

Introduction to Machine Learning

Christos Dimitrakakis

September 17, 2024

Outline

The problems of Machine Learning (1 week)

- Introduction

Estimation

- Answering a scientific problem

- Pandas and dataframes

- Single variable models

- Two variable models

Statistics, validation and model selection

Course summary

- Course Contents

Reading for this week

- Reading

The problems of Machine Learning (1 week)

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Reading for this week

Reading

Machine Learning And Data Mining

The nuts and bolts

- ▶ Models
- ▶ Algorithms
- ▶ Theory
- ▶ Practice

Workflow

- ▶ Scientific question
- ▶ Formalisation of the problem
- ▶ Data collection
- ▶ Analysis and model selection

Types of statistics / machine learning problems

- ▶ Classification
- ▶ Regression
- ▶ Density estimation

Machine learning

Data Collection

- ▶ Downloading a clean dataset from a **repository**
- ▶ **Scraping** data from the web
- ▶ Conducting a **survey**
- ▶ Performing **experiments**, and obtaining measurements.

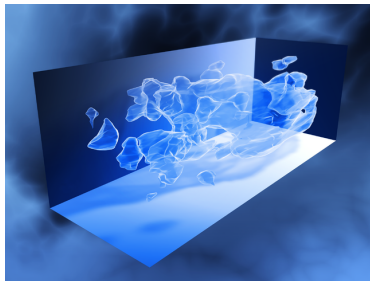
Modelling

- ▶ Simple: the bias of a coin
- ▶ Complex: a language model.
- ▶ The model depends on the data and the problem

Algorithms and Decision Making

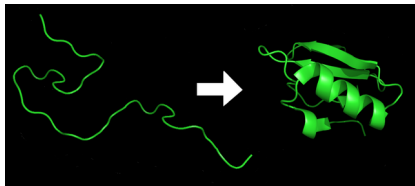
- ▶ We want to use models to make decisions.
- ▶ Decisions are made every step of the way.
- ▶ Both humans and algorithms can make decisions.

