

Lecture 1: Introduction

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TÉCNICO
LISBOA

Deep Structured Learning Course, Fall 2020

Course Website

[https://andre-martins.github.io/pages/
deep-structured-learning-ist-fall-2020.html](https://andre-martins.github.io/pages/deep-structured-learning-ist-fall-2020.html)

There I'll post:

- Syllabus
- Lecture slides
- Literature pointers
- Homework assignments
- ...

Outline

① Introduction

② Class Administrativa

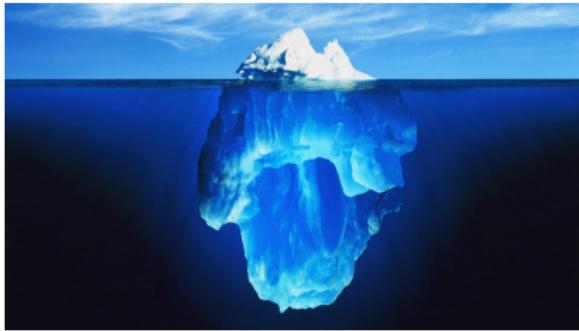
③ Recap

Linear Algebra

Probability Theory

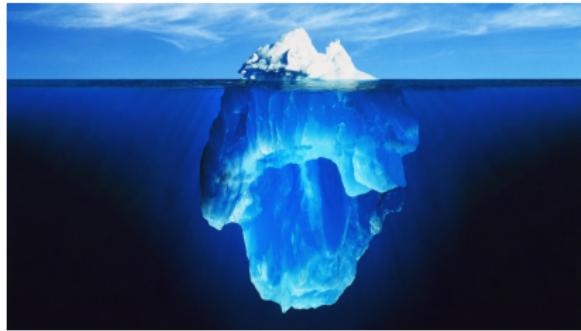
Optimization

What is “Deep Learning”?



- Neural networks?
- Neural networks with many hidden layers?
- Anything beyond shallow (linear) models for statistical learning?
- Anything that learns representations?
- A form of learning that is really intense and profound?

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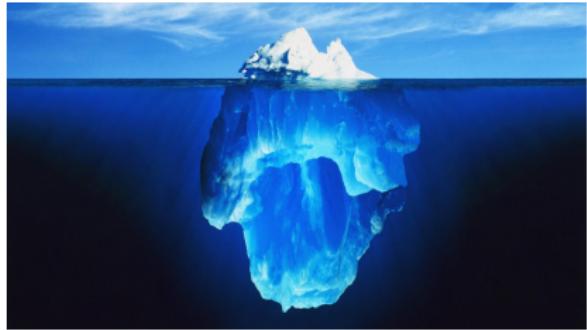
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Where is the “Structure”?



- In the **input** objects (text, graphs, images, ...)
- In the **outputs** we want to predict (parsing, graph labeling, image segmentation, ...)
- In our **model** (convolutional networks, attention mechanisms)
- Related: **latent structure** (typically a way of encoding prior knowledge into the model)

This Course: “Deep Learning + Structure”



Why Did Deep Learning Become Mainstream?

Lots of recent breakthroughs:

- Object recognition
- Speech and language processing
- Chatbots and dialog systems
- Self-driving cars
- Machine translation
- Solving games (Atari, Go)

No signs of slowing down...



Microsoft's Deep Learning Project Outperforms Humans In Image Recognition



Michael Thomsen, CONTRIBUTOR

I write about tech, video games, science and culture. [FULL BIO](#) ▾

Opinions expressed by Forbes Contributors are their own.

**Big Data
on AWS**

Microsoft's new breakthrough: AI that's as good as humans at listening... on the phone

Microsoft's new speech-recognition record means professional transcribers could be among the first to lose their jobs to artificial intelligence.



By Liam Tung | October 19, 2016 -- 10:10 GMT (11:10 BST) | Topic: [Innovation](#)

A closer look at Google Duplex

Google's appointment booking AI wowed the crowd and raised concern at I/O

No problem. I'll make you an appointment and
update you soon.

Who is wearing glasses?

man



woman

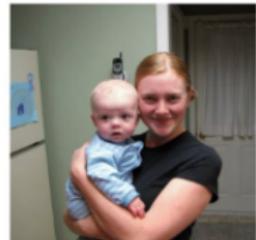


Where is the child sitting?

fridge



arms



Is the umbrella upside down?

yes



no



How many children are in the bed?

2



1



The Great A.I. Awakening

How Google used artificial intelligence to transform Google Translate, one of its more popular services — and how machine learning is poised to reinvent computing itself.

BY GIDEON LEWIS-KRAUS DEC. 14, 2016



Google unleashes deep learning tech on language with Neural Machine Translation

Posted Sep 27, 2016 by Devin Coldewey, Contributor



Systran launches neural machine translation engine in 30 languages

Language barriers represent one of the biggest challenges to develop business strategies among global markets. Now, thanks to advances in artificial intelligence and machine translation, these barriers are being broken down.



By Eileen Brown for Social Business | November 24, 2016 -- 13:49 GMT (3:49 GMT) | Topic: Artificial Intelligence

Siri and Alexa Are Fighting to Be Your Hotel Butler

By Hui-yong Yu and Spencer Soper

March 22, 2017, 9:00 AM GMT Updated on March 22, 2017, 2:13 PM GMT

- Hotels are new frontier for voice-command technologies
- Wynn Las Vegas was first to install Alexa devices in December





AlphaGo Beats Go Human Champ: Godfather Of Deep Learning Tells Us Do Not Be Afraid Of AI

21 March 2016, 10:16 am EDT By [Aaron Mamiit](#) Tech Times



Last week, Google's artificial intelligence program

Last week, Google's artificial intelligence program AlphaGo **dominated** its match with South Korean world Go champion Lee Sedol, winning with a 4-1 score.

The achievement stunned artificial intelligence experts, who previously thought that Google's computer program would need at least 10 more years before developing enough to be able to beat a human world champion.

A robot wrote this entire article. Are you scared yet, human?

We asked GPT-3, OpenAI's powerful new language generator, to write an essay for us from scratch. The assignment? To convince us robots come in peace

- For more about GPT-3 and how this essay was written and edited, please read our editor's note below



Why Now?

Why does deep learning work now, but not 20 years ago?

Many of the core ideas were there, after all.

But now we have:

- more data
- more computing power
- better software engineering
- a few algorithmic innovations (many layers, ReLUs, better initialization and learning rates, dropout, LSTMs, convolutional nets)

“But It’s Non-Convex”

Why does gradient-based optimization work at all in neural nets despite the non-convexity?

