## Machine Learning An introduction



Troels C. Petersen (NBI)

"Statistics is merely a quantisation of common sense - Machine Learning is a sharpening of it!"

What is ML?

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Under all circumstances, ML allows the analysis and understanding of data, that is complex in terms of both size, dimensionality, quality, and relations [TP].

## Why ML?

## The Data "Deluge"

Shown is the total amount of data created, captured, and copied.


However, only a small portion ( $\sim 2 \%$ ) of this data is stored for a longer period of time.

## ML and the Data "Deluge"

The amount of data in the world is growing very fast.

In order to consider this data, Machine Learning (ML) has become a standard tool.

This is due to the easy access to large data sets, but also the growth in data storage and processing capabilities.

By now ML can also consider text, images, sound, etc.

## The Economist

## The data deluge

AND HOW TO HANDLE IT: A 14-PAGE SPECIAL REPORT


Humans vs. ML

## Dimensionality and Complexity

Humans are good at seeing/ understanding data in few dimensions! However, as dimensionality grows, complexity grows exponentially ("curse of dimensionality"), and humans are generally not geared for such challenges.

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| :--- | :--- | :--- |
| Linear | Humans: <br> Computers: | Humans: <br> Computers: |
| Non- <br> linear | Humans: <br> Computers: | Humans: <br> Computers: |

Computers, on the other hand, are OK with high dimensionality, albeit the growth of the challenge, but have a harder time facing non-linear issues.

However, through smart algorithms, computers have learned to deal with it all! That is essentially what Machine Learning has enabled!

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Humans \& Computers are good at seeing / understanding linear data in few dimensions:


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## Dimensionality and Complexity

However, when the dimensionality goes beyond 3D, we are lost, even for simple linear data. Computers are not...

Shown is the famous Fisher Iris dataset: 150 irises ( 3 kinds) with 4 measurements for each.

4 dimensional data!


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## Two main ingredients

# Two main ingredients: <br> 1. Solutions exists <br> 2. How to find them 

# Solutions exists 

(Technically called Universal Approximation Theorems)

## Where to separate?

Look at the red and green points, and imagine that you wanted to draw a curve that separates these.


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This could be an example:


Generally, we want to find a function that does this well! But how to write such a function?

## Universal Approx. Theorems

A simple function can be obtained simply by asking a lot of questions:
Question: Is B $>0.23$ ?
Answer: Yes $\rightarrow$ Red Answer: No $\rightarrow$ Blue

This question is illustrated in the drawing by the horizontal line with red and blue on the sides.

A Decision Tree consists of asking many such questions, corresponding to setting a lot of lines.


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In the drawing $\mathrm{k}=3$, leading to a rather "ragged" border.

However, increasing the number of neighbours considered to $\mathrm{k}=30$ gives a more smooth border.

This method is called "k-nearest neighbours".


## Universal Approx. Theorems

Other methods are based on entirely different principles.

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There is a wealth of different methods.

The main idea is, that they are all capable of getting close to the optimal solution.


## Universal Approx. Theorems

Such approximations typically entails a large amount of parameters, for which the UATs give no recipe on how to find - only that such a construction is possible.


## Universal

## Approximation Theorems

Theorem 5.1.1 (Universal Approximation Theorem) ${ }^{10}$ Let $\sigma$ be a nonconstant, bounded, and monotone-increasing continuous function. Let $I_{m_{0}}$ denote the $m_{0}$-dimensional unit hypercube $[0,1]^{m_{0}}$. The space of continuous functions on $I_{m_{0}}$ is denoted as $C\left(I_{m_{0}}\right)$. Then given any function $f \in C\left(I_{m_{0}}\right)$ and $\epsilon>0$ there exists a set of real constants $a_{i}, b_{i}$ and $w_{i j}$, where $i=1, \ldots, m_{1}$ and $j=1, \ldots, m_{0}$ such that we may define

$$
\begin{equation*}
F\left(x_{1}, \ldots, x_{m_{0}}\right)=\sum_{i=1}^{m_{1}} a_{i} \sigma\left(\sum_{j=1}^{m_{0}} w_{i j} x_{j}+b_{i}\right) \tag{5.6}
\end{equation*}
$$

as an approximate realization of the function $f$; that is,

$$
\begin{equation*}
\left|F\left(x_{1}, \ldots, x_{m_{0}}\right)-f\left(x_{1}, \ldots, x_{m_{0}}\right)\right|<\epsilon \tag{5.7}
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for all $x_{1}, x_{2}, \ldots, x_{m_{0}}$ that lie in the input space.

