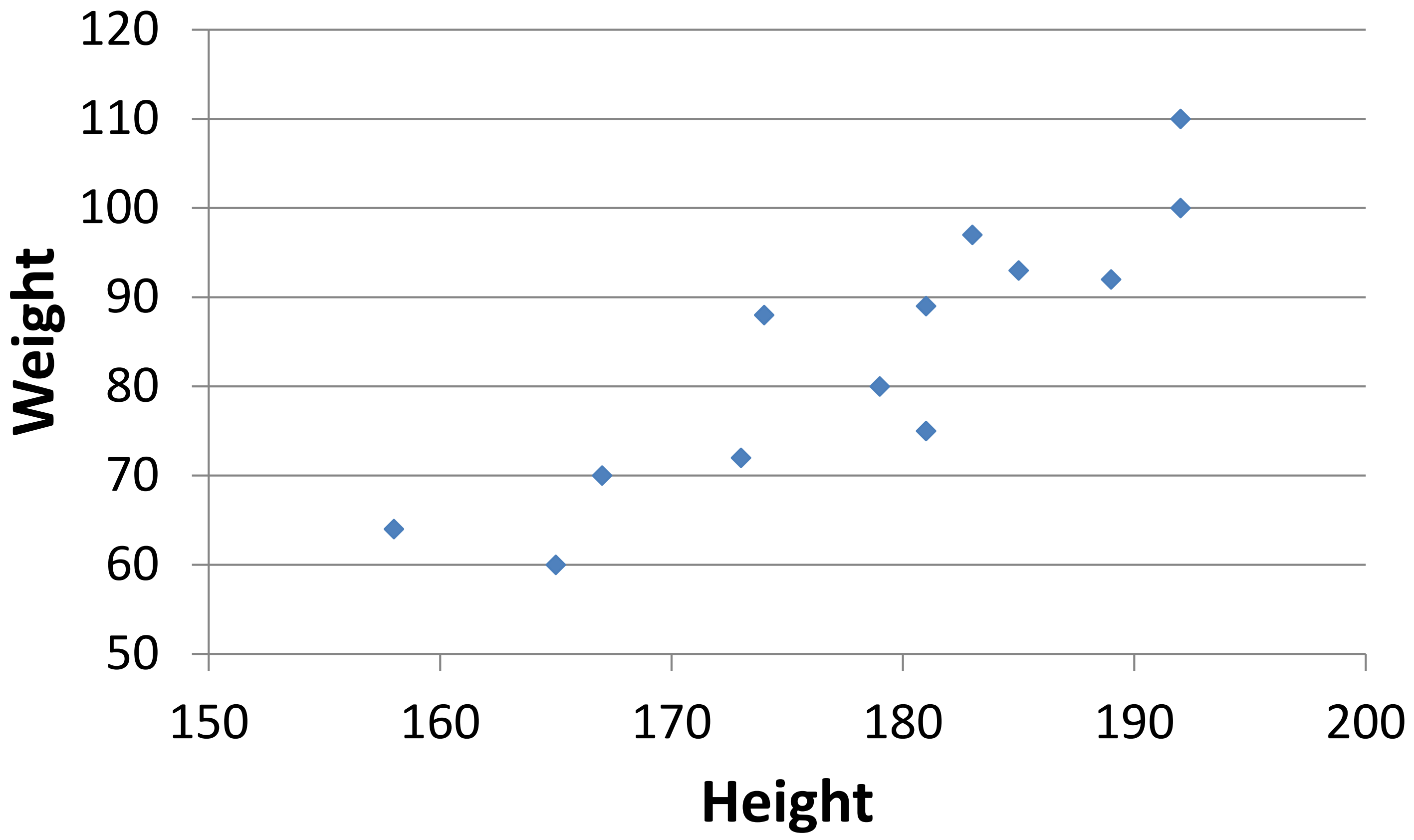
- Train a machine to learn the relationship between pre-defined *input* or *independent* variables and a chosen *output* or *dependent* variable

- Train a machine to *predict* an *output* or *dependent* variable from *input* or *independent* variables based on data

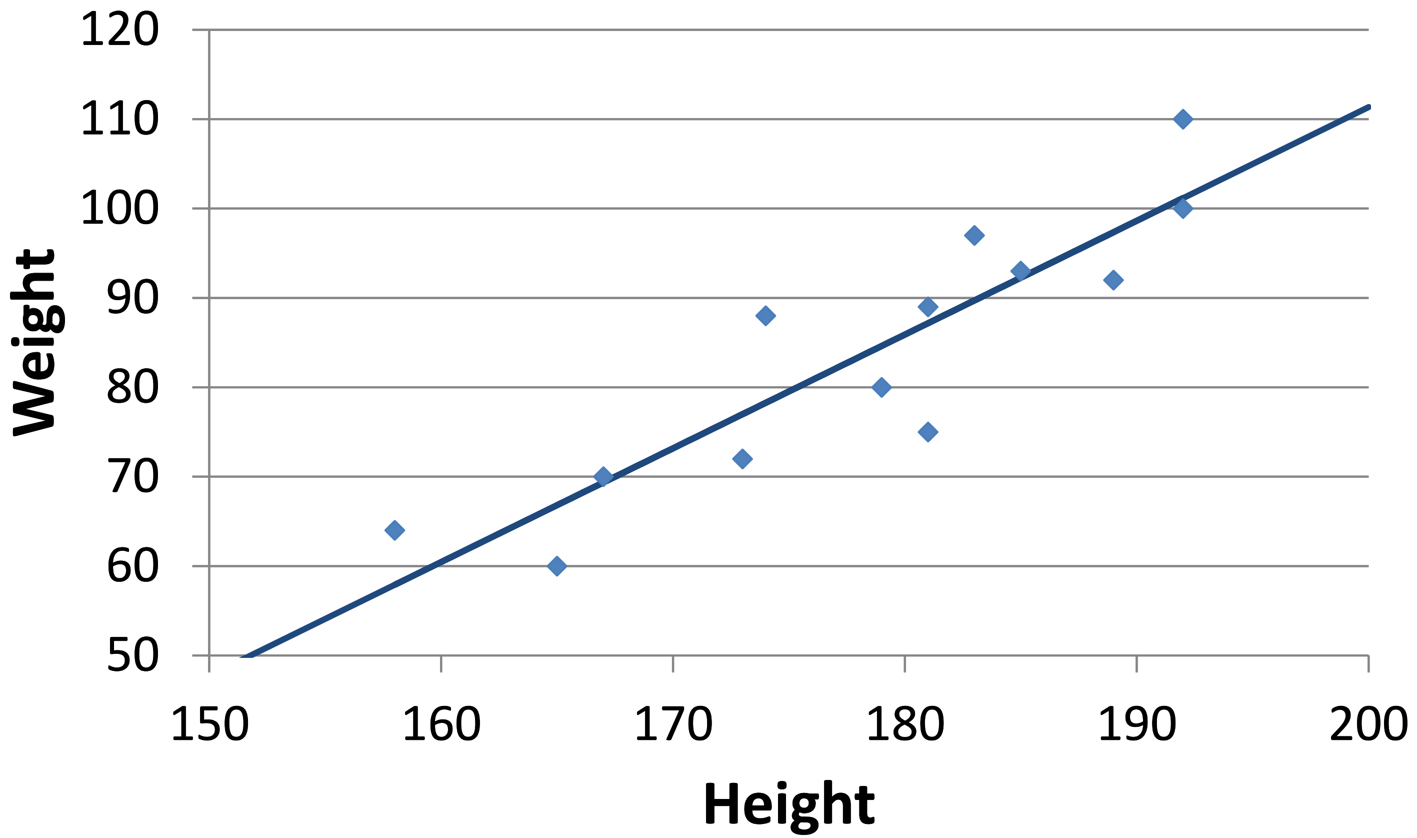
What is machine learning?



Example – regression

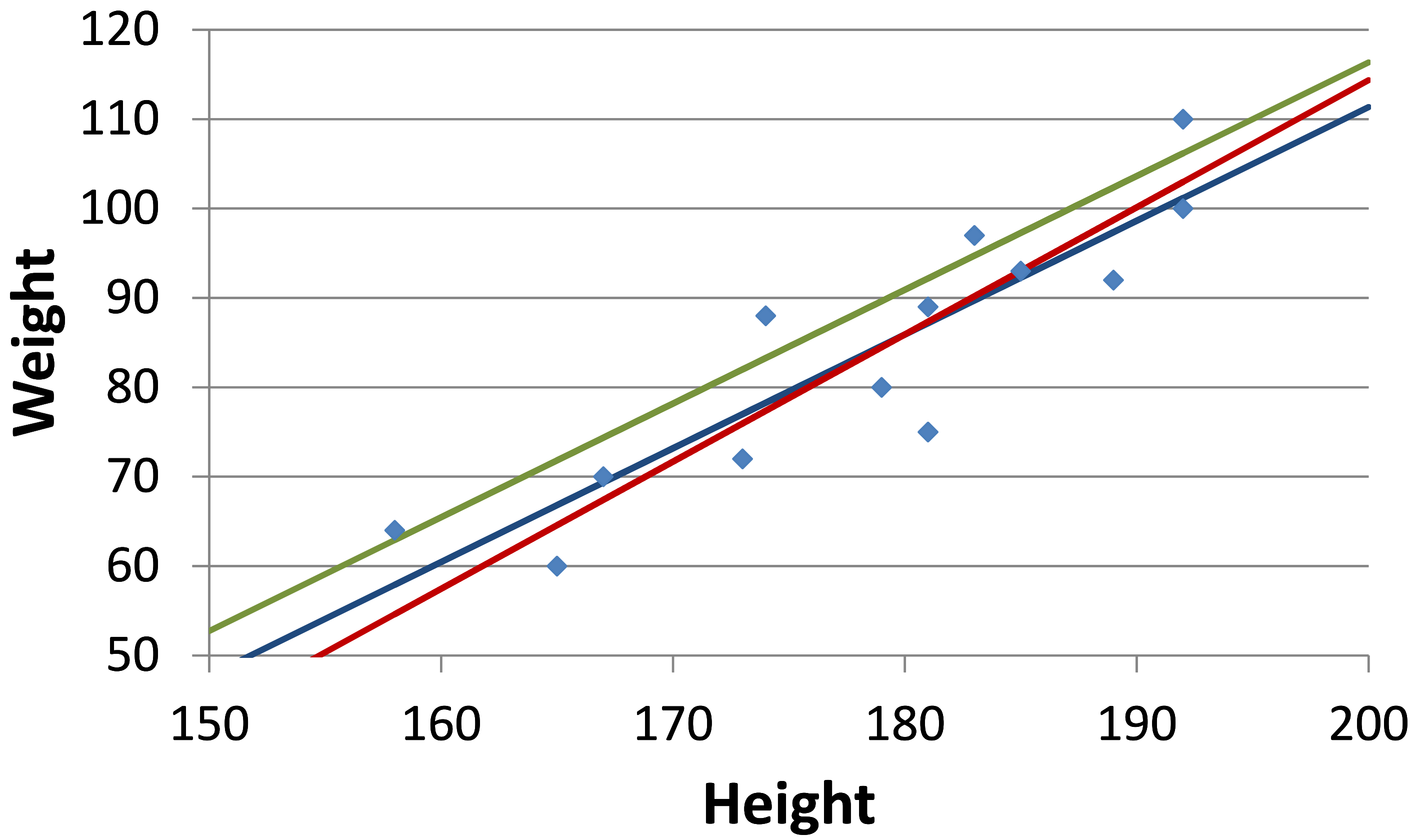


Example – regression



$$\hat{y} = w_0 + w_1 x$$

Example – regression



$$\hat{y} = w_0 + w_1 x$$

Parameter optimization

- Need a performance measure $P(w, x, y)$

$$MSE(w, x, y) = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i(w, x_i) - y_i)^2$$

$$MAD(w, x, y) = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i(w, x_i) - y_i|$$

- Solve $\min_w MSE(w, x, y)$ or $\min_w MAD(w, x, y)$

What is machine learning?