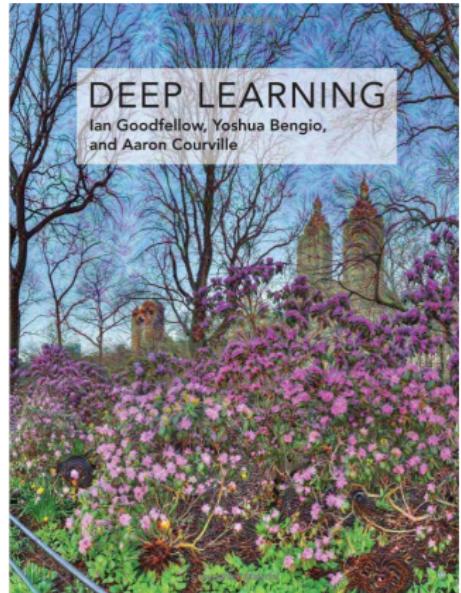
One possible, partial answer:

- there are generally many hidden units
- there are many ways a neural net can approximately implement the desired input-output relationship
- we only need to find one

Recommended Books

Main book:

- **Deep Learning.** Ian Goodfellow, Yoshua Bengio, and Aaron Courville. MIT Press, 2016. **Chapters available at** <http://deeplearningbook.org>



Recommended Books

Secondary books:

- **Machine Learning: a Probabilistic Perspective.** Kevin P. Murphy. MIT Press, 2013.
- **Introduction to Natural Language Processing.** Jacob Eisenstein. MIT Press. 2019.
- **Linguistic Structured Prediction.** Noah A. Smith. Morgan & Claypool Synthesis Lectures on Human Language Technologies. 2011.

Tentative Syllabus

- Sep 23 Introduction and Course Description
- Sep 30 Linear Classifiers
- Oct 7 Feedforward Neural Networks
- Oct 14 Representation Learning and Convolutional Networks
- Oct 21 Neural Network Toolkits (Pytorch)
- Oct 28 Linear Sequence Models
- Nov 4 Recurrent Neural Networks
- Nov 11 Structured Prediction and Graphical Models
- Nov 18 Sequence-to-Sequence Learning
- Nov 25 Attention Mechanisms and Explainability
- Dec 2 Deep Reinforcement Learning
- Dec 9 Deep Generative Models (VAEs, GANs)
- January Final Projects

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What This Class Is About

- Introduction to deep learning
- Introduction to structured prediction
- **Goal:** after finishing this class, you should be able to:
 - Understand how deep learning works without magic
 - Understand the intuition behind deep structured learning models
 - Apply the learned techniques on a practical problem (NLP, vision, ...)
- **Target audience:**
 - MSc/PhD students with basic background in ML and good programming skills

What This Class Is Not About

It's **not** about:

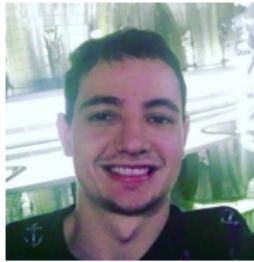
- Just playing with a deep learning toolkit without learning the fundamental concepts
- Introduction to ML (see Mário Figueiredo's **Statistical Learning** course and Jorge Marques' **Estimation and Classification** course)
- Optimization (check João Xavier's **Non-Linear Optimization** course)
- Natural Language Processing
- ...

Prerequisites

- Calculus and basic linear algebra
- Basic probability theory
- Basic knowledge of machine learning
- Programming (Python & PyTorch preferred)
- Helpful: basic optimization

Course Information

- **Instructor:** André Martins
- **TA:** Marcos Treviso
- **Location:** Fully remote (Zoom link in Piazza)
- **Schedule:** Wednesdays 14:30–17:30 (tentative)
- **Communication:**
piazza.com/tecnico.ulisboa.pt/fall2020/pdeecdsl



Grading

- 3 homework assignments: **60%**
 - Theoretical questions & implementation
 - Late days: 10% penalization each late day
- Final project (in groups of 2–3): **40%**
 - Final class presentations

Final Project

- **Possible idea:** apply a deep learning technique to a structured problem relevant to your research (NLP, vision, robotics, ...)
- Otherwise, pick a project from a list of suggestions
- Must be finished this semester
- Four evaluation stages: project proposal (10%), midterm report (10%), final report (10%, conference paper format), class presentation (10%)
- List of project suggestions will be made available soon

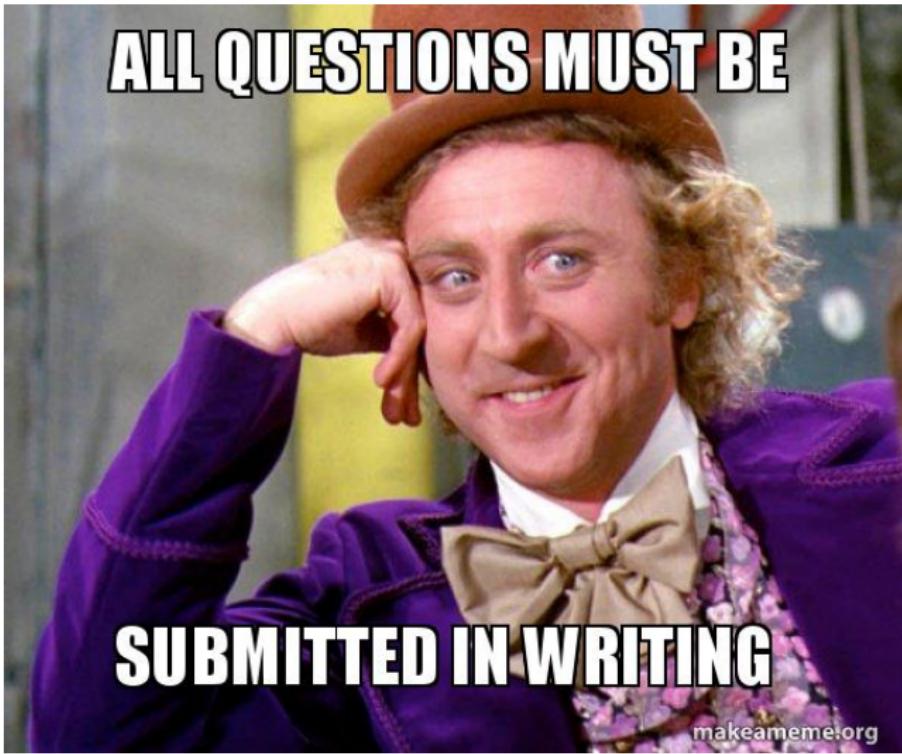
Collaboration Policy

- Assignments are individual
- Students may discuss the questions, as long as they write their own answers and their own code
- If this happens, acknowledge with whom you collaborate!
- Zero tolerance on plagiarism!!
- Always credit your sources!!!

Caveat

- This is the third year I'm teaching this class
- ... which means you're the third batch of students taking it :)
- **Constructive feedback will be highly appreciated (and encouraged!)**

Questions?



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Quick Background Recap

Slide credits: Prof. Mário Figueiredo (taken from his LxMLS class)



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- Linear algebra provides (among many other things) a compact way of representing, studying, and solving linear systems of equations

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- Example: the system

$$\begin{aligned}4x_1 - 5x_2 &= -13 \\-2x_1 + 3x_2 &= 9\end{aligned}$$

can be written compactly as $\boxed{Ax = b}$, where

$$A = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix}, \quad b = \begin{bmatrix} -13 \\ 9 \end{bmatrix},$$

and can be solved as

$$x = A^{-1}b = \begin{bmatrix} 1.5 & 2.5 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} -13 \\ 9 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}.$$

Notation: Matrices and Vectors

- $A \in \mathbb{R}^{m \times n}$ is a **matrix** with m rows and n columns.

