Machine learning – Block 1(a)

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Department of Statistics, Uppsala University

Autumn 2022

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?

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

Artificial intelligence (AI), the ability of a digital computer or computer-controlled robot to perform tasks commonly associated with intelligent beings. – Encyclopedia Brittanica

What is Artificial General Intelligence?

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

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:

1. Strong AI
2. General AI
3. Full AI

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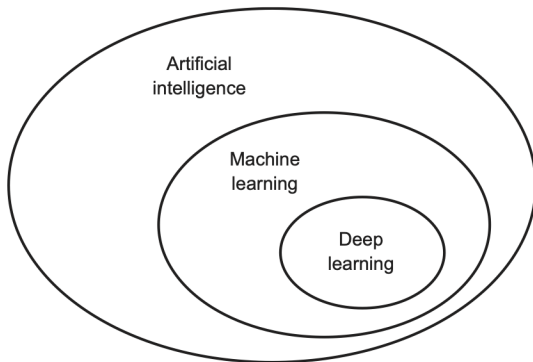
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Learning from data. – Hastie, Tibshirani, Friedman (2009)

What is Machine Learning?

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

Computer Science and Machine Learning

Figure: A new paradigm? (Chollet, 2018, Figure 1.2)
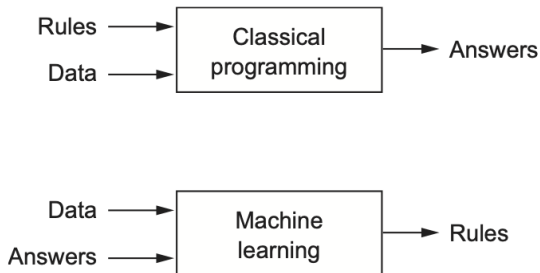
Statistics and Machine Learning

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.	$\mathbf{x}$ $p \times n$: 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)

Different flavors of ML

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

Questions?

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Section 2

Course information

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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 (1 block)
    - Tree-based methods (1 block)
    - Neural Networks (3 block)
  - Unsupervised learning (2 blocks)
  - Reinforcement learning (1 block)

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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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  6. 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.

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  Learning by doing

- Machine learning = Statistics + Computer Science
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- We will mark and return each assignment within 10 working days.

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- Course information
- Introduction to Supervised Learning
  - Example: Logistic regression
- Optimization in Machine Learning

Figure: Workload last year to pass (G)

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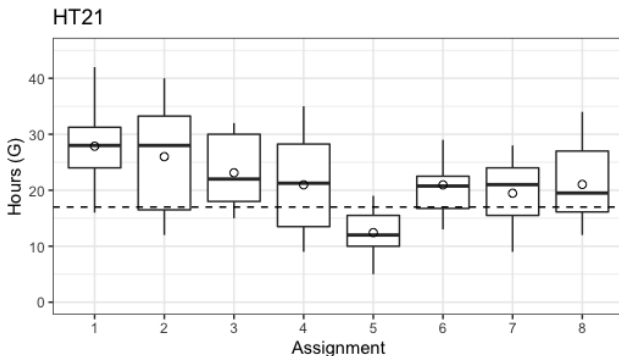 — Example: Logistic
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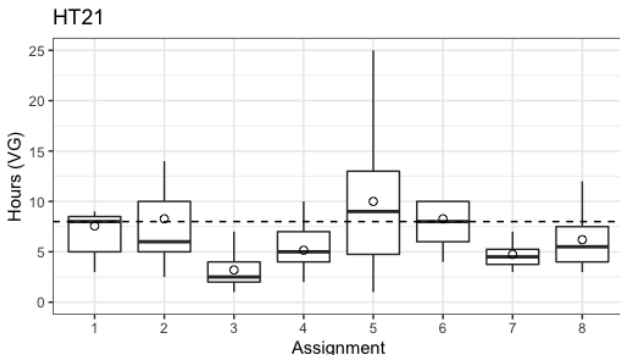
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- Project oral presentation (10-15 minutes)

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- The project should result in a 4 page report (PDF) using the ICML LaTeX template (see course page).
- Project oral presentation (10-15 minutes)
- Mini-project and master thesis:
  - The mini-project can be used to explore thesis project
  - Master thesis proposals in November

Practicalities

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- If the course is too easy - reach out to me!

Course improvements since last year

- More even (and lower) burden (hopefully)
- General updates of unclear parts in assignments
- *Note!* There can be some new bugs after these updates.
- Three Zoom sessions Wednesday-Friday (1h) instead of a 2h session on campus
- Introduction to each assignment the first Zoom session.
- Industry guest lecture (Erik Fredlund)
- More on AI and fairness (Holli Sargeant)

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Section 3

Introduction to Supervised Learning

Supervised learning

Figure: Relationship between appartment size and price (source)

Ground living area partially explains sale price of apartments

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
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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

- Is this e-mail message spam (1) or not (0)?

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Logistic regression and classification

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Logistic regression is a workhorse in classification problems.

Logistic regression

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

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

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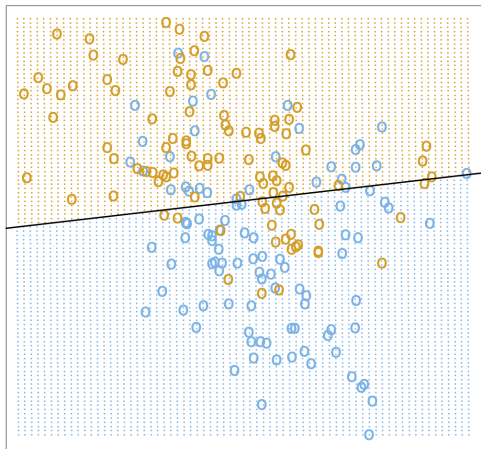
Logistic regression: Prediction

- 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:

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

Logistic regression: Example

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

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.

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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...

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)
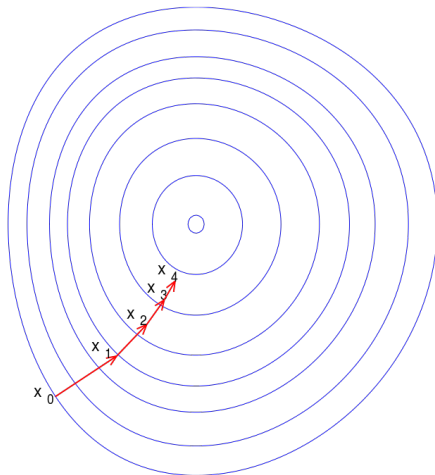
Why Gradient Descent?

- Gradient Descent is a poor algorithm
  (Newtons method, Iteratively Reweighted Least Squares
  are 'better')

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Why Gradient Descent?

- Gradient Descent is a poor algorithm
  (Newtons method, Iteratively Reweighted Least Squares
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- 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

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

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. $\sum_t^\infty \eta_t^2 < \infty$

Mini-batch gradient descent

- Can we estimate the gradient better?

Mini-batch gradient descent

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- 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

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

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

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

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