Machine Learning

Lecture 1.1:
Introduction and probability theory

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Based on slides made by Jes Frellsen.

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IT UNIVERSITY OF COPENHAGEN

Welcome to the

Machine Learning and

Advanced Machine Learning

courses!

Outline of lecture

Course overview

Introduction to Machine Learning

Probability Theory (repetition)

Who are the teachers?

Sami: lecturer

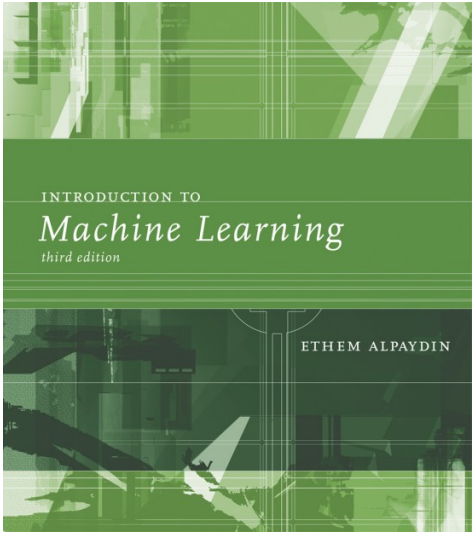
Sanne: lecturer

Stella: lecturer

Najmeh: lecturer

TAs: Stefan (ML), Viktor (ML), and Luis (AML).

Textbooks



Main textbook: “Alpaydin”

- A good textbook for introducing ML
- Fits well to this course
- Not too heavy if compared to e.g. Bishop’s book.

Course structure

- **Weekly activities** in the **first 10 weeks**:
  - **Lecture 1**: Mondays at 12:00–14:00 (Aud 1; except W37 when in Aud3)
  - **Exercises (ML)**: Thursdays at 12:00–14:00 (Anders–Jeppe: 2A52, Ji–Ziming: 2A54)
  - **Exercises (AML)**: Wednesdays at 14:00–16:00 (3A52)
  - **Lecture 2**: Thursdays at 10:00–12:00 (Aud 1; except W37,W40,W45 when in Aud3)
  - **Mandatory Exercises (ML)**: Mondays at 14:00–16:00 (Anders–Jeppe: 2A52, Ji–Ziming: 3A18)
  - **Mandatory Exercises (AML)**: Fridays at 12:00–14:00 (3A52)
- The **last 4 weeks**: project in groups of 2–3 persons.
  - Part of the final exam
  - Will count towards you final grade together with the oral exam
- **Communication** will happen through the **LearnIT** page
  - The **course outline** gives a overview of the course
  - **Separate section for each week** below (detailed reading plan, exercises etc.)
  - **Student forum** for Q&A

Preparation for Weekly Activities

- **How to prepare for weekly activities?**
  - **We do not assume that you have read before the lectures**, but we expect that you have looked at the material.
  - We do not expect you to have solved the exercises before the Wed/Thu exercise session.
  - You have to have solved the exercises before the Fri/Mon mandatory exercise session.

Mandatory activities

- **9 mandatory exercise sessions**
  - You have to **offer** to present at least 50% of the exercises on average during the course.
  - **Before** you come to the mandatory exercises on Mondays (ML) or Fridays (AML) you have to fill in the checklist on the LearnIT page.
  - The TA will select who presents the exercise.
  - *If you have indicated that you can present an exercise and you have not done the exercises you fail this mandatory activity.*
- You need to **pass the mandatory activities to go to the exam**.
- If you have not passed before the project starts: an **oral test**

Exam

The exam exists of two parts:

- A **4 week project** to be done in groups and be handed in by the end of the semester (more information later)
  - ML: Covers many of the subjects that we discussed in the first 10 weeks
  - AML: You will implement a recent machine learning method from a research article.
- A **20 min oral exam** about the project and the topics of the course.