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- A matrix with 1 row and n columns is called a **row vector**.

Matrix Transpose and Products

- Given matrix $A \in \mathbb{R}^{m \times n}$, its **transpose** A^T is such that $(A^T)_{i,j} = A_{j,i}$.

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- Transpose of sum: $(A + B)^T = A^T + B^T$.

Norms

- The **norm** of a vector is (informally) its “magnitude.” Euclidean norm:

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- Notable case: the ℓ_∞ norm, $\|x\|_\infty = \max\{|x_1|, \dots, |x_n|\}$.
- Notable case: the ℓ_0 “norm” (not): $\|x\|_0 = |\{i : x_i \neq 0\}|$.

Special Matrices

- The **identity matrix** $I \in \mathbb{R}^{n \times n}$ is a square matrix such that

$$I_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases} \quad I = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

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- Upper triangular matrix: $(j < i) \Rightarrow A_{i,j} = 0$.
- Lower triangular matrix: $(j > i) \Rightarrow A_{i,j} = 0$.

Eigenvalues, eigenvectors, determinant, trace

- A vector $x \in \mathbb{R}^n$ is an **eigenvector** of matrix $A \in \mathbb{R}^{n \times n}$ if

$$Ax = \lambda x,$$

where $\lambda \in \mathbb{R}$ is the corresponding **eigenvalue**.

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Matrix Inverse

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Matrix Inverse

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- ...matrix B , such that $AB = BA = I$, denoted $B = A^{-1}$.

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- There are many algorithms to compute A^{-1} ; general case, computational cost $O(n^3)$.

Quadratic Forms and Positive (Semi-)Definite Matrices

- Given matrix $A \in \mathbb{R}^{n \times n}$ and vector $x \in \mathbb{R}^n$,

$$x^T A x = \sum_{i=1}^n \sum_{j=1}^n A_{i,j} x_i x_j \in \mathbb{R}$$

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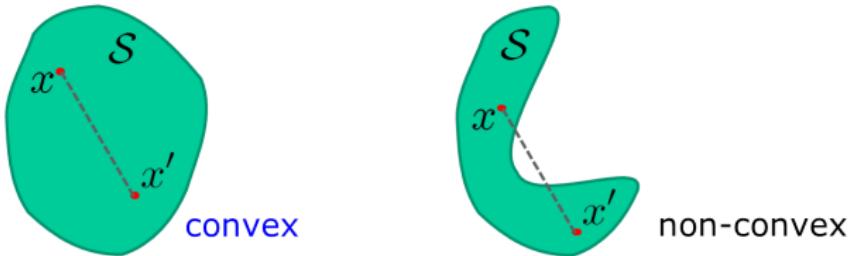
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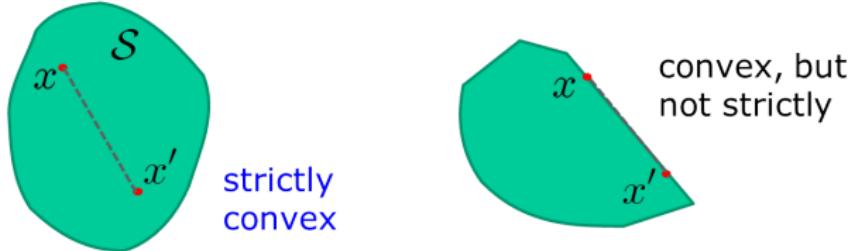
Convex Sets

Convex and strictly convex sets

\mathcal{S} is **convex** if $x, x' \in \mathcal{S} \Rightarrow \forall \lambda \in [0, 1], \lambda x + (1 - \lambda)x' \in \mathcal{S}$



\mathcal{S} is **strictly convex** if $x, x' \in \mathcal{S} \Rightarrow \forall \lambda \in (0, 1), \lambda x + (1 - \lambda)x' \in \text{int}(\mathcal{S})$



Convex Functions

Convex and strictly convex functions

Extended real valued function: $f : \mathbb{R}^N \rightarrow \bar{\mathbb{R}} = \mathbb{R} \cup \{+\infty\}$

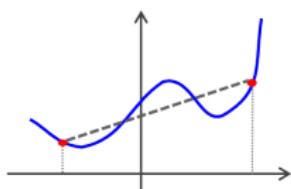
Domain of a function: $\text{dom}(f) = \{x : f(x) \neq +\infty\}$

f is a convex function if

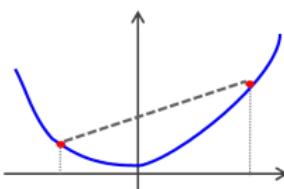
$$\forall \lambda \in [0, 1], x, x' \in \text{dom}(f) \quad f(\lambda x + (1 - \lambda)x') \leq \lambda f(x) + (1 - \lambda)f(x')$$

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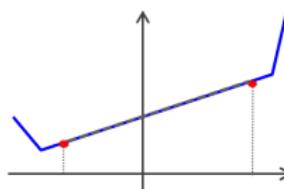
$$\forall \lambda \in (0, 1), x, x' \in \text{dom}(f) \quad f(\lambda x + (1 - \lambda)x') < \lambda f(x) + (1 - \lambda)f(x')$$



