## Lecture 1: Introduction

André Martins, Francisco Melo, Mário Figueiredo

## fit técnico <br> LISBOA

Deep Learning Course, Winter 2022-2023

## Deep Learning Course

- A new MSc-level course
- Offered jointly by DEEC and DEI
- MSc programs: MEEC, MECD, MEIC-A, MEIC-T
- 350 students enrolled this year! (192 DEEC, 158 DEI).


## Course Website(s)

## DEEC:

https:
//fenix.tecnico.ulisboa.pt/disciplinas/AProf/2022-2023/1-semestre

DEI:
https://fenix.tecnico.ulisboa.pt/disciplinas/AP-Dei/2022-2023/
1-semestre
There we can find:

- Syllabus
- Lecture slides
- Literature pointers
- Practical and homework assignments
- Announcements


## Instructors

- Main instructors: André Martins (DEI Alameda), Francisco Melo (DEI Tagus), Mário Figueiredo (DEEC)
- Practical classes: Andreas Wichert, Ben Peters, Chrysoula Zerva, Gonçalo Correia, João Fonseca, João Santinha, José Moreira, Margarida Campos, Tomás Costa
- Location \& schedule: see course webpage in Fenix (previous slide)
- Office hours: see information in Fenix
- Communication:
piazza.com/tecnico.ulisboa.pt/fall2022/c88

> Please register in Piazza!!

## Outline

## (1) Introduction

(2) Class Administrativia
(3) Recap

Linear Algebra
Probability Theory Refresher
Optimization
(4) Introduction to Machine Learning

## What is ""Deep Learning"?



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


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## Why Did Deep Learning Become Mainstream?

Lots of recent breakthroughs:

- Object recognition
- Speech and language processing (Transformers, BERT, GPT-3)
- Machine translation
- Chatbots and dialog systems
- Self-driving cars
- Solving games (Atari, Go, StartCraft II)
- Protein design (AlphaFold)

No signs of slowing down...


# Microsoft's Deep Learning Project Outperforms Humans In Image Recognition 

Michael Thomsen, contributor
I write about tech, video games, sclence and culture. FULL BIO $\vee$

## Microsoft's new breakthrough: Al 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

Who is wearing glasses? man


Is the umbrella upside down?


Where is the child sitting?
fridge

arms


How many children are in the bed?


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.

## Google unleashes deep learning tech on language with Neural Machine Translation

Posted Sep 27, 2016 by Devin Coldewey, Contributor



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



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



## 'It will change everything': DeepMind's AI makes gigantic leap in solving protein structures

Google's deep-learning program for determining the 3D shapes of proteins stands to transform biology, say scientists.

Ewen Callaway
v) f


A protein's function is determined by its 3D shape. Credit: DeepMind

## AlphaFold's new rival? Meta AI predicts shape of $\mathbf{6 0 0}$ million proteins

Microbial molecules from soil, seawater and human bodies are among the planet's least understood.

Ewen Callaway

- $f$ -


The ESM Metagenomic Atlas contains structural predictions for 617 million proteins. Credit: ESM Metagenomic Atlas (CC BY 4.0)

## How to use DALL•E 2 to turn your wildest imaginations into tangible art

Al art platform, DALL•E 2, creates images from text descriptions in seconds. In this article, we show you how to get the results you desire.



## Why Now?

Why does deep learning work now, but not 30 years ago?

Many of the core ideas were there, after all.

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Why does deep learning work now, but not 30 years ago?

Many of the core ideas were there, after all.

But now we have:

- more data
- more computing power
- (much) better software engineering (e.g. auto-diff)
- some algorithmic innovations: many layers, ReLUs, better learning algorithms, dropout, CNNs, LSTMs, transformers, etc.
All of these will be covered in this course.


## "But It's Non-Convex"

For many years (1990-2010), NNs were not popular in machine learning, because they were hard to learn.

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For many years (1990-2010), NNs were not popular in machine learning, because they were hard to learn.