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## Summary:

Neural Networks etc. can approximate functions in any dimension very well!

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## Universal Approx. Theorems

One main ingredient behind ML are Universal Approximation Theorems (UAT).
These imply that Neural Networks can approximate a very wide variety of functions given simple function constraints and enough degrees of freedom.

This typically entails a large amount of weights, for which the UATs give no recipe on how to find - only that such a construction is possible.

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## Part of this course is learning how to find these!

Decision Trees and K-Nearest Neighbour algorithms are also capable of "universal approximation" (i.e. have forms of UATs).

A UAT has also been worked out for Graph Neural Networks... in 2020!

## Universal Approx. Theorems

Regarding UATs, as far as learning is concerned, whether the class is really universal or not is not overly important:

If one assumes that there is no noise in the training set, then there will still be infinitely many functions that passes through all training points and not all of them will have the same error on an unseen point (i.e. the test set).

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Thus, one can ask for what sort of functions the approximation applies. All differentiable functions? Typically, NNs are restricted to this class. All continuous functions ? All measurable functions? All computable functions?

As it turns out, the real deal is characterising that class of functions that can be approximated.

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As it turns out, the real deal is characterising that class of functions that can be approximated.

However, we don't really care about that - we simply assume, that with enough liberty/complexity, the functions can approximate what we want.

# How to find these 

(Technically called Stochastic Gradient Descent)

## Stochastic Gradient Descent

The way to obtain the parameters/ weights of ML algorithms, is generally by Stochastic Gradient Descent.

This "back propagation" algorithm works by computing the gradient of the loss function (to be optimised) with respect to each weight using the chain rule.

One thus computes the gradient one layer at a time, iterating backwards from the last layer (avoiding redundancies). See Goodfellow et al. for details.


Goodfellow, Ian; Bengio, Yoshua; Courville, Aaron (2016). "6.5 Back-Propagation and Other Differentiation Algorithms". Deep Learning. MIT Press. pp. 200-220. ISBN 9780262035613.

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The gradient descent is made stochastic (and fast) by only considering a fraction (called a "batch") of the data, when calculating the step in the search for optimal parameters for the algorithm. This allow for stochastic jumping, that avoids local (false) minima.


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- Batch gradient descent
- Mini-batch gradient Descent
- Stochastic gradient descent



## Ingredients for ML

So now we know that at least in principle:

- a solution exists (Universal Approximation Theorem) and
- that it can be found (Stochastic Gradient Descent).

But this does not in reality make us capable of getting ML results.

We (at least) also need:

- actual functions/algorithms for making approximations
- knowledge about how to tell them what to learn
- a scheme for how to use the data we have available


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We (at least) also need:

- actual functions/algorithms for making approximations Boosted Decision Trees (BDTs) \& Neural Networks (NNs)
- knowledge about how to tell them what to learn Loss functions (and now to minimise these)
- a scheme for how to use the data we have available Training, validation, and testing samples \& Cross Validation


## Types of ML

# Unsupervised vs. Supervised Classification vs. Regression 

Machine Learning can be supervised (you have correctly labelled examples) or unsupervised (you don't)... [or reinforced]. Following this, one can be using ML to either classify (is it A or B ?) or for regression (estimate of X ).


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## Target of ML

## Classification



REALITY

STATISTICAL DECISION:

|  | Null is True | Null is False |
| ---: | :---: | :---: |
| Do Not Reject Null | $1-\alpha$ <br> Correct | $\beta$ <br> Type II error |
| Reject Null | $\alpha$ <br> Type I error | $1-\beta$ <br> Correct |
|  |  |  |

## Classification



## Machine Learning typically enables

 a better separation between hypothesisDECISION:

Reject Null

| $\alpha$ | $1-\beta$ |
| :---: | :---: |
| Type I error | Correct |

## Hypothesis testing

Hypothesis testing is like a criminal trial. The basic "null" hypothesis is Innocent (called $\mathrm{H}_{0}$ ) and this is the hypothesis we want to test, compared to an "alternative" hypothesis, Guilty (called $\mathrm{H}_{1}$ ).