non-convex



convex
strictly convex



convex, not strictly

Outline

① Introduction

② Class Administrativia

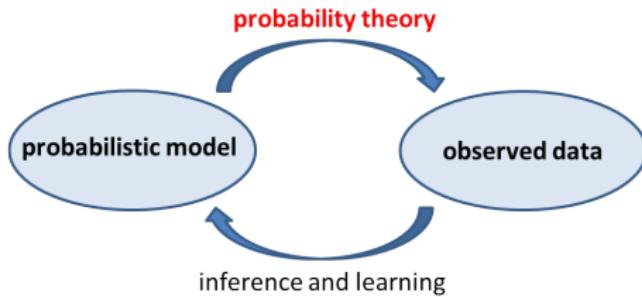
③ Recap

Linear Algebra

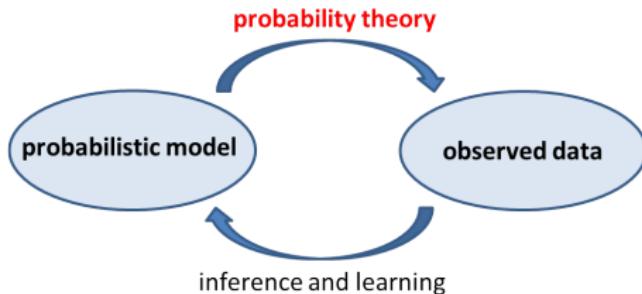
Probability Theory

Optimization

Probability theory

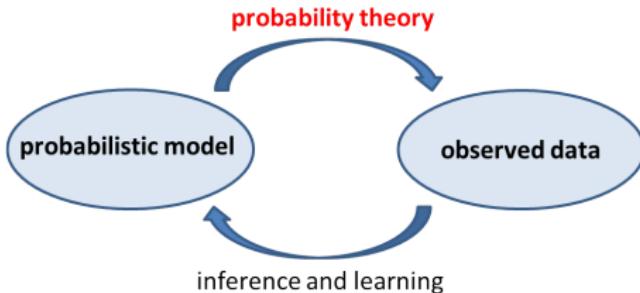


Probability theory



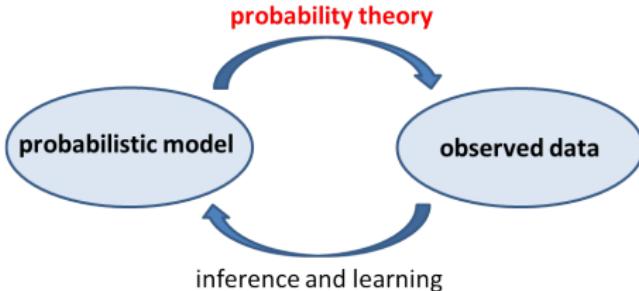
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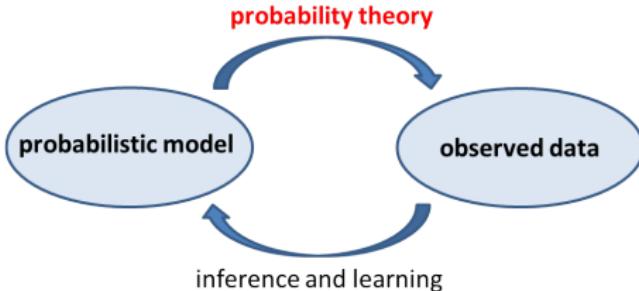
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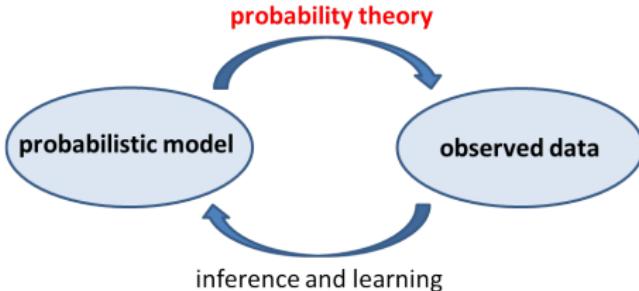
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- ...thus also learning, decision making, inference, ...

What is probability?

- Classical definition: $\mathbb{P}(A) = \frac{N_A}{N}$

...with N mutually exclusive equally likely outcomes,
 N_A of which result in the occurrence of event A .

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Example: $\mathbb{P}(\text{randomly drawn card is } \clubsuit) = 13/52$.

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- Subjective probability: $\mathbb{P}(A)$ is a degree of belief.

de Finetti, 1930s

...gives meaning to $\mathbb{P}(\text{"Tomorrow it will rain"})$.

Key concepts: Sample space and events

- **Sample space** \mathcal{X} = set of possible outcomes of a random experiment.

Examples:

- Tossing two coins: $\mathcal{X} = \{HH, TH, HT, TT\}$
- Roulette: $\mathcal{X} = \{1, 2, \dots, 36\}$
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- An **event** A is a subset of \mathcal{X} : $A \subseteq \mathcal{X}$.

Examples:

- “exactly one H in 2-coin toss”: $A = \{TH, HT\} \subset \{HH, TH, HT, TT\}$.
- “odd number in the roulette”: $B = \{1, 3, \dots, 35\} \subset \{1, 2, \dots, 36\}$.
- “drawn a ♠ card”: $C = \{A\heartsuit, 2\heartsuit, \dots, K\heartsuit\} \subset \{A\clubsuit, \dots, K\diamondsuit\}$

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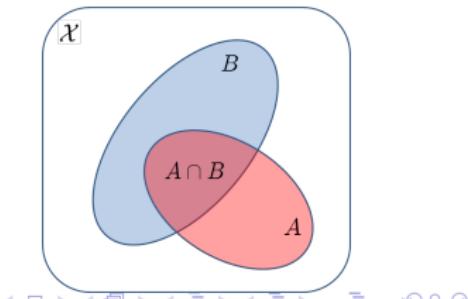
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- From these axioms, many results can be derived. Examples:
 - $\mathbb{P}(\emptyset) = 0$
 - $C \subset D \Rightarrow \mathbb{P}(C) \leq \mathbb{P}(D)$
 - $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B) - \mathbb{P}(A \cap B)$
 - $\mathbb{P}(A \cup B) \leq \mathbb{P}(A) + \mathbb{P}(B)$ (union bound)

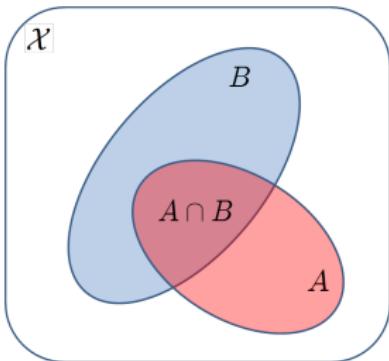


Conditional Probability and Independence

- If $\mathbb{P}(B) > 0$, $\mathbb{P}(A|B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}$ (**conditional prob. of A given B**)

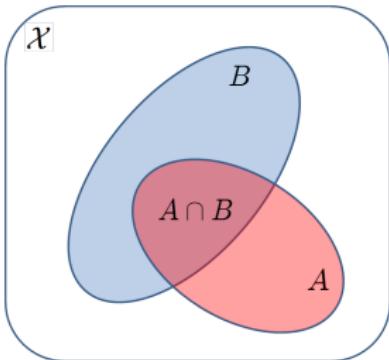
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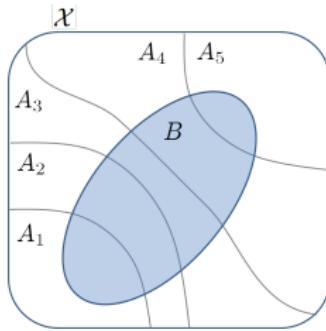
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Bayes Theorem

- Law of total probability: if A_1, \dots, A_n are a partition of \mathcal{X}

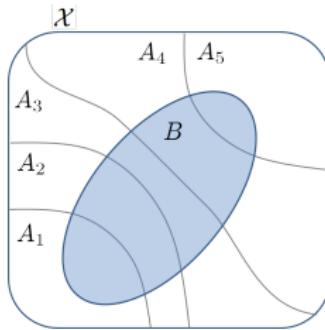
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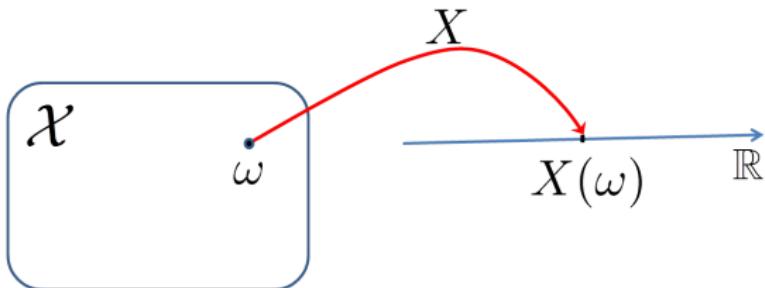


