Machine learning fundamentals

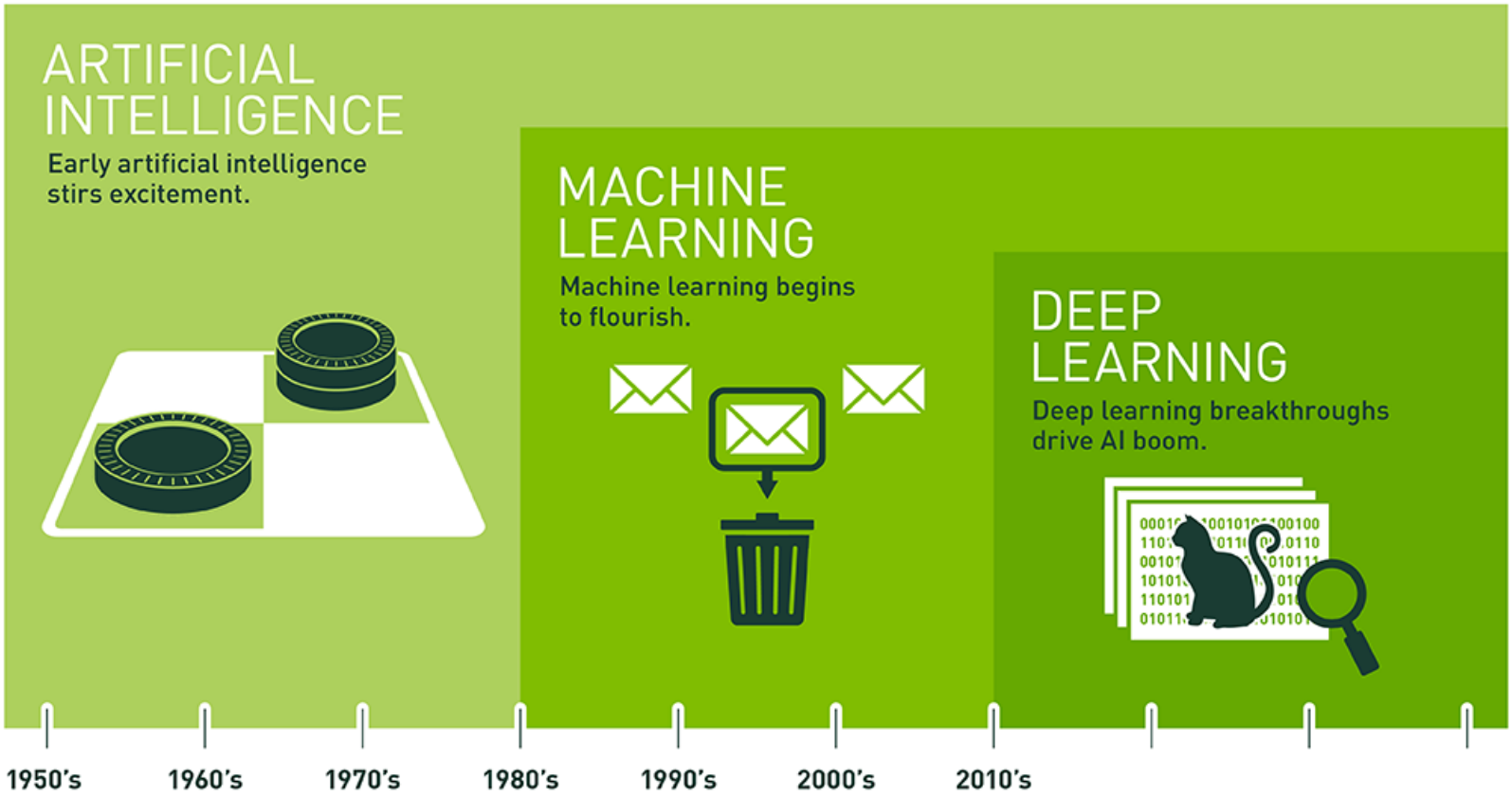
Deep learning course for industry

Mitko Veta

Eindhoven University of Technology
Department of Biomedical Engineering

2020

Historical perspective



Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

Figure source: nvidia.com

Course overview

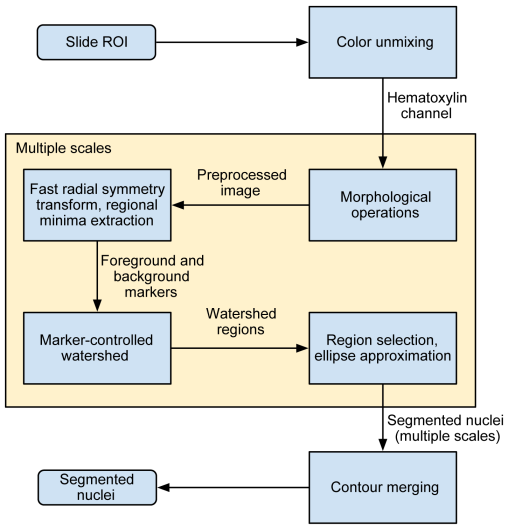
- 09.30 - 10.15 Machine learning fundamentals
- 10.30 - 11.15 From linear models to deep neural networks
- 11.30 - 12.00 Convolutional neural networks
- *Lunch break*
- 13.00 - 14.00 Training neural networks in your web browser

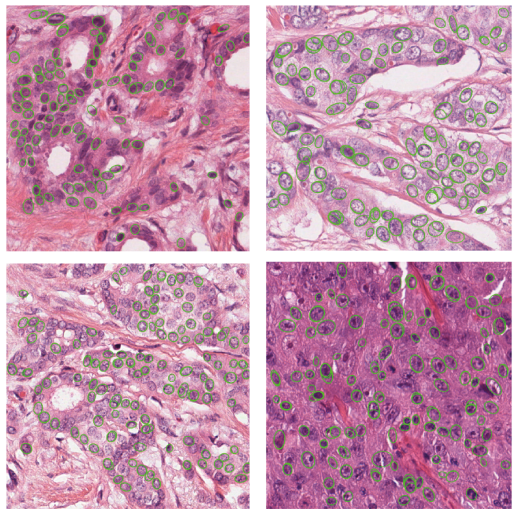
Learning goals

- Define machine learning.
- Introduce the conceptually simple yet practically useful linear model.
- Discuss the central challenge of machine learning: generalisation.

An example from my past work: nuclei area measurement

2010-2011: An image processing pipeline of (mainly) mathematical morphology operators (e.g. the watershed algorithm).



