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Machine learning – Block 1(a)

Måns Magnusson
Department of Statistics, Uppsala University

Autumn 2022

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



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This block

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



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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?

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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 Britannica



What is Artificial General Intelligence?

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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



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What is Machine Learning?

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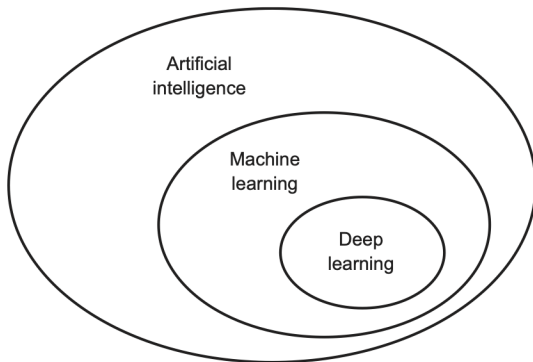
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Learning from data. – Hastie, Tibshirani, Friedman (2009)



What is Machine Learning?

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



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

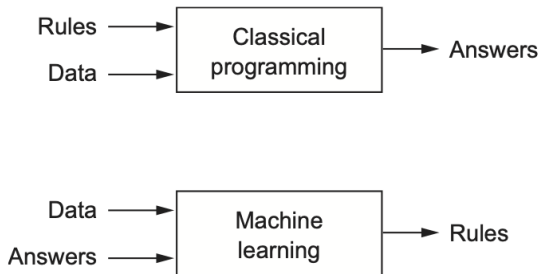




Figure: Regression vs. Pure Predictions (Efron, 2020, Table 5)

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)

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Different names for the same things

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- 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)



Different names for the same things

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 2. Time series regression (ML) vs. Scalar-on-function regression (Stats)



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 4. Weights (ML) vs. Parameters (Stats)



Different names for the same things

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 1. Time series classification (ML) vs. Functional data classification (Stats)
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 3. Learning (ML) vs. Estimation (Stats)
 4. Weights (ML) vs. Parameters (Stats)
 5. Features (ML) vs. Covariates (Stats)



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Different flavors of ML

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



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Questions?

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Questions?



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- What is AI and ML?
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Section 2

Course information



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Course information

The aims of this course are that you should:

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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,

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Course Outline

Two main parts:

- What is AI and ML?
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- Introduction to Supervised Learning
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- 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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 - Mini-project on a supervised project (2-3 students)



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Exact dates and details; see the course page.



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Core Content

- What is AI and ML?
- **Course information**
- Introduction to Supervised Learning
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- 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).
 - Three Zoom computer lab sessions (optional)



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 - Three Zoom computer lab sessions (optional)
- 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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Lectures

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- Present overall theory and content (overview)



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 1. Jonas Wallin, Lund University (regularization)



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 6. Väinö Yrjänäinen, UU (word embeddings)



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Examination

- What is AI and ML?
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- To pass (G): All labs, mini-project, and project review need to be passed (70%)



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- To pass with distinction (VG): 6/10 VG points
- 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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Computer Assignments

- Main part of the course
Learning by doing
- Machine learning = Statistics + Computer Science
Hence a lot of programming



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- All assignments 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!**



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- We will mark and return each assignment within 10 working days.



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Computer Assignments

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- Zoom sessions:
 1. First lab each week will include a 15 min introduction
 2. Our focus: Help during computer labs - less focus on written feedback
 3. **Ask questions!** This is **your** time.



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Figure: Workload last year to pass (G)

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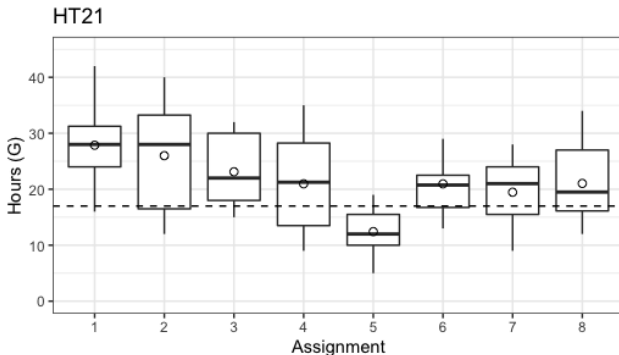
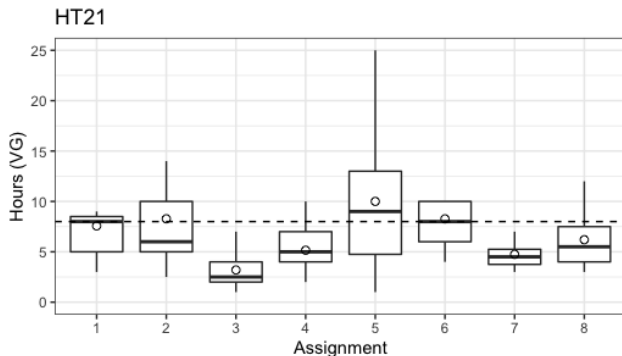




Figure: Workload last year to pass with distinction (VG)





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Mini-project

- See project instructions on webpage for details.