- Bayes' theorem: if $\{A_1, \dots, A_n\}$ is a partition of \mathcal{X}

$$\mathbb{P}(A_i|B) = \frac{\mathbb{P}(B \cap A_i)}{\mathbb{P}(B)} = \frac{\mathbb{P}(B|A_i) \mathbb{P}(A_i)}{\sum_j \mathbb{P}(B|A_j) \mathbb{P}(A_j)}$$

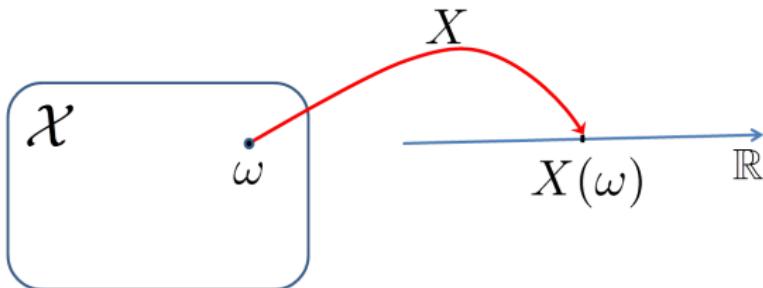
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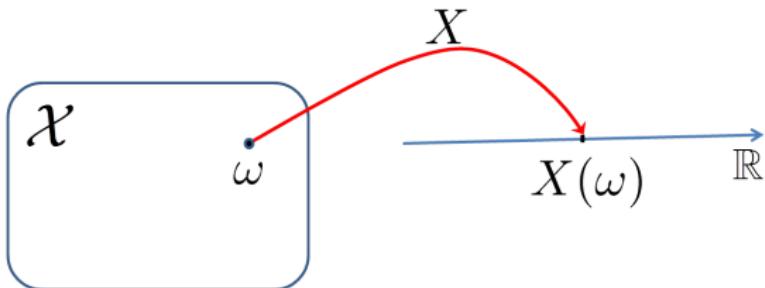
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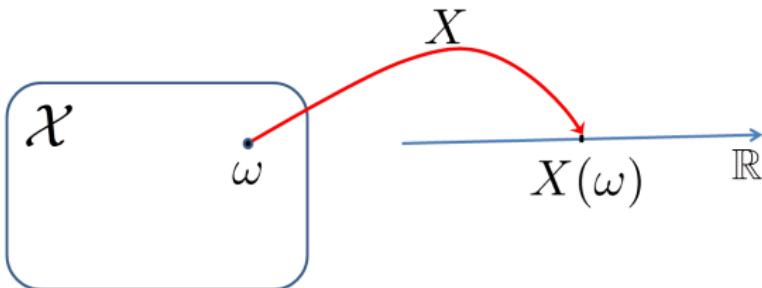
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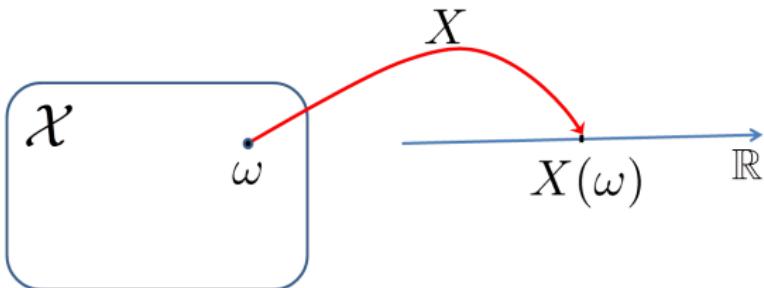
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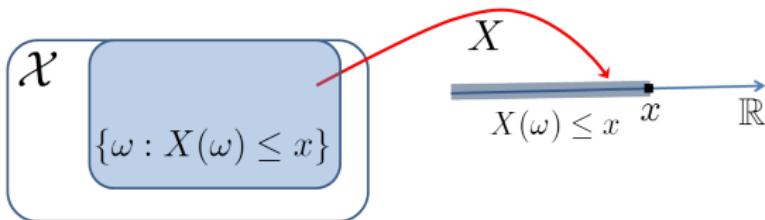
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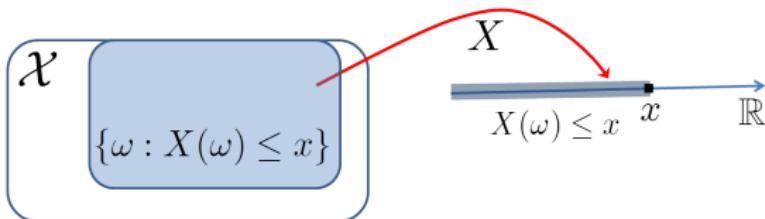
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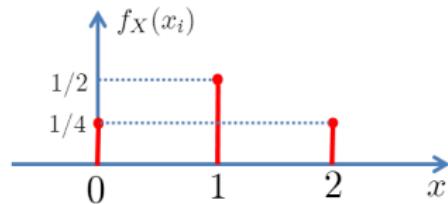
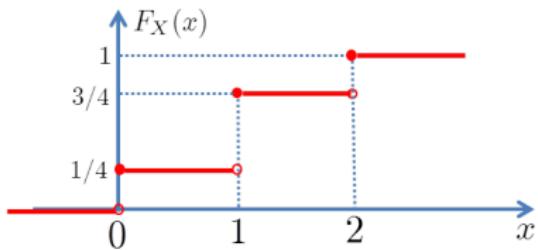


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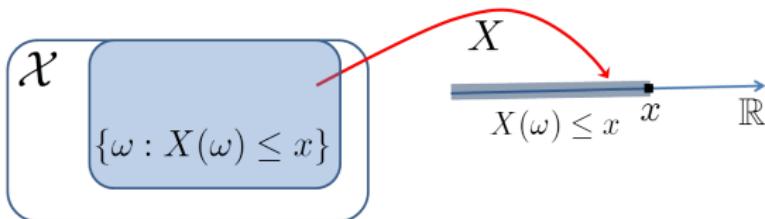


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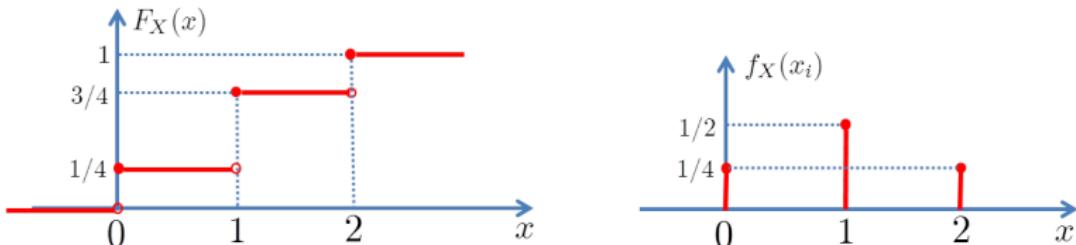