The main problems in machine learning and statistics



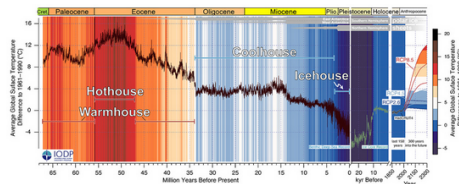
Matter

Dark

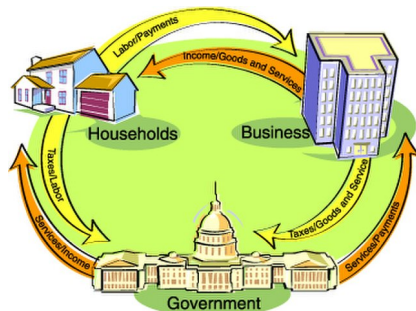


Protein Folding

Christos Dimitrakakis



Climate Modelling



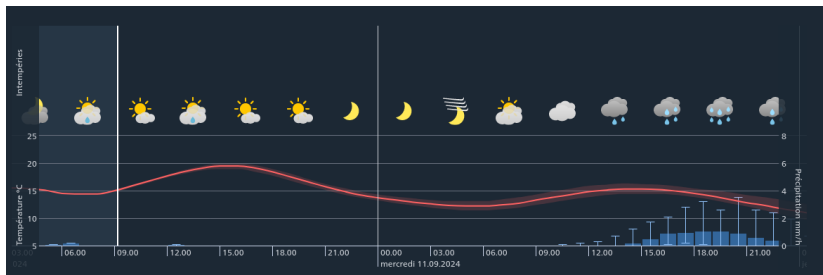
Economic Policy

Introduction to Machine Learning

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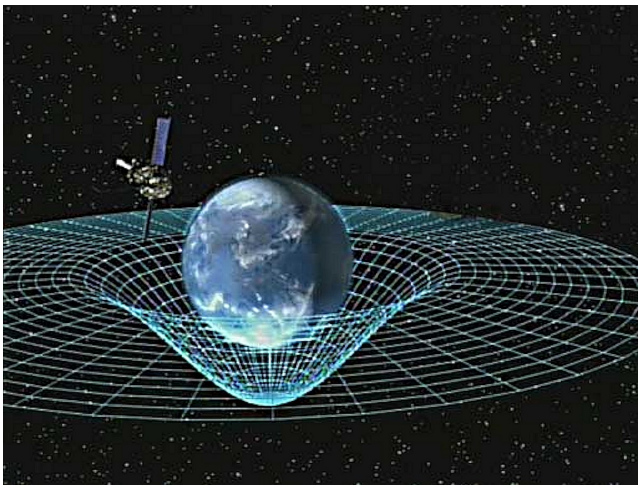
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Prediction



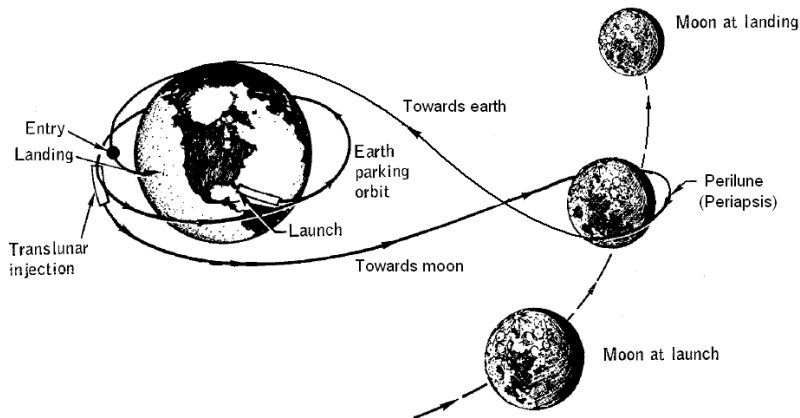
- ▶ Will it rain tomorrow?
- ▶ How much will bitcoin be worth next year?
- ▶ When is the next solar eclipse?

Inference



- ▶ What is the law of gravitation?
- ▶ Where is the spaceship now?
- ▶ Does my poker opponent have two aces?

Decision Making



- ▶ What data should I collect?
- ▶ Which model should I use?
- ▶ Should I fold, call, or raise in my poker game?
- ▶ How can I get a spaceship to the moon and back?

./fig/artemis.gif

The need to learn from data

Problem definition

- ▶ What problem do we need to solve?
- ▶ How can we formalise it?
- ▶ What properties of the problem can we learn from data?

Data collection

- ▶ **Why** do we need data?
- ▶ **What** data do we need?
- ▶ How **much** data do we want?
- ▶ **How** will we collect the data?

Modelling and decision making

- ▶ How will we **compute** something useful?
- ▶ How can we use the model to make **decisions**?

Course Material

Moodle

- ▶ Assignments and project
- ▶ Additional reading material
- ▶ Asking questions

Course Github

- ▶ `https://github.com/olethrosdc/machine-learning-neuch/tree/main/BSc`
- ▶ .org files for notes, PDF for slides
- ▶ source code for examples



Assignment, teaching and questions

Assignments and project

- ▶ Individual Weekly assignments in the first half
- ▶ Group project in the second half
- ▶ Project presentation
- ▶ No exam.

Other questions

- ▶ Use Moodle for technical/administrative questions: That way everybody gets the same information.
- ▶ Use email for personal problems or extra help, if the moodle is not enough.
- ▶ Complicated questions can be answered at the next lecture

Office hours

- ▶ Fridays 13:00-14:00: book with an email to avoid clashes.
- ▶ Email me for an appointment outside those hours.

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Problem definition

- ▶ Example: Health, weight and height

Example (Health questions regarding height and weight)

- ▶ What is a normal height and weight?
- ▶ How are they related to health?
- ▶ What variables affect height and weight?