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

One possible, partial answer (this is an open research topic)

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


## One turning point: AlexNet

- Alex Krizhevsky, Ilya Sutskever, Geoffrey Hinton; 2012


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- Large CNN, much deeper than anything else at the time
- Used parallel processing (one of the first uses of GPUs in NNs)
- Convinced many people that deep learning would change the field.


## 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:

- Artificial Intelligence Engines: A Tutorial Introduction to the Mathematics of Deep Learning. James Stone. Sebtel Press, 2019.
- Dive into Deep Learning. Aston Zhang, Zach Lipton, Mu Li, Alex Smola (https://d2l.ai/)
- Deep Learning with Python. François Chollet. Manning Publications, 2017.
- Machine Learning - A Journey to Deep Learning with Exercises and Answers. Andreas Wichert and Luis Sa-Couto, 2021
- Probabilistic Machine Learning. Kevin P. Murphy (https://probml.github.io/pml-book/)


## Tentative Syllabus

| Week 1 | Introduction and Course Description |
| :--- | :--- |
|  | Linear Classifiers I (linear regression, perceptron) |
| Week 2 | Linear Classifiers II (logistic regression, regularization) |
| Week 3 | Neural Networks I |
| Week 4 | Neural Networks II |
|  | Representation Learning and Auto-Encoders |
| Week 5 | Convolutional Networks |
|  | Recurrent Neural Networks and LSTMs |
| Week 6 | Sequence-to-Sequence Models and Attention Mechanisms <br>  <br> Week 7 7 |
|  | Self-Supervised Learning (BERT, GPT3, etc.) <br> Interpretability and Fairness |

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## What This Class Is About

- Introduction to deep learning (DL)
- Goal: after finishing this class, you should be able to:
$\checkmark$ Understand how DL works (it's not magic)
$\checkmark$ Understand the math and intuition behind DL models
$\checkmark$ Apply DL on practical problems (language, vision, ...)
- Target audience:
$\checkmark$ MSc students with basic background in probability theory, linear algebra, programming.
$\checkmark$ Useful: background in machine learning.


## What This Class Is Not About

- Just playing with DL toolkits, without learning the fundamental concepts
- Introduction to machine learning (other courses by DEEC and DEI)
- Natural language processing (another course offered by DEI)
- Computer vision (another course offered by DEEC)
- Optimization (other courses by DEEC and DEI)


## Prerequisites

- Calculus and basic linear algebra
- Basic probability theory
- Basic knowledge of machine learning (preferred, but not required)
- Programming (Python \& PyTorch, preferred but not required)


## Course Information

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## Schedule (DEI Alameda/Tagus)

|  | Mon 11/21 | Tue 11/22 | Wed 11/23 | Thu 11/24 | Fri 11/25 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 07:00 |  |  |  |  |  |
|  |  |  |  |  |  |
| 08:00 |  |  |  |  |  |
|  | 68:30-10:30 |  |  |  |  |
| 09:00 |  |  |  |  |  |
|  |  |  |  |  |  |
| 10:00 |  |  |  |  |  |
|  |  |  |  |  |  |
| 11:00 |  |  |  |  |  |
|  |  |  |  | $11730-13: 50$ |  |
| 12:00 |  |  |  |  |  |
|  |  |  |  | 1-29 |  |
| 13:00 |  |  |  |  |  |
|  | $1{ }^{13: 30-15: 00}$ |  |  | 13330-159 13:30-15. |  |
| 14:00 | -29 |  |  | $\begin{array}{\|l\|l} \mathrm{T} & \mathrm{~T} \\ \mathrm{QA} \end{array}$ | $14: 00-14: 00-94: 00-$ |
|  |  |  | $L^{1430-16} / \frac{14: 30-16}{}$ |  | $\begin{array}{\|l\|l\|l} \hline \mathrm{L} & \mathrm{~L} & \mathrm{~L} \\ \mathrm{EE} & \mathrm{~F} 2 & \mathrm{F4} \\ \hline \end{array}$ |
| 15:00 | $15: 00-16: 30$ | $\begin{aligned} & 15: 00-17: 00 \\ & T \end{aligned}$ | F2 F3 |  |  |
| 16:00 | 1-29 |  |  | $\begin{aligned} & 15: 30-17: 00 \\ & \mathrm{~L} \\ & 0-21 \end{aligned}$ | $\left\|\begin{array}{ll} 15: 30-173 & 15: 30-172 \\ E & L \\ E 5 & F 2 \end{array}\right\|$ |
| 17:00 |  |  |  |  | 17:00-18: 17:00-18. |
|  |  |  | 17:30-19: $17.30-18$. |  | $\begin{array}{l\|l} \mathrm{L} & \mathrm{~L} \\ \mathrm{~F} 2 & \mathrm{~F} \end{array}$ |
| 18:00 |  |  | L L <br> EF $\mathrm{F3}$ |  |  |
|  |  |  |  |  |  |
| 19:00 |  |  |  |  |  |
|  |  |  |  |  |  |
| 20:00 |  |  |  |  |  |