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- Probability mass function (discrete RV): $f_X(x) = \mathbb{P}(X = x)$,

$$F_X(x) = \sum f_X(x_i).$$

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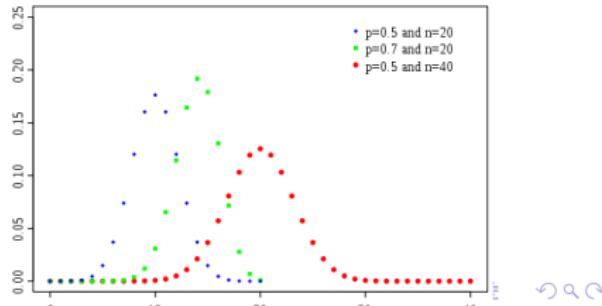
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Binomial coefficients
("n choose x"):

$$\binom{n}{x} = \frac{n!}{(n - x)! x!}$$



More Important Discrete Random Variables

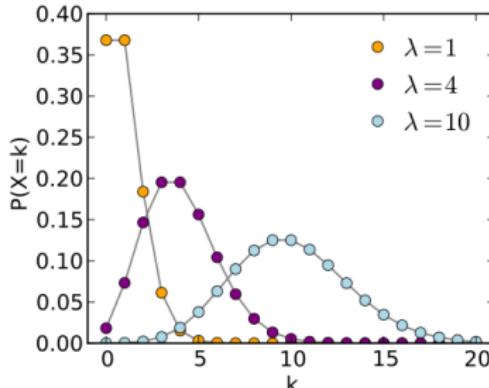
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- **Poisson(λ)**: $X \in \mathbb{N} \cup \{0\}$, pmf $f_X(x) = \frac{e^{-\lambda} \lambda^x}{x!}$

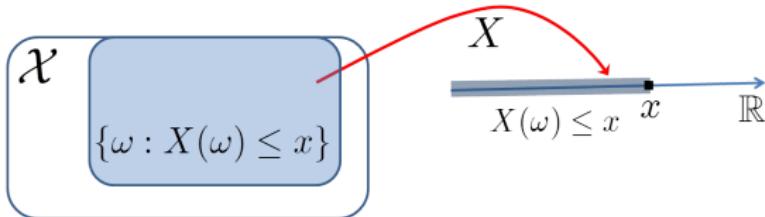
Notice that $\sum_{x=0}^{\infty} \frac{\lambda^x}{x!} = e^{\lambda}$, thus $\sum_{x=0}^{\infty} f_X(x) = 1$.

“...probability of the number of independent occurrences in a fixed (time/space) interval if these occurrences have known average rate”



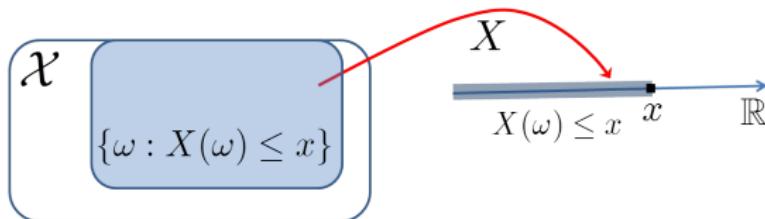
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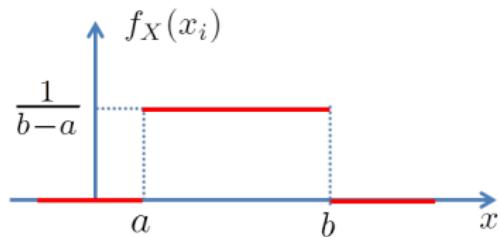
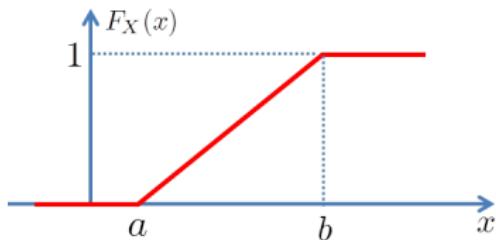


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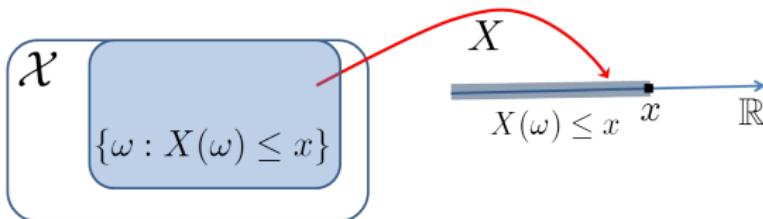


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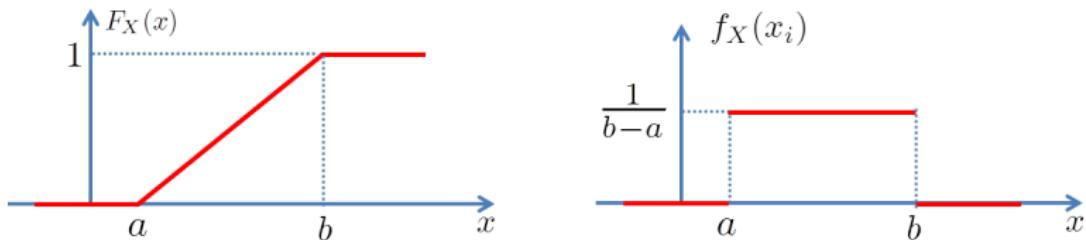


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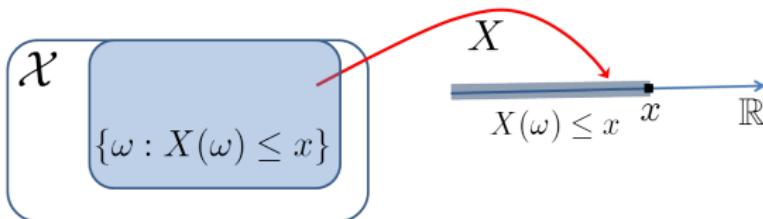
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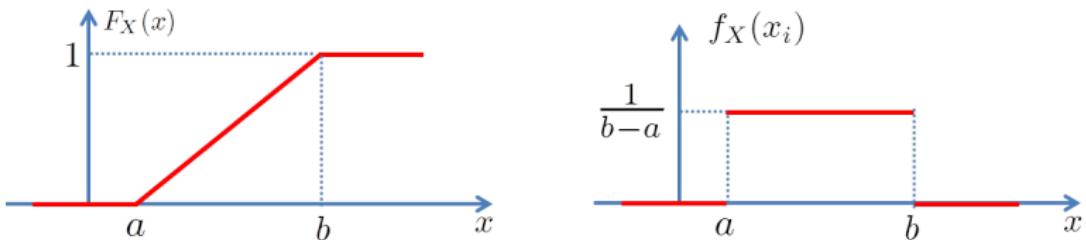
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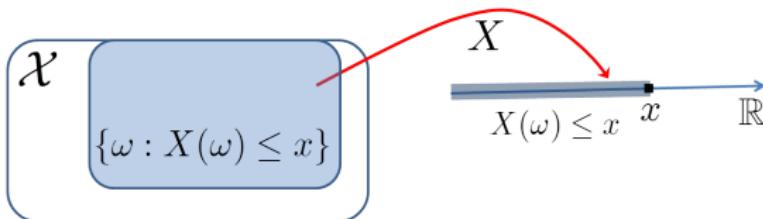