Define a research question

Find a **non-sensitive** variable that we can easily measure via a survey, e.g. related to sleep, smoking, exercise, food, politics, sports, hobbies etc.

- ▶ Discuss in small groups and post suggestions
- ▶ We then vote for what to measure

Data collection

Think about **which variables** we need to collect to answer our **research question**.

Necessary variables

The variables we need to know about

- ▶ Weight
- ▶ Height
- ▶ Dependent: (health/vote/opinion/salary)

Auxiliary variables

Measurable factors related to the variables of interest

Possible confounders

Hidden factors that might affect variables

Class data and variables

- ▶ The class enters their data into the excel file.



- ▶ Pay attention to the variables we wish to measure

Privacy

- ▶ Is the use of a pseudonym sufficient to hide your identity?

Variables

The class data looks like this

First Name	Gender	Height	Weight	Age	Nationality	Smoking
Lee	M	170	80	20	Chinese	10
Fatemeh	F	150	65	25	Turkey	0
Ali	Male	174	82	19	Turkish	0
Joan	N	5'11	180	21	American	4

- ▶ \mathbf{X} : Everybody's data
- ▶ \mathbf{x}_t : The t -th person's data
- ▶ $x_{t,k}$: The k -th feature of the t -th person.
- ▶ \mathbf{x}_k : Everybody's k -th feature

Raw versus neat data

- ▶ Neat data: $\mathbf{x}_t \in \mathbb{R}^n$
- ▶ Raw data: web pages, handwritten text, graphs, data packets, with missing/incorrect values, etc

Types of learning problems

Unsupervised learning (unconditional estimation)

- ▶ Predict the **gender** of an unknown individual.
- ▶ Predict the **height**.
- ▶ Predict the **height and weight**?

Supervised learning problems (conditional estimation)

- ▶ Classification: Can we predict gender from height/weight?
- ▶ Regression: Can we predict weight from height and gender?
- ▶ In both cases we predict **output** variables from **input** variables

Variables

- ▶ **Input** variables: aka features, predictors, independent variables
- ▶ **Output** variables: aka response, dependent variables, labels, or targets.
- ▶ The input/output dichotomy only exists in **some prediction problems**.

Python pandas for data wrangling

Reading class data

```
import pandas as pd
X = pd.read_excel("data/class.xlsx")
X["First Name"]
```

- ▶ Array columns correspond to features
- ▶ Columns can be accessed through namesx

Summarising class data

```
X.hist()
import matplotlib.pyplot as plt
plt.show()
```

Pandas and DataFrames

- ▶ Data in pandas is stored in a **DataFrame**
- ▶ DataFrame is **not the same** as a numpy array.

Core libraries

```
import pandas as pd
import numpy as np
```

Series: A sequence of values

```
# From numpy array:
s = pd.Series(np.random.randn(3), index=["a", "b", "c"])
# From dict:
d = {"a": 1, "b": 0, "c": 2}
s = pd.Series(d)
# accessing elements
s.iloc[2] #element 2
s.iloc[1:2] #elements 1,2
s.array # gets the array object
s.to_numpy() # gets the underlying numpy array
```

DataFrames

Constructing from a numpy array

```
data = np.random.uniform(size = [3,2])
df = pd.DataFrame(data, index=["John", "Ali", "Sumi"],
    columns=["X1", "X2"])
```

