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Machine learning – Block 1(a)

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Autumn 2022

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This block

- What is AI and Machine Learning?
- Course Information and Practicalities
- Introduction to Supervised Learning
- (Stochastic) Gradient Descent
- Regularization

Section 1

What is AI and ML?

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What exactly is machine learning and artificial intelligence?

The word "AI" is often used quite loosely:

> To briefly explain how Linear Regression helped us reverse engineer the BSR equation, let's break it down. Linear Regression is an AI equation that finds the proper coefficients for an equation by sorting through massive amounts of data. The equation looks something like BSR = X(a)+ Y(b) + Z(c)..... and so and and so forth.

What is Artificial Intelligence?

Artificial intelligence (AI), sometimes called machine intelligence, is intelligence demonstrated by machines, unlike the natural intelligence displayed by humans and animals. – Wikipedia

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What is Artificial General Intelligence?

Artificial general intelligence (AGI) is the hypothetical intelligence of a machine that has the capacity to understand or learn any intellectual task that a human being can. – Wikipedia

Also called:

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Artificial super intelligence (ASI) is "any intellect that greatly exceeds the cognitive performance of humans in virtually all domains of interest" – Nick Bostrom

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What is Machine Learning?

Machine Learning is the field of study that gives the computer the ability to learn without being explicitly programmed. – Arthur Samuel (1959)

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E. – Tom Mitchell (1998)

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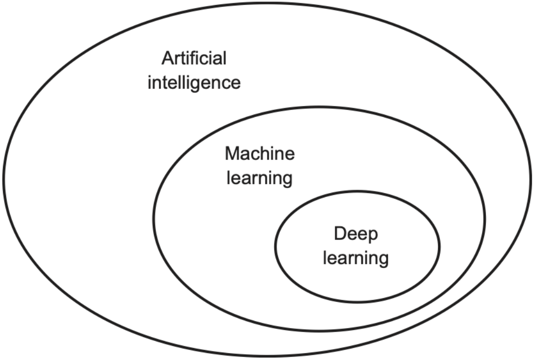
Learning from data. – Hastie, Tibshirani, Friedman (2009)

What is Machine Learning?

Figure: ML, AI and DL (Chollet, 2018, Figure 1.1)



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- What is AI and ML?
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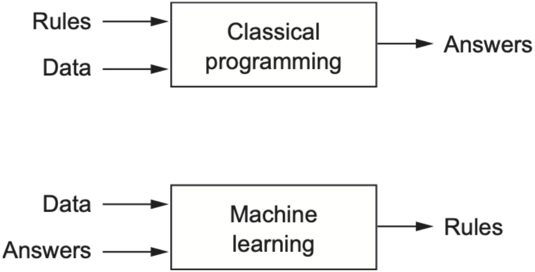
  - Example: Logistic regression
- Optimization in Machine Learning

Computer Science and Machine Learning

Figure: A new paradigm? (Chollet, 2018, Figure 1.2)



Statistics and Machine Learning

Figure: Regression vs. Pure Predictions (Efron, 2020, Table 5)

Table 5. A comparison checklist of differences between traditional regression methods and pure prediction algorithms.

	Traditional regressions methods	Pure prediction algorithms
1.	Surface plus noise models (continuous, smooth)	Direct prediction (possibly discrete, jagged)
2.	Scientific truth (long-term)	Empirical prediction accuracy (possibly short-term)
3.	Parametric modeling (causality)	Nonparametric (black box)
4.	Parsimonious modeling (researchers choose covariates)	Anti-parsimony (algorithm chooses predictors)
5.	**x** $p \times n$: with $p \ll n$ (homogeneous data)	$p \gg n$, both possibly enormous (mixed data)
6.	Theory of optimal inference (mle, Neyman–Pearson)	Training/test paradigm (Common Task Framework)

Different names for the same things

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  4. Weights (ML) vs. Parameters (Stats)
  5. Features (ML) vs. Covariates (Stats)

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Different flavors of ML

- Supervised learning
- Unsupervised learning
  - Self-(un)supervised learning
- Reinforcement learning

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Questions?

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Section 2

Course information

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The aims of this course are that you should:

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1. get a good knowledge of a large number of machine learning models,
2. become able to use methods for evaluating and improving predictive models,
3. become able to handle big data,
4. become able to train and use machine learning models in R,
5. become able to train and use neural networks using Keras/TensorFlow.
6. become able to describe and discuss ethical aspects of big data and black box-models,

Course Outline

Two main parts:

- Core Content (8 lecture blocks):
  - Supervised learning (5 blocks)
    - Introduction, statistical learning (1 block)
    - Tree-based methods (1 block)
    - Neural Networks (3 block)
  - Unsupervised learning (2 blocks)
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Exact dates and details; see the course page.