Innocence is initially assumed, and this hypothesis is only rejected, if enough evidence proves otherwise, i.e. that the probability of innocence is very small ("beyond reasonable doubt"). This is summarised in a Contingency Table:

|  | Truly innocent <br> $\left(\mathbf{H}_{0}\right.$ is true) | Truly guilty <br> (H1 is true) |
| :---: | :---: | :---: |
| Acquittal | Right decision | Wrong decision |
| (Accept $\mathbf{H}_{0}$ ) | True Positive (TP) | False Negative (FN) |
| Conviction <br> (Reject $\mathbf{H}_{0}$ ) | Wrong decision | Right decision |
| False Positive (FP) | True Negative (TN) |  |

The rate of FP and FN are correlated, and one can only choose one of these!

## Measuring separation



## Simple case



## ROC CURVE



## ROC CURVE



## ROC CURVE



## ROC CURVE



## Which metric to use?

There are a ton of metrics in hypothesis testing, see below. However, those in the boxes below are the most central ones.

One metric - not mentioned here - is the Area Under the Curve (AUC), which is simply an integral of the ROC curve (thus 1 is perfect score). This is sometimes used to optimise performance (loss), but not great!

|  |  | True condition |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | Total population | Condition positive | Condition negative | $\text { Prevalence }=\frac{\Sigma \text { Condition positive }}{\Sigma \text { Total population }}$ | Accuracy (ACC) = <br> $\frac{\Sigma \text { True positive }+\Sigma \text { True negative }}{\Sigma \text { Total population }}$ |
|  | Predicted condition positive | True positive | False positive, Type I error | Positive predictive value (PPV), <br> Precision = <br> $\Sigma$ True positive <br> $\bar{\Sigma}$ Predicted condition positive | False discovery rate $($ FDR $)=$ <br> $\Sigma$ False positive <br> $\bar{\Sigma}$ Predicted condition positive |
|  | Predicted condition negative | False negative, <br> Type II error | True negative | False omission rate (FOR) = <br> $\Sigma$ False negative <br> $\overline{\sum \text { Predicted condition negative }}$ | Negative predictive value (NPV) = <br> $\Sigma$ True negative <br> $\bar{\Sigma}$ Predicted condition negative |
|  |  | True positive rate (TPR), Recall, Sensitivity, probability of detection, Power $=\frac{\Sigma \text { True positive }}{\Sigma \text { Condition positive }}$ | False positive rate (FPR), Fall-out, probability of false alarm $=\frac{\Sigma \text { False positive }}{\Sigma \text { Condition negative }}$ | Positive likelihood ratio (LR+) $=\frac{\text { TPR }}{\text { FPR }}$ | Diagnostic odds $\quad F_{1}$ score $=$ ratio (DOR) |
|  |  | False negative rate (FNR), Miss rate $=\frac{\Sigma \text { False negative }}{\Sigma \text { Condition positive }}$ | Specificity (SPC), Selectivity, True negative rate (TNR) $=\frac{\Sigma \text { True negative }}{\Sigma \text { Condition nearive }}$ | Negative likelihood ratio (LR-) $=\frac{\mathrm{FNR}}{\mathrm{TNR}}$ | $=\frac{L R_{+}}{L R-}$ |

https:/ / en.wikipedia.org/ wiki/ Receiver_operating_characteristic

## Matthew's Correlation Coefficient

Given a Contingency Table:

|  | Got well | Remained ill |
| :---: | :---: | :---: |
| Medicin | 28 | 5 |
| No Medicin | 19 | 9 |

One of the commonly used measures of separation the MCC, which (in this case) is the Pearson $\varrho$, and related to the ChiSquare:

$$
\mathrm{MCC}=\frac{T P \times T N-F P \times F N}{\sqrt{(T P+F P)(T P+F N)(T N+F P)(T N+F N)}}
$$

Read more at:
https://en.wikipedia.org/wiki/Phi_coefficient
However, when optimising an algorithm and giving continuous scores in the range $] 0,1[$, there are other things to consider (see talk on Loss Functions).

## The linear analysis case

## Simple Example

Problem: You want to figure out a method for getting sample that is mostly male! Solution: Gather height data from 10000 people, Estimate cut with $95 \%$ purity!


## Simple Example

Additional data: The data you find also contains shoe size! How to use this? Well, it is more information, but should you cut on it?


Height


Shoe size

The question is, what is the best way to use this (possibly correlated) information!

## Simple Example

So we look if the data is correlated, and consider the options:

## Cut on each var? <br> Poor efficiency!

Advanced cut?
Clumsy and hard to implement

Combine var? Smart and promising




The latter approach is the Fisher discriminant!
It has the advantage of being simple and applicable in many dimensions easily!

