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

Machine learning – Block 1(a)

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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?

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.

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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?

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?

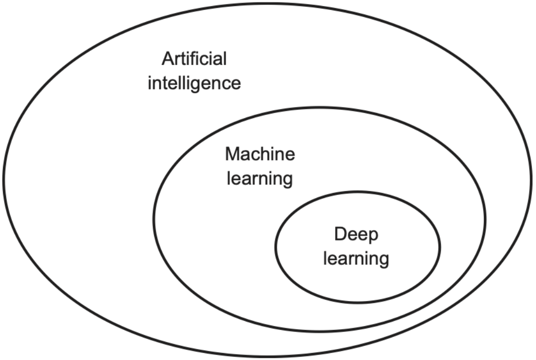
Machine Learning is the field of study that gives the computer the ability to learn without being explicitly programmed. – Arthur Samuel (1959)

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)

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

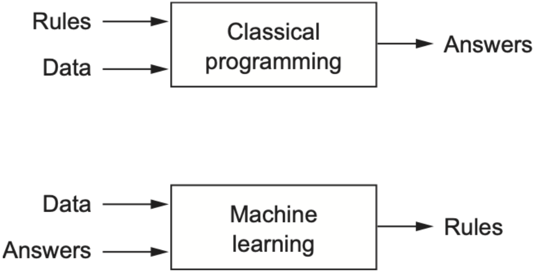
What is Machine Learning?

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

- Machine learning has developed in parallel with Statistics
- Common with different names for the same thing:
  1. Time series classification (ML) vs. Functional data classification (Stats)
  2. Time series regression (ML) vs. Scalar-on-function regression (Stats)
  3. Learning (ML) vs. Estimation (Stats)
  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

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Section 2

Course information

Course information

The aims of this course are that you should:

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)
- Assignments (8 individual assignments)
- Mini-project on a supervised project (2-3 students)

Exact dates and details; see the course page.

Core Content

- One-two lectures/computer labs (approx. 2-4h)
  - Lecture(s): present overall theory and content (overview)
  - Computer labs(s): Hands on help with the assignment if you get stuck. Start before the computer assignment!
- Ask questions!
- Online video material and reading assignments (approx. 2-3h, 50-90 pages a week)
- *Note!* There might be some overlap between reading instructions.
- An individual computer assignment (approx. 14-16h). Deadline Sundays 23.59.
- Recommended workflow for each block
  - Do the reading assignments
  - Attend the lecture (optional) to ask questions!
  - Watch the videos (although, optional)
  - Do the computer assignment

Examination

1. To pass (G): All labs, mini-project, and project review need to be passed (70%)
2. To pass with distinction (VG): 6/10 VG points
3. Each assignment has an extra (VG) task worth 1 VG point.
4. The mini-project is worth 2 VG-points (if it is passed with distinction).
5. Ph.D. students: I suggest you get VG to pass the course. Make the project a potential paper.

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Computer Assignments

1. Main part of the course
   Learning by doing
2. Machine learning = Statistics + Computer Science
   Hence a lot of programming
3. Both implementation of core components and state-of-the-art methods
4. *Warning!* There might be bugs in the assignments! Don't hesitate to ask questions!
5. All labs can be turned in a three times. 2nd deadline last day of course. 3rd deadline approx 2-4 weeks after the course. If failed, resubmit right away!
6. We will mark and return each assignment within 10 working days.
7. *Important!* Don't write your name anywhere and do the assignment evaluation!
8. *Important!* Don't show your assignment to any other student. But feel free to discuss!

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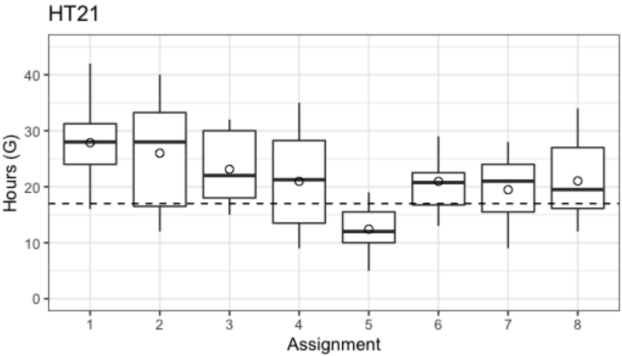
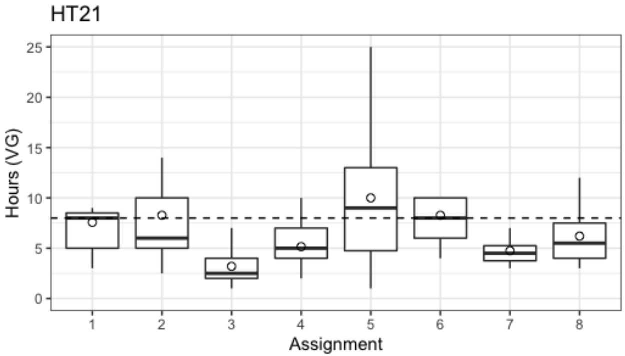
Computer Assignments