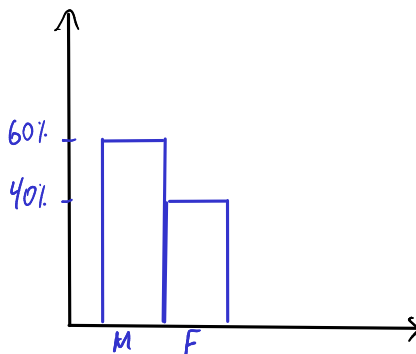
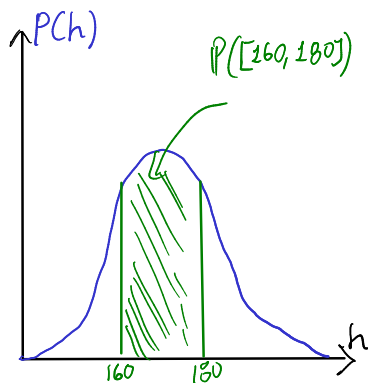
Constructing from a dictionary

```
d = { "one": pd.Series([1, 2], index=["a", "b"]),
      "two": pd.Series([1, 2, 3], index=["a", "b", "c"])}
df = pd.DataFrame(d)
```

Access

```
X["First Name"] # get a column
X.loc[2] # get a row
X.at[2, "First Name"] # row 2, column 'first name'
X.loc[2].at["First Name"] # row 2, element 'first name' of the series
X.iat[2,0] # row 2, column 0
```

Modelling single variables

Figure: $x \in \mathbb{N}$ Figure: $x \in \mathbb{R}$

Means using python

Example (Calculating the mean of our class data)

```
X.mean() # gives the mean of all the variables through pandas.core.f
X["Height"].mean()
np.mean(X["Weight"])
```

- ▶ The mean here is **fixed** because we calculate it on the same data.
- ▶ If we were to **collect new data** then the answer would be different.

Example (Calculating the mean of a random variable)

```
import numpy as np
X = np.random.gamma(170, 1, size=20)
X.mean()
np.mean(X)
```

- ▶ The mean is **random**, so we get a different answer everytime.

One variable: expectations and distributions

Definition (The expected value)

- ▶ Ω : random outcome space

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- ▶ Random variable $x : \Omega \rightarrow \mathbb{R}$, and $\omega \sim P$

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$$\mathbb{E}_P[x] = \sum_{\omega \in \Omega} x(\omega)P(\omega)$$

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Definition (The sample mean)

- ▶ **i.i.d.** variables $x_1, \dots, x_t, \dots, x_T$: with $x_t = x(\omega_t)$, $\omega_t \sim P$.

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Definition (The sample mean)

- ▶ **i.i.d.** variables $x_1, \dots, x_t, \dots, x_T$: with $x_t = x(\omega_t)$, $\omega_t \sim P$.
- ▶ The sample mean of x_1, \dots, x_T is

$$\frac{1}{T} \sum_{t=1}^T x_t$$

The sample mean is $O(1/\sqrt{T})$ -close $\mathbb{E}_P[x_t]$ with high probability.

Reminder: expectations of random variables

A gambling game

What are the expected winnings if you play this game?

- ▶ [a] With probability 1%, you win 100 CHF
- ▶ [b] With probability 40%, you win 20 CHF.
- ▶ [c] Otherwise, you win nothing

Solution

Reminder: expectations of random variables

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- ▶ Let x be the amount won, then $x(a) = 100$, $x(b) = 20$, $x(c) = 0$.

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$$\mathbb{E}_P(x) = \sum_{\omega \in \{a,b,c\}} x(\omega)P(\omega) = x(a)P(a) + x(b)P(b) + x(c)P(c)$$

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- ▶ $P(c) = 59\%$, as $P(\Omega) = 1$. Substituting,
- $$\mathbb{E}_P(x) = 1 + 8 + 0 = 9.$$

Models

Models as summaries

- ▶ They summarise what we can see in the data
- ▶ The ultimate model of the data **is** the data

Models as predictors

- ▶ They make predictions about things **beyond** the data
- ▶ This requires some assumptions about the **data-generating process**.

Example models

- ▶ A numerical mean
- ▶ A linear classifier
- ▶ A linear regressor
- ▶ A deep neural network
- ▶ A Gaussian process
- ▶ A large language model

Estimates and decisions

We always need to make decisions based on some **estimates**.