- Letures: 2 per week (Alameda: Tue \& Thur; Tagus: Mon \& Thur)
- Practical shifts (see Fenix) - pick your slots and register as a group! (more later)


## Schedule (DEEC Alameda)



- Lectures: 2 per week (shift 1: Mon \& Thur; shift 2: Tue \& Thur)
- Practical shifts (see Fenix): pick your slots and register as a group! (more later!)


## Grading

- 2 homework assignments: $50 \%$
- Minimal grade: 8
- Theoretical questions \& implementation
- Groups of 2 - you need to register your group in Fenix!
- Some of the practicals will be Q\&A about these assignments, so please join the practicals as a group
- Submission through Fenix
- No late days allowed
- Final exam: 50\%
- Minimal grade: 8


## Registering Your Group in Fenix

- Pick a group of 2
- Register in Fenix
- Deadline: Sunday, November 27, at 23:59
- Use Piazza to find group mates
- Can't find a group?

Tell the instructors by November 28 (in Piazza); we'll find a solution.

## Collaboration Policy

- Assignments should be done within each group
- Students may discuss the questions across groups, 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!!!


## Questions?



## Today's Roadmap

- Linear Algebra (only skim over)
- Probability Refresher (only skim over)
- Optimization
- Introduction to Machine Learning
- "Deep Learning Superheroes"
- Supervised, Unsupervised, Reinforcement Learning
- Classification and Regression


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## Notation: Matrices and Vectors

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

$$
A=\left[\begin{array}{ccc}
A_{1,1} & \cdots & A_{1, n} \\
\vdots & \ddots & \vdots \\
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- A (column) vector is a matrix with $n$ rows and 1 column.
- A matrix with 1 row and $n$ columns is called a row vector.


## Matrix Transpose and Matrix Products

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


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- Given matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$, their product is

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- Inner product between vectors $x, y \in \mathbb{R}^{n}$ :

$$
\begin{gathered}
\langle x, y\rangle=x^{T} y=y^{T} x=\sum_{i=1}^{n} x_{i} y_{i} \\
{\left[\begin{array}{c}
x_{1} \\
\vdots \\
x_{n}
\end{array}\right]^{T}\left[\begin{array}{c}
y_{1} \\
\vdots \\
y_{n}
\end{array}\right]=\left[x_{1}, \ldots, x_{n}\right]\left[\begin{array}{c}
y_{1} \\
\vdots \\
y_{n}
\end{array}\right]=\sum_{i=1}^{n} x_{i} y_{i}}
\end{gathered}
$$

## Outer and Hadamard Products

- Outer product between vectors $x \in \mathbb{R}^{n}$ and $y \in \mathbb{R}^{m}$ :

$$
\begin{gathered}
x y^{\top} \in \mathbb{R}^{n \times m}, \quad \text { where }\left(x y^{\top}\right)_{i, j}=x_{i} y_{j} \\
x y^{T}=\left[\begin{array}{c}
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\end{array}\right]
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- Hadamard/Schur product between vectors $x, y \in \mathbb{R}^{n}:(x \odot y)_{i}=x_{i} y_{i}$,

$$
\left[\begin{array}{c}
x_{1} \\
\vdots \\
x_{n}
\end{array}\right] \odot\left[\begin{array}{c}
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## Properties of Matrix Products and Transposes

