Introduction to Machine Learning

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Outline

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 machine learning / statistics problems

- Classification
- Regression
- Density estimation
- Clustering

Machine learning

Data Collection

- Downloading a clean dataset from a repository
- Performing a survey
- Scraping data from the web
- Deploying sensors, performing experiments, and obtaining measurements.

Modelling (what we focus on this course)

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

Algorithms and Decision Making

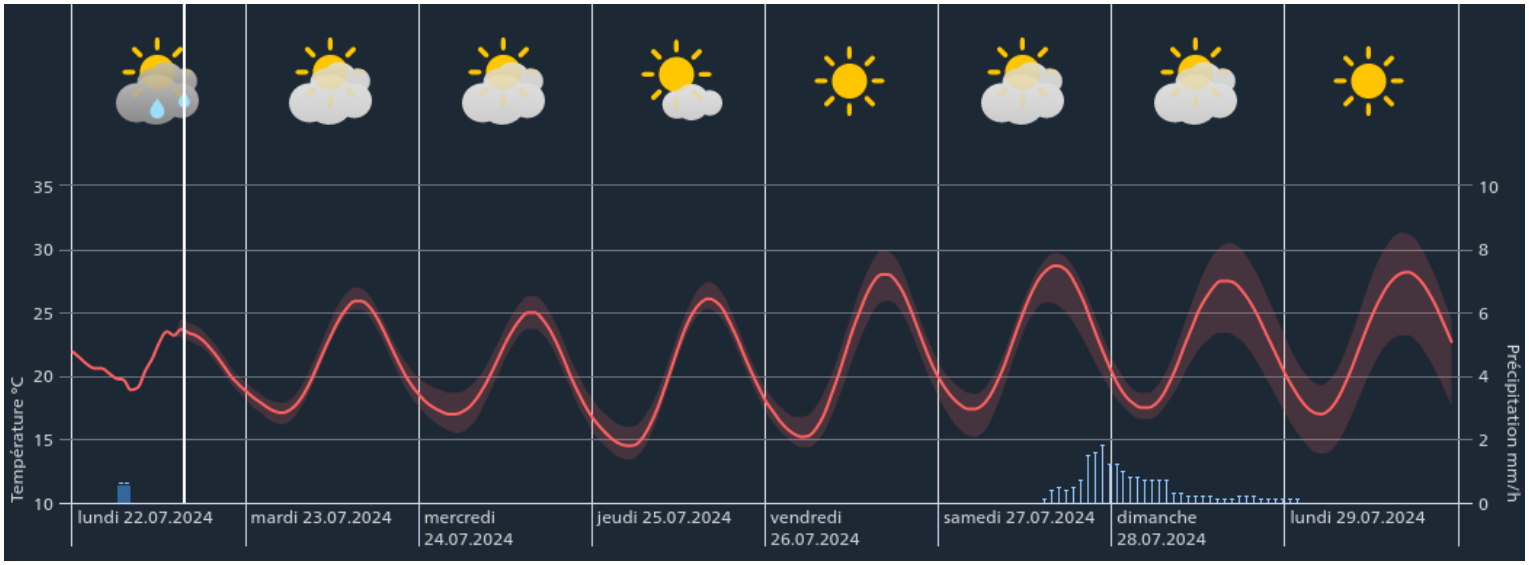
- We want to use models to make decisions.
- Decisions are made every step of the way.
- Decisions are automated algorithmically.

The main problems in machine learning and statistics

- Inference (what is going on now? what happened in the past?)
- Prediction (of the future, from the past)
- Decision making (what should we do to achieve our goals?)