Intended learning outcome

After the course, the student should be able to:

- **Discuss**, clearly **explain**, and **reflect** upon central machine learning concepts and algorithms.
- **Choose among** and **make use** of the most important machine learning approaches in order to apply (match) them to practical problems.
- **Implement** abstractly specified machine learning methods in an imperative programming language (Python)
- **Combine** and **modify** machine learning methods to **analyse** practical dataset and **covey** the results.

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  - **Main learning activity:** project
  - **Main evaluation:** project and oral exam

What is this course not?

- It is not a *deep learning* course
- It is not a Tensorflow / PyTorch / scikit-learn course

Outline of lecture

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Introduction to Machine Learning

Probability Theory (repetition)

What is *Machine Learning*?

Picture from: https://history-computer.com/ModernComputer/thinkers/Samuel.html

What is *Machine Learning*?

The term was coined by Arthur Lee Samuel in the 1950s.

> "Programming computers to learn from experience should eventually eliminate the need for much of this detailed programming effort."

(Samuel, 1959)

This quote is often loosely rephrased into the definition

> Machine learning is the field of study that gives computers the ability to learn without being explicitly programmed

(e.g. Wikipedia)

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What is the difference between ML and stats?

- Stats is mainly concerned with estimation
- ML is mainly concerned with prediction

Picture from: https://history-computer.com/ModernComputer/thinkers/Samuel.html

A brief history of machine learning

Bishop (2009)

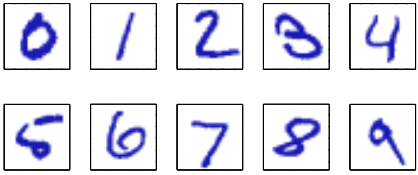
- **First Generation**: Expert systems[1] (1970s and 1980s)
  - Rule based (hand crafted by humans)
  - **Drawback:** Combinatorial explosion
- **Second Generation:** "Black-box" statistical models (1980s and 1990s)
  - Neural networks, Support Vector Machines
  - **Drawback:** Difficult to incorporate domain knowledge
- **Third Generation:** Integration of domain knowledge using the language of probability theory (1990s and 2000s)
  - Bayesian framework, efficient scalable inference algorithms
  - Ability to quantify uncertainties
  - **Drawback:** High computational complexity
- **Forth Generation:** Deep Learning (2010s)
  - Driven by faster computers and larger data sets
  - **Drawback:** Challenging to quantify uncertainties

[1] Aka *Symbolic Artificial Intelligence* or **Good Old-Fashioned Artificial Intelligence**

Example of machine learning: hand-written digit recognition

Task: Given an input image $\mathbf{x} \in \mathbb{R}^{28\times 28}$ produce the identity of the digit $t \in \{0, 1, \ldots, 9\}$.

- $\mathbf{x}$: input or feature vector
- t: target, output or label (vector)



The ML approach: from a **training set**

$$\mathcal{D} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_N, t_N)\}$$

tune the parameters $\mathbf{w}$ of an adaptive model y such that $y_{\mathbf{w}}(\mathbf{x}) = t$.

This is called the **training** or **learning** phase.

Figure(s) from Bishop.

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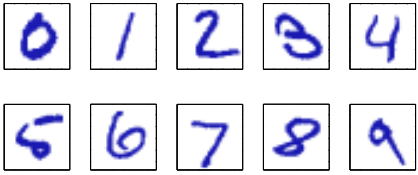

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This is called the **training** or **learning** phase.

When the model is learned, we can evaluate it on a **test set**.

Generalization: the ability to correctly categorize new examples (not in the training set)

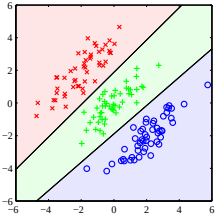
Feature extraction: Pre-processing of the training and test data, e.g. normalization, standardization, dimensionality reduction...

Figure(s) from Bishop.

