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Machine learning – Block 1(a)

Måns Magnusson
Department of Statistics, Uppsala University

Autumn 2024

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?

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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:

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

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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

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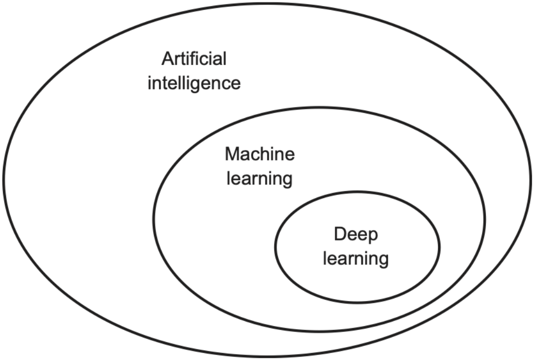
Learning from data. – Hastie, Tibshirani, Friedman (2009)

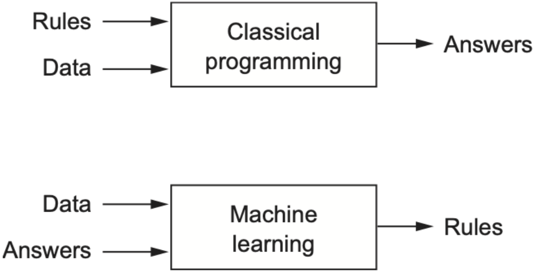
What is Machine Learning?

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



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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- 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)

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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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The aims of this course are that you should:

Course information

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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:

- 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.

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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).
  - 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.

Lectures

- Present overall theory, concepts and content (overview)

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

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  1. Jonas Wallin, Lund University (regularization)

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- No lectures after 19th/20th of December

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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.
- Reassesement 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
- Machine learning = Statistics + Computer Science
  Hence a lot of programming

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

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- Don't write your name anywhere!

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  2. Our focus: Help during computer labs - less focus on written feedback
  3. Ask questions! This is your time.

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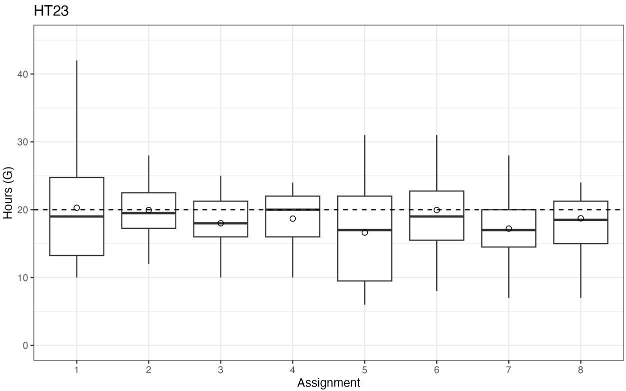

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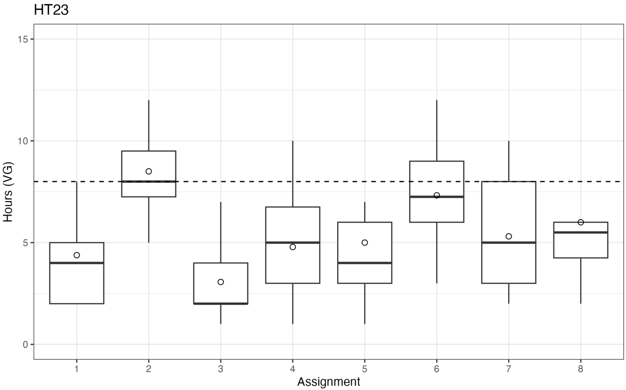
Figure: Workload last year to pass with distinction (VG)



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- Supply step 2 proposal at the end of block 6.

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Mini-project

- See project instructions on webpage for details.
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- 2-3 students.
- Supply step 1 proposal at the end of block 3.
- Supply step 2 proposal at the end of block 6.
- Project will last two weeks (half time) - but start earlier. Good case to show potential employers.
- Recommended data: Images, text or tabular data (e.g. avoid time series).
- Feel free to build upon the Bayesian project (e.g. compare with Bayesian methods).
- 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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- The first author is corresponding author

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- Recommended data: Images, text or tabular data (e.g. avoid time series).
- Feel free to build upon the Bayesian project (e.g. compare with Bayesian methods).
- 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)
- The first author is corresponding author
- Mini-project and master thesis:
  - The mini-project can be used to explore thesis project

Practicalities

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  - Additional articles, tuturials, videos etc. posted on course (github) homepage
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  - Mandatory and optional material: Overlap exists!
- If you have complaint - reach out to me in assignment evaluations!