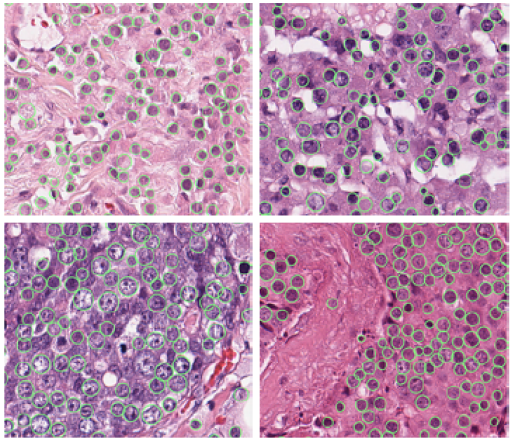


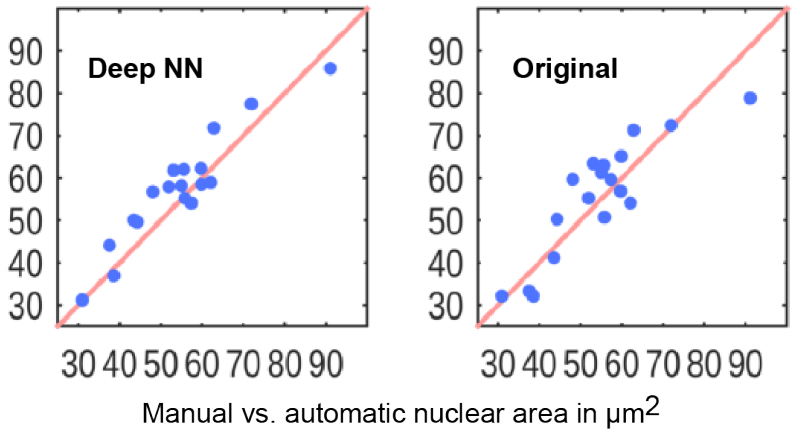
The design and validation of the processing pipeline took the better part of a year.

Figure source: Veta et al. PLOS ONE 2012

An example from my past work: nuclei area measurement

2015: A deep neural network for nuclei area measurement.





The the training and validation of the deep neural network model took less than a week.

The results were more accurate than the the original method.

Figure source: Veta et al. MICCAI 2016

The central premise of machine learning

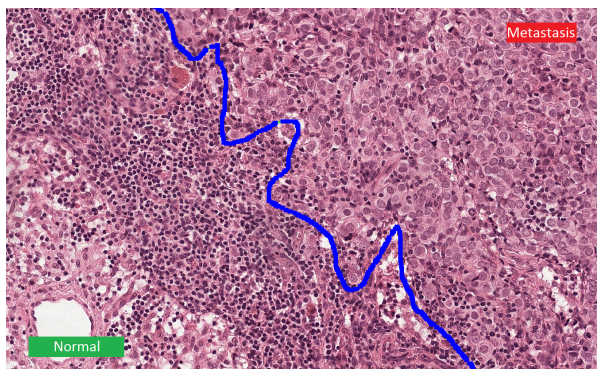
Learn "computer programs" from examples instead of manually writing rules.

The central premise of machine learning

Learn "computer programs" from examples instead of manually writing rules.

Advantage: the same method (e.g. a neural network) can be used to solve a variety of different problems.

Siberian hustky vs. eskimo dog



Normal vs. metastases

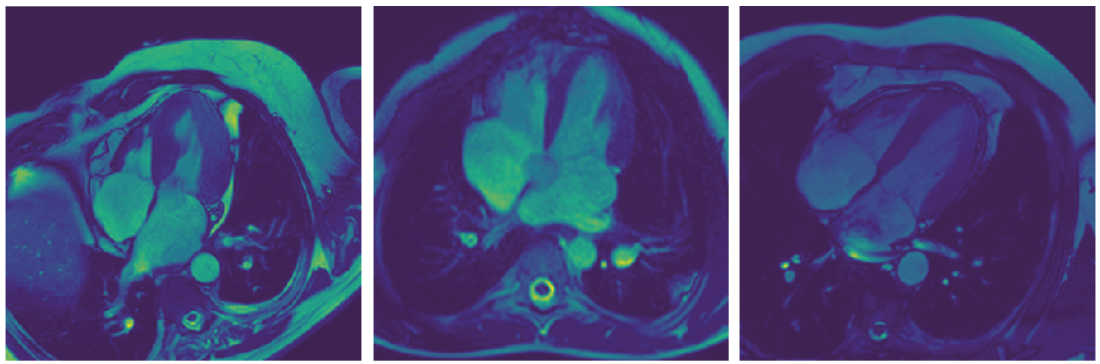
Figures source: (left) Szegedy et al. arXiv 2014, (right) camelyon16.grand-challenge.org

What are the "examples"?

Depends on the particular problem and task.

Dataset: cardiac MRI images.
Task: detect if a specific pathology is present in each image.

In this case, every image is an example and is associated with a binary target: 0 = "healthy", 1 = "diseased" (i.e. we want to classify each image as "healthy" or "diseases").