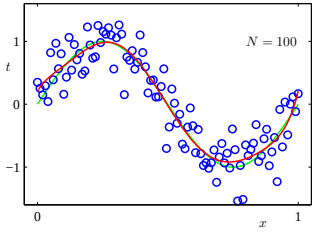
Categories of Machine Learning (I)

Supervised learning: $\mathcal{D} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$

Classification

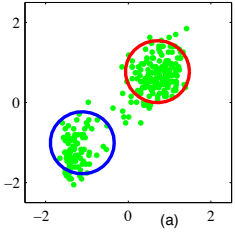


Regression

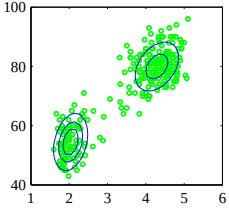


Unsupervised learning: $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$

Clustering



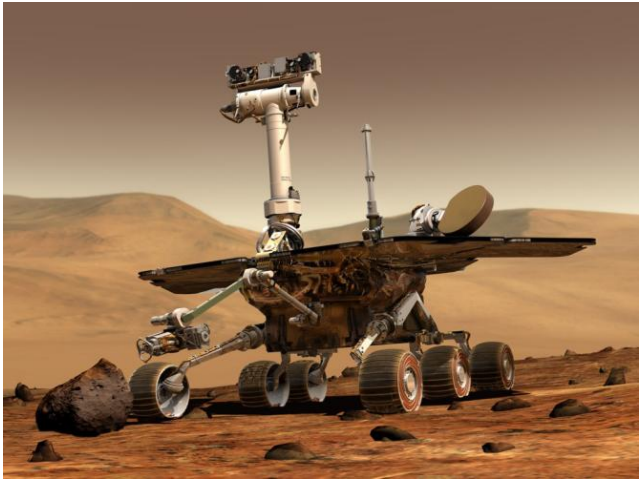
Density estimation



Figure(s) from Bishop.

Categories of Machine Learning (II)

Reinforcement learning: find suitable actions in a given situation to maximize a reward.



Picture from: https://photojournal.jpl.nasa.gov/catalog/PIA04413

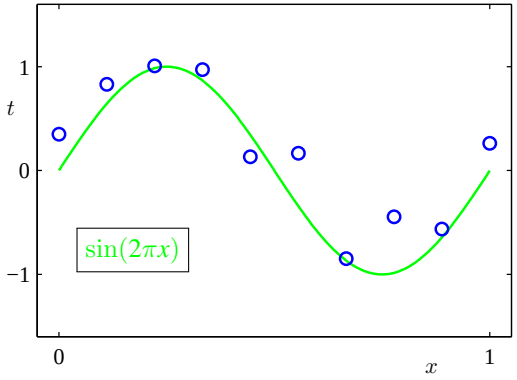
Categories of Machine Learning (II)

Reinforcement learning: find suitable actions in a given situation to maximize a reward.

Picture from: https://medicalfuturist.com/alphago-artificial-intelligence-in-healthcare

Example: Polynomial Regression

Assume we are given a dataset $\mathcal{D} = \{(x_1, t_1), \ldots, (x_N, t_N)\}$ where $x_n, t_n \in \mathbb{R}$ and $N = 10$.



We want to fit the data using a polynomial function

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \sum_{j=1}^{M} w_j x^j$$

Figure(s) from Bishop.

Outline of lecture

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Introduction to Machine Learning

Probability Theory (repetition)

Sample spaces and outcomes

The **sample space** for an **experiment** is a **set**, where

- each element of the sample space is an **outcome** of the **experiment**, and
- all possible **outcomes** are included in the set.

A **sample space** is typically denoted Ω.

Example (Coin flipping)

The experiment of flipping a coin has two possible outcomes: heads and tails.
The sample space for this experiment is $\Omega = \{\mathsf{H}, \mathsf{T}\}$.