Previous observations

data (x,y)

Learn model parameters w from data

Observation

features (x)

$f(w,x)$

Prediction/
Classification

output (y)

Machine learning tasks

- Regression ($f\colon \mathbb{R}^n \to \mathbb{R}$)
- Classification ($f\colon \mathbb{R}^n \to \{0, \ldots, k\}$)
- Density estimation $p(y|x)$
- Imputation of missing values
- Denoising
- Density estimation $p(x)$
- …

Supervised
(with label)

Unsupervised
(without label)

Machine learning methods

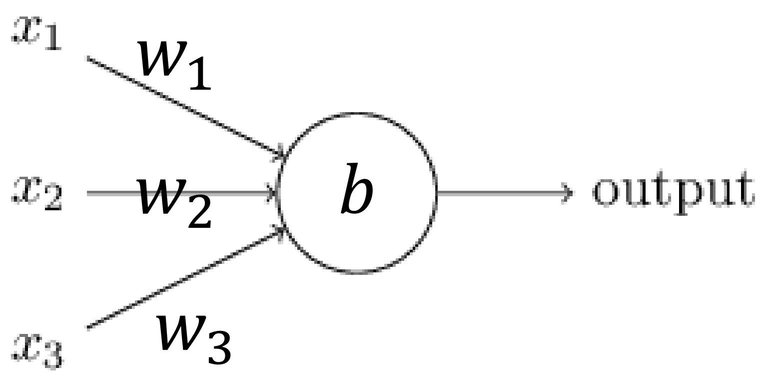
- (Logistic) regression
- Nearest neighbor classification
- Support vector machines
- Decision trees & random forest
- (Deep) neural networks
  - Feedforward neural networks
  - Convolutional neural networks
  - ...
- …

Supervised learning steps

1. Collect data
2. Choose model
3. Optimize parameters
4. Predict for new observations

(Deep) neural networks

Perceptron



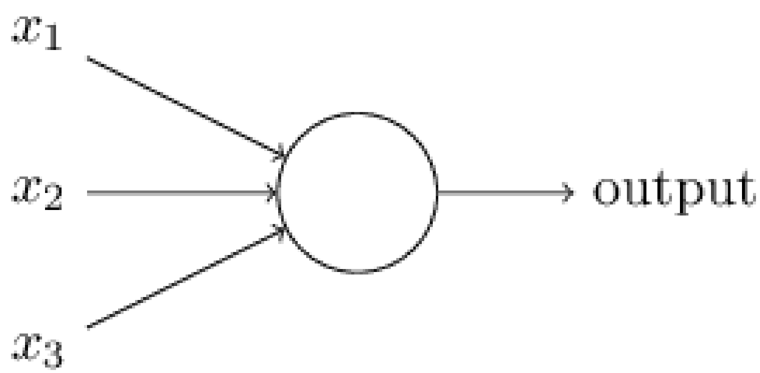
$$\text{output} = \begin{cases} 0 & \text{if } w^T x + b < 0 \\ 1 & \text{if } w^T x + b \geq 0 \end{cases}$$

weights

biases (thresholds)

Perceptron - example

Decision making: shall I go to the festival?

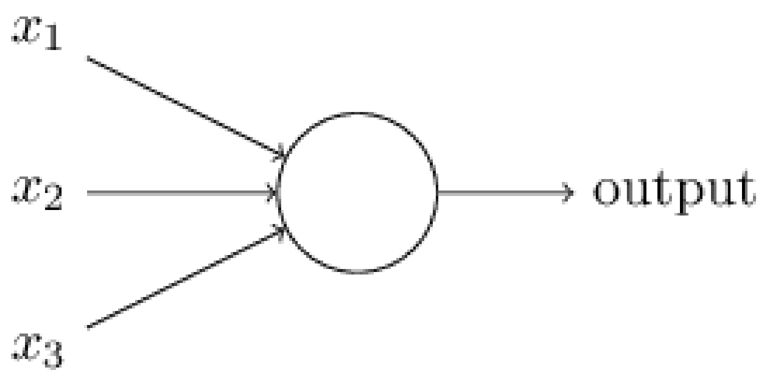


- x_1= is it not raining?
- x_2= are my friends going?
- x_3= is the festival within biking distance?

I go to the festival if and only if it is not raining.

Perceptron - example

Decision making: shall I go to the festival?

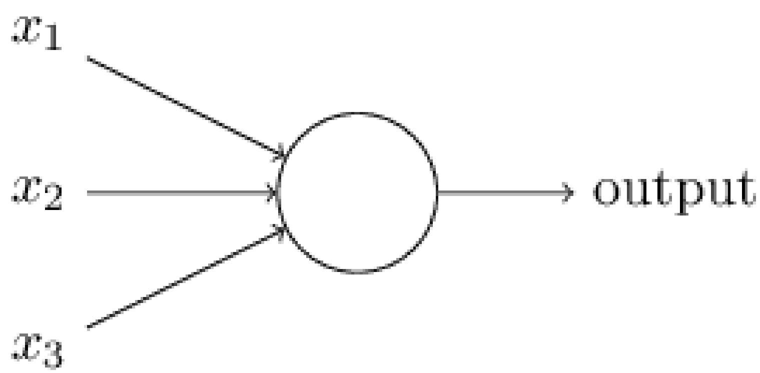


- x_1= is it not raining?
- x_2= are my friends going?
- x_3= is the festival within biking distance?

I go to the festival if it is not raining, OR (if my friends are going AND it is within biking distance)

Perceptron - example

Decision making: shall I go to the festival?

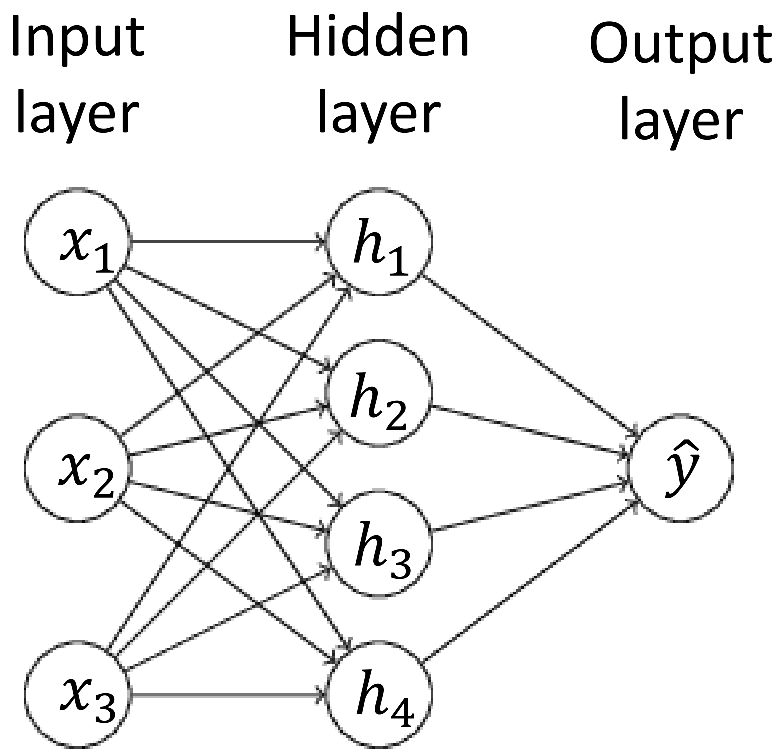


- x_1= is it not raining?
- x_2= are my friends going?
- x_3= is the festival within biking distance?

If $x_1 = 1 \vee (x_2 = 1 \wedge x_3 = 1)$ then y = 1, 0 otherwise

Perceptrons can learn AND and OR

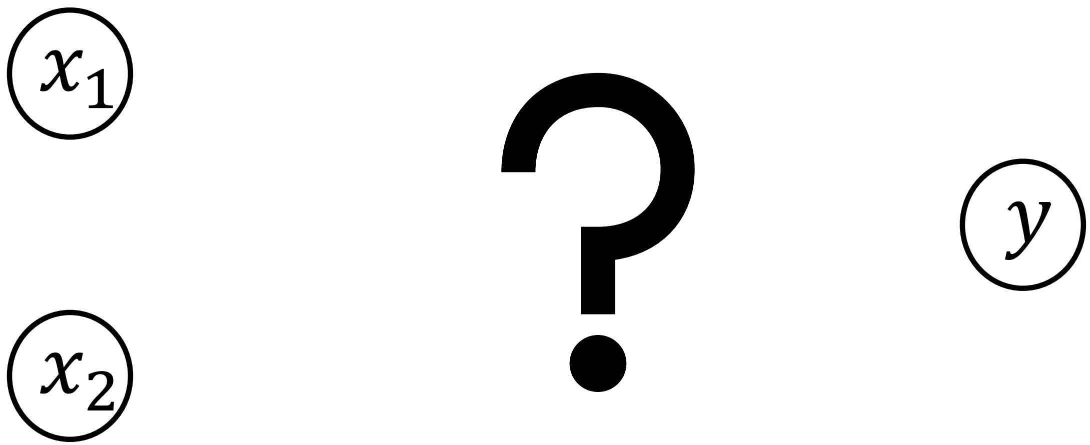
Neural network (NN)



$$h_i = \begin{cases} 1 & if\ w_i^T x + b_i \geq 0 \\ 0 & if\ w_i^T x + b_i < 0 \end{cases}$$

$$\hat{y} = \begin{cases} 1 & if\ w_5^T h + b_5 \geq 0 \\ 0 & if\ w_5^T h + b_5 < 0 \end{cases}$$

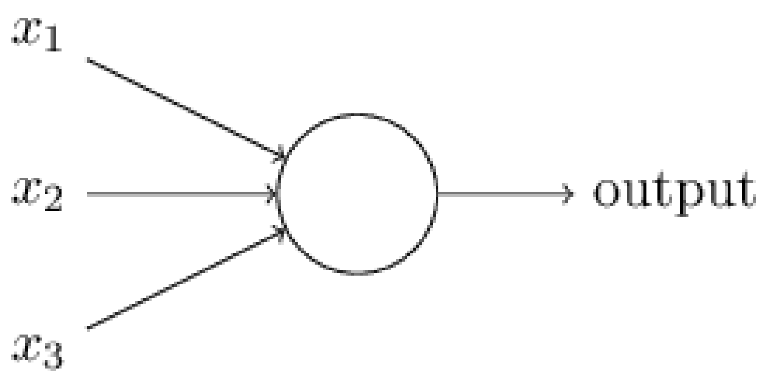
Can we learn XOR?