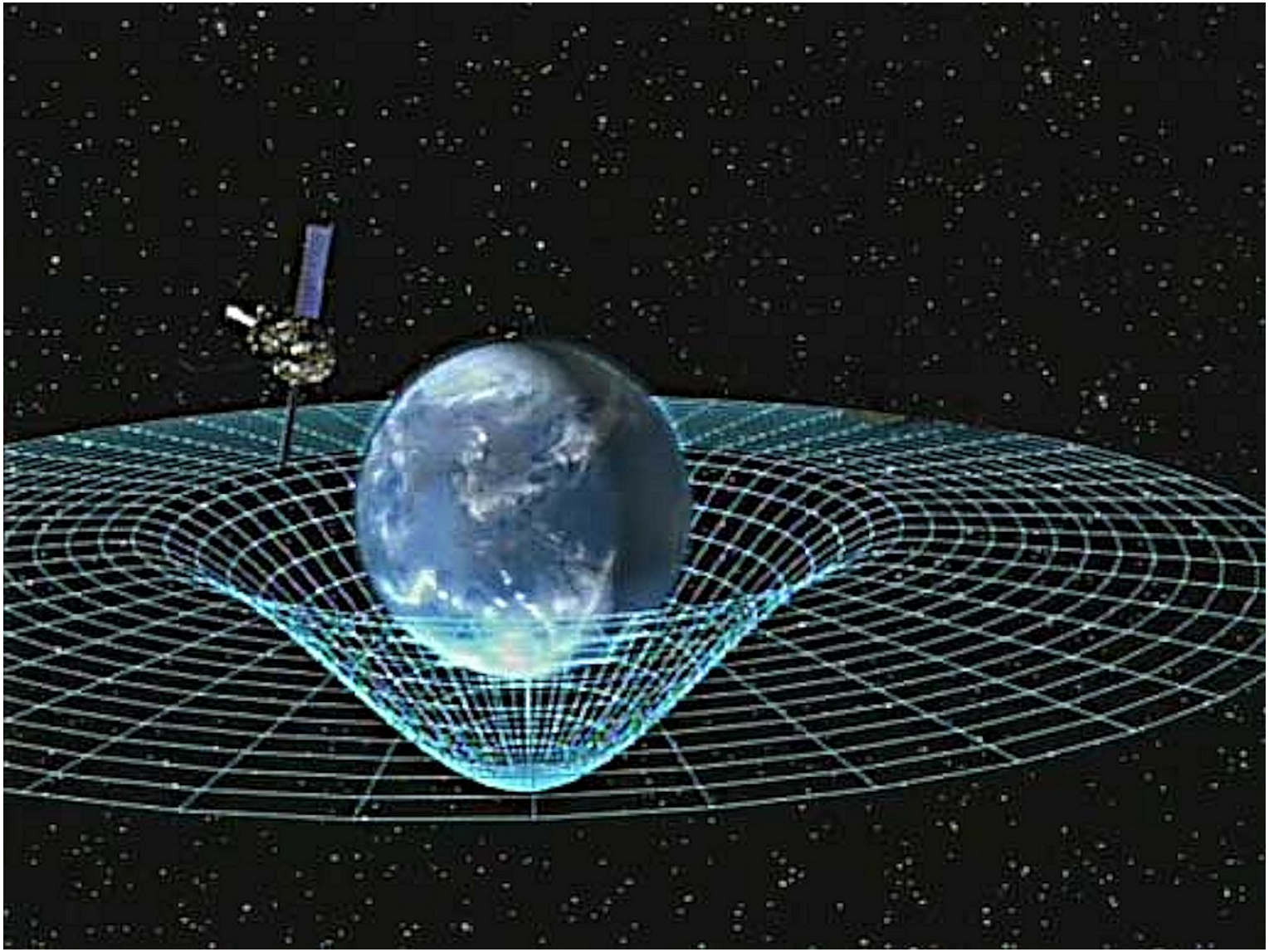
Sometimes each problem can be solved in isolation, but we usually have to partially solve all problems at the same time.