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- Transpose of product: $(A B)^{T}=B^{T} A^{T}$.
- 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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\|x\|_{2}=\sqrt{\langle x, x\rangle}=\sqrt{x^{\top} x}=\sqrt{\sum_{i=1}^{n} x_{i}^{2}}
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- More generally, the $\ell_{p}$ norm of a vector $x \in \mathbb{R}^{n}$, where $p \geq 1$,

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- Notable case: the $\ell_{1}$ norm, $\|x\|_{1}=\sum_{i}\left|x_{i}\right|$.
- Notable case: the $\ell_{\infty}$ norm, $\|x\|_{\infty}=\max \left\{\left|x_{1}\right|, \ldots,\left|x_{n}\right|\right\}$.


## Special Matrices

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

$$
I_{i j}=\left\{\begin{array}{cc}
1 & i=j \\
0 & i \neq j
\end{array} \quad I=\left[\begin{array}{cccc}
1 & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 1
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- Properties: $\left(A^{-1}\right)^{-1}=A, \quad\left(A^{-1}\right)^{T}=\left(A^{T}\right)^{-1}, \quad(A B)^{-1}=B^{-1} A^{-1}$
- There are many algorithms to compute $A^{-1}$; general case, computational cost $O\left(n^{3}\right)$.


## Quadratic Forms and Positive (Semi-)Definite Matrices

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

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# Outline 

## (1) Introduction

(2) Class Administrativia
(3) Recap

Linear Algebra
Probability Theory Refresher
Optimization
(4) Introduction to Machine Learning

## Probability theory



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- The study of probability has roots in games of chance (dice, cards, ...)
- Natural tool to model uncertainty, information, knowledge, belief, ...
- ...thus also learning, 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 $A$.

Example: $\mathbb{P}($ randomly drawn card is $\boldsymbol{\%})=13 / 52$.
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- Subjective probability: $\mathbb{P}(A)$ is a degree of belief. de Finetti, 1930s ...gives meaning to $\mathbb{P}$ ("Tomorrow it will rain").


## Key concepts: Sample space and events

- Sample space $X=$ set of possible outcomes of a random experiment. Examples:
- Tossing two coins: $X=\{H H, T H, H T, T T\}$
- Roulette: $\mathcal{X}=\{1,2, \ldots, 36\}$
- Draw a card from a shuffled deck: $X=\{A \&, 2 \boldsymbol{\downarrow}, \ldots, Q \diamond, K \diamond\}$.


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- Draw a card from a shuffled deck: $X=\{A \boldsymbol{\alpha}, 2 \boldsymbol{\phi}, \ldots, Q \diamond, K \diamond\}$.
- An event $A$ is a subset of $X: A \subseteq X$.

Examples:

- "exactly one H in 2-coin toss": $A=\{T H, H T\} \subset\{H H, T H, H T, T T\}$.
- "odd number in the roulette": $B=\{1,3, \ldots, 35\} \subset\{1,2, \ldots, 36\}$.
- "drawn a $\odot$ card" : $C=\{A \odot, 2 \odot, \ldots, K \odot\} \subset\{A \&, \ldots, K \diamond\}$


## Kolmogorov's Axioms for Probability

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


Conditional Probability and Independence

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- Example: $\mathcal{X}=$ " 52 cards", $A=\{3 @, 3 \boldsymbol{\$}, 3 \diamond, 3 \uparrow\}$, and $B=\{A \odot, 2 \odot, \ldots, K \bigcirc\} ;$ then, $\mathbb{P}(A)=1 / 13, \mathbb{P}(B)=1 / 4$

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\mathbb{P}(A \mid B) & =\mathbb{P}(" 3 " \mid " \cap \text { " })=\frac{1}{13}=\mathbb{P}(A)
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## Law of Total Probability and Bayes Theorem

- Law of total probability: if $A_{1}, \ldots, A_{n}$ are a partition of $X$

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

$$
F_{X}(x)=\sum_{x_{i} \leq x} f_{X}\left(x_{i}\right)
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Can be written compactly as $f_{X}(x)=p^{x}(1-p)^{1-x}$.