If $x_1 = 1$ XOR $x_2 = 1$ then $y = 1$

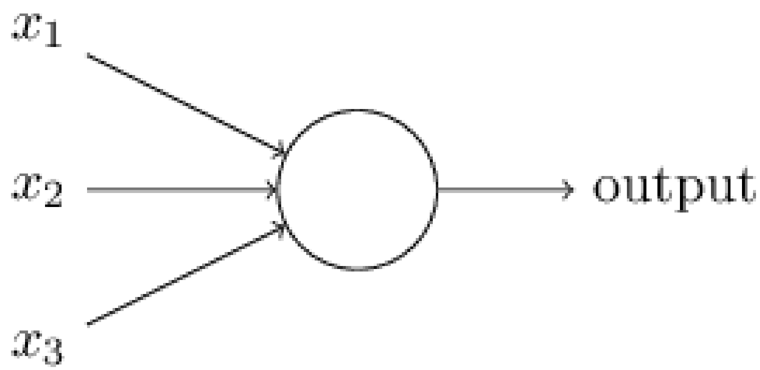
If $(x_1 = 1$ OR $x_2 = 1)$ AND NOT $(x_1 = 1$ AND $x_2 = 1)$ then $\hat{y} = 1$

Activation function: sigmoid



$$\text{output} = \begin{cases} 0 & \text{if } w^T x + b < 0 \\ 1 & \text{if } w^T x + b \geq 0 \end{cases}$$

Activation function: sigmoid

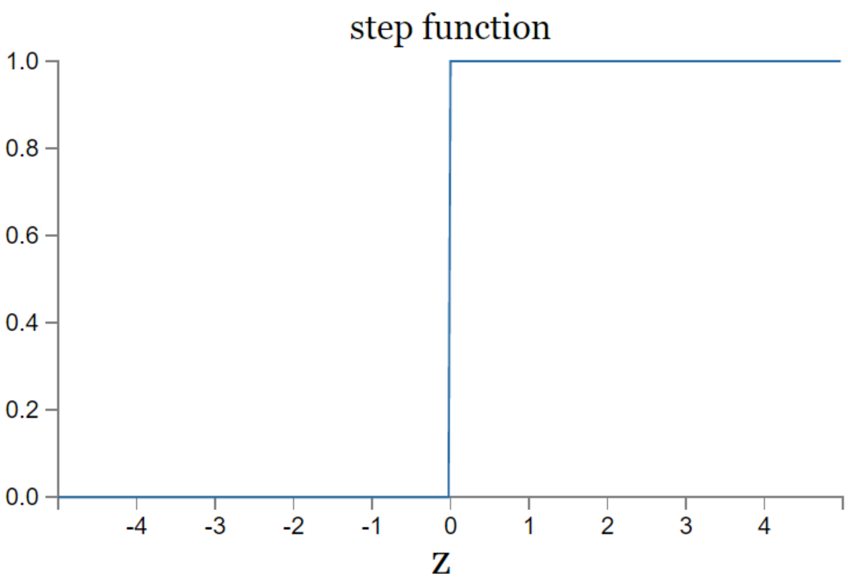


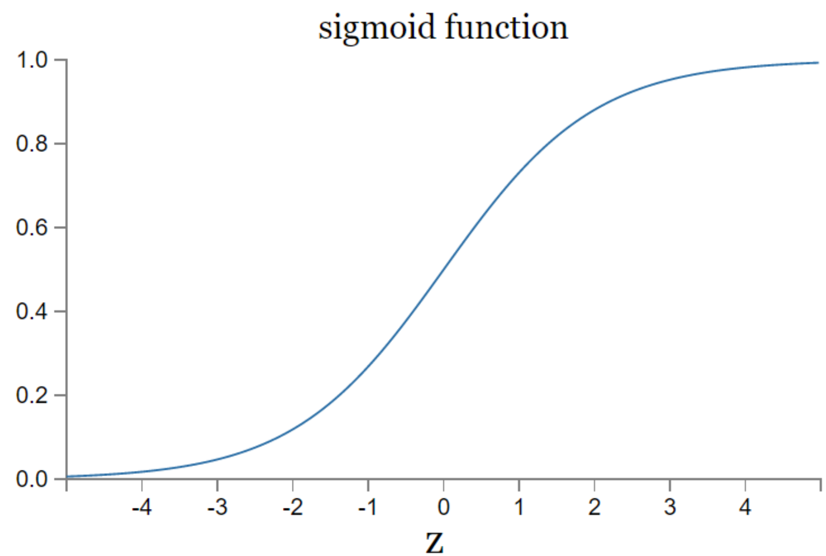
$$\text{output} = f(w^T x + b)$$

Activation function

Most frequently used is the sigmoid function:

$$f(w^T x - b) = \frac{1}{1 + e^{w^T x + b}}$$


step function
1.0
0.8
0.6
0.4
0.2
0.0
-4
-3
-2
-1
0
1
2
3
4
Z


sigmoid function
1.0
0.8
0.6
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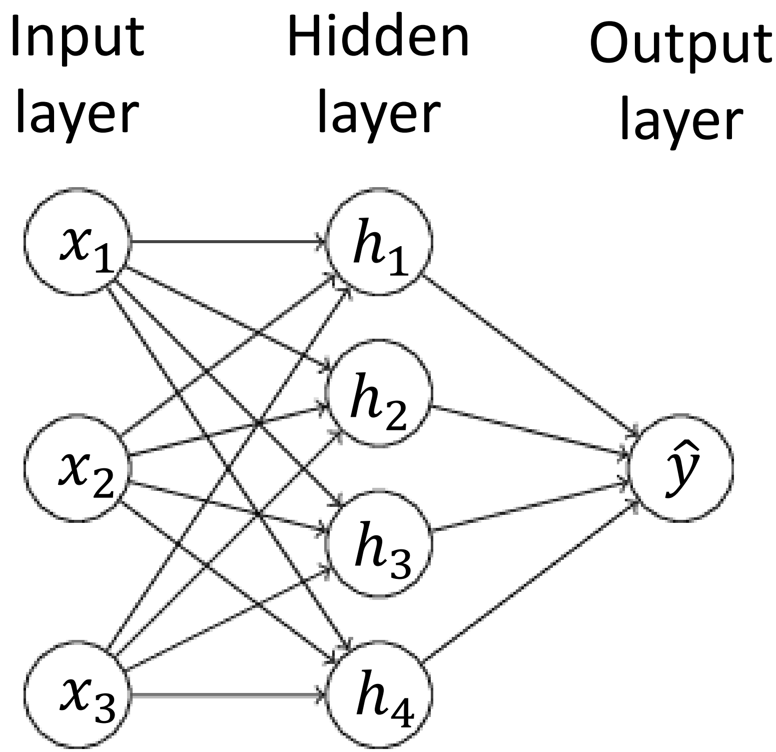
Neural network (NN)



$$h_i = f(w_i^T x + b_i)$$

$$\hat{y} = f(w_5^T h + b_5)$$

$$\hat{y} = f(w_1, \dots, w_5, b_1, \dots, b_5, x)$$

Goal: find W and b that minimize $P(y, \hat{y}) = P(y, x, W, b)$
where P is a performance measure
measuring the distance between y and $\hat{y}$

Universal approximation theorem

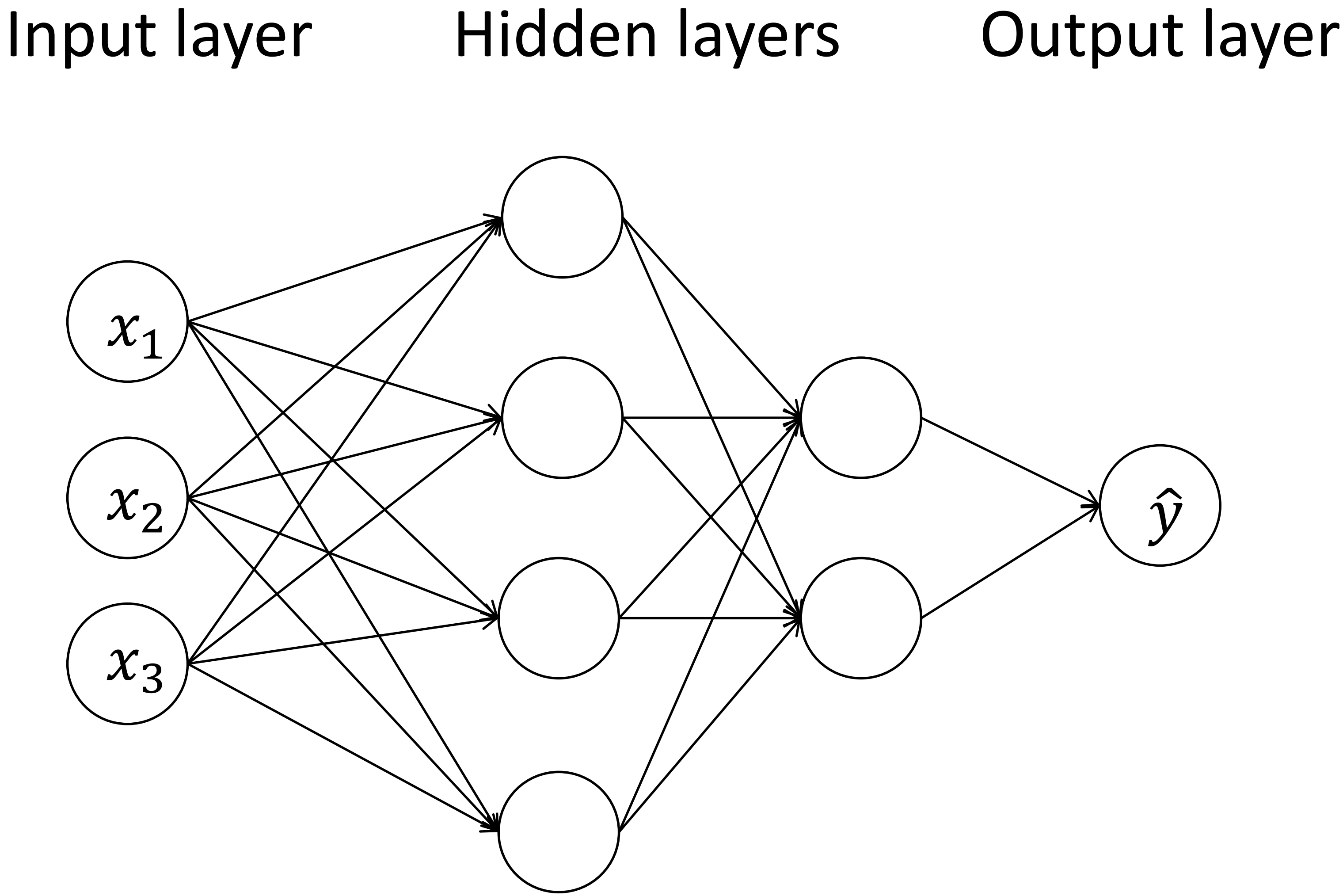
The theorem basically says:

A feedforward network with a single hidden layer containing a finite number of neurons can approximate any nonconstant, bounded and continuous function with arbitrary closeness, as long as there are enough hidden nodes.