Figure: Workload last year to pass (G)



Computer Assignments

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



Mini-project

- See project instructions on webpage for details.
- Supervised problem of choice on real data.
- 2-3 students.
- Supply a half-page project proposal of data and problem at the end of block 6.
- Project will last two weeks (half time) - but start earlier.
- Approximate 40 hours of work *per student*.
- The project should result in a 4 page report (PDF) using the ICML LaTeX template (see course page).
- Project oral presentation (10-15 minutes)

Practicalities

- Course page: Github – please do a PR if something is wrong!
- Acknowledgements: Måns Thulin, Josef Wilzén, Anders Eklund
- Schedule: Time Edit/Studium
- Assignments: Studium
- Literature
  - Hastie, Tibshirani & Friedman (2009). *Elements of Statistical Learning*.
  - Chollet & Allaire (2018) *Deep Learning with R*.
  - Goodfellow, Bengio & Courville (2017) *Deep Learning*.
  - Sutton and Barto (2020) *Reinforcement learning: An introduction*
  - Additional articles, tuturials, videos etc. posted on course (github) homepage

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Course improvements since last time

- More even burden (hopefully)
- General updates of unclear parts in assignments
- *Note!* There can be some new bugs after these updates.

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Section 3

Introduction to Supervised Learning

Supervised learning

Figure: Relationship between appartment size and price (source)

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

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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.
- 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)?
- Image recognition/classification
- Image object traction (position in a video)
- Will this patient recover from their illness or not?
- Does this fingerprint belong to an employee or not?
- Does this customer have stable finances or not?
- Face recognition
- Is this tumour malign (1) or not (0)?

Logistic regression and classification

When the y_i in a regression problem is binary (or more generally, categorical), it becomes a classification problem.

The question that the model tries to answer is: does this observation belong to class 0 or class 1?

Logistic regression is a workhorse in 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.

Assume that $Y_1, \dots, Y_N$ are independent with $Y_i \sim Bernoulli(\pi_i)$.

$Y_i \in 0, 1$ with success probability π_i and $\mu_i = E(Y_i) = \pi_i$.

- The natural parameter of the binomial distribution is

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

  called the logit or log odds.

- 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

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

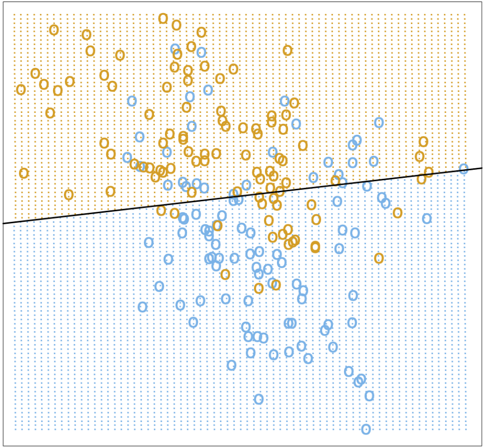
Logistic regression: Prediction

- 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

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.

Section 4

Optimization Algorithms for 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

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

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

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

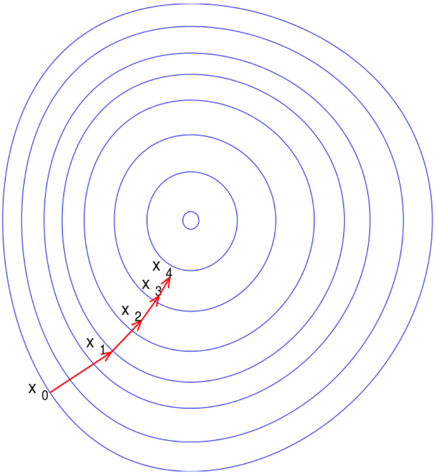
2. $L(\theta)$ needs to be differentiable

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')
- 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.
- Think survey sampling – 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 $\nabla L(\theta, \mathbf{X}, \mathbf{y})$
- Epochs vs. Iterations

Stochastic Gradient Descent

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- Learning rate η_t is important
- We need to reduce η_t over time
- Will it converge to an optimum?
- 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?
- 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 the velocity – the rolling mean of gradients
- Additional hyperparemeter α to control velocity

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

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

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SGD with momentum, Intuition

Figure: SGD with momentum, Intuition (CC)

SGD with momentum

Example of SGD with momentum here.

Adam and RMSprop

- Want the optimizer to adapt to the learning rate η_t to individual parameters
- Common approaches are
  - RMSprop
  - Adaptive Moment Estimation (Adam)