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- Binomial RV: $X \in\{0,1, \ldots, n\}$ (sum on $n$ Bernoulli RVs)

$$
f_{X}(x)=\operatorname{Binomial}(x ; n, p)=\binom{n}{x} p^{x}(1-p)^{(n-x)}
$$

## Important Discrete Random Variables

- Uniform: $X \in\left\{x_{1}, \ldots, x_{K}\right\}, \operatorname{pmf} f_{X}\left(x_{i}\right)=1 / K$.
- Bernoulli RV: $X \in\{0,1\}$, pmf $f_{X}(x)=\left\{\begin{array}{cc}p & \Leftarrow x=1 \\ 1-p & \Leftarrow x=0\end{array}\right.$

Can be written compactly as $f_{X}(x)=p^{x}(1-p)^{1-x}$.

- Binomial RV: $X \in\{0,1, \ldots, n\}$ (sum on $n$ Bernoulli RVs)

$$
f_{X}(x)=\operatorname{Binomial}(x ; n, p)=\binom{n}{x} p^{x}(1-p)^{(n-x)}
$$

Binomial coefficients
(" $n$ choose $x$ "):

$$
\binom{n}{x}=\frac{n!}{(n-x)!x!}
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## Continuous Random Variables

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- Uniform: $f_{X}(x)=\operatorname{Uniform}(x ; a, b)=\left\{\begin{array}{rll}\frac{1}{b-a} & \Leftarrow & x \in[a, b] \\ 0 & \Leftarrow & x \notin[a, b]\end{array}\right.$ (previous slide).


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- Gaussian: $f_{X}(x)=\mathcal{N}\left(x ; \mu, \sigma^{2}\right)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} e^{-\frac{(x-\mu)^{2}}{2 \sigma^{2}}}$



## Expectation of Random Variables

- Expectation: $\mathbb{E}(X)=\left\{\begin{array}{cl}\sum_{i} x_{i} f_{X}\left(x_{i}\right) & X \in\left\{x_{1}, \ldots, x_{K}\right\} \subset \mathbb{R} \\ \int_{-\infty}^{\infty} x f_{X}(x) d x & X \text { continuous }\end{array}\right.$


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

Expectation of Functions of Random Variables

- $\mathbb{E}(g(X))=\left\{\begin{aligned} \sum_{i} g\left(x_{i}\right) f_{X}\left(x_{i}\right) & X \text { discrete, } g\left(x_{1}\right) \\ \int_{-\infty}^{\infty} g(x) f_{X}(x) d x & X \text { continuous }\end{aligned}\right.$

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- Example: Gaussian variance, $\mathbb{E}\left((X-\mu)^{2}\right)=\sigma^{2}$.
- Probability as expectation of indicator, $1_{A}(x)= \begin{cases}1 & \multirow{1}{*}{\in A} \\ 0 & \Leftarrow x \notin A\end{cases}$

$$
\mathbb{P}(X \in A)=\int_{A} f_{X}(x) d x=\int 1_{A}(x) f_{X}(x) d x=\mathbb{E}\left(1_{A}(X)\right)
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## Two (or More) Random Variables

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## Conditionals and Bayes' Theorem

- Conditional pmf (discrete RVs):

$$
f_{X \mid Y}(x \mid y)=\mathbb{P}(X=x \mid 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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- 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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- Marginals: $f_{X}(0)=\frac{1}{5}+\frac{2}{5}=\frac{3}{5}$,

$$
f_{X}(1)=\frac{1}{10}+\frac{3}{10}=\frac{4}{10},
$$

$$
f_{Y}(0)=\frac{1}{5}+\frac{1}{10}=\frac{3}{10}, \quad f_{Y}(1)=\frac{2}{5}+\frac{3}{10}=\frac{7}{10}
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| :---: | :---: | :---: |
| $X=0$ | $2 / 3$ | $4 / 7$ |
| $X=1$ | $1 / 3$ | $3 / 7$ |


| $f_{Y \mid X}(y \mid x)$ | $Y=0$ | $Y=1$ |
| :---: | :---: | :---: |
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## An Important Multivariate RV: Multinomial