(Video of intuition behind proof: https://www.youtube.com/watch?v=Ijqkc7OLenI)

But is it learnable?

Deep neural network (DNN)



Why DNNs?

- Allows learning of complex functions
- Can deal with the curse of dimensionality (more input variables than samples)
- Allows for parallellizing computations

Recognizing handwritten digits

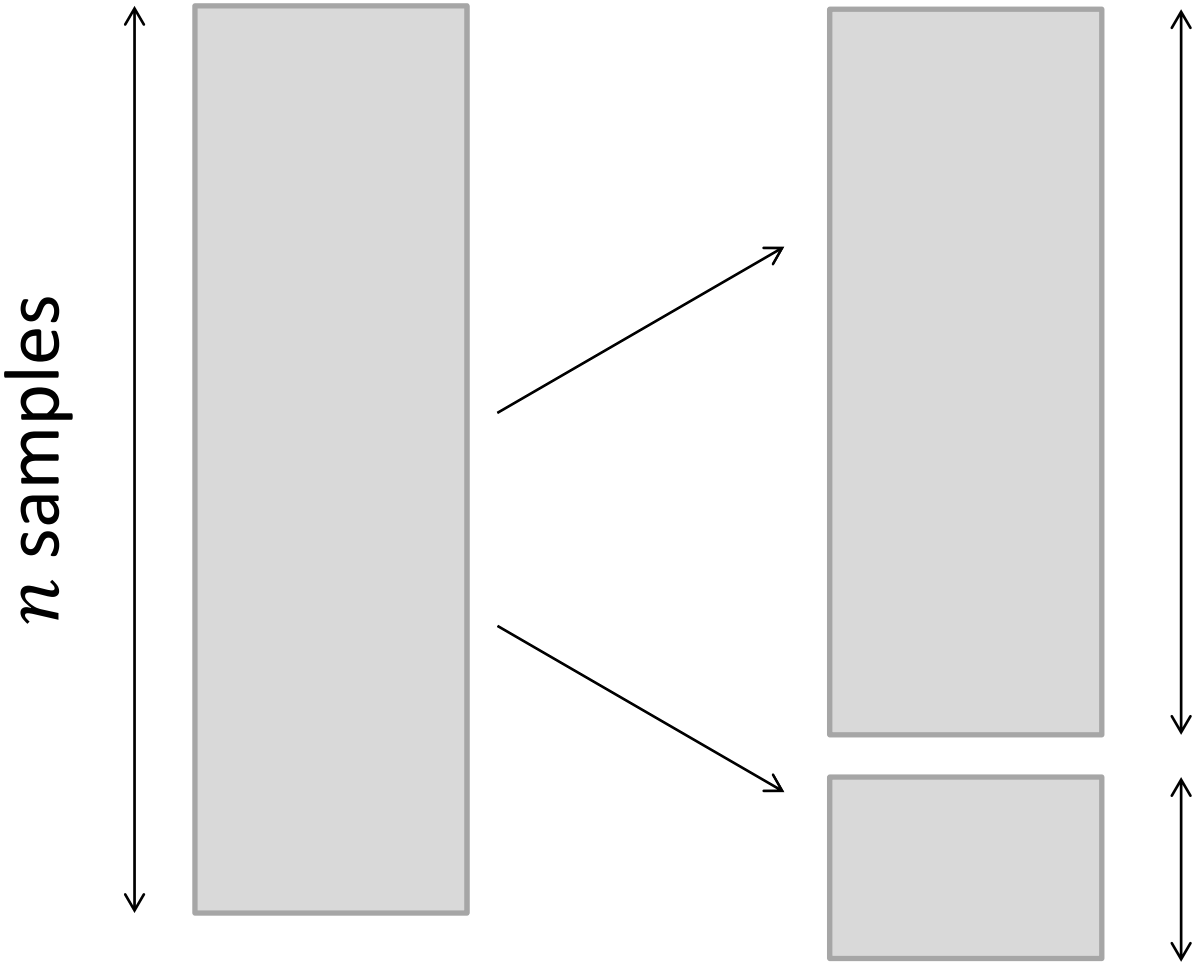
Supervised learning steps

1. Collect data
2. Choose model
3. Optimize parameters
4. Predict for new observations

Training

- Given n samples with input variables x and output y
- Find optimal w and b: minimize $P(w, b, x, y)$
- *Generalization:* the ability to perform well on previously unobserved inputs.

Train and test



Training data

τn samples

Minimize

$P(w, b, x^{\text{train}}, y)$

Test data

$(1-\tau)n$ samples

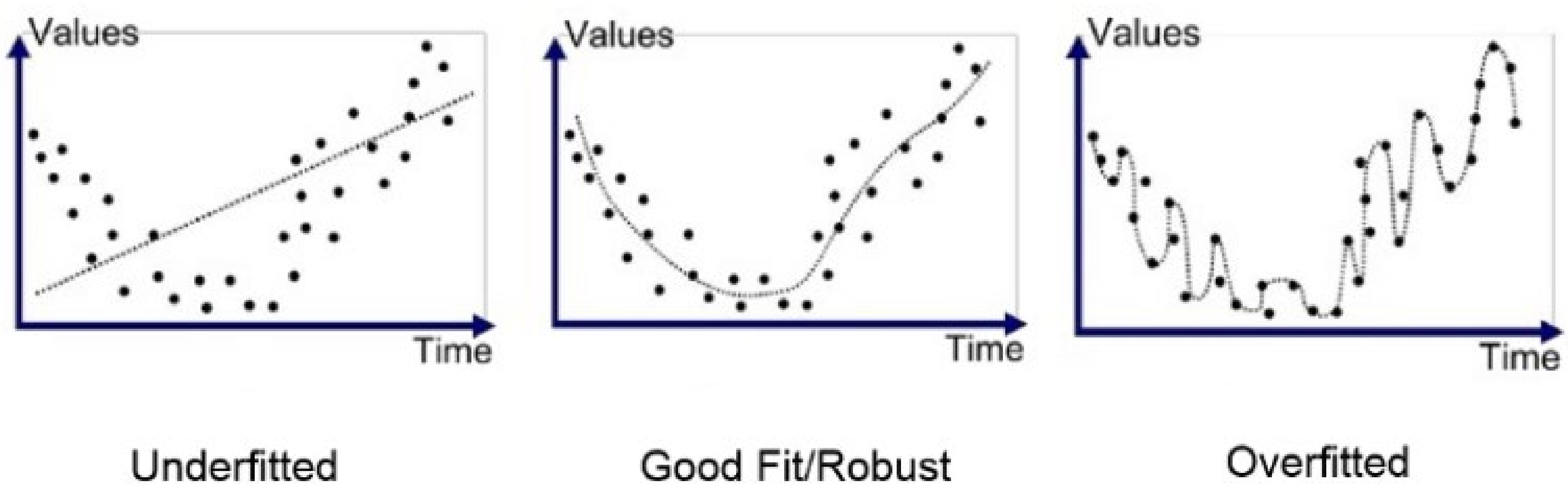
Evaluate $P(w, b, x^{\text{test}}, y)$

Train and test

- Training: minimize train error $P(w, b, x^{\text{train}}, y)$
- Testing: evaluate test error $P(w, b, x^{\text{test}}, y)$
- In general: $P\left(w, b, x^{\text{test}}, y\right) > P(w, b, x^{\text{train}}, y)$
- Goal: $P\left(w, b, x^{\text{test}}, y\right) - P\left(w, b, x^{\text{train}}, y\right)$ small

Under- and overfitting & capacity

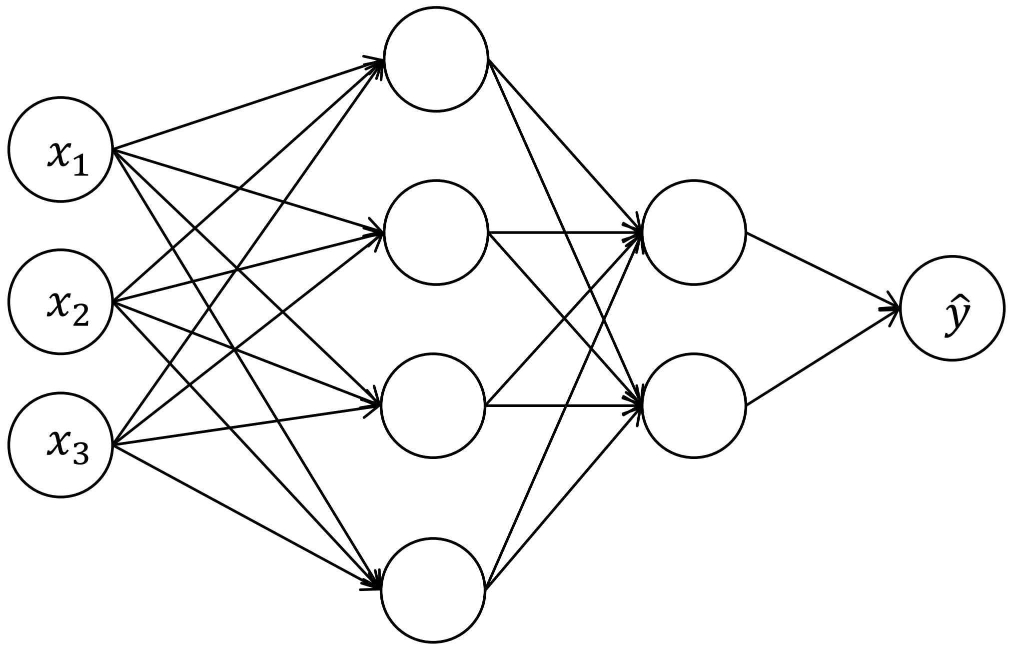
- *Underfitting*: large $P(w, b, x^{\text{train}}, y)$
- *Overfitting*: large $P\left(w, b, x^{\text{test}}, y\right) - P(w, b, x^{\text{train}}, y)$