Core Content

- Each block consist of:
  - Online video material (optional)
  - Reading assignments (approx. 2-4h, 50-90 pages a week)
  - One-two Lecture(s) (optional)
  - An individual computer assignment (approx. 14-16h).
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- Reading: Mandatory and optional (overlap)
- Recommended workflow for each block
  - Do the reading assignments
  - Watch the videos (optional)
  - Attend the lecture (optional) to ask questions.
  - Do the computer assignment
  - Attend the zoom lab session (optional) to ask questions.

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- Present overall theory, concepts and content (overview)

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  5. Väinö Yrjänäinen, UU (word embeddings)

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- Each assignment has an extra (VG) task worth 1 VG point.
- The mini-project is worth 2 VG-points (if it is passed with distinction).
- Ph.D. students: I suggest you get VG to pass the course. Make the project a potential paper.
- Reassesment of grades (supply form to course admin)
- Failing the course: You will need to redo all assignments and mini-project.

Computer Assignments

- Main part of the course
  Learning by doing
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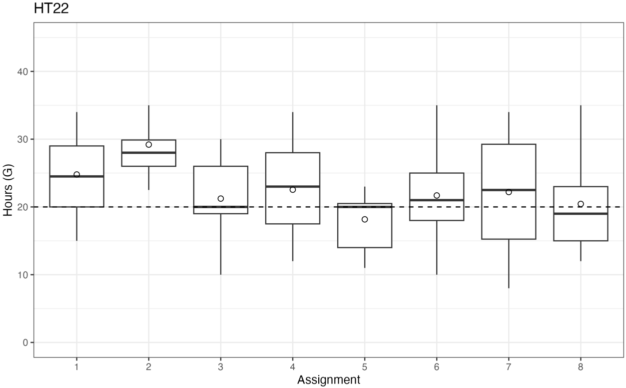

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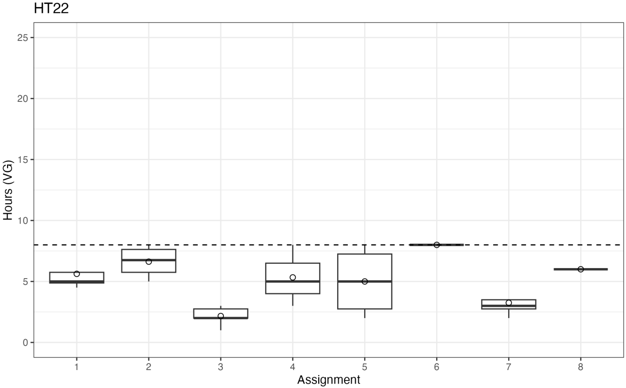
Figure: Workload last year to pass with distinction (VG)



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- Recommended data: Images, text or tabular data.
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- Mini-project and master thesis:
  - The mini-project can be used to explore thesis project
  - Master thesis proposals in November

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Practicalities

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Course improvements since last year

- More even (and lower) burden (hopefully)
- General updates of unclear parts in assignments
- Added points to the assignments.
- *Note!* There can be some new bugs after these updates.
- New lectures (and maybe VG-assignments) on generative AI (mainly LLMs)

Questions?

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Section 3

Introduction to Supervised Learning

Supervised learning

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- What is AI and ML?
- Course information
- Introduction to Supervised Learning
  - — Example: Logistic regression
- Optimization in Machine Learning

Figure: Relationship between appartment size and price (source)

Problem: We want to predict the price of a new apartment.

Supervised learning

- General problem: We have *training* data

$$\mathbf{d} = \{(y_i, \mathbf{x}_i), i = 1, ..., n\}.$$

- $\mathbf{x}_i$ = features/input/predictors/features/independent variables
- y_i = labels/output/dependent variable
- We want to *learn* a function $\hat{y} = f(x_{new})$ with as good performance as possible.

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- We want to *learn* a function $\hat{y} = f(x_{new})$ with as good performance as possible.
- Regression problems: $y_i \in \mathbb{R}$
- Classification problems: $y_i \in a, b, c, ...$ where $a, b, c...$ are discrete classes.

Example of supervised problems

Any examples of applications?

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Logistic regression is a workhorse for classification problems.