- Multinomial: $X=\left(X_{1}, \ldots, X_{K}\right), X_{i} \in\{0, \ldots, n\}$, such that $\sum_{i} X_{i}=n$,

$$
\left.\left.\begin{array}{rl}
f_{X}\left(x_{1}, \ldots, x_{K}\right)= & \left\{\begin{array}{c}
\binom{n}{x_{1} x_{2} \cdots x_{K}} p_{1}^{x_{1}} p_{2}^{x_{2}} \cdots p_{k}^{x_{K}} \\
0
\end{array}\right. \\
\Leftarrow \sum_{i} x_{i}=n \\
& \Leftarrow \sum_{i} x_{i} \neq n
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n \\
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Parameters: $p_{1}, \ldots, p_{K} \geq 0$, such that $\sum_{i} p_{i}=1$.

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- 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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$$
x_{i}=\text { number of outcomes with } i \text { dots. Of course, } \sum_{i} x_{i}=n .
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- For $n=1$, sometimes called categorical or multinoulli.

For $n=1$, one and only one $x_{i}=1$, others are 0 , thus $\binom{n}{x_{1} \cdots}=1$.

## An Important Multivariate RV: Gaussian

- Multivariate Gaussian: $X \in \mathbb{R}^{n}$,

$$
f_{X}(x)=\mathcal{N}(x ; \mu, C)=\frac{1}{\sqrt{\operatorname{det}(2 \pi C)}} \exp \left(-\frac{1}{2}(x-\mu)^{T} C^{-1}(x-\mu)\right)
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## Covariance, Correlation, and all that...

- Covariance between two RVs:

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- $X \Perp Y \Leftrightarrow f_{X, Y}(x, y)=f_{X}(x) f_{Y}(y) \stackrel{\Rightarrow}{\nLeftarrow} \operatorname{cov}(X, Y)=0$
- Covariance matrix of multivariate $\mathrm{RV}, X \in \mathbb{R}^{n}$ :

$$
\operatorname{cov}(X)=\mathbb{E}\left[(X-\mathbb{E}(X))(X-\mathbb{E}(X))^{T}\right]=\mathbb{E}\left(X X^{T}\right)-\mathbb{E}(X) \mathbb{E}(X)^{T}
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## Covariance, Correlation, and all that...

- Covariance between two RVs:

$$
\operatorname{cov}(X, Y)=\mathbb{E}[(X-\mathbb{E}(X))(Y-\mathbb{E}(Y))]=\mathbb{E}(X Y)-\mathbb{E}(X) \mathbb{E}(Y)
$$

- Relationship with variance: $\operatorname{var}(X)=\operatorname{cov}(X, X)$.
- $X \Perp Y \Leftrightarrow f_{X, Y}(x, y)=f_{X}(x) f_{Y}(y) \underset{\nLeftarrow}{\nRightarrow} \operatorname{cov}(X, Y)=0$
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- Covariance of Gaussian RV, $f_{X}(x)=\mathcal{N}(x ; \mu, C) \Rightarrow \operatorname{cov}(X)=C$


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- If $f_{X}(x)=\mathcal{N}(x ; \mu, C)$ and $Y=C^{-1 / 2}(X-\mu)$, then $f_{Y}(y)=\mathcal{N}(y ; 0, I)$.


## Entropy and all that...

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- If $f_{X}(x)=\mathcal{N}\left(x ; \mu, \sigma^{2}\right)$, then $h(X)=\frac{1}{2} \log \left(2 \pi e \sigma^{2}\right)$.