Under- and overfitting & capacity

- *Underfitting*: large $P(w, b, x^{\text{train}}, y)$
- *Overfitting*: large $P\left(w, b, x^{\text{test}}, y\right) - P(w, b, x^{\text{train}}, y)$
- *Capacity*: a model's ability to fit a wide range of functions

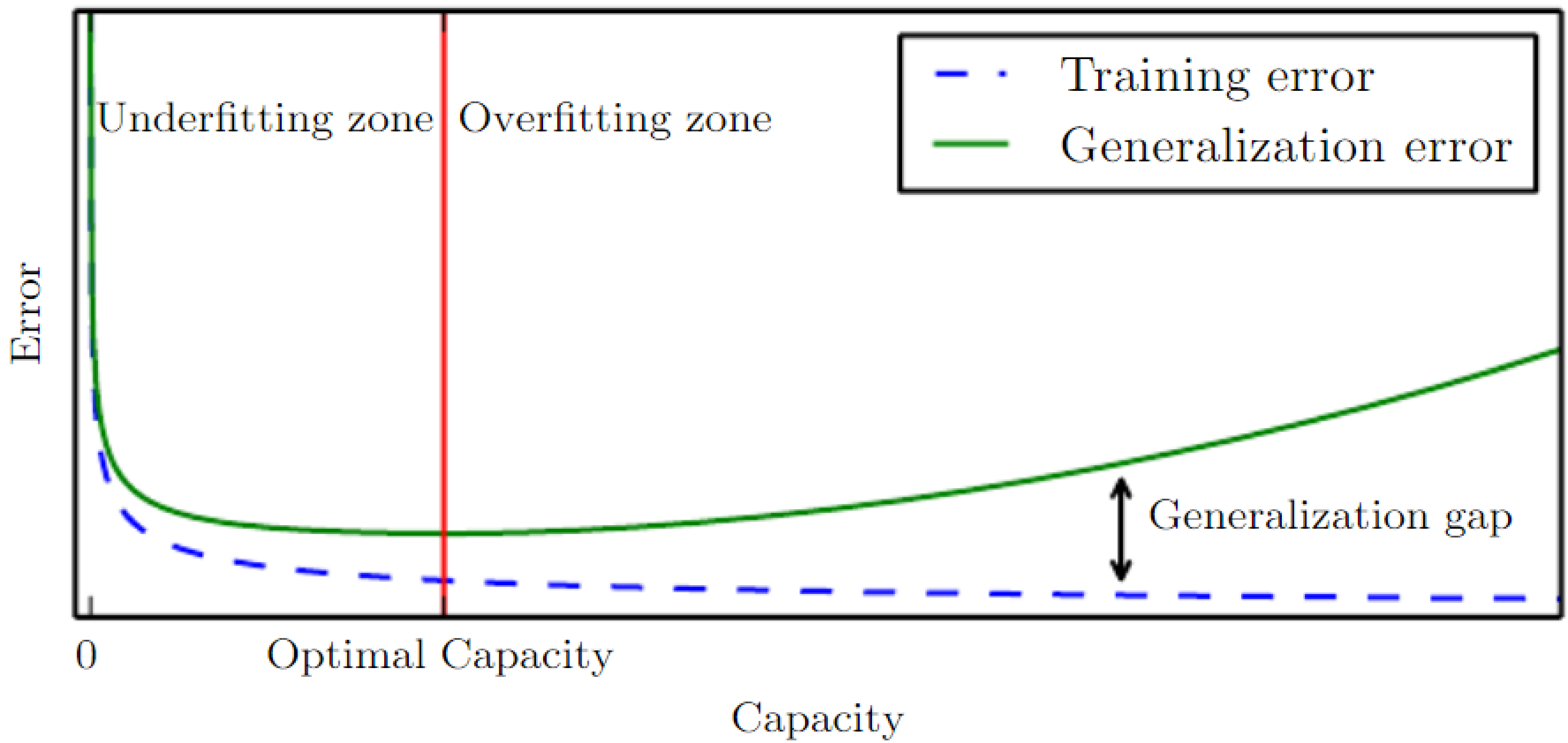
Capacity of your DNN



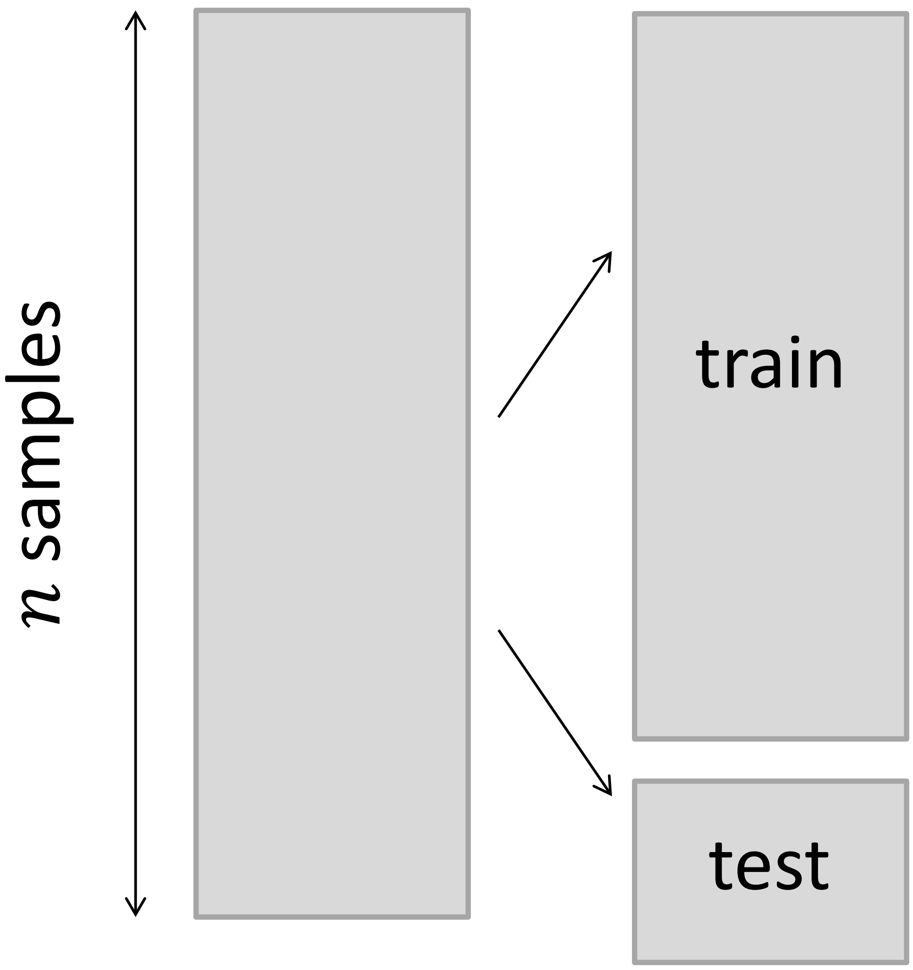
- How many layers?
- How many nodes in each layer?

→ *hyperparameter optimization*

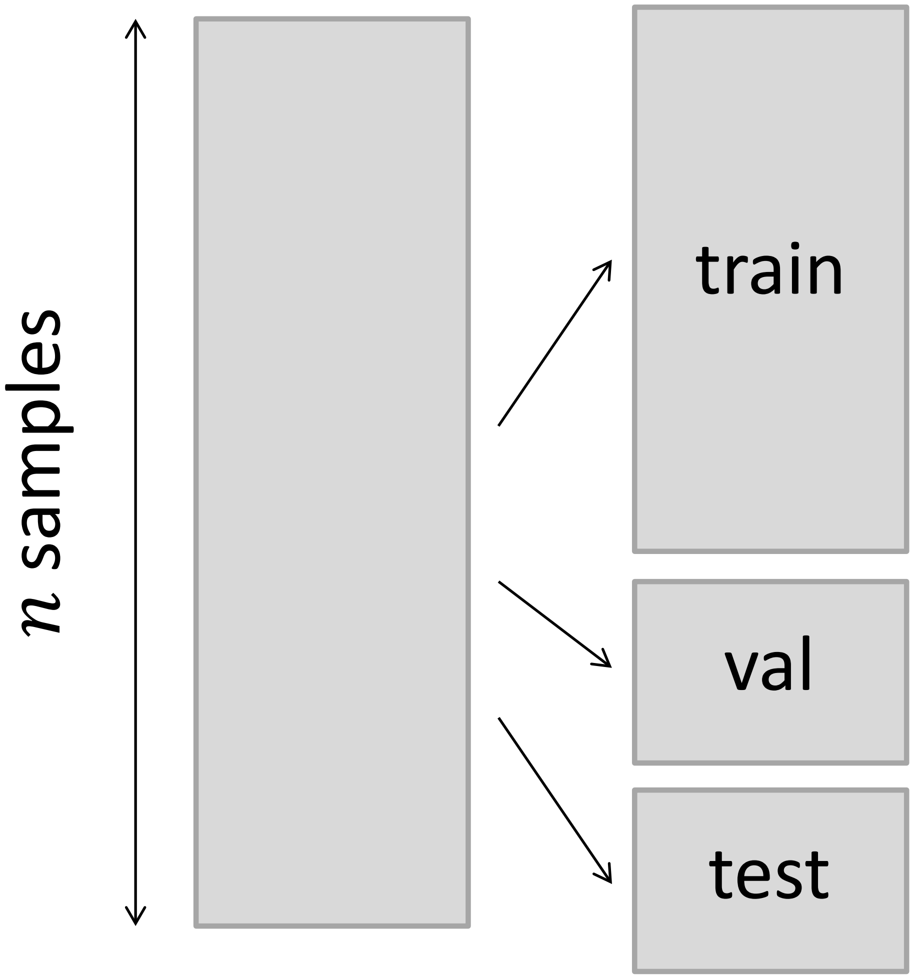
Under- and overfitting & capacity



Train and test



Train, validation and test



Hyperparameter optimization

Given a set of hyperparameters H.