Prediction



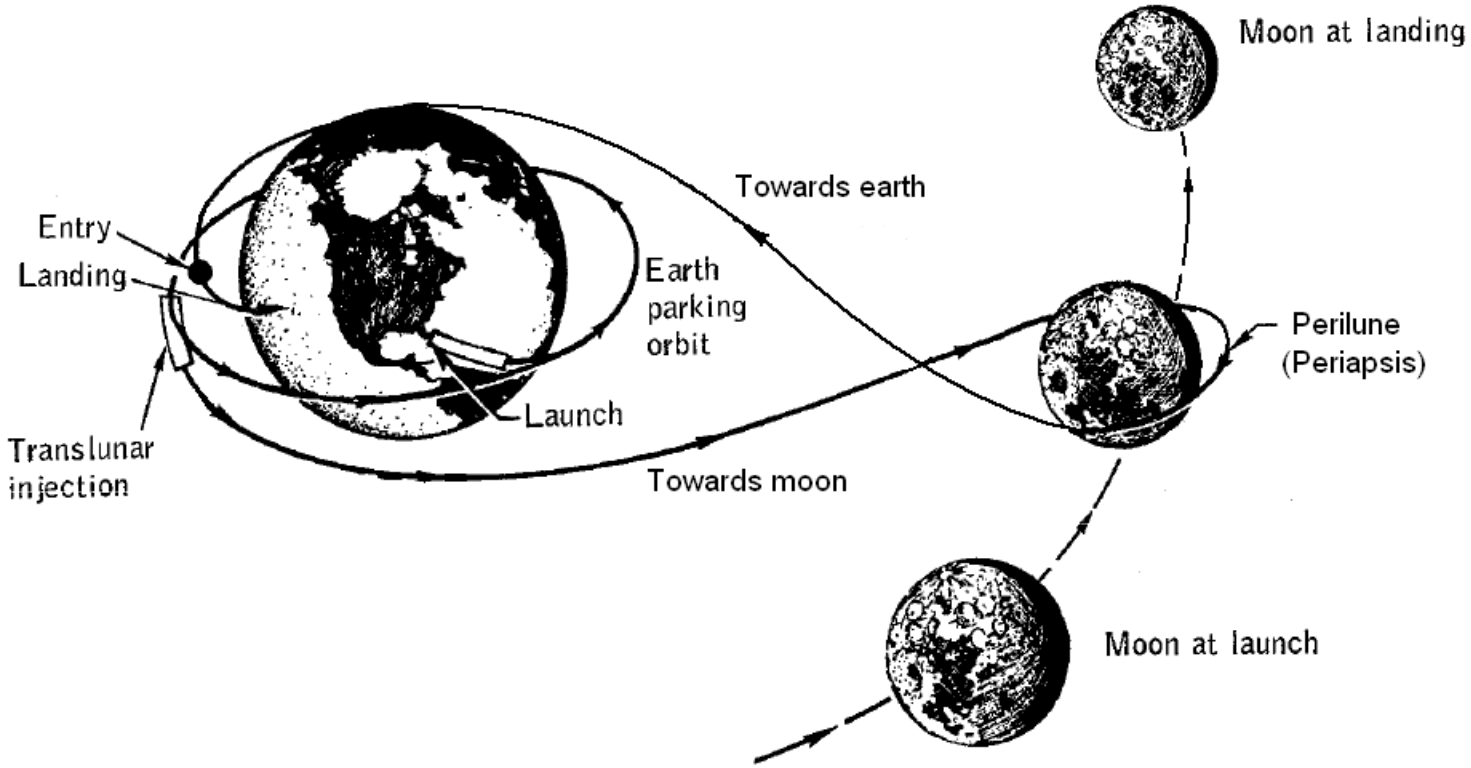
- Will it rain tomorrow?
- How much will bitcoin be worth next year?
- When is the next solar eclipse?

Inference



- Does my poker opponent have two aces?
- What is the law of gravitation?

Decision Making



`./fig/artemis.gif`

- Should I go hiking tomorrow?
- Should I buy some bitcoins?
- Should I fold, call, or raise in my poker game?
- How can I get a spaceship to the moon and back?

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?

Problem definition

- Health, weight and height

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?

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
- Health issue:

Auxiliary variables

Factors related to height, weight a aitnd health

Possible confounders

Other factors that might affect health outcomes, unrelated to height and weight

Class data

- The class enters their data into the excel file.

Mean estimation

- What is the average height/disease prevalence?
- What is the expected height/disease prevalence in the general population?

Supervised learning problems:

- 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

Input variables

Also called features, predictors, independent variables

Output variables

Also called response, or dependent variables.

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	Brtish	4

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

Raw versus neat data

- Neat data: $x_t \in \mathbb{R}^n$
- Raw data: text, graphs, missing values, etc

