Introduction to Machine Learning

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Outline

The problems of Machine Learning (1 week)

Introduction

Estimation

Statistics, validation and model selection

Course summary

Reading for this week

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
- Reinforcement learning

The nuts and bolts

- Models
- Algorithms
- Theory
- Practice

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)

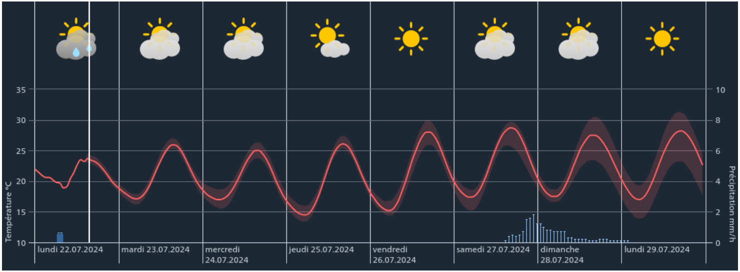
- Simple: the bias of a coin
- Complex: a language model.
- The model depends on the data and the problem

Algorithms and Decision Making

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

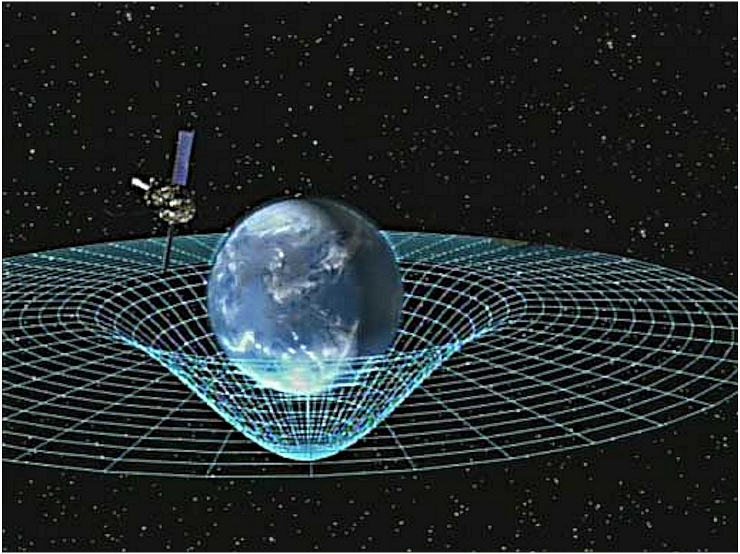
The main problems in machine learning and statistics

Prediction



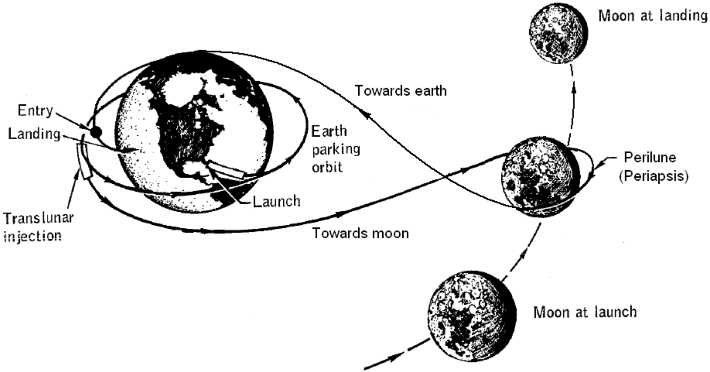
- Will it rain tomorrow?
- How much will bitcoin be worth next year?
- When is the next solar eclipse?

Inference



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

Decision Making



./fig/artemis.gif

- 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?

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

- 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?

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.

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

Input variables

Also called features, predictors, independent variables

Output variables

Also called response, dependent variables, labels, or targets.

General problems

The input/output dichotomy only exists in some problems.

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

Modelling variables

Predicting...