Logistic regression

When analysing binary data $y_1, \dots, y_N$, we usually assume that the Y_i follow binomial (or Bernoulli) distributions.

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$$g(\pi_i) = \log\left(\frac{\pi_i}{1-\pi_i}\right),$$

called the logit or log odds.

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- A GLM using this link function is called logistic regression, but other link functions are also often used in practice. Many times we use likelihood functions

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Logistic regression

There are two equivalent formulas for logistic regression:

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_0+\beta_1 x_{i1}+\beta_2 x_{i2}+\cdots+\beta_p x_{ip}, \qquad i = 1,\ldots,N$$

and

$$\pi_i = \frac{\exp\left(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}\right)}{1+\exp\left(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}\right)}.$$

Logistic regression: Prediction

- We *train* a logistic regression model using MLE using the training data.
- Our estimation/traing output the MLE $\hat{\theta}$
- We the compute $\hat{p}_i = g^{-1}(\hat{\theta} x_{new})$ a for a new observation
- We use a decision rule to predict value 0 or 1:

$$\hat{y}_i(\hat{p}_i) = \begin{cases} 1, & \text{if } \hat{p}_i \geq 0.5 \\ 0, & \text{otherwise} \end{cases}$$

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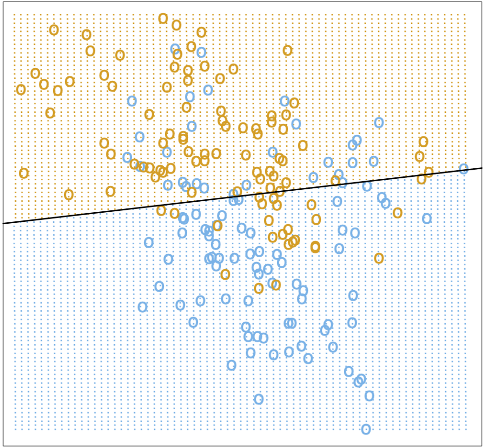
- What is AI and ML?
- Course information
- Introduction to Supervised Learning
  - Example: Logistic regression
- Optimization in Machine Learning

Logistic regression: Example

Figure: Decision boundry with two covariates (Hastie et al, 2009, Figure 2.1)



An example: Spam and Ham

E-mail Spam
An e-mail provider what to help classify e-mails as spam (1) or ham (0). They have many previous e-mails that customers have already classified as spam, and e-mails people have responded (ham). They want to predict if a new, unseen e-mail is spam or ham.

Questions?

Questions?

Section 4

Optimization in Machine Learning

Training of ML algorithms

1. Training is usually done by minimizing the objective/loss/cost function $L(\theta)$ for $\theta \in \mathbf{R}^P$.
2. Example: Logistic regression, here we can use the negative log-likelihood as loss function:

$$L(\theta, \mathbf{y}, \mathbf{X}) = -\log \prod_{i=1}^{N} p_i^{y_i} (1 - p_i)^{1-y_i} \,,$$

where

$$\log \frac{p_i}{1 - p_i} = \mathbf{x}_i \theta \,,$$

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3. In Machine Learning: P and N might be very large...

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Gradient Decent

1. The workhorse of Machine Learning

$$\theta_t = \theta_{t-1} - \eta \nabla L(\theta_{t-1}, \mathbf{X}, \mathbf{y}),$$

where

$$\nabla f(p) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(p) \\ \vdots \\ \frac{\partial f}{\partial x_n}(p) \end{bmatrix}$$

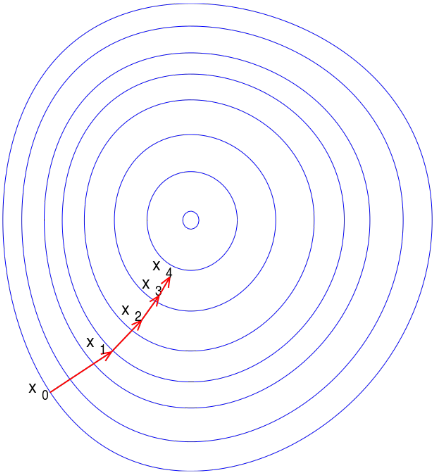
2. $L(\theta)$ needs to be differentiable

Gradient Descent Analogy

Figure: Gradient Descent Analogy (source)

Gradient Descent (cont.)

Figure: Gradient Descent (source)



Why Gradient Descent?

- Gradient Descent is a poor algorithm
  (Newtons method, Iteratively Reweighted Least Squares are 'better')
- So why is gradient descent relevant?