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Mini-project

- See project instructions on webpage for details.
- Supervised problem of choice on real data.
- 2-3 students.



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- See project instructions on webpage for details.
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- Supply a half-page project proposal of data and problem at the end of block 6.



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- See project instructions on webpage for details.
- **Supervised problem** of choice on real data.
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- 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*.



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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)



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- 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)
- 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

- Course page: Github – please do a PR if something is wrong!

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 - Chollet & Allaire (2018) *Deep Learning with R*.
 - Goodfellow, Bengio & Courville (2017) *Deep Learning*.
 - Sutton and Barto (2020) *Reinforcement learning: An introduction*
 - Additional articles, tutorials, videos etc. posted on course (github) homepage
 - Mandatory and optional material: Overlap exists!



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



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Course improvements since last year

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

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Section 3

Introduction to Supervised Learning



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Supervised learning

Figure: Relationship between apartment size and price ([source](#))



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



- General problem: We have *training* data

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

- \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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- \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: $y_i \in a, b, c, \dots$ where a, b, c, \dots are discrete classes.



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Example of supervised problems

- What is AI and ML?
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- Is this e-mail message spam (1) or not (0)?



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 - Image recognition/classification



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 - Will this patient recover from their illness or not?



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- Face recognition



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- Is this tumour malign (1) or not (0)?



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Logistic regression and classification

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



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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?



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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.



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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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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 $Y_i \sim \text{Bernoulli}(\pi_i)$.



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

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



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$Y_i \in 0, 1$ 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**.



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- 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.



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Logistic regression

There are two equivalent formulas for **logistic regression**:

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

and

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



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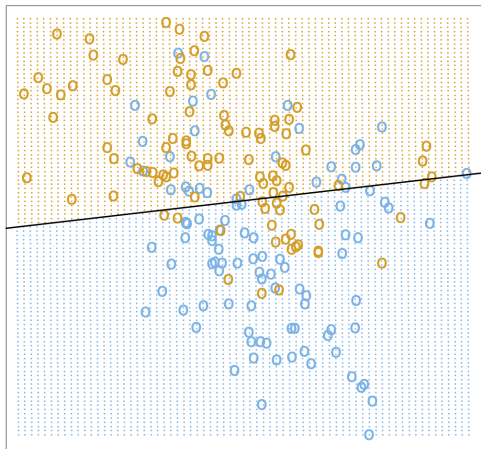
- We *train* a logistic regression model using MLE using the training data.
- Our estimation/training output the MLE $\hat{\theta}$
- We then compute $\hat{p}_i = g^{-1}(\hat{\theta}x_{new})$ for a new observation
- We use a **decision rule** to predict value 0 or 1:

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



Logistic regression: Example

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



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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.





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Section 4

Optimization in Machine Learning



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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



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Gradient Descent Analogy

Figure: Gradient Descent Analogy ([source](#))

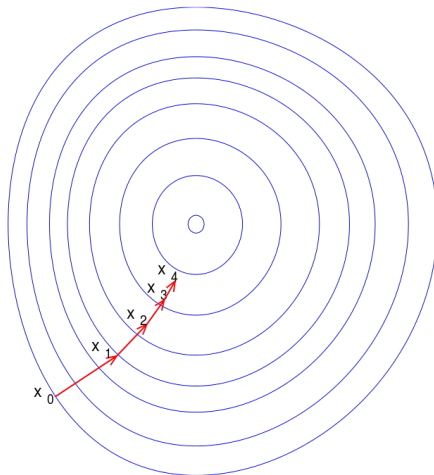




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Gradient Descent (cont.)

Figure: Gradient Descent ([source](#))





Why Gradient Descent?

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



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- Gradient Descent is a poor algorithm (Newton's 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



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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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- *Note!*
We need to have an unbiased estimator for $\nabla L(\theta, \mathbf{X}, \mathbf{y})$
- What is an iteration?
- Epochs vs. Iterations



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Stochastic Gradient Descent

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



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- 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

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- Can we estimate the gradient better?



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- 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 hyperparameter 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)





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SGD with momentum

Example of SGD with momentum [here](#).



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Adaptive Moment Estimation (Adam)

- Adapt η_t to individual parameters

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

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

- 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