Instance $h \in H$ describes no. and size of layers.

for $h \in H$ do:

  train network by minimizing $P(h, w, b, x^{\text{train}}, y)$

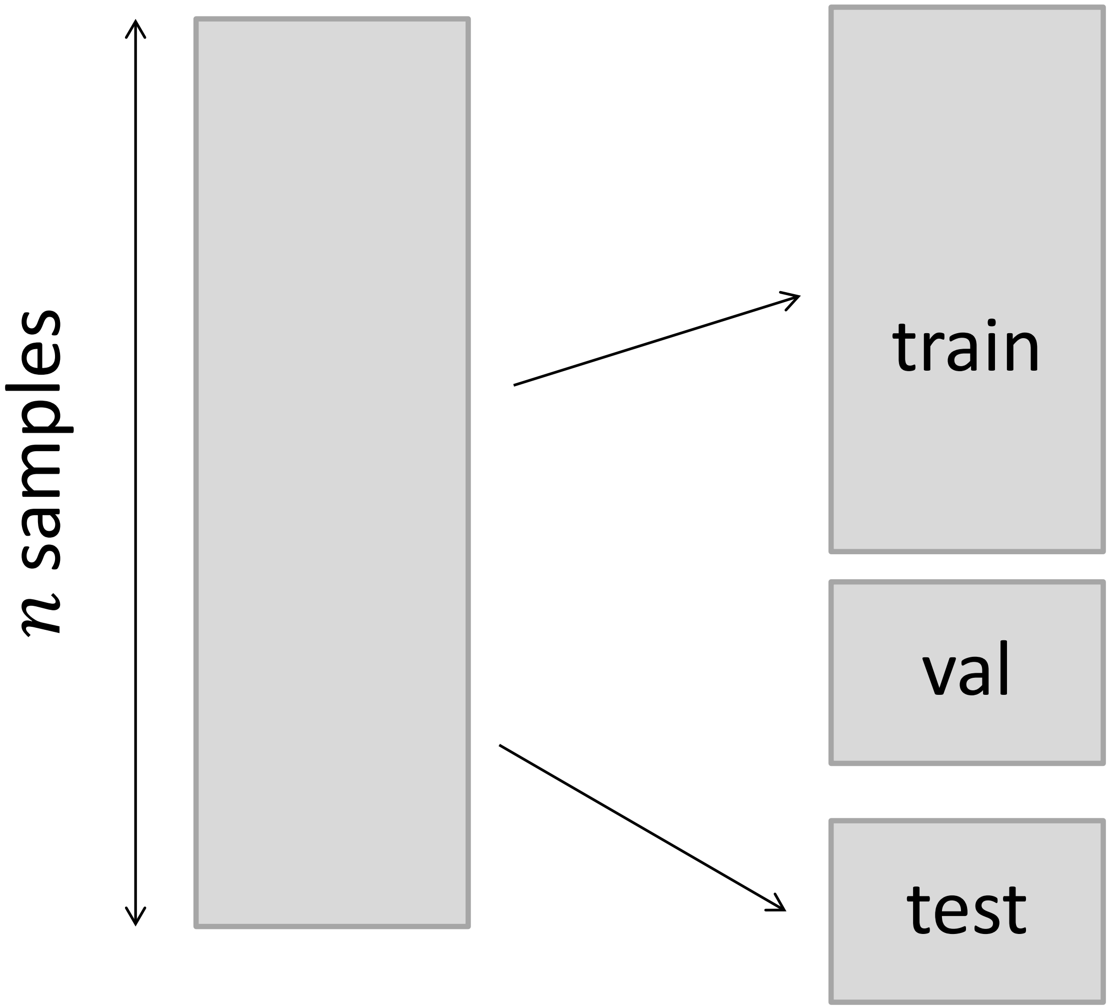
  gives $P(h, w^h, b^h, x^{\text{val}}, y)$

choose $h^* = \text{argmin}_h\{P(h, w^h, b^h, x^{\text{val}}, y)\}$

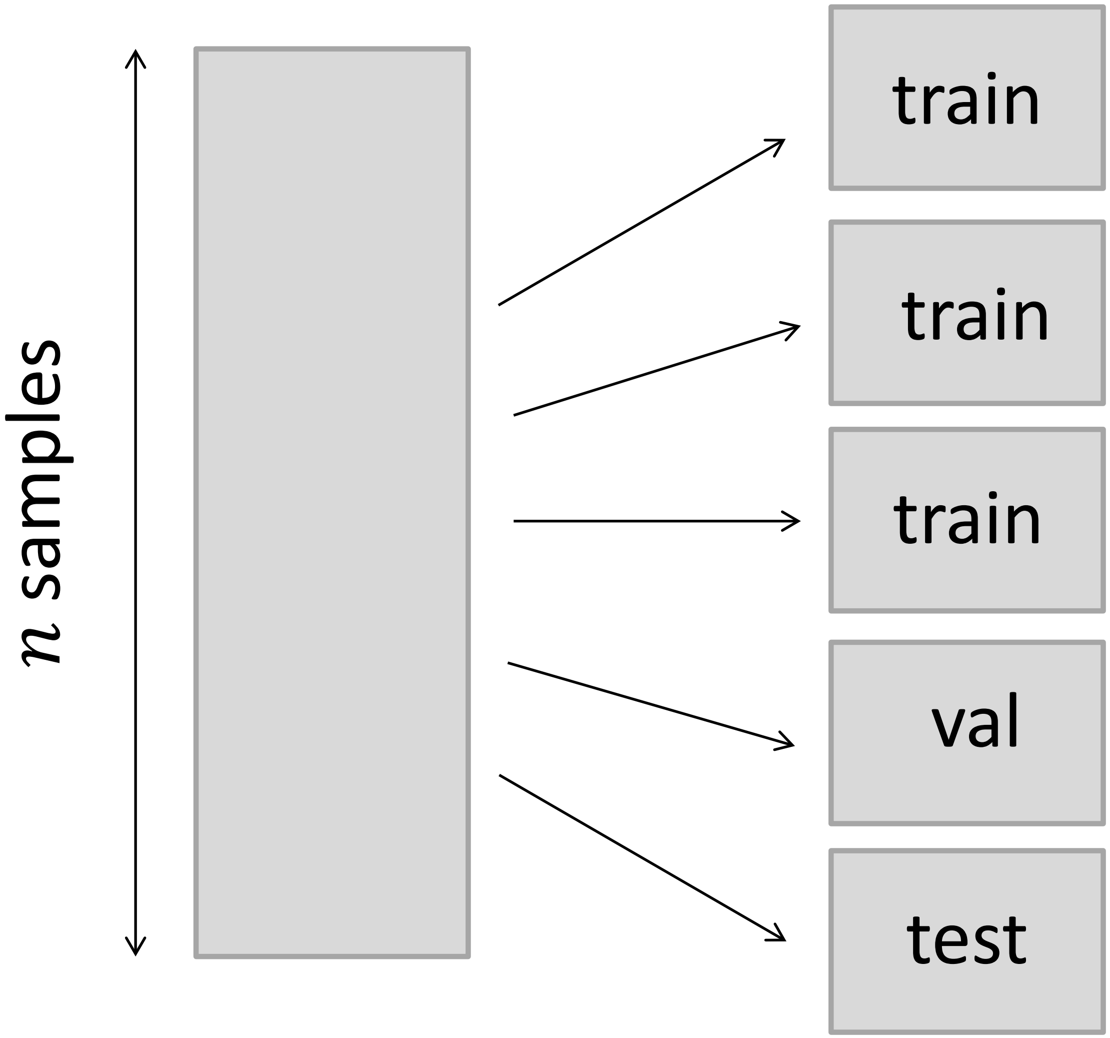
evaluate $P(h^*, w^{h^*}, b^{h^*}, x^{\text{test}}, y)$

(w^h and b^h are the optimized parameters for a network with hyperparameters h)

