IMS135 Machine learning and data-driven modelling in mechanics

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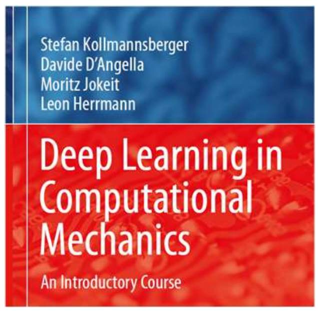
Aim:
The course includes evaluation and application of machine learning and data-driven modelling for problems in mechanics, solid mechanics and fluid dynamics.

Main course book:



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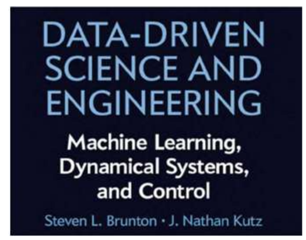

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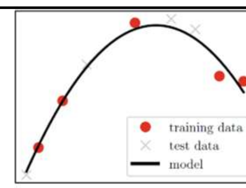
Week 1-4:

"Traditional course", lectures and tutorial sessions (mainly supervision)

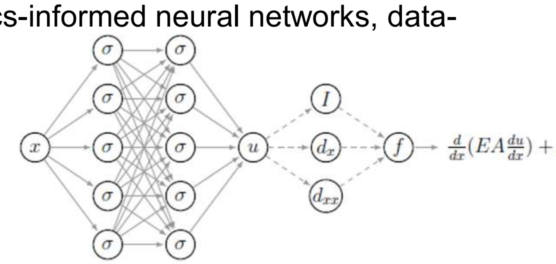


From the main book

machine learning, optimization techniques, regularization, neural networks, activation functions, deep learning, automatic differentiation, physics-informed neural networks, data-driven inference, data-driven identification

Complemented with

singular value decomposition, reduced order model, model discovery…



Python programming, PyTorch

Assessment 4.5hp:
computer assignment: model reduction, presentation in front of screen, before w3
exam 4.5hp (in computer room with Python)

Supervisors: Johan Friemann(johan.friemann@chalmers.se), Lars Davidson (lada@chalmers.se), Magnus Ekh (magnus.ekh@chalmers.se)

Syllabus for IMS135 Machine learning and data-driven modelling in mechanics (instructure.com)

IMS135 Machine learning and data-driven modelling in mechanics

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Week 5-8:

Projects where methods are applied to mechanics

Solid mechanics

Fluid mechanics

***A*ssessment:** project presentations 3hp

Supervisors: Magnus Ekh, Johan Friemann, Lars Davidson, …

AI: simulation of human intelligence processes by machines/computer systems that can perform tasks that typically require human intelligence. E.g. understanding natural language, recognizing patterns, solving complex problems, making decisions, and learning from experience.

ML: enables machines to learn and improve from experience (large datasets) to make predictions/decisions. It's about developing algorithms and models that allow computers to learn patterns from data and make predictions or decisions based on that learning.

Deep Learning is a subfield of machine learning and artificial intelligence that focuses on creating and training neural networks with many layers, also known as deep neural networks. The term "deep" refers to the depth of the network, meaning the number of layers it has.

Machine learning algorithm relies on a large amount of data that is observed in nature, handcrafted by humans, or generated by another algorithm

1. dataset
2. cost function
3. optimization procedure
4. parameterized model

Burkov. *The Hundred-Page Machine Learning Book*

2.2 Data structure

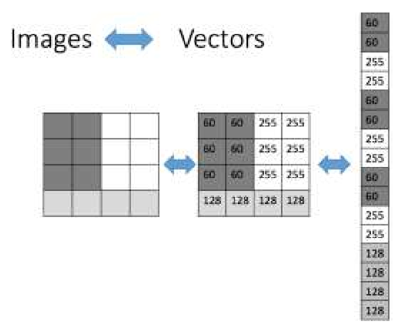
Design matrix

$$
X = \begin{array}{c} \\ \text{example } 1 \\ \text{example } 2 \\ \vdots \\ \text{example } m \end{array}
\begin{array}{c}
\begin{array}{cccc} \text{feature } 1 & \text{feature } 2 & \cdots & \text{feature } n \end{array} \\
\left[\begin{array}{cccc} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{array}\right]
\end{array}
$$

Example:

- snapshots of temperature/displacement/velocity/ … field

Example: grey scale images, 50x50 pixels -> row/column with 2500 features



2.2 Data structure

Design matrix

$$X = \begin{array}{c} \\ \text{example } 1 \\ \text{example } 2 \\ \vdots \\ \text{example } m \end{array} \begin{array}{c} \begin{array}{cccc} \text{feature } 1 & \text{feature } 2 & \cdots & \text{feature } n \end{array} \\ \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix} \end{array}$$

Data is divided into subsets:
- training set (usually 90%)
- test set (usually 10%).