## Kullback-Leibler divergence

Kullback-Leibler divergence (KLD) between two pmf:

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D\left(f_{X} \| g_{X}\right)=\sum_{x=1}^{K} f_{X}(x) \log \frac{f_{X}(x)}{g_{X}(x)}
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Positivity: $D\left(f_{X} \| g_{X}\right) \geq 0$ $D\left(f_{X} \| g_{X}\right)=0 \Leftrightarrow f_{X}(x)=g_{X}(x)$, almost everywhere

## Recommended Reading

- A. Maleki and T. Do, "Review of Probability Theory", Stanford University, 2017 (https://tinyurl.com/pz7p9g5)
- L. Wasserman, "All of Statistics: A Concise Course in Statistical Inference", Springer, 2004.


# Outline 

## (1) Introduction

(2) Class Administrativia
(3) Recap

Linear Algebra
Probability Theory Refresher
Optimization
(4) Introduction to Machine Learning

## Minimizing a function

- We are given a function $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$.
- Goal: find $x^{*}$ that minimizes $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$.


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- Local minimum: for any $\left\|x-x^{*}\right\| \leq \delta \Rightarrow f\left(x^{*}\right) \leq f(x)$.
- Are local minima also global minima?


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- $f$ is a strictly convex function, if, for any $\lambda \in] 0,1\left[\right.$, and any $x, x^{\prime}$,

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non-convex

convex
strictly convex

convex, not strictly

## Relationship Between Convexity and Minimization

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## Gradients and Minimization

- Given $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ (differentiable), the gradient of $f$ at $x$ :

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\nabla f(x)=\left[\begin{array}{c}
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local max

saddle point


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- Relationship between Hessian and convexity:
$\checkmark$ Positive semi-definite Hessian $\Leftrightarrow f$ is convex
$\checkmark$ Positive definite Hessian $\Leftrightarrow f$ is strictly convex.


## More on Gradients

- Gradient of quadratic form $f(x)=x^{T} A x: \nabla f(x)=\left(A+A^{T}\right) x$


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- If $g(x)=f(A x)$, then $\nabla g(x)=A^{T} \nabla f(A x)$


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- If $g(x)=f(a \odot x)$, then $\nabla g(x)=a \odot \nabla f(a \odot x)$
- In simple cases, we can find minima analytically: $f(x)=\|A x-y\|_{2}^{2}$

$$
\nabla f(x)=2 A^{T}(A x-y)=0 \Rightarrow x^{*}=\left(A^{T} A\right)^{-1} A^{T} y
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$$

- Choosing the step-size: crucial for convergence and performance.
- GD may work well, or not so well. There are many ways to improve it.



## Recommended Reading

- Z. Kolter and C. Do, "Linear Algebra Review and Reference", Stanford University, 2015 (https://tinyurl.com/44x2qj4)


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## Machine Learning

Tom Mitchell's definition:

- "A computer program is said to learn from experience $E$ with respect to some class of tasks $T$ and performance measure $P$ if its performance at tasks in $T$, as measured by $P$, improves with experience $E$."
- In a nutshell: learn from data; improve performance with experience

This comes in many flavours:

- Supervised learning
- Unsupervised learning
- Self-supervised learning
- Reinforcement learning
- Active learning

Formulate the problem; get data; learn the model from the data; evaluate.

## Example Tasks

Binary classification: given an e-mail: is it spam or not-spam?
Multi-class classification: given a news article, determine its topic (politics, sports, etc.)

Regression: how much time a person will spend reading this article?

https://www.approximatelycorrect.com/2020/10/26/
superheroes-of-deep-learning-vol-1-machine-learning-yearning/

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## Let's Start Simple

- Example 1 - sequence: $\star \diamond$; ;
- Example 2 - sequence: $\star \diamond \triangle$;
- Example 3 - sequence: $\star \triangle \boldsymbol{\varphi}$;
- Example 4 - sequence: $\diamond \triangle$;
label: -1
label: -1
label: +1
label: +1
(Credits: Ryan McDonald)


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- New sequence: $\star \diamond \circ$; label ?
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(Credits: Ryan McDonald)