Estimate the bias of a coin

- ▶ I give you a coin that, lands with some fixed probability on heads.
- ▶ You are allowed to experiment with the coin.
- ▶ I will pay you **1 CHF** if you guess the throw correctly
- ▶ Otherwise you pay me **x CHF**.
- ▶ How much should I ask you to **pay** for the bet to be **fair**?
- ▶ What do you need to **know** to determine this?

Example (If the coin is fair)

- ▶ If the coin is fair, then you only have 50% probability of guessing correctly.
- ▶ If you bet x CHF, your expected return is x

The Bernoulli distribution

Definition (Bernoulli distribution)

We say that $x \in \{0, 1\}$ has Bernoulli distribution with parameter θ and write

$$x \sim \text{Bernoulli}(\theta),$$

when

$$\mathbb{P}(x) = \begin{cases} \theta & x = 1 \\ 1 - \theta & x = 0. \end{cases}$$

Example (Applications of the Bernoulli distribution)

- ▶ A biased coin flip.
- ▶ Classification errors.

Exercise: The expected value

If x is Bernoulli with parameter θ , then what is the expected value of

- ▶ The variable $f(x) = x$?
- ▶ The variable $g(x) = x^2$?

Two-variable models

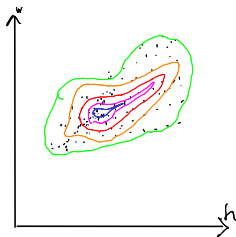


Figure: $x \in \mathbb{R}^2$

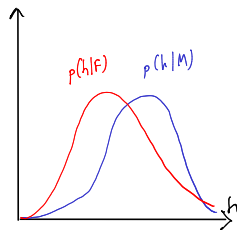
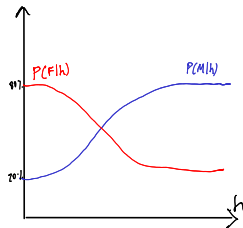
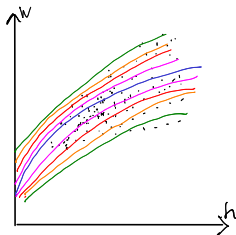


Figure: $x \in \mathbb{N} \rightarrow y \in \mathbb{R}$



Predicting y from x , discrete case.

Consider two variables, x, y . We can either care about

- ▶ $\mathbb{E}[y|x]$ the expectation of y for all x .
- ▶ $\mathbb{P}[y|x]$ the distribution of y for all x .

Probability table for $P(x, y)$

$P(x, y)$	$y = 0$	$y = 1$
$x = 0$	54%	6%
$x = 1$	16%	24%

- ▶ How can we graph this?
- ▶ What is $P(x)$?

Conditional probability table for $P(y|x)$

$P(y x)$	$y = 0$	$y = 1$
$x = 0$	90%	10%
$x = 1$	40%	60%

- ▶ What is $\mathbb{E}[y | x]$?

Distributions of two variables

In this setting, both x and y have a Bernoulli distribution. If we use a model whereby x is sampled first, and then y , then we can define two Bernoulli distributions. The first, for x is unconditional, while the second, for y , depends on the value of x :

$$\begin{aligned}x &\sim \text{Bernoulli}(\theta) \\ y \mid x &\sim \text{Bernoulli}(\phi_x).\end{aligned}$$

In our example, $\phi_0 = 0.1$ and $\phi_1 = 0.6$.

Homework

Probability table for $P(x, y)$

$P(x, y)$	$y = -1$	$y = 0$	$y = 1$
$x = 0$	10%	20%	10%
$x = 1$	30%	20%	10%

Given the above table, calculate

- ▶ $P(x)$
- ▶ The conditional probability table for $P(y|x)$.
- ▶ $\mathbb{E}[y|x]$ for all values of x .