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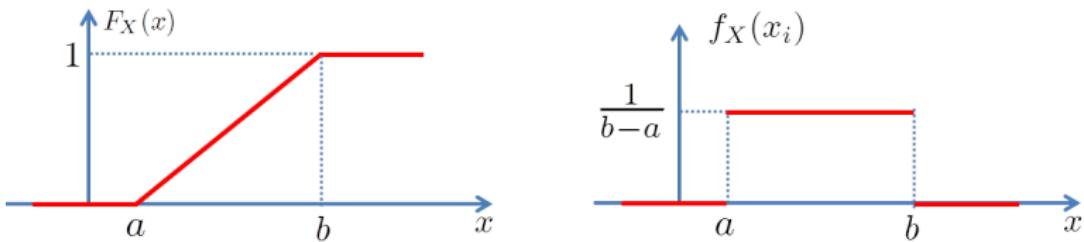
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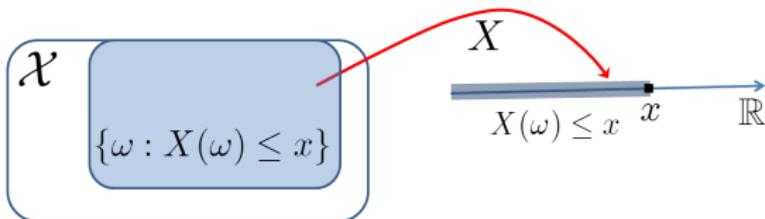


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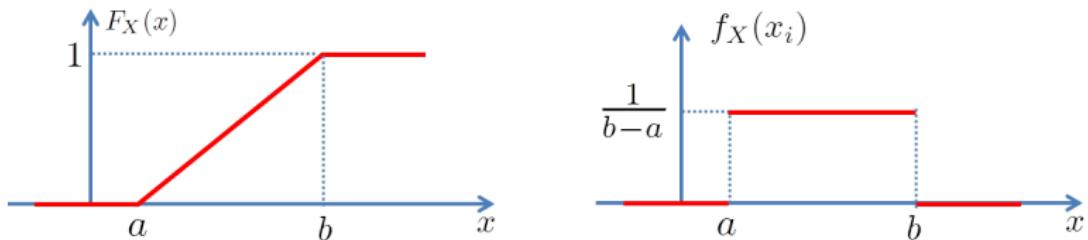
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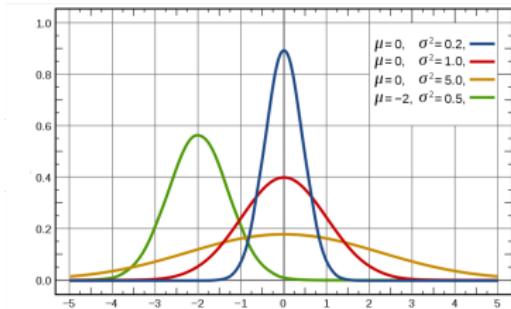
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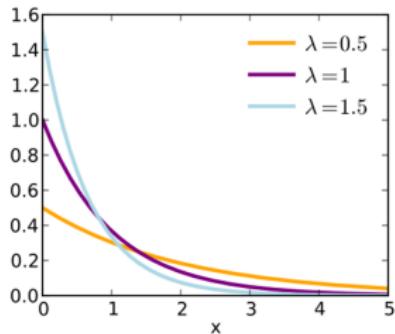
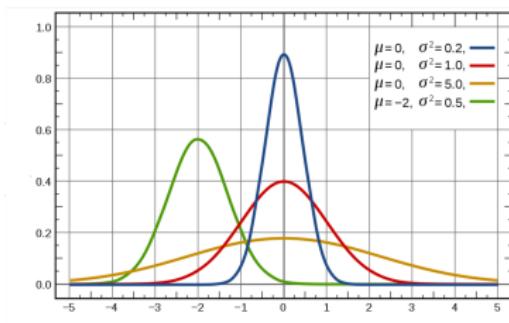
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- Linearity of expectation:

$$\mathbb{E}(X + Y) = \mathbb{E}(X) + \mathbb{E}(Y); \quad \mathbb{E}(\alpha X) = \alpha \mathbb{E}(X), \quad \alpha \in \mathbb{R}$$

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- Marginalization: $f_Y(y) = \begin{cases} \sum\limits_x f_{X,Y}(x,y), & \text{if } X \text{ is discrete} \\ \int_{-\infty}^{\infty} f_{X,Y}(x,y) dx, & \text{if } X \text{ continuous} \end{cases}$

- Independence:

$$X \perp\!\!\!\perp Y \Leftrightarrow f_{X,Y}(x,y) = f_X(x) f_Y(y) \stackrel{\Rightarrow}{\not\Leftarrow} \mathbb{E}(XY) = \mathbb{E}(X)\mathbb{E}(Y).$$

Conditionals and Bayes' Theorem

- Conditional pmf (discrete RVs):

$$f_{X|Y}(x|y) = \mathbb{P}(X = x | Y = y) = \frac{\mathbb{P}(X = x \wedge Y = y)}{\mathbb{P}(Y = y)} = \frac{f_{X,Y}(x,y)}{f_Y(y)}.$$

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- Bayes' theorem: $f_{X|Y}(x|y) = \frac{f_{Y|X}(y|x) f_X(x)}{f_Y(y)}$ (pdf or pmf).
- Also valid in the mixed case (e.g., X continuous, Y discrete).

Joint, Marginal, and Conditional Probabilities: An Example

- A pair of binary variables $X, Y \in \{0, 1\}$, with joint pmf:

$f_{X,Y}(x,y)$	$Y = 0$	$Y = 1$
$X = 0$	1/5	2/5
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$X = 1$	1/3	3/7

$f_{Y X}(y x)$	$Y = 0$	$Y = 1$
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An Important Multivariate RV: Multinomial

- **Multinomial:** $X = (X_1, \dots, X_K)$, $X_i \in \{0, \dots, n\}$, such that $\sum_i X_i = n$,

$$f_X(x_1, \dots, x_K) = \begin{cases} \binom{n}{x_1 \ x_2 \ \dots \ x_K} p_1^{x_1} p_2^{x_2} \cdots p_k^{x_k} & \Leftrightarrow \sum_i x_i = n \\ 0 & \Leftrightarrow \sum_i x_i \neq n \end{cases}$$

$$\binom{n}{x_1 \ x_2 \ \dots \ x_K} = \frac{n!}{x_1! x_2! \cdots x_K!}$$

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- Generalizes the binomial from binary to K -classes.
- **Example:** tossing n independent fair dice, $p_1 = \cdots = p_6 = 1/6$.
 x_i = number of outcomes with i dots. Of course, $\sum_i x_i = n$.