Probability Function

Definition

A **probability function** P on a **finite sample space** Ω assigns to each event A in Ω **a number** $P(A)$ **in** $[0, 1]$ such that

i. $P(\Omega) = 1$, and

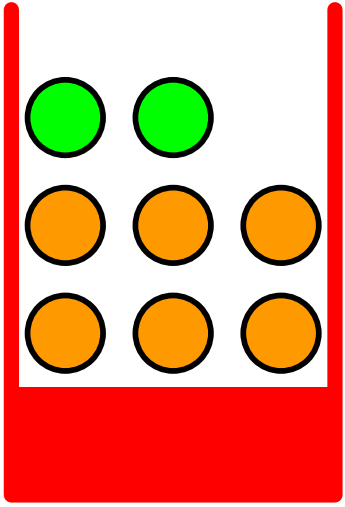
ii. $P(A \cup B) = P(A) + P(B)$ if A and B are **disjoint** (**called the additive property**).

The number $P(A)$ is called the probability that A occurs.

The additive rule implies that

$$P(A \cup B \cup C) = P(A \cup B) + P(C) = P(A) + P(B) + P(C).$$

Frequentist Notion of Probability



Apples and oranges

Frequentist definition of probability:

The probability of an event is the number of times the event occurs out of the total number of trails, as the number of trials goes to infinity.

One trial: Pick a random fruit from a new box containing apples and oranges.

$$P(F = a) = \frac{n_a}{N} \text{ as } N \to \infty$$

Figure(s) from Bishop.

Probability as a measure of uncertainty

We can all agree that the probability of **heads** is $\frac{1}{2}$ for a toss of a fair coin.

Here are to common justifications

1. **Frequency argument:**

$$\text{probability} = \text{relative frequency obtained in a long sequence of tosses,}$$

   i.e. $P(H) = \frac{n_H}{N}$ as $N \to \infty$..

2. **Symmetry or exchangeability argument:**

$$\text{probability} = \frac{\text{number of favorable cases}}{\text{number of possibilities}}$$

   assuming equally likely possibilities, i.e. $P(H) = \frac{1}{2}$.

The frequents argument involves the hypothetical notion of a long sequence of experiments.

The symmetry argument allow us to assign probability to a singe experiment.

Picture from gurmeet.net

Bayesian Notion of Probability

In the Bayesian statistics, probability is used as a measure of uncertainty.

What is the probability of Denmark winning the World Cup in 2022?

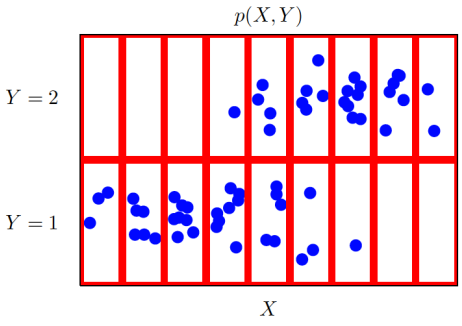
How uncertain am I that Denmark will win the World Cup?

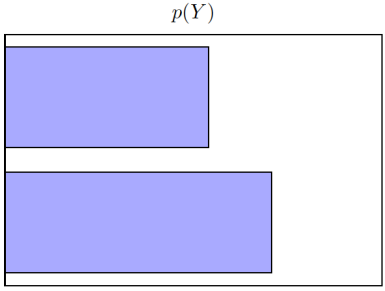
What is the probability that the Arctic ice cap will have melted by the end of the century?

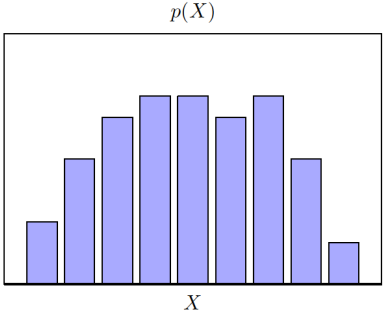
How uncertain am I about the rate of ice loss?