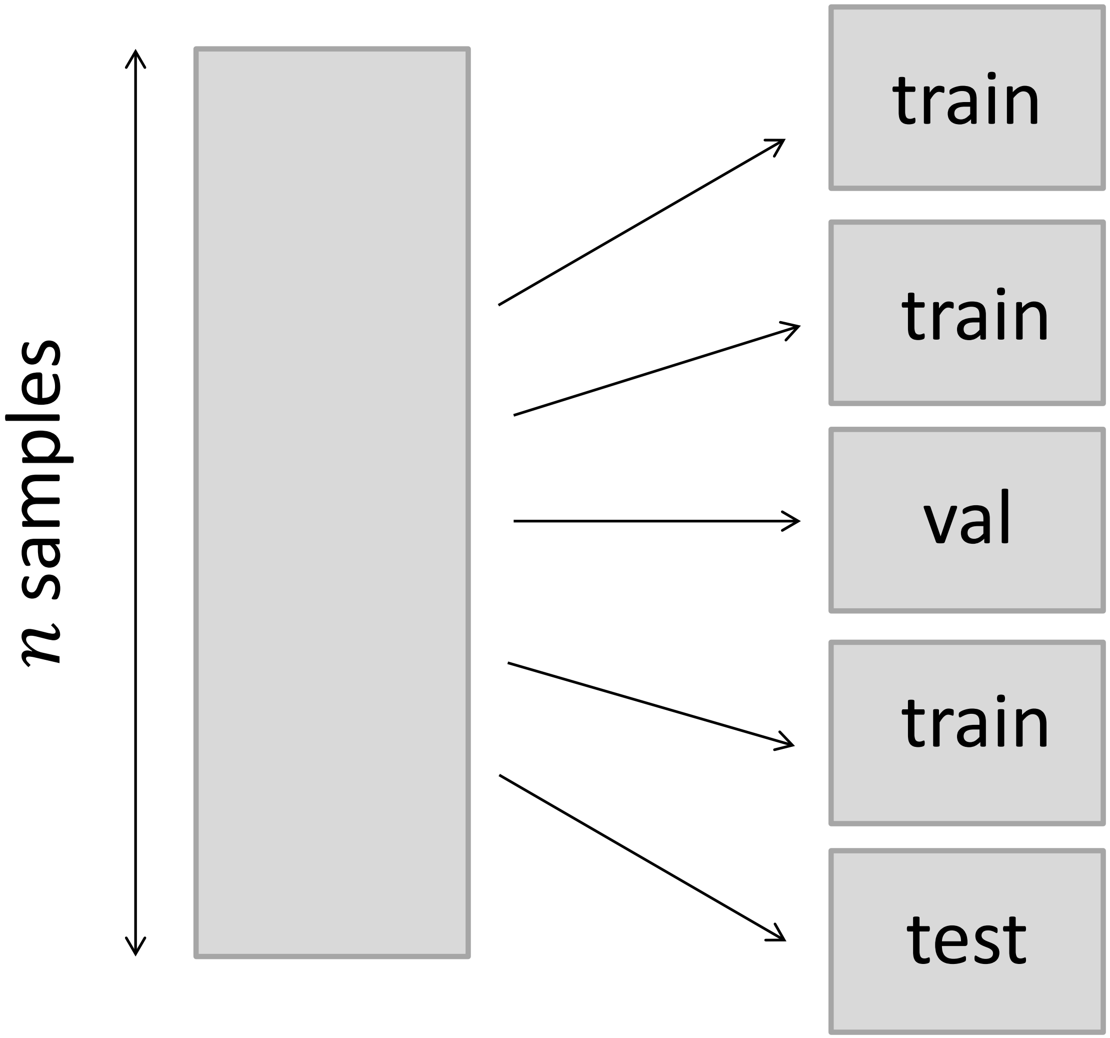
k-fold cross validation



k-fold cross validation



k-fold cross validation



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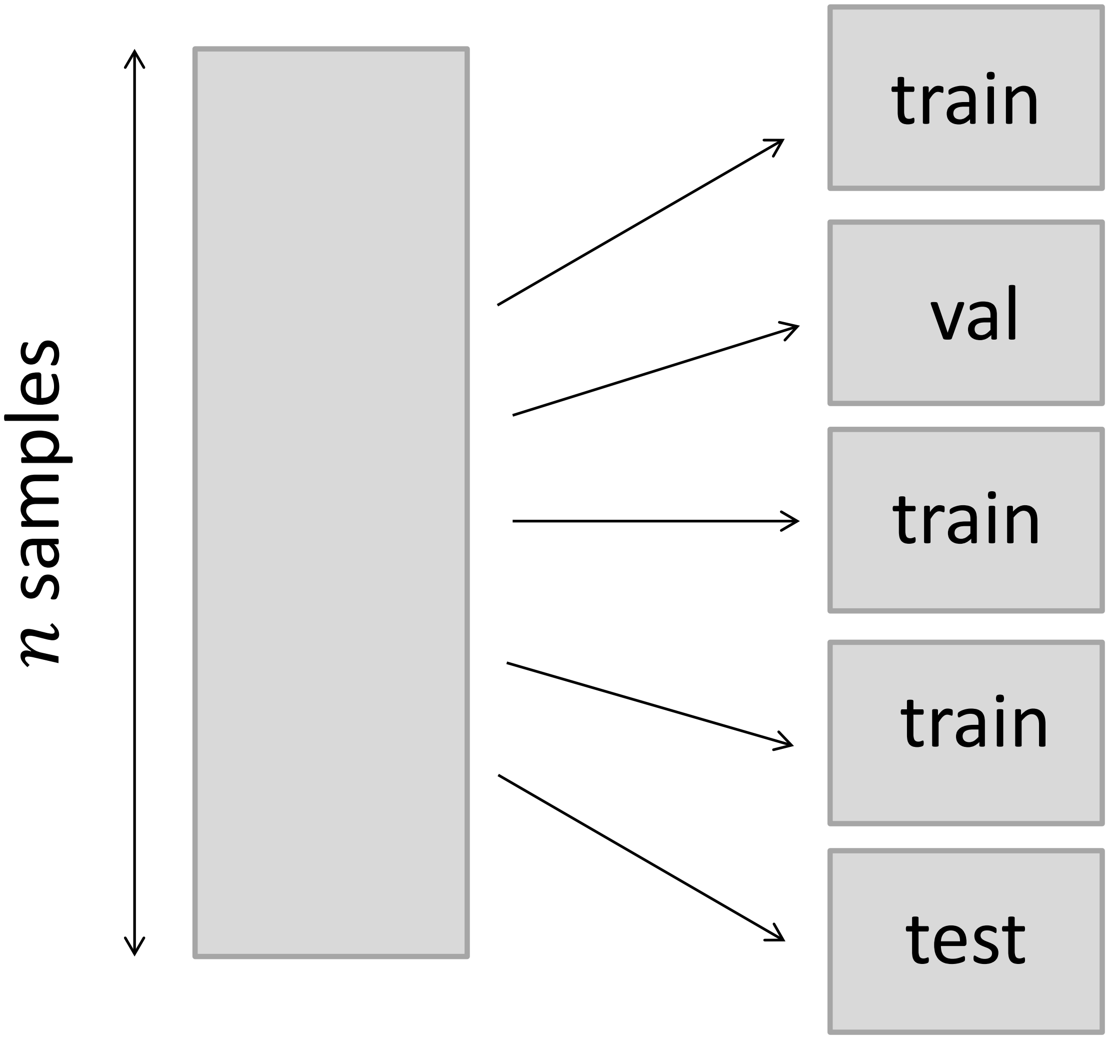

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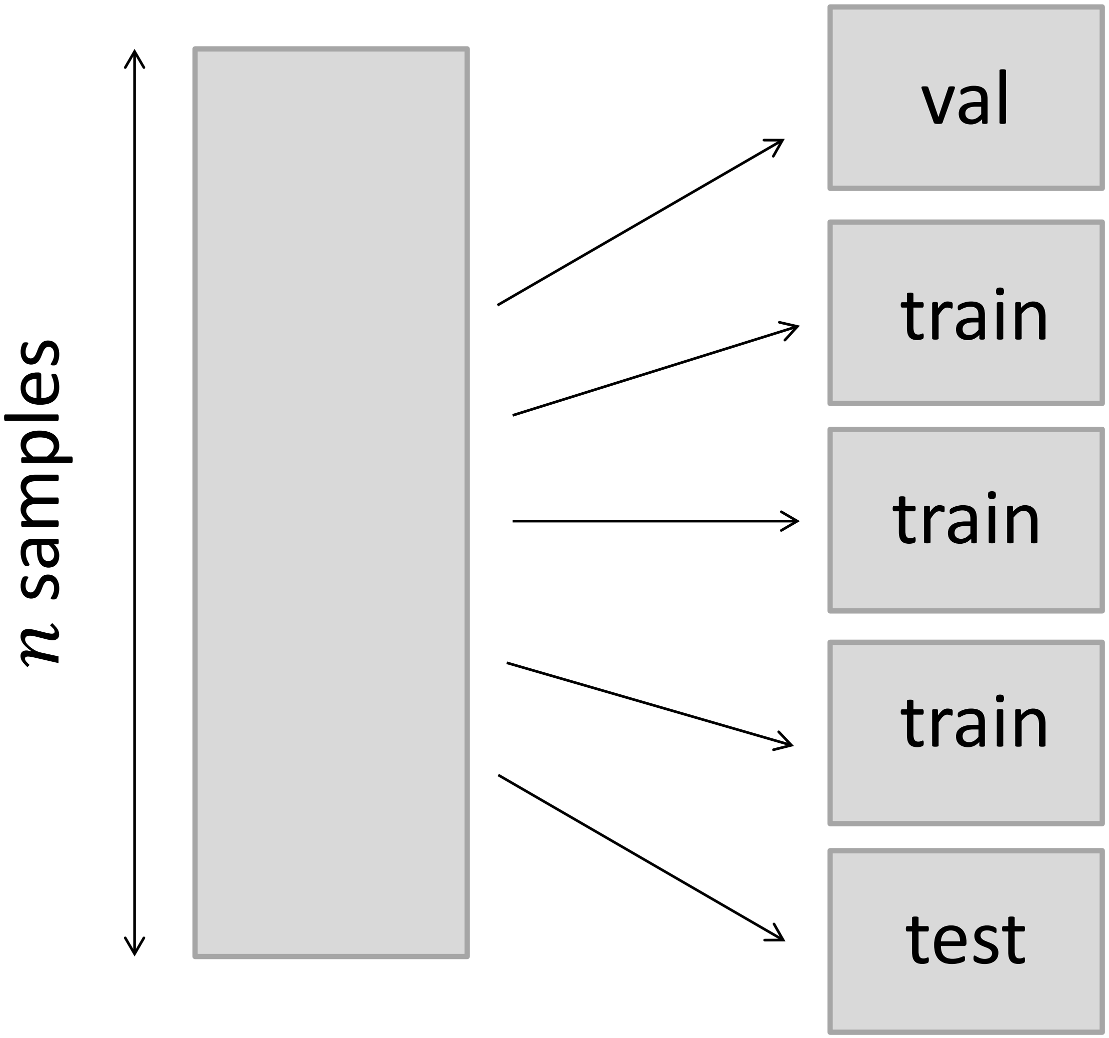
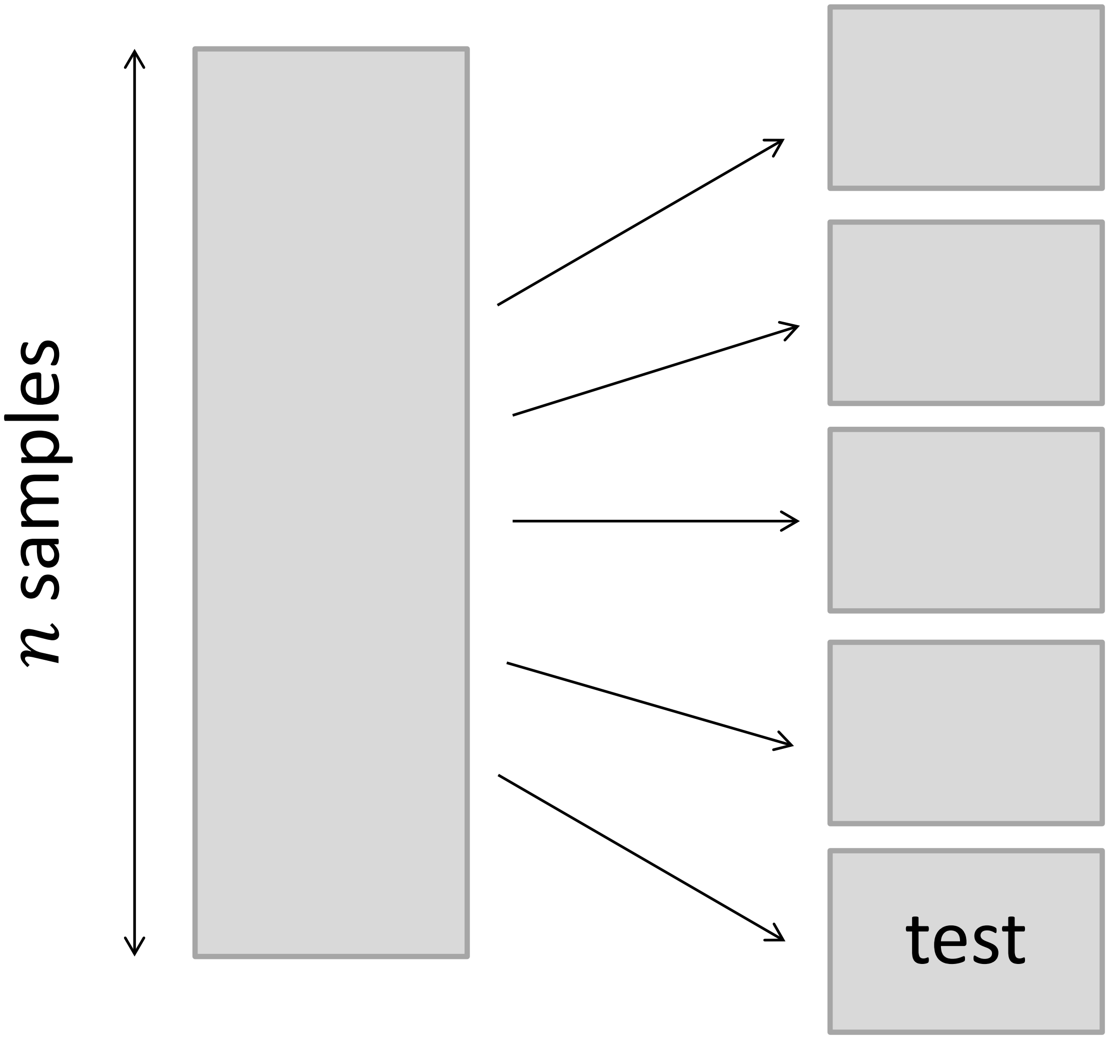


k-fold cross validation



- Train k times
- Different x^{val} for each fold
- Average P over the k folds

Why DNNs?