Why Gradient Descent?

- Gradient Descent is a poor algorithm
  (Newtons method, Iteratively Reweighted Least Squares are 'better')
- So why is gradient descent relevant?
- The two benefits with Gradient Descent:
  1. Only uses the gradient—scales to large P
  2. Can scale to large data with Stochastic Gradient Descent—scales to large N

Stochastic Gradient Descent

- Many loss functions (and gradients) are a sum over N observations (e.g. log-likelihoods).
- We can estimate $\nabla L(\theta, X_i, y_i)$ by choosing a random observation (with index i)

$$E(\nabla L(\theta, X_i, y_i)) = \frac{1}{Z}\nabla L(\theta, \mathbf{X}, \mathbf{y}),$$

  for some constant Z.
- Goal – we want to estimate a total.
- This give us the following algorithm:

$$\theta_t = \theta_{t-1} - \eta_t \hat{\nabla} L(\theta_{t-1}, X_i, y_i),$$

  where i is random sampled index.
- *Note!*
  We need to have an unbiased estimator for $\nabla L(\theta, \mathbf{X}, \mathbf{y})$
- What is an iteration?

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- What is an iteration?
- Epochs vs. Iterations

Stochastic Gradient Descent

- Learning rate η_t is important
- Will it converge to an optimum?

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Stochastic Gradient Descent

- Learning rate η_t is important
- Will it converge to an optimum?
- We need to reduce η_t over time
- Robbins–Monro (1951) conditions:
  1. $\eta_t \geq 0 \ \forall t \geq 0$
  2. $\sum_t^\infty \eta_t = \infty$
  3. $\sum_t^\infty \eta_t^2 < \infty$

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Mini-batch gradient descent

- Can we estimate the gradient better?

Mini-batch gradient descent

- Can we estimate the gradient better?
- We take a mini-batch of size B:

$$\theta_t = \theta_{t-1} - \eta_t \nabla L(\theta, \mathbf{X}_{(S)_i}, y_{(S)_i}),$$

  where $(S)_i$ is a set of random sample (without replacement) indices and $|(S)_i| = B$.
- B is usually set to optimize hardware

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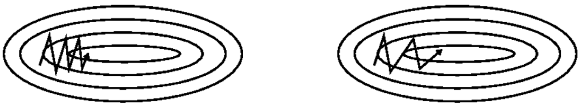
SGD with momentum

- SGD can be slow to converge due to 'jumping' behaviour
- Can improve behaviour using momentum – the rolling mean of gradients
- Additional hyperparemeter α to control the momentum

$$m_t = \alpha m_{t-1} + \eta_t \hat{\nabla} L(\theta_{t-1}, X_i, y_i)\,,$$

$$\theta_t = \theta_{t-1} - m_t,$$

Figure: SGD with momentum



(a) SGD without momentum (b) SGD with momentum

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SGD with momentum, Intuition

Figure: SGD with momentum, Intuition (CC)

SGD with momentum

Example of SGD with momentum here.

Adaptive Moment Estimation (Adam)

- Adapt η_t to individual parameters

$$m_t = \beta_1 m_{t-1} + (1-\beta_1)\hat{\nabla} L(\theta_{t-1}, X_i, y_i)$$
$$v_t = \beta_1 v_{t-1} + (1-\beta_2)\hat{\nabla} L(\theta_{t-1}, X_i, y_i)^2$$

- Bias correction

$$\hat{m}_t = \frac{m_t}{1-\beta_1}$$
$$\hat{v}_t = \frac{v_t}{1-\beta_2}$$

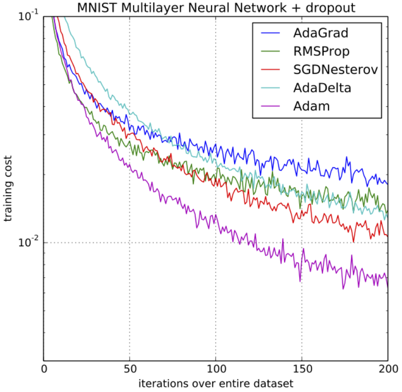
- Update

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon}\hat{m}_t,$$

- Common values: $\beta_1 = 0.9$, $\beta_2 = 0.999$, and $\epsilon = 10^{-8}$
- RMSprop is another (similar) alternative

Adam

Figure: The Adam Optimizer (Kingma and Ba, 2014)



For convergence proofs, see:
Defossez et al (2020) A Simple Convergence Proof of Adam and Adagrad