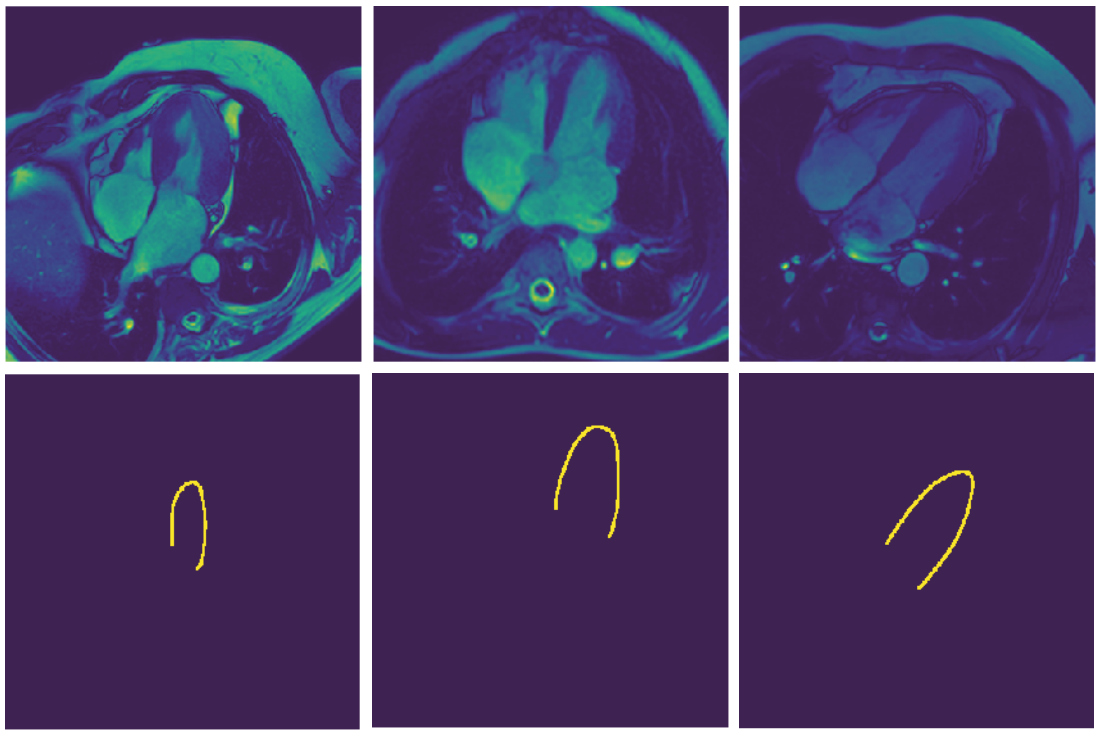


diseased diseased healthy

What are the "examples"?

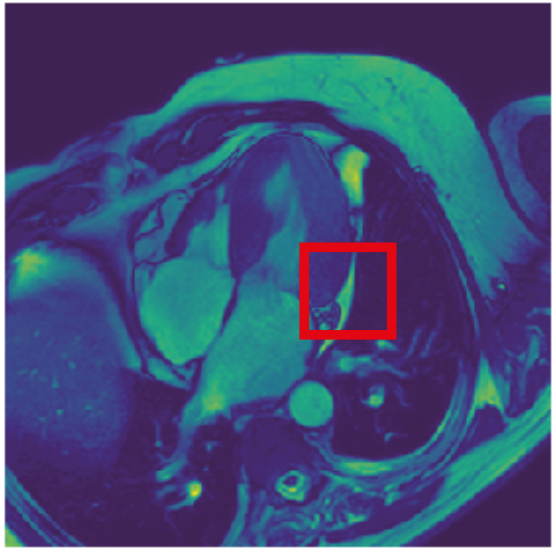
Dataset: cardiac MRI images.
Task: Segment the contours of the left ventricle

In this case, each pixel is an example and is associated with a binary target: 0 = "background", 1 = "contour".



How are the "examples" represented?

Traditionally with feature extraction:



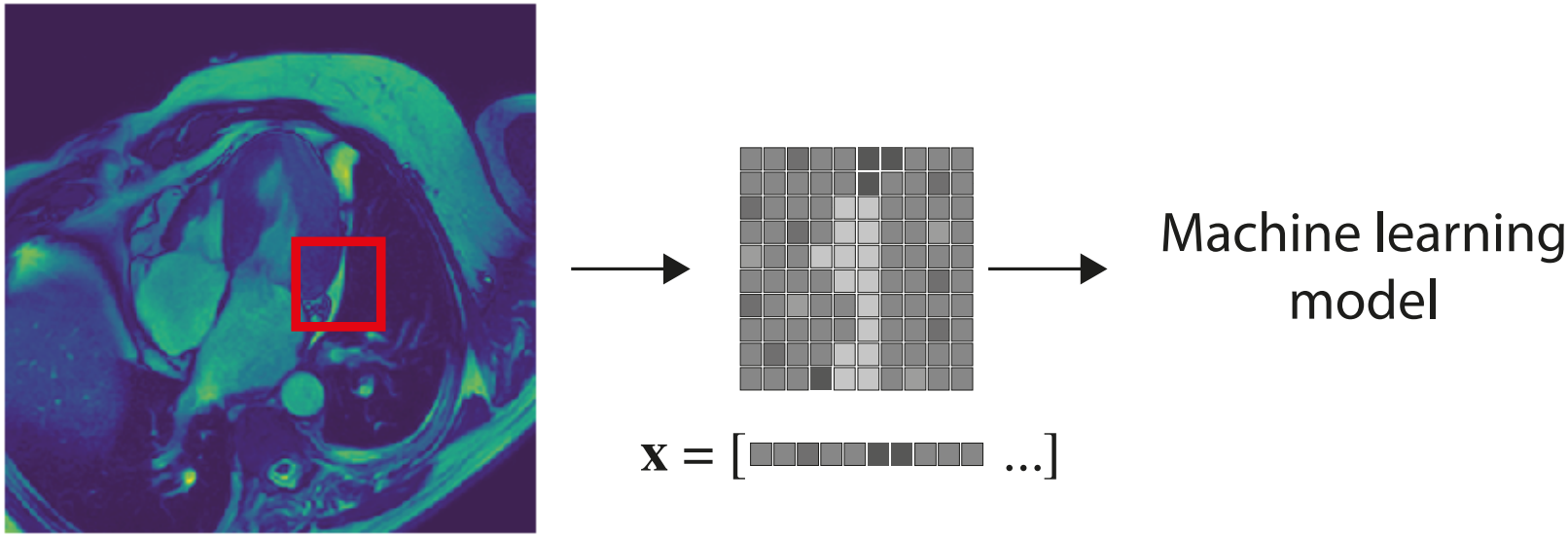
Intensity features
Texture features
Shape features
...

Machine learning model

$$\mathbf{x} = [\mathbf{x}_{\text{intensity}}\ \mathbf{x}_{\text{texture}}\ \mathbf{x}_{\text{shape}} \ldots]$$

How are the "examples" represented?

With raw pixel values (the *de facto* standard for deep learning):



In summary...

In order to design a machine learning algorithm for a specific task we are given a dataset of examples represented by $\mathbf{x}_i$.

Each example is (optionally) associated with a target y_i.