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## Separating data

Fisher's friend, Anderson, came home from picking Irises in the Gaspe peninsula... 180 MULTIPLE MEASUREMENTS IN TAXONOMIC PROBLEMS

Table I


## Fisher's Linear Discriminant

You want to separate two types / classes (A and B) of events using several measurements.

Q: How to combine the variables?
A: Use the Fisher Discriminant:

$$
\mathcal{F}=w_{0}+\vec{w} \cdot \vec{x}
$$

Q: How to choose the values of $w$ ? $\underline{\text { A }}$ : Inverting the covariance matrices:

$$
\vec{w}=\left(\boldsymbol{\Sigma}_{A}+\boldsymbol{\Sigma}_{B}\right)^{-1}\left(\vec{\mu}_{A}-\vec{\mu}_{B}\right)
$$

This can be calculated analytically, and incorporates the linear correlations into the separation capability.

Iris Data (red=setosa,green=versicolor,blue=virginica)


## Fisher's Linear Discriminant

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Q: How to combine the variables?
A: Use the Fisher Discriminant:
Iris Data (red=setosa,green=versicolor,blue=virginica)
ments are given. We shall first consider the question: What linear function of the four measurements

$$
X=\lambda_{1} x_{1}+\lambda_{2} x_{2}+\lambda_{3} x_{3}+\lambda_{4} x_{4}
$$

will maximize the ratio of the difference between the specific means to the standard deviations within species? The observed means and their differences are shown in Table II. Q: How to choose the values of $w$ ? A: Inverting the covariance matrices:

$$
\vec{u}=\left(\sum A+\sum B\right)^{-1}(\vec{\mu} A-\vec{\mu} B)
$$

This can be calculated analytically, and incorporates the linear correlations into the separation capability.


Petal.Width

## Fisher's Linear Discriminant

## Executive summary:

Fisher's Discriminant uses a linear combination of variables to give a single variable with the maximum possible separation (for linear combinations!).


It is for all practical purposes a projection (in a Euclidian space)!

## Fisher's Linear Discriminant

The details of the formula are outlined below:
You have two samples, $A$ and $B$, that you want to separate.

For each input variable (x), you calculate the mean ( $\mu$ ), and form a vector of these.

$$
\vec{w}=\left(\Sigma_{A}+\Sigma_{B}\right)^{-1}\left(\vec{\mu}_{A}-\vec{\mu}_{B}\right)
$$

Using the input variables (x), you calculate the covariance matrix ( $\Sigma$ ) for each species (A/B), add these and invert.

Given weights (w), you take your input variables (x) and combine them linearly as follows:

$$
\mathcal{F}=w_{0}+\vec{w} \cdot \vec{x}
$$

$F$ is what you base your decision on.

## The non-linear case

## Non-linear cases

While the Fisher Discriminant uses all separations and linear correlations, it does not perform optimally, when there are non-linear correlations present:


If the PDFs of signal and background are known, then one can use a likelihood. But this is very rarely the case, and hence one should move on to the Fisher. However, if correlations are non-linear, more "tough" methods are needed...

## (Boosted) Decision Trees

Can become very complex.
Good for discrete problems. "Good for all problems!!!"

Not always highest efficiency, though...

Boosting adds to separation.


* Example decision tree on a simple algorithm for predicting survival of Titanic!


## Boosted Decision Trees (BDT)



Decision tree learning uses a decision tree as a predictive model which maps observations about an item to conclusions about the item's target value. It is one of the predictive modelling approaches used in statistics, data mining and machine learning.
[Wikipedia, Introduction to Decision Tree Learning]

## Boosted Decision Trees

A decision tree divides the parameter space, starting with the maximal separation. In the end each part has a probability of being signal or background.

- Works in $95+\%$ of all problems!
- Fully uses non-linear correlations.

But BDTs require a lot of data for training, and is sensitive to overtraining.

Overtraining can be reduced by limiting the number of nodes and number of trees.


## Boosting

There is no reason, why you can not have more trees. Each tree is a simple classifier, but many can be combined!

To avoid N identical trees, one assigns a higher weight to events that are hard to classify, i.e. boosting:


Boost weight


## Neural Networks

Can become very complex.
Good for continuous problems.
Sometimes hard to train!

Very versatile approach that can also be applied to images, text, etc.

Easily produces multiple outputs.