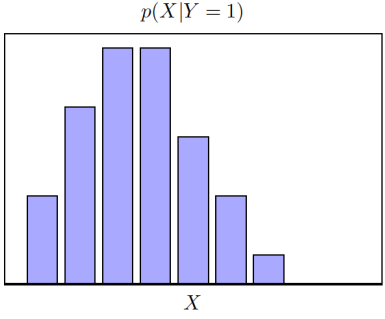
Pictures from wikipedia.org and ecochiccayman.com

Distribution of Two Variables, Discrete





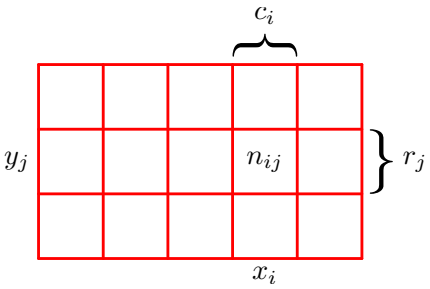




Probability theory

Joint probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$



Figure(s) from Bishop.

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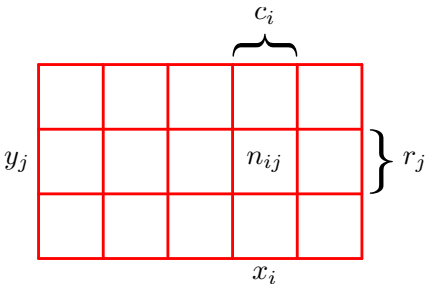
Marginal probability

$$p(X = x_i) = \frac{c_i}{N}$$



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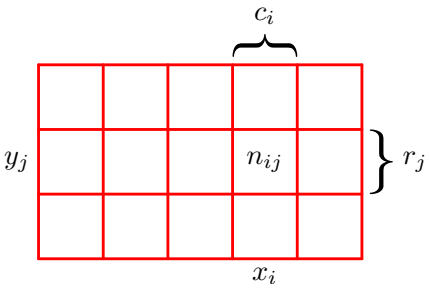
$$p(X = x_i) = \frac{c_i}{N} = \frac{\sum_j n_{ij}}{N}$$



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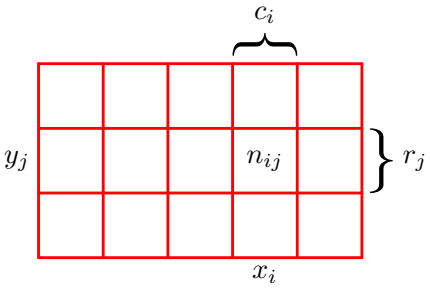

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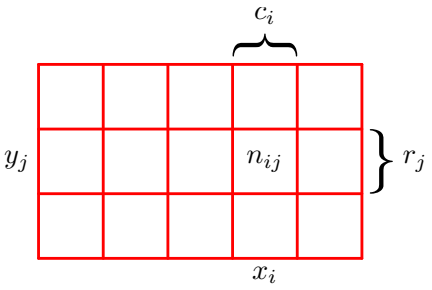

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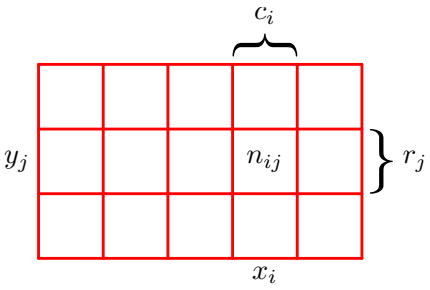
Conditional probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$



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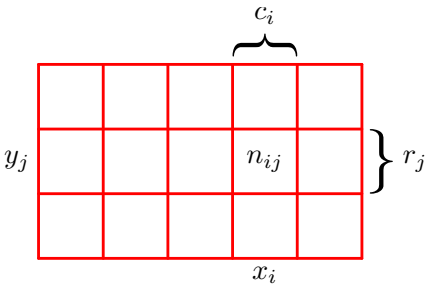

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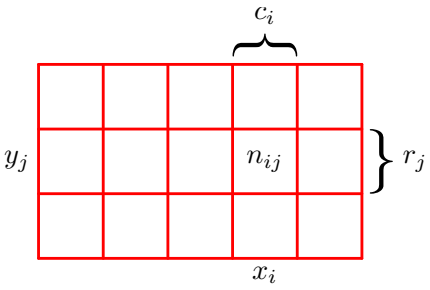

Conditional probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

We can then derive the **product rule**

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N}$$

Figure(s) from Bishop.