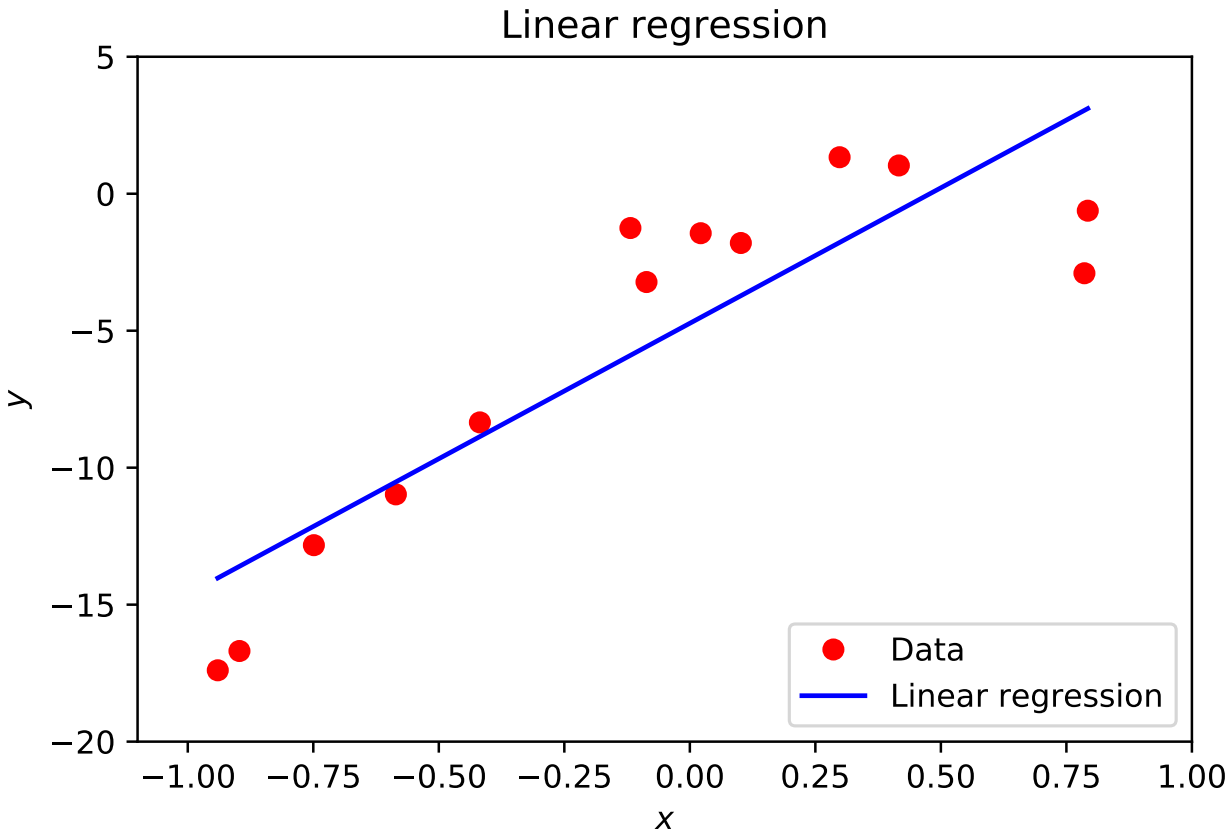
The target can be categorical, such as class membership (e.g. $y_i = \{0, 1\}$), or continuous (e.g. area, volume etc.).

Types of machine learning

- Unsupervised machine learning: given a dataset x_i, find "some interesting properties".
  - Clustering: find groupings of x_i
  - Density estimation: find $p(x_i)$
  - Generative models.
  - ...
- Supervised machine learning: given a training dataset $\{x_i, y_i\}$, predict $\hat{y}_i$ of previously unseen samples.
  - Regression: the target variables y_i are continuous.
  - Classification: the target variables y_i are continuous.
  - ...

A simple machine learning model for regression

The predictions $\hat{y}_i$ are a linear combination of the inputs:



$$\hat{y} = \hat{w}_0 + \sum_{j=1}^{p} x_j \hat{w}_j$$

Linear models are surprisingly useful and common

Fetal weight estimate from ultrasound imaging:

fetal weight $= \hat{w}_0 + \hat{w}_1 \times$ femur len. $+ \hat{w}_2 \times$ abdominal circ. $+ \hat{w}_3 \times$ head circ.

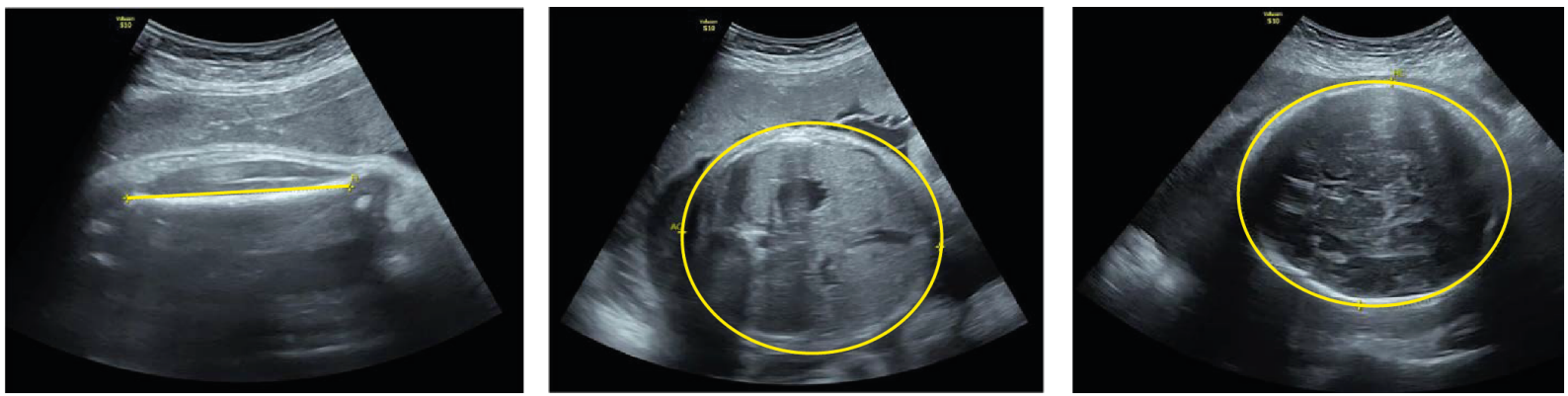


Figure source: my daughter

Linear model

- Input vector $\boldsymbol{x}^T = (x_1, x_2, \ldots, x_p)$.
- Output y predicted using the model

$$\hat{y} = \hat{w}_0 + \sum_{j=1}^{p} x_j \hat{w}_j$$

- In vector form

$$\hat{y} = \hat{\boldsymbol{w}}^T \boldsymbol{x} = \boldsymbol{x}^T \hat{\boldsymbol{w}}$$

- We assume that w_0 is in $\boldsymbol{w}$ and 1 is included in $\boldsymbol{x}$.

Linear model fit by least squares

- We need to find coefficients $\hat{w}_i$ which minimise the error estimated with the **residual sum of squares**

$$\mathrm{RSS}(\boldsymbol{w}) = \sum_{i=1}^{N} (y_i - \boldsymbol{x}_i^T \boldsymbol{w})^2$$

  assuming N input-output pairs (the dataset).
- $\mathrm{RSS}(\boldsymbol{w})$ is a quadratic function.
- A minimum always exists.