Important with test set for model predictions and measure of model performance.

2.3 Types of learning

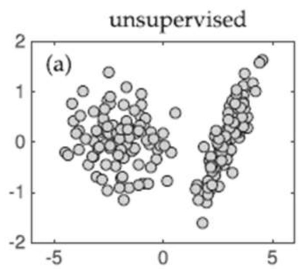
Supervised learning (most common):
-the algorithm is processing a labeled dataset. Next to the design matrix,
the data set comprises a output data (labels/values) for each example/snapshot.

Examples of the input and output of a desired model are explicitly given, and regression methods are used to find the best model for the given output data, via optimization.
This model is then used for prediction/classification using new data.

Example see introduction.ipynb

Unsupervised learning:

to find a structure or, more precisely, the probability distribution in the provided data. The data is not labeled and therefore no explicit prediction is possible. However, it can be very useful to apply unsupervised learning to large datasets in order to find inherent structures or repeating patterns in the data.



Example see introduction.ipynb

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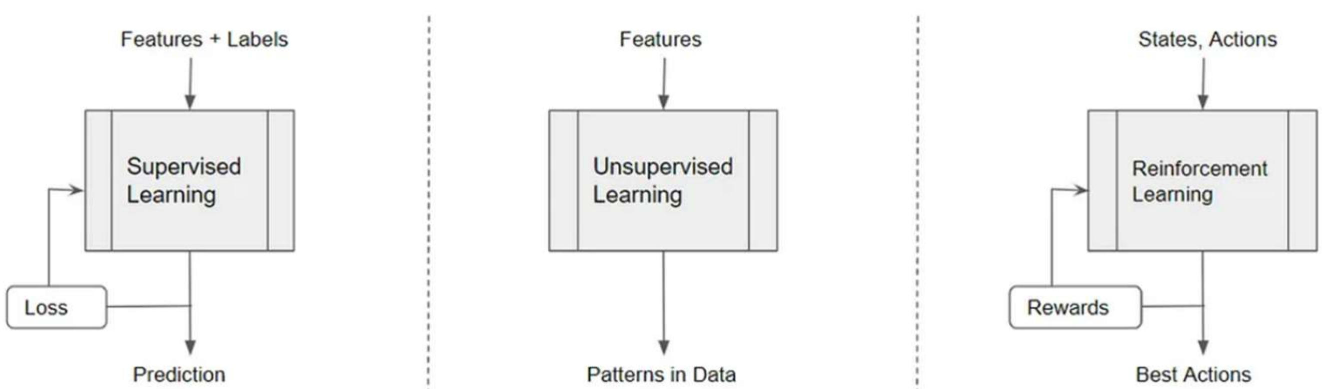
Reinforcement learning
An algorithm that interacts with an environment to learn a certain decision behavior maximizing the expected average reward [Bur19]. It is used for problems involving sequential decision-making in order to fulfill a long-term goal.



From: towardsdatascience.com

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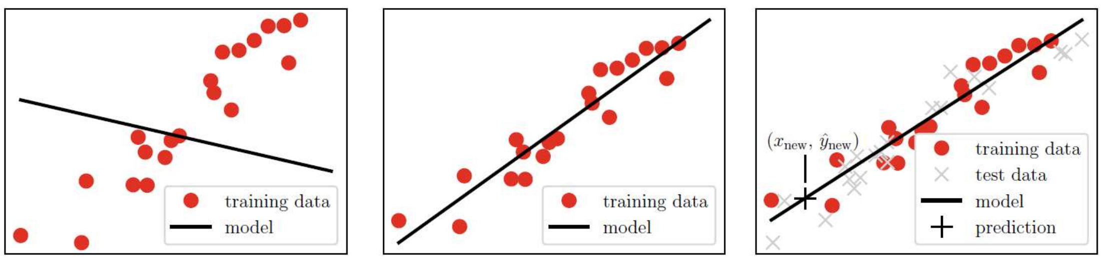
2.4 Machine learning tasks

Regression:
Regression is a supervised learning problem with the goal of predicting a numerical value. Basically, a regression algorithm outputs a function that maps a given input to an output, usually in form of a real number. An example is the prediction of house prices based on certain criteria like the area, number of rooms, or the age of the house.