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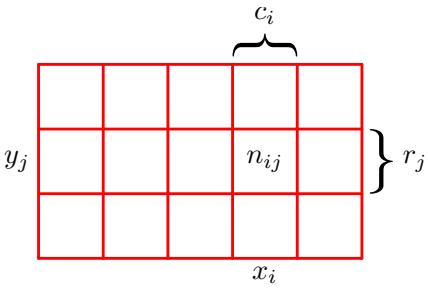


Conditional probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

We can then derive the **product rule**

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N}$$
$$= p(Y = y_j | X = x_i) P(X = x_i)$$

Figure(s) from Bishop.

The rules of probability and Bayes theorem

The Rules of Probability

sum rule
$$p(X) = \sum_Y p(X, Y)$$

product rule
$$p(X, Y) = p(Y|X)p(X)$$

From these rules follows:

Bayes' theorem

$$p(Y|X) = \frac{p(X|Y)p(Y)}{P(X)} \quad \text{where} \quad p(X) = \sum_Y p(X|Y)p(Y)$$

Continuous case: Probability densities

A **probability density** $p(x)$ over $x \in \mathbb{R}$ must satisfy

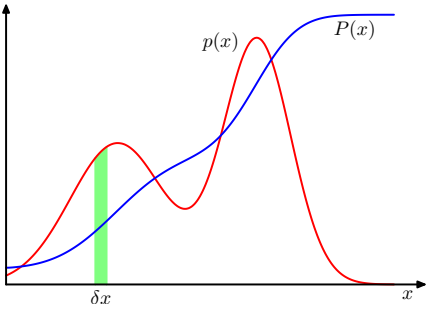
$$p(x) \geq 0 \quad \text{and} \quad \int_{-\infty}^{\infty} p(x)\,\mathrm{d}x = 1$$

The probability of x lying on the interval (a, b) is

$$p(x \in (a, b)) = \int_{a}^{b} p(x)\,\mathrm{d}x$$

The **cumulative distribution function** (CDF) is defined as

$$P(z) = p(x \in (-\infty, z)) = \int_{-\infty}^{z} p(x)\,\mathrm{d}x$$



The **sum and product rules** also apply to densities

$$p(x) = \int p(x, y)\,\mathrm{d}y \quad \text{and} \quad p(x, y) = p(y|x)p(x)$$

Figure(s) from Bishop.

Expectations

The **expected value** of a function $f(x)$ under a discrete probability mass function or continuous density, both denoted by $p(x)$,

$$\mathrm{E}[f] \equiv \sum_x p(x) f(x) \qquad \text{or} \qquad \mathrm{E}[f] \equiv \int_x p(x) f(x).$$

The **conditional expectation** can be written as

$$\mathrm{E}_x[f|y] \equiv \sum_x p(x|y) f(x).$$

We can approximate the expected value by using **samples** of x drawn from $p(x)$, i.e,

$$\mathrm{E}[f] \simeq \frac{1}{N} \sum_{n=1}^{N} f(x_n).$$

Variance and covariance

The **variance** of $f(x)$ (under $p(x)$) is defined as

$$\begin{aligned}\mathrm{var}[f] &\equiv \mathrm{E}\left[(f(x) - \mathrm{E}[f(x)])^2\right] \\ &= \mathrm{E}[f(x)^2] - \mathrm{E}[f(x)]^2,\end{aligned}$$

and measures the variability of $f(x)$ around its mean.