Linear model fit by least squares

- $\boldsymbol{y} = [y_1, y_2, \ldots, y_N]^T$ is the vector formed from the N output values and $\boldsymbol{X}$ is an $N \times p$ matrix where each row corresponds to one example $\boldsymbol{x}_i$

$$\text{RSS}(\boldsymbol{w}) = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})$$

- If $\boldsymbol{X}^T\boldsymbol{X}$ is non-singular there exists a unique solution given by

$$\hat{\boldsymbol{w}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

Linear model fit by least squares

- For each input $\boldsymbol{x}_i$ there corresponds the fitted output

$$\hat{y}_i = \hat{y}_i(\boldsymbol{x}_i) = \hat{\boldsymbol{w}}^T \boldsymbol{x}_i$$

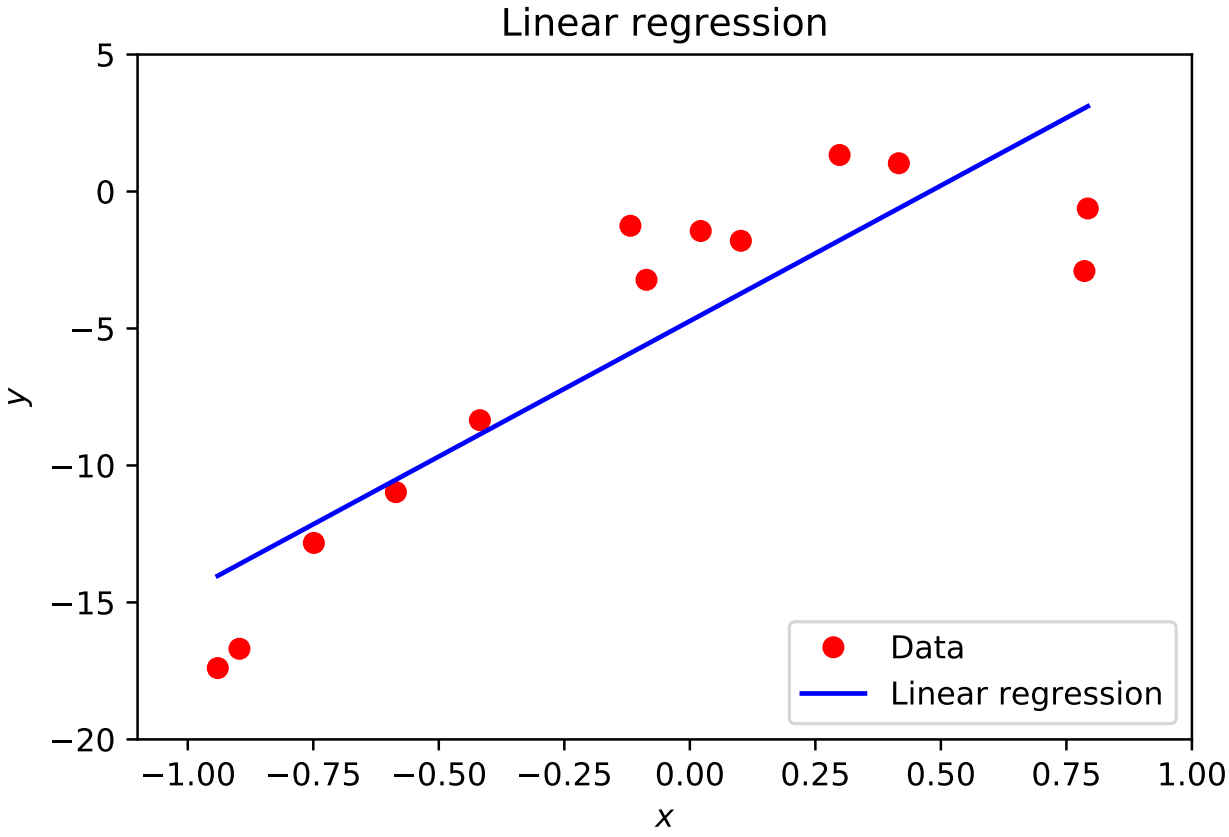
.

- This is called "making a prediction" for $\boldsymbol{x}_i$.
- The entire fitted surface (hyperplane) is fully characterised by the parameter vector $\hat{\boldsymbol{w}}$.
- After fitting the model, we can "discard" the training dataset.

The ML workflow (thus far)

- Collect dataset $\{\mathbf{x}_i, y_i\}$.
- Assume a model for $\hat{y}$.
- Decide on an **error/loss function** that measures the "goodness of fit" of $\hat{y}$ to $\{\mathbf{x}_i, y_i\}$.
- Fit the model to the data with an optimisation procedure (e.g. gradient-based optimisation).

But what if a linear model is not enough?



$$\hat{y} = \hat{w}_0 + \sum_{i=1}^{p} x_i \hat{w}_i$$
$$\hat{y} = \boldsymbol{x}^T \hat{\boldsymbol{w}}$$

Polynomial regression

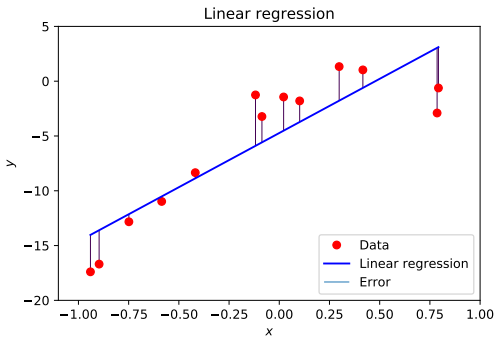
- The linear regression algorithm can be generalised to include all polynomial functions instead of just the linear ones.
- Moving to degree two we obtain: $\hat{y} = b + w_1 x + w_2 x^2$.

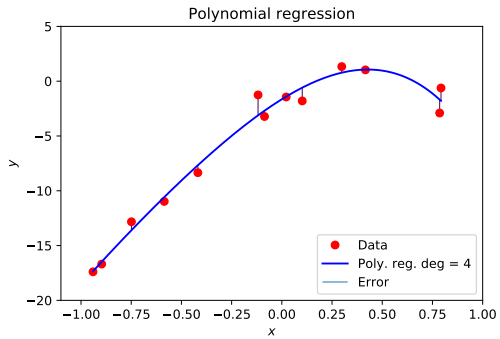
Polynomial regression

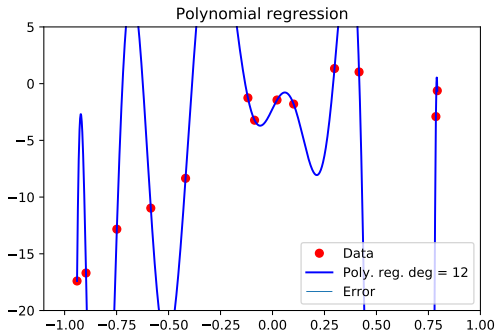
- The linear regression algorithm can be generalised to include all polynomial functions instead of just the linear ones.
- Moving to degree two we obtain: $\hat{y} = b + w_1 x + w_2 x^2$.
  - **This can be seen as adding a new feature x^2.**
  - In fact, we can generalise this approach to create all sorts of hypothesis spaces, e.g.: $\hat{y} = b + w_1 x + w_2 \sin(x) + w_3 \sqrt{x}$.
- The **output** is still a **linear** function of the parameters, so it can be fitted with least squares.