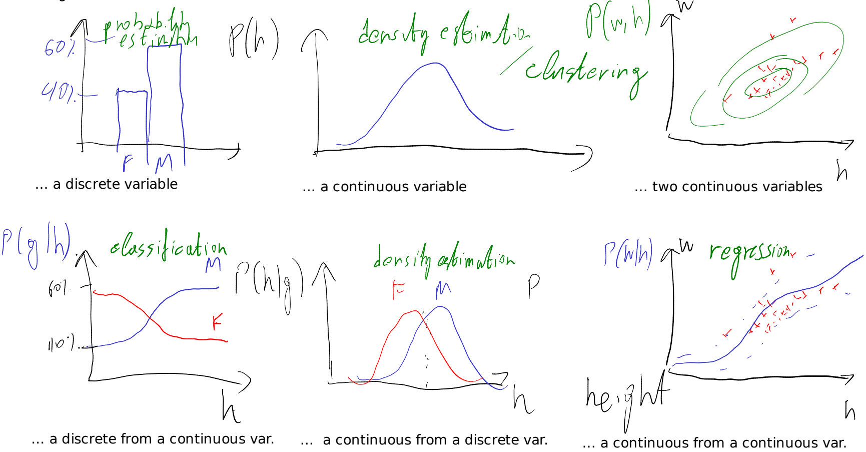


Figure: Basic learning problems

Directed graphs for modelling relationships

We can always summarise the type of model we want through a graph. In directed graphs we always have to specify a direction between linked variables.

Single variable

x

Regression

$w \longrightarrow h$

Classification

$w \longrightarrow g$

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

Example (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"])
```

- 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)

Assume $x : \Omega \to \mathbb{R}$, and $\omega_t \sim P$

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

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

One variable: expectations and distributions

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Definition (The sample mean)

The sample mean of $x_1, \dots, x_T$ is

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

Under P, the sample mean is $O(1/\sqrt{T})$-close to the expected value $\mathbb{E}_P[x_t]$.

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?

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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,

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

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

The simplest model: A mean

Predicting y from x.

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.

Models x discrete, y discrete

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

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

- Conditional probability table for $P(x, y)$

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

- What is $P(x)$?

x discrete, y continuous

- Collection of probability distributions.

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

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

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

Populations, samples, and distributions

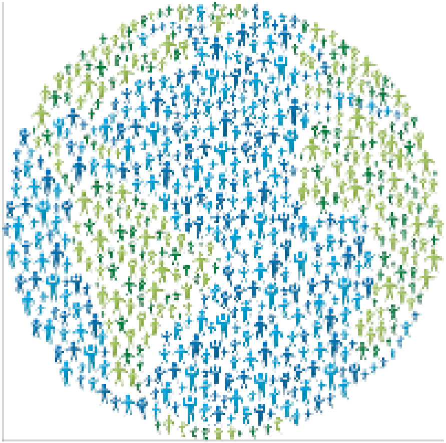

Figure: The world population

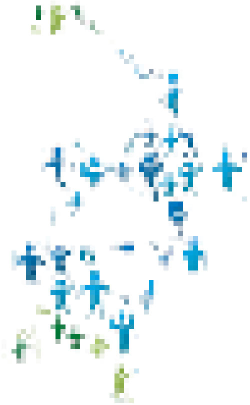

Figure: A sample

Statistical assumptions

Independent, Identically Distributed data

- $\omega_t \sim P$: individuals $\omega_t \in \Omega$ are drawn from some distribution P
- $\boldsymbol{x}_t \triangleq \boldsymbol{x}(\omega_t)$ 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 $\Omega = \{\omega_1, \omega_2, \ldots, \omega_N\}$
- A subset $S \subset \Omega$ of size $T < N$ is selected with a uniform distribution, i.e. so that

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

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

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

Robust models of the mean

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

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
- Can be mapped into classification by binning.

Unsupervised learning

The general goal is learning the data distribution.

Density estimation

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

Special case: Compression

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

Special case: Clustering

- Input data $x_1, \ldots, x_T$.
- Estimate latent cluster labels c_t to model the distribution of x as

a mix over densities p_c.

$$p(x_t) = \sum_c P(c_t = c) p_c(x_t)$$

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

Reading for this week

ISLP Chapter 1