The **covariance** of two random variables x and y is defined as

$$\begin{aligned}\mathrm{cov}[x, y] &\equiv \mathrm{E}_{x,y}\left[(x - \mathrm{E}[x])(y - \mathrm{E}[y])\right] \\ &= \mathrm{E}[xy] - \mathrm{E}[x]\mathrm{E}[y],\end{aligned}$$

and measures the extend to which x and y vary together

Examples of Probability Distributions

We will review two **parametric distributions**, that are used as a building blocks in machine learning methods:

- Binomial distribution (Discrete)
- Gaussian distribution (Continous)

A distribution is said to be parametric, if it can be described using **a finite set of parameters**.

Binomial distribution

Figure(s) from Bishop.

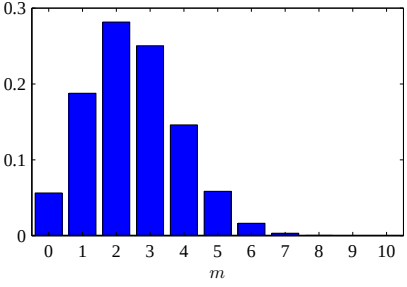
Now suppose that we perform N **Bernoulli trials**, e.g. $N = 10$ coin tosses.

What is the probability of obtaining m **successes in** N **trials**?
E.g. $m = 3$ heads in $N = 10$ trials.

$$\mathrm{Bin}(m|N,\mu) = \binom{N}{m}\mu^m(1-\mu)^{N-m}$$
$$\mathrm{E}[E] = N\mu$$
$$\mathrm{var}[m] = N\mu(1-\mu)$$

Picture from gurmeet.net

$\mathrm{Bin}(m|N=10,\mu=0.25)$

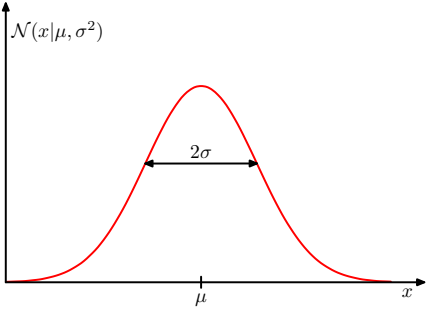


The Gaussian distribution

The **Gaussian** is widely used in ML and is defined by

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

where μ is the **mean** and σ^2 is the **variance**.



Law of Large Numbers

Law of Large Numbers

The law of large numbers says that the mean of i.i.d. samples

$$\bar{x}_n = \frac{1}{n}\left(x_1 + x_2 + \ldots + x_n\right)$$

converges to the expected value, or

$$\bar{x}_n \longrightarrow E\{\bar{X}_n\}, \qquad \text{as } n \to \infty.$$

(What are the required conditions?)

Central limit theorem

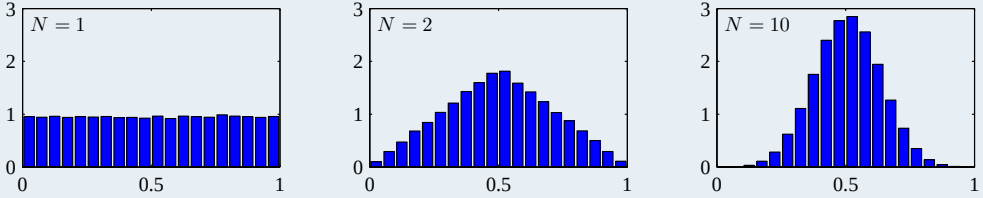
Figure(s) from Bishop.

Central limit theorem

The distribution of the sum of N i.i.d. random variables **becomes increasingly Gaussian as N grows**.

N uniform $[0, 1]$ random variables

The distribution of the mean $(x_1 + \cdots + x_N)/N$ for the N variables $x_1, \ldots, x_N \sim \mathcal{U}(0, 1)$:



Figure(s) from Bishop.

Next lecture

- Introduction to Supervised learning

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