Polynomial regression

A comparison of a linear, degree-4, and degree-12 polynomials as predictors

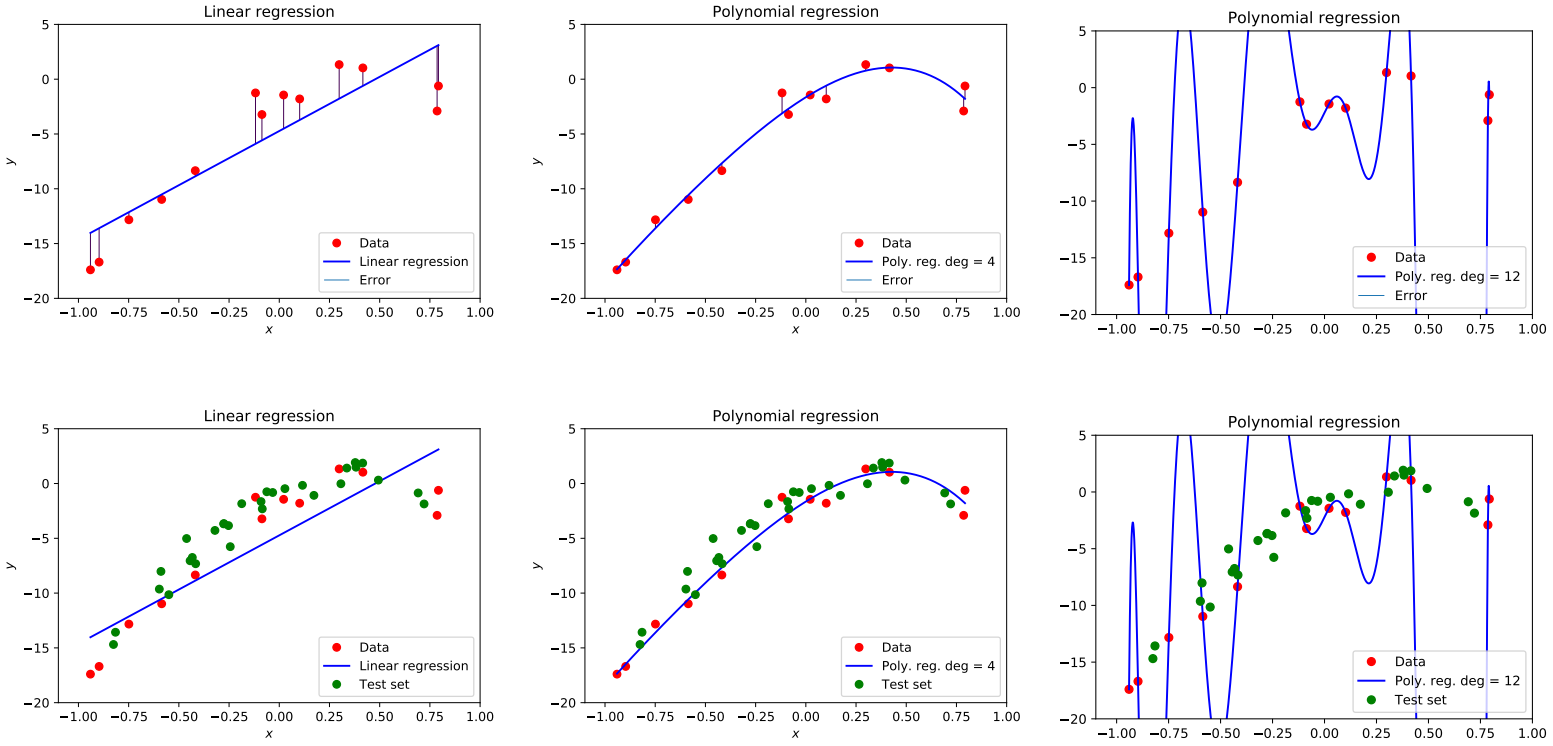






Polynomial regression

A comparison of a linear, degree-4, and degree-12 polynomials as predictors

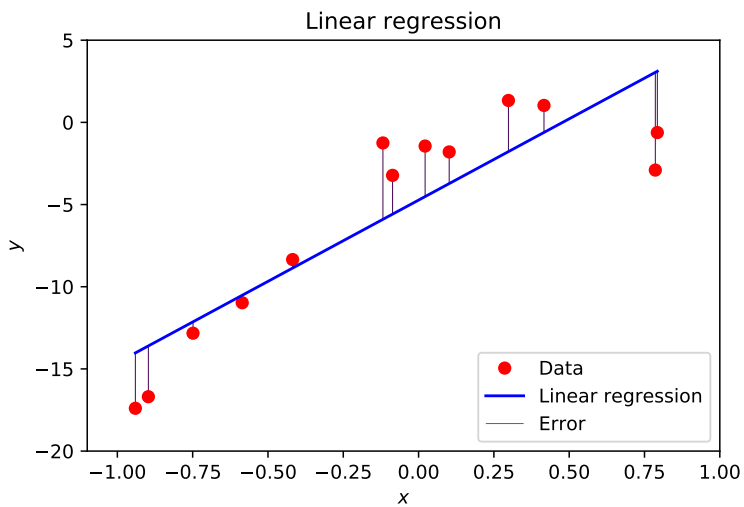


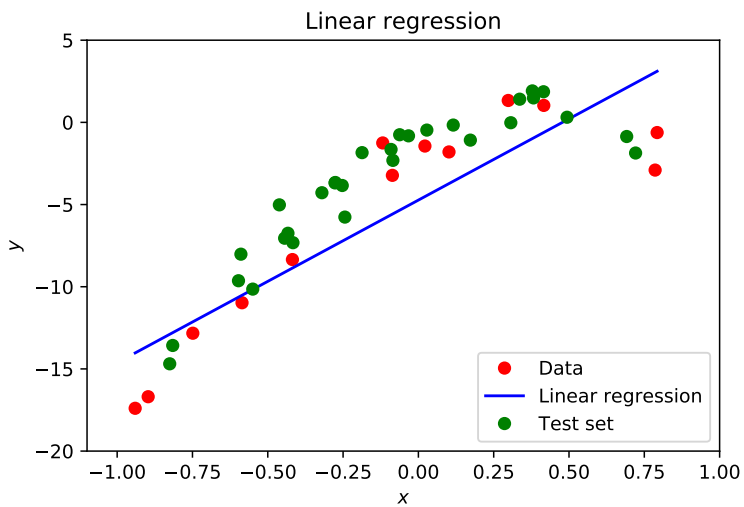
Generalisation

- The central challenge in machine learning is to design an algorithm that will **perform well on new data** (different from the training set data).
- This ability is called **generalisation**.