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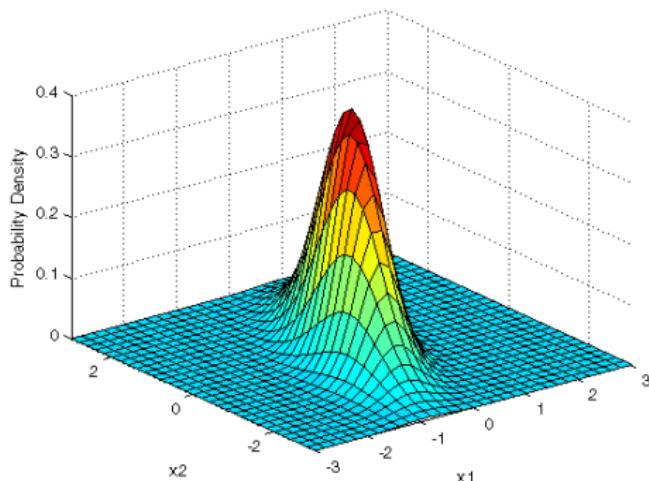
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- Covariance of Gaussian RV, $f_X(x) = \mathcal{N}(x; \mu, C) \Rightarrow \text{cov}(X) = C$

More on Expectations and Covariances

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- ...thus, if $Z_n = \frac{Y_n - \mu}{\sigma}$

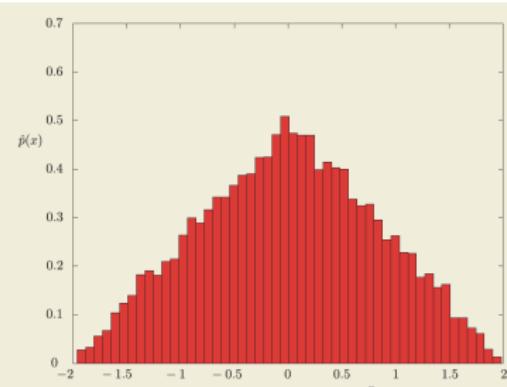
$$\mathbb{E}[Z_n] = 0 \quad \text{var}(Z_n) = 1$$

- Central limit theorem (CLT): under some mild conditions on X_1, \dots, X_n

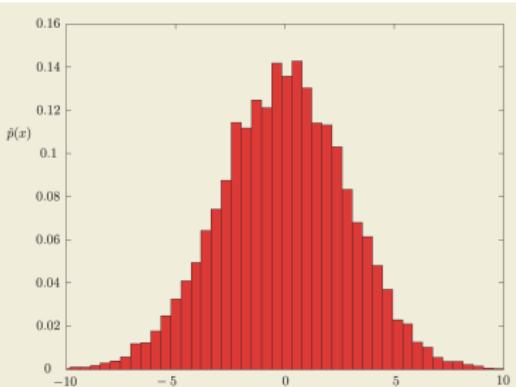
$$\lim_{n \rightarrow \infty} Z_n \sim \mathcal{N}(0, 1)$$

Central Limit Theorem

Illustration



Sum of two i.i.d variables from a uniform in [-1,1]



Sum of twenty five i.i.d r.v from a uniform in [-1,1]

Important Inequalities

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- **Chebyshev's inequality:** $\mu = \mathbb{E}(Y)$ and $\sigma^2 = \text{var}(Y)$, then

$$\mathbb{P}(|Y - \mu| \geq s) \leq \frac{\sigma^2}{s^2}$$

...simple corollary of Markov's inequality, with $X = |Y - \mu|^2$, $t = s^2$

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- Implication for correlation:

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Examples: $\mathbb{E}(X)^2 \leq \mathbb{E}(X^2) \Rightarrow \text{var}(X) = \mathbb{E}(X^2) - \mathbb{E}(X)^2 \geq 0$.

$\mathbb{E}(\log X) \leq \log \mathbb{E}(X)$, for X a positive RV.

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Entropy and all that...

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Kullback-Leibler divergence

Kullback-Leibler divergence (KLD) between two pmf:

$$D(f_X \| g_X) = \sum_{x=1}^K f_X(x) \log \frac{f_X(x)}{g_X(x)}$$

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Positivity: $D(f_X \| g_X) \geq 0$

$$D(f_X \| g_X) = 0 \Leftrightarrow f_X(x) = g_X(x), \text{ almost everywhere}$$

Mutual information

Mutual information (MI) between two random variables:

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MI is a measure of dependency between two random variables

Recommended Reading

- K. Murphy, “Machine Learning: A Probabilistic Perspective”, MIT Press, 2012.
- L. Wasserman, “All of Statistics: A Concise Course in Statistical Inference”, Springer, 2004.

Outline

① Introduction

② Class Administrativa

③ Recap

Linear Algebra

Probability Theory

Optimization

Minimizing a function

- We are given a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$.
- Goal: find x^* that minimizes $f : \mathbb{R}^n \rightarrow \mathbb{R}$.
- Global minimum: for any $x \in \mathbb{R}^n$, $f(x^*) \leq f(x)$.
- Local minimum: for any $\|x - x^*\| \leq \delta \Rightarrow f(x^*) \leq f(x)$.

Are these global minima ?

- No, (local minima, saddle points, . . .)

Iterative descent methods

Goal: find the minimum/minimizer of $f : \mathbb{R}^d \rightarrow \mathbb{R}$

- Proceed in **small steps** in the **optimal direction** till a **stopping criterion** is met.
- **Gradient descent:** updates of the form: $x^{(t+1)} \leftarrow x^{(t)} - \eta_{(t)} \nabla f(x^{(t)})$

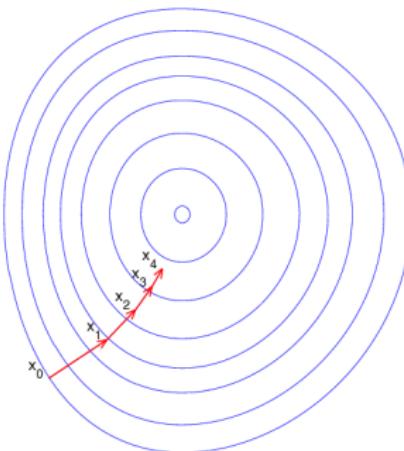


Figure: Illustration of gradient descent. The blue circles correspond to the function values at different points, while the red lines correspond to steps taken in

Convex functions

Pro: Guarantee of a global minima ✓



Figure: Illustration of a convex function. The line segment between any two points on the graph lies entirely above the curve.

Non-Convex functions

Pro: No guarantee of a global minima \times

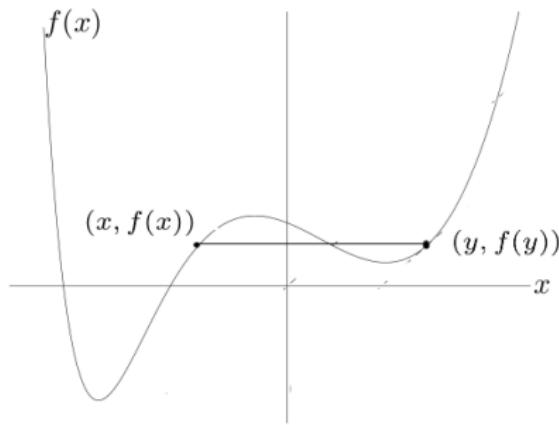


Figure: Illustration of a non-convex function. Note the line segment intersecting the curve.

Thank you!

Questions?



References I