Two variables: conditional expectation

The height of different genders

The conditional expected height

$$\mathbb{E}[h \mid g = 1] = \sum_{\omega \in \Omega} h(\omega) P[\omega \mid g(\omega) = 1]$$

The empirical conditional expectation

$$\mathbb{E}[h \mid g = 1] \approx \frac{\sum_{t: g(\omega_t)=1} h(\omega_t)}{|\{t : g(\omega_t) = 1\}|}$$

Python implementation

Two variables: conditional expectation

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Python implementation

```
h[g==1] / sum(g==1)
## alternative
import numpy as np
np.mean(h[g==1])
```

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Populations, samples, and distributions

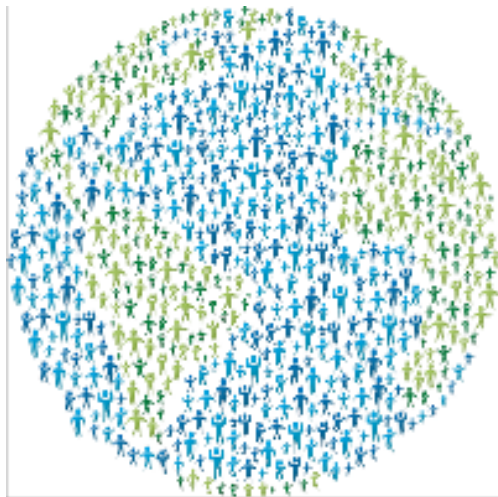


Figure: The world population



Figure: A sample

Statistical assumptions

Independent, Identically Distributed data

- ▶ $\omega_t \sim P$: individuals $\omega_t \in \Omega$ are drawn from some **distribution** P
- ▶ $\mathbf{x}_t \triangleq \mathbf{x}(\omega_t)$ are some **features** of the t -th individual
- ▶ Here we are interested in properties of the **unknown** distribution P .

Representative sample from a fixed population

- ▶ Finite population $\Omega = \{\omega_1, \omega_2, \dots, \omega_N\}$
- ▶ A subset $S \subset \Omega$ of size $T < N$ is selected with a **uniform distribution**, i.e. so that

$$P(S) = T/N, \quad \forall S \subset \Omega.$$

- ▶ Here we are interested in statistics of the **unknown** population Ω .
- ▶ We assume an underlying distribution P for convenience.
- ▶ We can try both cases essentially the same.

Learning from data

Unsupervised learning

- ▶ Given data x_1, \dots, x_T .
- ▶ Learn about the data-generating process.
- ▶ Example: Estimation, compression, text/image generation

Supervised learning

- ▶ Given data $(x_1, y_1), \dots, (x_T, y_T)$
- ▶ Learn about the relationship between x_t and y_t .
- ▶ Example: Classification, Regression

Online learning

- ▶ Sequence prediction: At each step t , predict x_{t+1} from x_1, \dots, x_t .
- ▶ Conditional prediction: At each step t , predict y_{t+1} from $x_1, y_1, \dots, x_t, y_t, x_{t+1}$

Reinforcement learning

Learn to act in an **unknown** world through interaction and rewards

Validating models

Training data

- ▶ Calculations, optimisation
- ▶ Data exploration

Validation data

- ▶ Fine-tuning
- ▶ Model selection

Test data

- ▶ Performance comparison

Simulation

- ▶ Interactive performance comparison
- ▶ White box testing

Real-world testing

- ▶ Actual performance measurement

Model selection

- ▶ Train/Test/Validate
- ▶ Cross-validation
- ▶ Simulation

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Models

- ▶ k-Nearest Neighbours.
- ▶ Linear models and perceptrons.
- ▶ Multi-layer perceptrons (aka deep neural networks).
- ▶ Bayesian Networks

Algorithms

- ▶ (Stochastic) Gradient Descent.
- ▶ Bayesian inference.

Reproducibility

- ▶ Modelling assumptions
- ▶ Interactions and feedback

Fairness

- ▶ Implicit biases in training data
- ▶ Fair decision rules and meritocracy

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ISLP Chapter 1