## Neural Networks (NN)



In machine learning and related fields, artificial neural networks (ANNs) are computational models inspired by an animal's central nervous systems (in particular the brain) which is capable of machine learning as well as pattern recognition. Neural networks have been used to solve a wide variety of tasks that are hard to solve using ordinary rule-based programming, including computer vision and speech recognition.
[Wikipedia, Introduction to Artificial Neural Network]

## Neural Networks

Neural Networks combine the input variables using a "activation" function $s(x)$ to assign, if the variable indicates signal or background.

The simplest is a single layer perceptron:

$$
t(x)=s\left(a_{0}+\sum a_{i} x_{i}\right)
$$

This can be generalised to a multilayer perceptron:

$$
\begin{aligned}
& t(x)=s\left(a_{i}+\sum a_{i} h_{i}(x)\right) \\
& h_{i}(x)=s\left(w_{i 0}+\sum w_{i j} x_{j}\right)
\end{aligned}
$$

Activation function can be any sigmoid function.

Training \& Over-training

## Test for simple over-training

In order to test for overtraining, half the sample is used for training, the other for testing:

```
TMVA overtraining check for classifier: BDT_0p0m_2e2mu
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## Real overtraining

The "real" limit of overtraining, is when the (Cross) Validation (CV) error starts to grow!


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## Methods (dis)advantages

## Method's (dis-)advantages

Another comparison is done in Elements of Statistical Learning II (ESL II), where linear methods are not included.

As can be seen, Neural Networks are "difficult" in almost all respects, but performant.

For trees, the case is almost the opposite.

However, I don't agree with the evaluation of the predictive power of trees.
At least not for normal structured data.

| Characteristic | Neural Nets | SVM | Trees | MARS | k-NN, <br> Kernels |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Natural handling of data of "mixed" type | $\nabla$ | $\nabla$ | A | A | $\nabla$ |
| Handling of missing values | $\nabla$ | $\nabla$ | A | A | A |
| Robustness to outliers in input space | $\nabla$ | $\nabla$ | A | $\nabla$ | A |
| Insensitive to monotone transformations of inputs | $\nabla$ | $\nabla$ | A | $\nabla$ | $\nabla$ |
| Computational scalability (large $N$ ) | $\nabla$ | $\nabla$ | A | A | $\nabla$ |
| Ability to deal with irrelevant inputs | $\nabla$ | $\nabla$ | A | A | $\nabla$ |
| Ability to extract linear combinations of features | A | A | $\nabla$ | $\nabla$ | * |
| Interpretability | $\nabla$ | $\nabla$ | $\checkmark$ | $\Delta$ | $\nabla$ |
| Predictive power | $\Delta$ | $\Delta$ | $\nabla$ | $\checkmark$ | $\Delta$ |

From ESL II, Chapter 10.7

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For tabular data, I disagree!

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| :--- | :---: | :---: | :---: | :---: | :---: |
| Natural handling of data <br> of "mixed" type | $\nabla$ | $\nabla$ | $\Delta$ | $\Delta$ | $\nabla$ |
| Handling of missing values | $\nabla$ | $\nabla$ | $\Delta$ | $\Delta$ | $\Delta$ |
| Robustness to outliers in <br> input space | $\nabla$ | $\nabla$ | $\Delta$ | $\nabla$ | $\Delta$ |
| Insensitive to monotone <br> transformations of inputs | $\nabla$ | $\nabla$ | $\Delta$ | $\nabla$ | $\nabla$ |
| Computational scalability <br> large $N$ ) | $\nabla$ | $\nabla$ | $\Delta$ | $\Delta$ | $\nabla$ |
| Ability to deal with irrel- <br> evant inputs | $\nabla$ | $\nabla$ | $\Delta$ | $\Delta$ | $\nabla$ |
| Ability to extract linear <br> combinations of features | $\Delta$ | $\Delta$ | $\nabla$ | $\nabla$ | $\Delta$ |
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| Prodictivo powor |  | $\xrightarrow{\square}$ | (V) | $\checkmark$ | A |

## Performance comparison

Left figure shows the distribution of signal and background used for test.
Right figure shows the resulting separation using various MVA methods.


The theoretical limit is known from the Neyman-Pearson lemma using the (known / correct) PDFs in a likelihood.
In all fairness, this is a case that is great for the BDT...

How to choose method?

## Which method to use?

There is no good/simple answer to this, though people have tried, e.g.:


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## What is Machine Learning?