Course improvements since last year

- New course book (I hope it works!)
- New lecture (maybe) on diffusion models

Questions?

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Section 3

Introduction to Supervised Learning

Supervised learning

- What is AI and ML?
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  - 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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- Is this e-mail message spam or not?

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Logistic regression is a workhorse for classification problems.

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

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

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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.

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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.

- 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

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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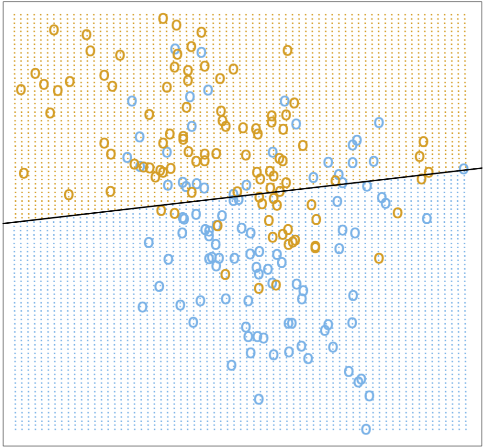
Logistic regression: Example

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



An example: E-mail classification

E-mail Spam
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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- What is AI and ML?
- Course information
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Training of ML algorithms

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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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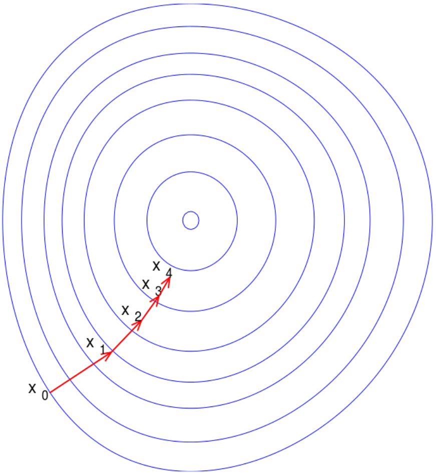
Gradient Descent Analogy

Figure: Gradient Descent Analogy (source)

Gradient Descent (cont.)

Figure: Gradient Descent (source)



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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).

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.

Stochastic Gradient Descent

- 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 $\nabla L(\theta, \mathbf{X}, \mathbf{y})$

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

Mini-batch gradient descent

- Can we estimate the gradient in a better way?

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 $|(S)_i| = B$.

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- B is usually set to optimize hardware

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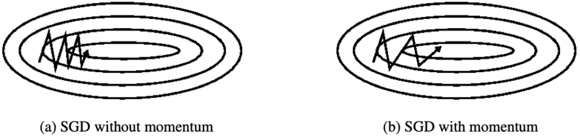
- SGD can be slow to converge due to 'jumping' behaviour
- Can improve behaviour using momentum – the rolling mean of gradients
- Additional hyperparemeter α to control the momentum

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

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

Figure: SGD with momentum



SGD with momentum, Intuition

Figure: SGD with momentum, Intuition (CC)

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SGD with momentum

Example of SGD with momentum here.

Adaptive Moment Estimation (Adam)

- Adapt η_t to individual parameters

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

- Bias correction
  (due to initialization at 0)

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

- 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 $\epsilon = 10^{-8}$

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Adaptive Moment Estimation (Adam)

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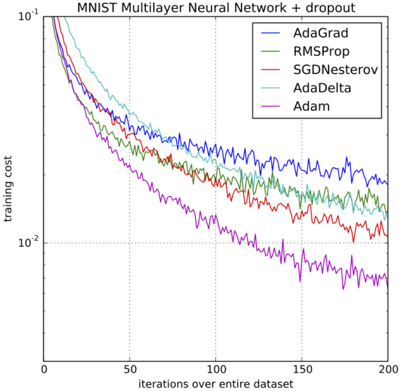
$$
\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t,
$$

- 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"