- Allows learning of complex functions
- Can deal with the curse of dimensionality
- Allows for parallellizing computations

When not to use DNNs?

- If a simpler model works at least as good
- If you know the underlying relationship (for example linear)

Dealing with overfitting

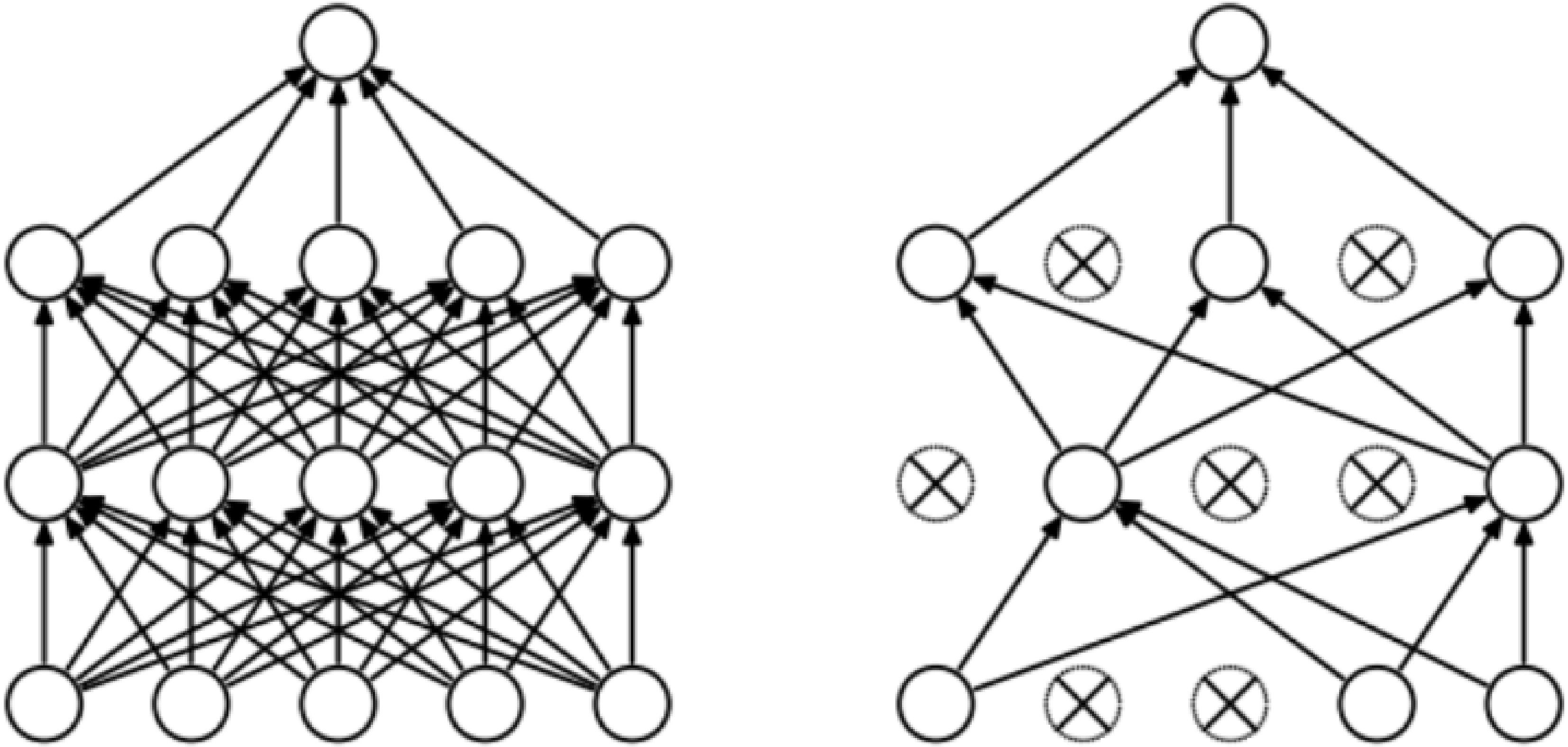
- Hyperparameter tuning
- Regularization

L1 and L2 regularization

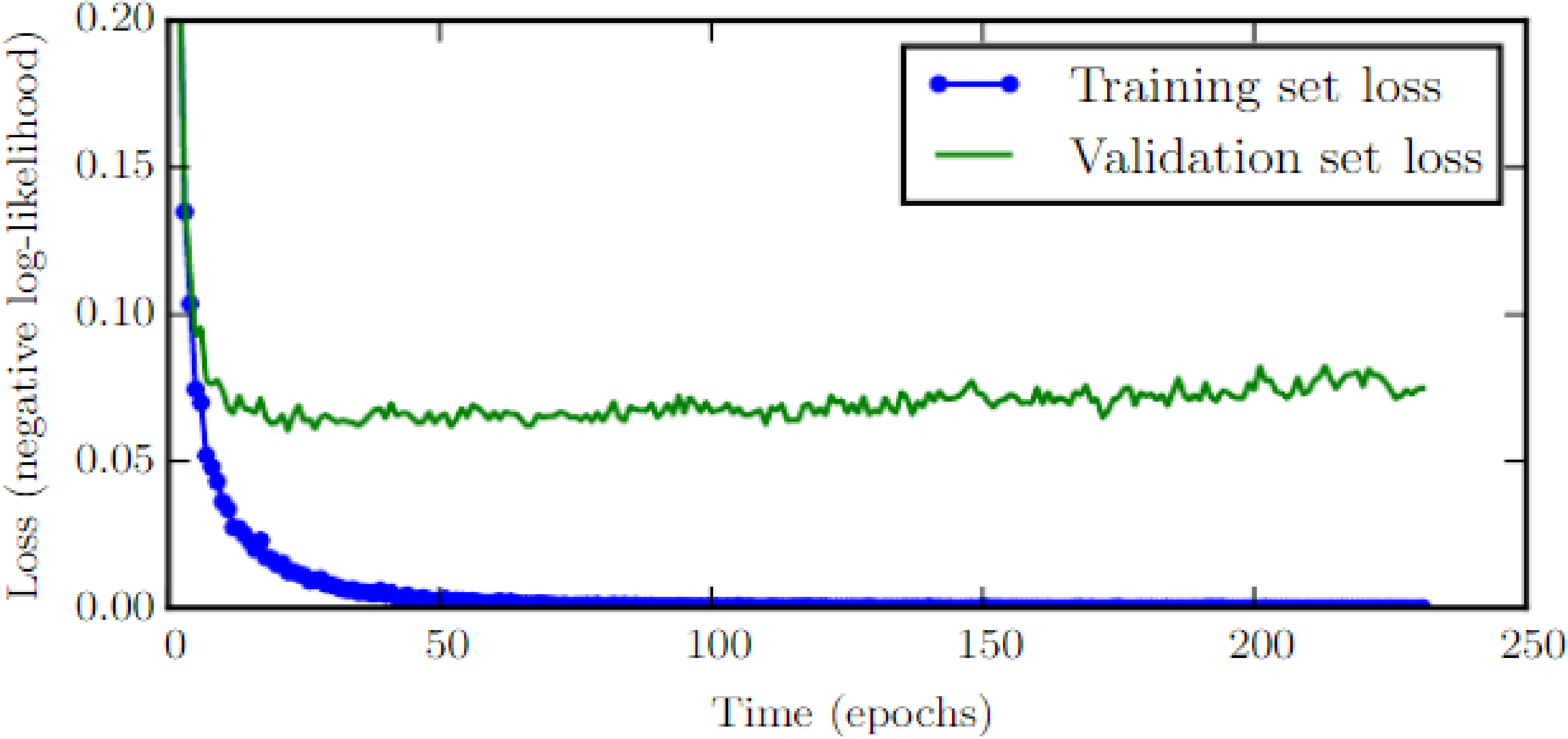
minimize $P\left(h, w, b, x^{\text{train}}, y\right) + \frac{\lambda}{m} L(w, b)$

- L1: $L(w, b) = |(w, b)|_1$
- L2: $L(w, b) = |(w, b)|_2$
- λ is a weighting factor
- m is the total number of parameters

Dropout



Early stopping



Summary

- What is machine learning?
- What is a perceptron?
- What is a (deep) neural network?
- Why use DNNs?
- What is underfitting, overfitting and capacity?
- How to train your model and optimize hyperparameters?
- How to use regularization to prevent overfitting?

Prepare for next week

- Install python
- Learn how to use python
- Read literature

Installing python (windows)

- Install miniconda (python3.6)

https://conda.io/miniconda.html

- Open the anaconda prompt
- Create an anaconda environment:

conda create –n DLcourse

- Activate the environment (not necessary after creating it, only the next time you start):

source activate DLcourse

- You're ready to go!

Installing python (linux)

- Install miniconda (python3.6)

https://conda.io/miniconda.html

- Open the command line
- Create an anaconda environment:

conda create –n DLcourse

- Activate the environment (not necessary after creating it, only next time you start):

source activate DLcourse

- You're ready to go!

Installing python (mac)

- Install miniconda (python3.6)

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- Open the command line
- Create an anaconda environment:

conda create –n DLcourse

- Activate the environment (not necessary after creating it, only next time you start):

source activate DLcourse

- You're ready to go!

Learning python

- https://www.learnpython.org/
- https://www.programiz.com/python-programming/tutorial

Further reading

http://neuralnetworksanddeeplearning.com :

- Chapter 1 up to and including “Perceptrons”

https://www.deeplearningbook.org/ :

- 5.1-5.3, 5.10-5.11
- 7.1, 7.8, 7.12