Generalisation

- During the training (learning) we aim at reducing the training error.
- If that is the end goal, we only have an optimisation problem, not a machine learning one.





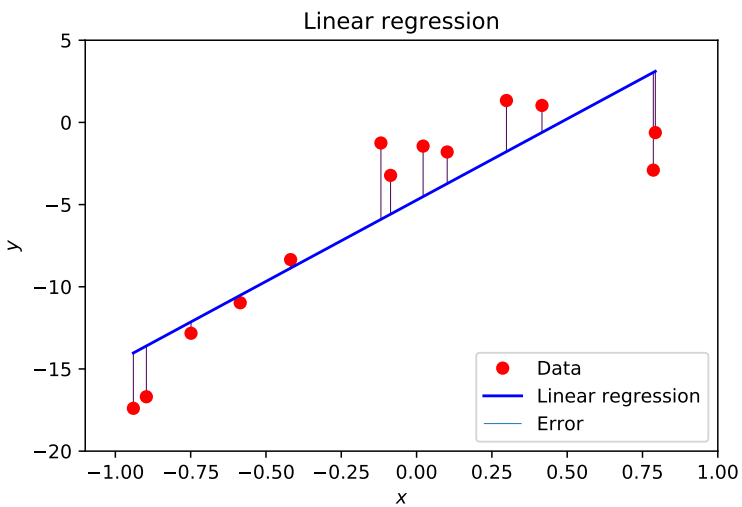
Example: Linear regression

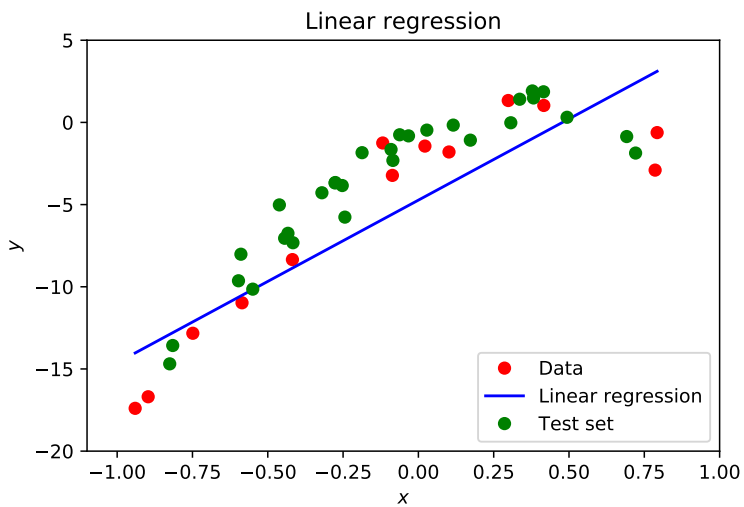
- Previously, we trained the model by minimising the training error

$$\frac{1}{m^{(\text{train})}} \left\| \boldsymbol{X}^{(\text{train})} \hat{\boldsymbol{w}} - \boldsymbol{y}^{(\text{train})} \right\|_2^2$$

- We would like actually to minimise the test error

$$\frac{1}{m^{(\text{test})}} \left\| \boldsymbol{X}^{(\text{test})} \hat{\boldsymbol{w}} - \boldsymbol{y}^{(\text{test})} \right\|_2^2$$





Statistical learning theory

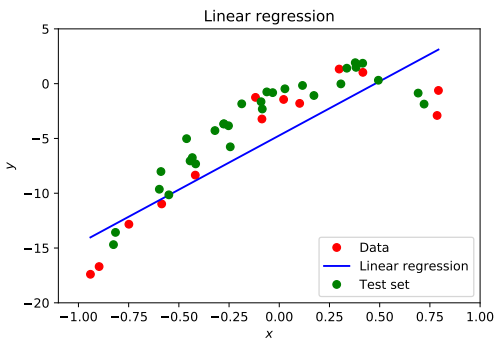
- **Statistical learning theory** provides methods to mathematically reason about the performance on the test set although we can observe only the training set.
- This is possible under some assumptions about the data sets
  - The training and test data are generated by drawing from a probability distribution over data sets. We refer to that as **data-generating process**.
  - **i.i.d. assumptions**
    - Examples in each data sets are **independent** from each other.
    - The training data set and the test data set are **identically distributed**, i.e., drawn from the same probability distribution.

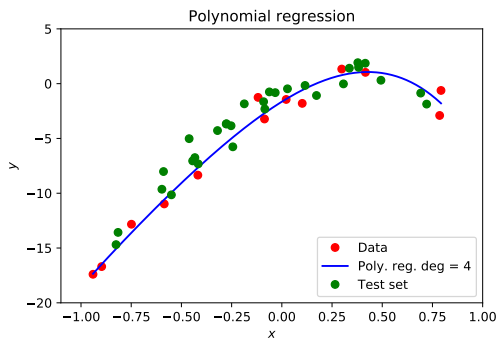
Underfitting and overfitting

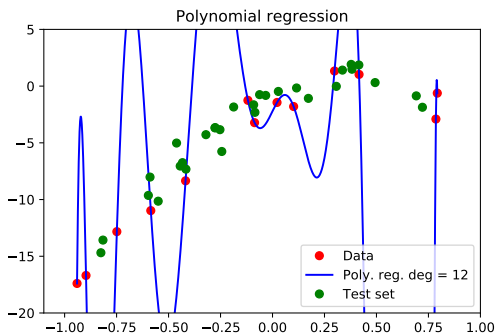
- The factor that determines how well a machine algorithm will perform is its ability to
  1. Make the training error small.
  2. Make the difference between the training and test error small.
- These two factors correspond to the two central challenges in machine learning: **underfitting** and **overfitting**.