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 elemets
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 s
X.iat[2,0] # row 2, column 0
```

Means using python

Calculating the mean of a random variable

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

Calculating the mean of our class data

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

One variable: expectations and distributions

Modelling the height

- Mean: models the expected value
- Variance: models the . . . variance
- Empirical distribution: models the distribution

The expected value and the mean

Assume $x_t : \Omega \to \mathbb{R}$, and $\omega \sim P$

- $x_1, \ldots, x_t, \ldots, x_T$: random i.i.d. variables
- Ω: random outcome space
- P: distribution of outcomes $\omega \in \Omega$
- $\mathbb{E}_p[x]$: expectation of x under P

$$\mathbb{E}_P[x_t] = \sum_{\omega \in \Omega} x_t(\omega) P(\omega) \approx \frac{1}{T} \sum_{t=1}^{T} x_t$$

- The sample mean is $O(1/\sqrt{T})$-close to the expected value.

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

A gambling game

What are the expected winnings if you play this game?

- [a] With probability 1%, you win 100 CHF
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Solution

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

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

- $P(c) = 59\%$, as $P(\Omega) = 1$. Substituting,

$$\mathbb{E}_P(x) = 1 + 8 + 0 = 9.$$

Populations, samples, and distributions

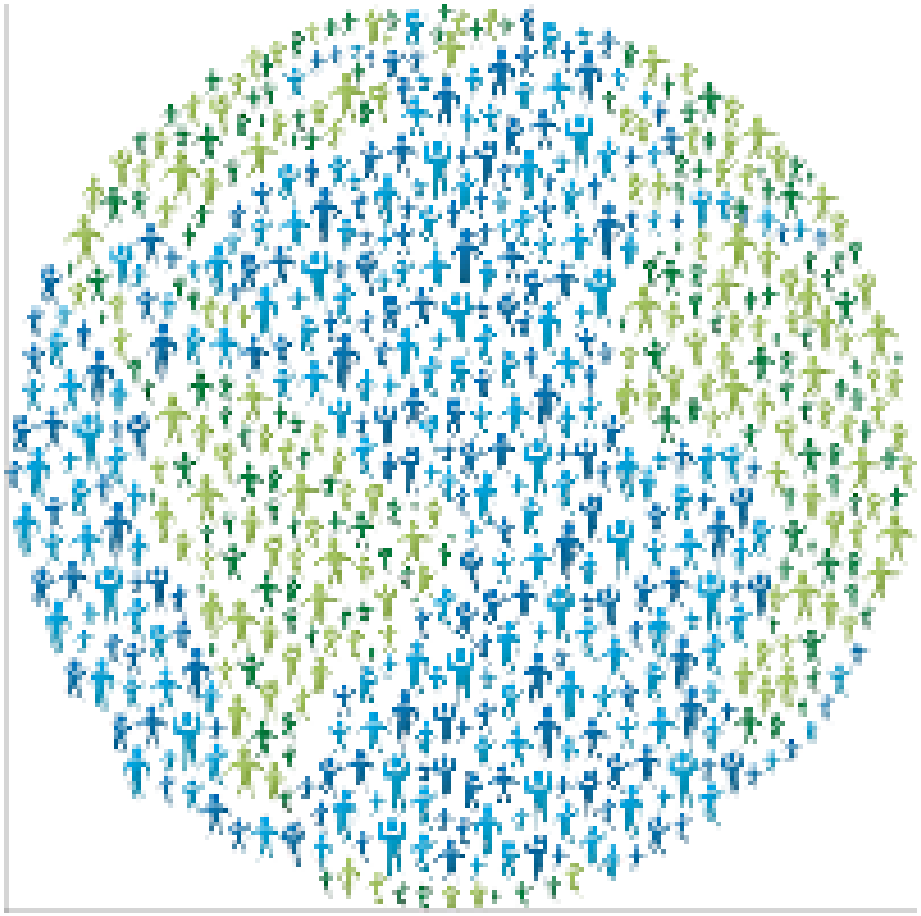

Figure: The world population

Figure: A sample

Statistical assumptions

We usually assume that individuals

Two variables: conditional expectation

The height of different genders

Learning from data

Unsupervised learning

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

Supervised learning

- Given data $(x_1, y_1), \ldots, (x_T, y_T)$
- 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 $x_1, \ldots, x_t$.
- Conditional prediction: At each step t, predict y_{t+1} from $x_1, y_1 \ldots, x_t, y_t, x_{t+1}$

Reinforcement learning

Learn to act in an unknown world through interaction and rewards

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 out of sample data
- This requires some assumptions about the data distribution.

Example models

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

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

The simplest model: A mean

Robust models of the mean

Model selection

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

Course Contents

Models

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

Algorithms

- (Stochastic) Gradient Descent.
- Bayesian inference.

Supervised learning

The general goal is learning a function $f : X \to Y$.

Classification

- Input data $x_t \in \mathbb{R}$, $y_t \in [m] = \{1, 2, \ldots, m\}$
- Learn a mapping f so that $f(x_t) = y_t$ for unseen data

Regression

- Input data x_t, y_t
- Learn a mapping f so that $f(x_t) = \mathbb{E}[y_t]$ for unseen data

Unsupervised learning

The general goal is learning the data distribution.

Compression

- Learn two mappings c, d
- $c(x)$ compresses an image x to a small representation z.
- $d(z)$ decompresses to an approximate image $\hat{x}$.

Density estimation

- Input data $x_1, \ldots, x_T$ from distribution with density p
- Problem: Estimate p.

Clustering

- Input data $x_1, \ldots, x_T$
- Assign each data x_t. to cluster label c_t.

Supervised learning objectives

- Data (x_t, y_t), $x_t \in X$, $y_t \in Y$, $t \in [T]$.
- i.i.d assumption: $(x_t, y_t) \sim P$ for all t.
- Supervised decision rule $\pi(a_t|x_t)$

Classification

- Predict the labels correctly, i.e. $a_t = y_t$.
- Have an appropriate confidence level

Regression

- Predict the mean correctly
- Have an appropriate variance around the mean

Unsupervised learning objectives

- Reconstruct the data well
- Be able to generate data

Reinforcement learning objectives

- Maximise total reward

Pitfalls

Reproducibility

- Modelling assumptions
- Distribution shift
- Interactions and feedback

Fairness

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

Privacy

- Accidental data disclosure
- Re-identification risk

ISLP Chapter 1