2.5 Example: Linear Regression 11



(a) Untrained model **(b)** Trained model **(c)** Prediction

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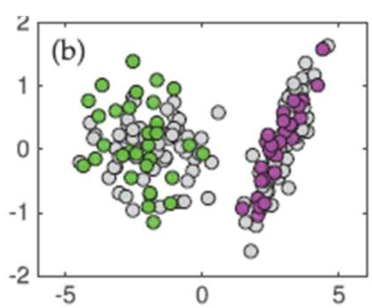
Classification:
A type of **supervised learning**. Instead of a numerical value, their output takes on a discrete form. In other words, a classification algorithm returns a function that assigns a category to the provided input. Logistic regression, support vector machines and decision trees.



Green and purple data = labelled training data

Goal: Classify grey data as green or purple

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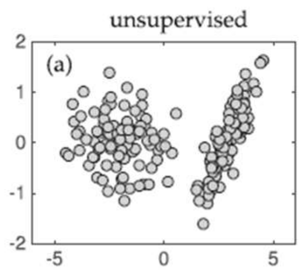
Clustering:

Clustering differs from classification and regression as it is an **unsupervised learning** task. The algorithm gives feedback about which parts of the data share similarities and therefore belong to the same cluster. A popular choice for clustering is the k-means algorithm that divides the incoming data into k different clusters of examples being close to each other.

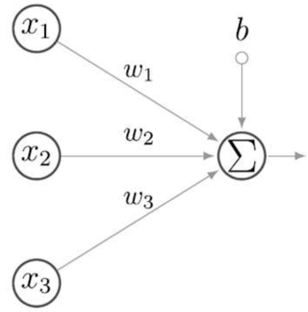


Find cluster for data (not labelled) to classify them

Planning of course:

- Dimensional reduction: singular value decomposition, principal component analysis, model reduction
- Regression, optimization
- Neural networks
- Physics informed neural networks
- Model discovery
- Projects

2.5 Example: Linear Regression



$$\hat{y} = \underbrace{w_1 x_1 + w_2 x_2 + w_3 x_3 + b}_{\underset{\sim}{w}^T \underset{\sim}{x} + b}$$

$\underset{\sim}{x}$ = input vector / features

$\hat{y}$ = target / output

$\left.\begin{array}{l} \underset{\sim}{w} = \text{weights (importance of features)} \\ b = \text{bias} \end{array}\right\}$ model parameters

Model performance

e.g. Mean Square Error $= \frac{1}{m} \sum_{i=1}^{m} (y_i - \hat{y}_i)^2 \approx$ cost function C

m = number of data points $\underset{\sim}{x}_i, y_i$ (snapshots)

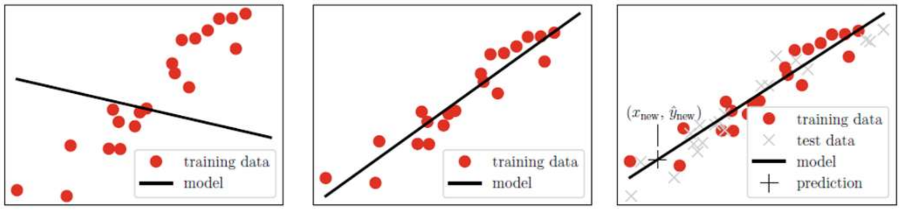
$$C(\underset{\sim}{w}, b) = \frac{1}{m} \sum_{i=1}^{m} \left(y_i - (\underset{\sim}{w}^T \underset{\sim}{x}_i + b)\right)^2$$

$$\Rightarrow \underset{\sim}{w}^*, b^* = \arg\left(\min C(\underset{\sim}{w}, b)\right)$$

Machine learning: use only training data points

$$\rightsquigarrow C(\underset{\sim}{w}, b) = \frac{1}{m_{train}} \sum_{i=1}^{m_{train}} \left(y_i - (\underset{\sim}{w}^T \underset{\sim}{x}_i + b)\right)^2$$

and test the error $\frac{1}{m_{test}} \sum_{i=1}^{m_{test}} \left(y_i^{(test)} - (\underset{\sim}{w}^T \underset{\sim}{x}_i^{(test)} + b)\right)^2$



(a) Untrained model (b) Trained model (c) Prediction

Fig. 2.2 Linear regression example. Left: The initial model does not fit the training data. Middle: Shows the model properly fitted to the training data. Right: The trained model is used to make a prediction $\hat{y}_{\mathrm{new}}$ for an unknown example x_{new}. Figures are inspired by [GBC16]