Underfitting and overfitting in polynomial estimation

- Models with low capacity are not up to the task.
- Models with high-capacity can solve a complex task, but when the capacity is too high for the concrete (training) task there is the danger of overfitting.



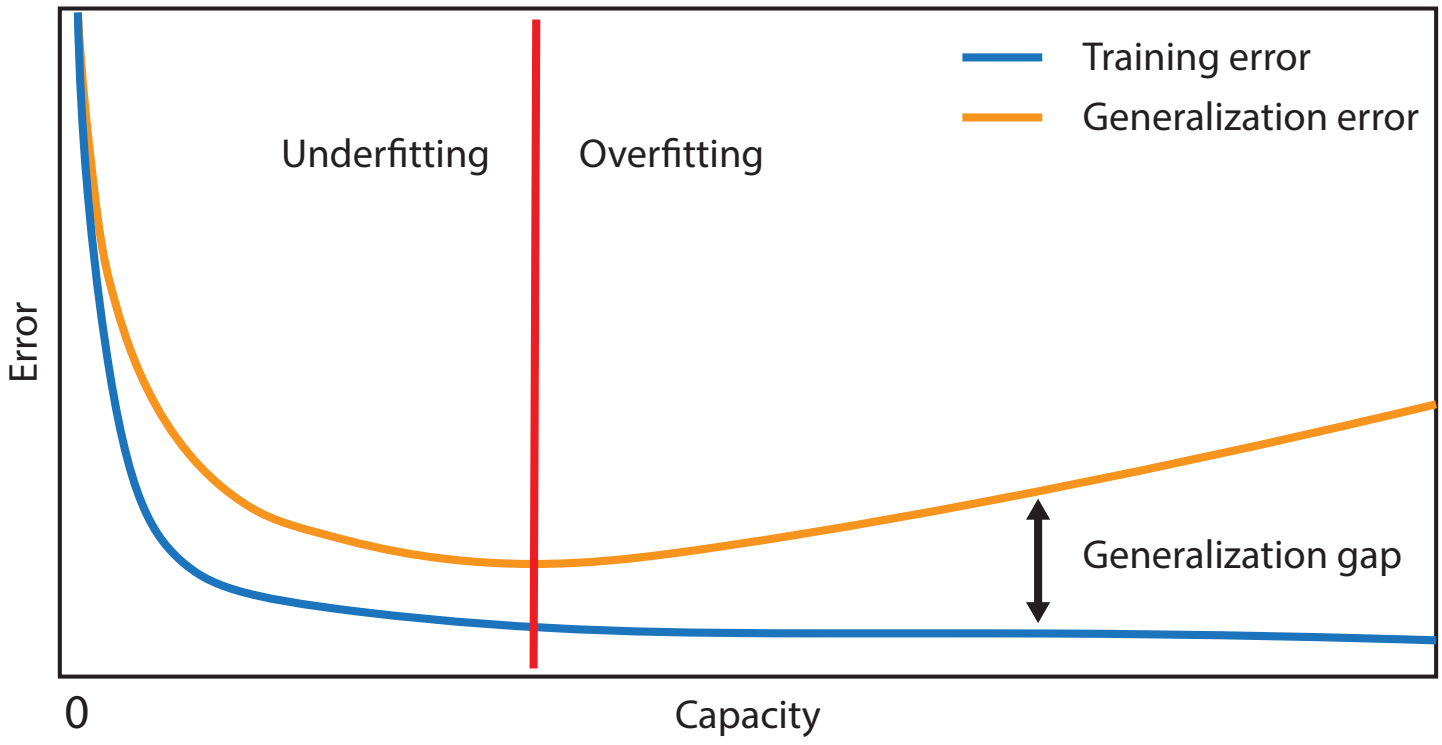




Generalisation and capacity

- Simpler functions generalise more easily, but we still need to choose a sufficiently complex hypothesis (function) to obtain small training error.
- Typically training error decreases with the increase of the model capacity until an (asymptotic) value is reached.
- The generalisation error is U-shaped with the capacity range split in an underfitting and an overfitting zone.

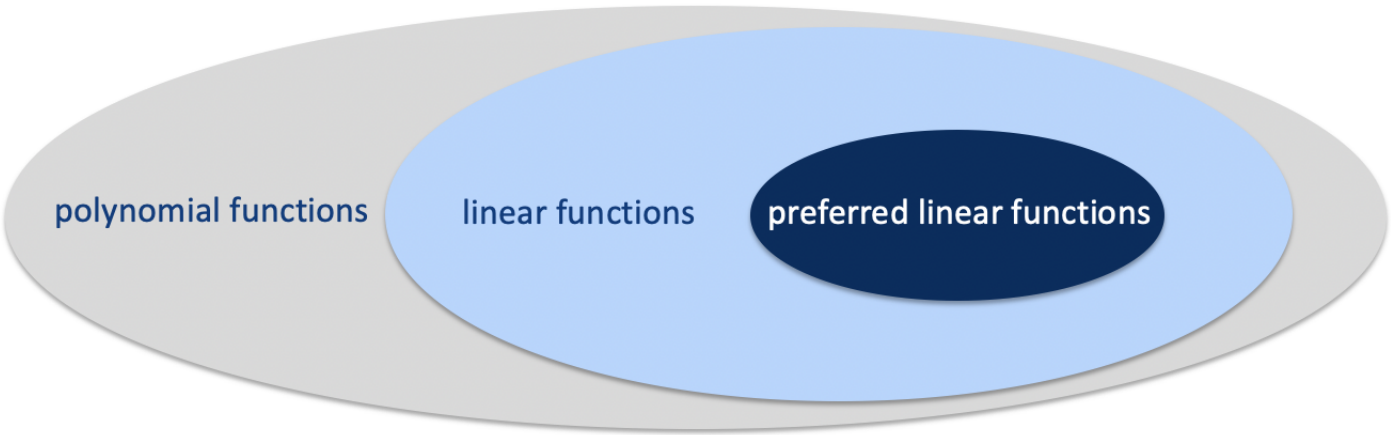
Generalisation and capacity



Regularisation

- In addition to increasing and decreasing of the hypothesis space, i.e., the capacity, we can influence the learning algorithm by **giving preference to one solution over another in the hypothesis space**.
- E.g., prefer smaller weights $\mathbf{w}$:

$$L(\mathbf{w}) = RSS(\mathbf{w}) + \lambda \mathbf{w}^\intercal \mathbf{w}$$



Summary

- Machine learning studies algorithms that learn from examples instead of relying on manually written rules.
- The linear model is conceptually simple but practically useful and can be seen as the basic building block of neural networks.
- The central challenge in machine learning is to find a model that will perform well on new data. This ability is called generalisation.