## Let's Start Simple

- Example 1 - sequence: $\star \diamond$;
- Example 2 - sequence: $\star \odot \triangle$;
- Example 3 - sequence: $\star \triangle \boldsymbol{\phi}$;
- Example 4 - sequence: $\diamond \triangle$;
label: -1
label: -1
label: +1
label: +1
- New sequence: $\star \diamond \circ$; label -1
- New sequence: $\star \diamond \wp$; label -1
- New sequence: $\star \triangle$; label ?
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- New sequence: $\star \diamond \diamond$; label -1
- New sequence: $\star \triangle \circ$; label ?

Why can we do this?
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## Let's Start Simple: Machine Learning

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- Example 4 - sequence: $\diamond \triangle$;
label: -1
label: -1
label: +1
label: +1
- New sequence: $\star \diamond \supset$; label -1

$$
\begin{gathered}
\text { Label -1 Label }+1 \\
P(-1 \mid \star)=\frac{\operatorname{count}(\star \text { and }-1)}{\operatorname{count}(\star)}=\frac{2}{3}=0.67 \text { vs. } P(+1 \mid \star)=\frac{\operatorname{count}(\star \text { and }+1)}{\operatorname{count}(\star)}=\frac{1}{3}=0.33 \\
P(-1 \mid \diamond)=\frac{\operatorname{count}(\diamond \operatorname{and}-1)}{\operatorname{count}(\diamond)}=\frac{1}{2}=0.5 \mathrm{vs} . P(+1 \mid \diamond)=\frac{\operatorname{count}(\diamond \text { and }+1)}{\operatorname{count}(\diamond)}=\frac{1}{2}=0.5 \\
P(-1 \mid \odot)=\frac{\operatorname{count}(\odot \text { and }-1)}{\operatorname{count}(\odot)}=\frac{1}{1}=1.0 \mathrm{vs} . P(+1 \mid \varnothing)=\frac{\operatorname{count}(\odot \text { and }+1)}{\operatorname{count}(\odot)}=\frac{0}{1}=0.0
\end{gathered}
$$

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## Let's Start Simple: Machine Learning

- Example 1 - sequence: $\star \diamond$;
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- Example 3 - sequence: $\star \triangle \boldsymbol{\phi}$;
- Example 4 - sequence: $\diamond \triangle$;
label: -1
label: -1
label: +1
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- New sequence: $\star \triangle$; label ?

$$
\begin{gathered}
\text { Label }-1 \quad \text { Label }+1 \\
P(-1 \mid \star)=\frac{\operatorname{count}(\star \text { and }-1)}{\operatorname{count}(\star)}=\frac{2}{3}=0.67 \text { vs. } P(+1 \mid \star)=\frac{\operatorname{count}(\star \text { and }+1)}{\operatorname{count}(\star)}=\frac{1}{3}=0.33 \\
P(-1 \mid \triangle)=\frac{\operatorname{count}(\triangle \text { and }-1)}{\operatorname{count}(\triangle)}=\frac{1}{3}=0.33 \mathrm{vs.} P(+1 \mid \triangle)=\frac{\operatorname{count}(\triangle \text { and }+1)}{\operatorname{count}(\triangle)}=\frac{2}{3}=0.67 \\
P(-1 \mid \circ)=\frac{\operatorname{count}(\circ \text { and }-1)}{\operatorname{count}(\circ)}=\frac{1}{2}=0.5 \mathrm{vs.} P(+1 \mid \circ)=\frac{\operatorname{count}(\circ \text { and }+1)}{\operatorname{count}(\circ)}=\frac{1}{2}=0.5
\end{gathered}
$$

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## Machine Learning

(1) Define a model/distribution of interest
(2) Make some assumptions if needed
(3) Fit the model to the data

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(1) Define a model/distribution of interest
(2) Make some assumptions if needed
(3) Fit the model to the data

- Model: $P($ label $\mid$ sequence $)=P\left(\right.$ label $_{\text {symbol }}^{1}, \ldots$ symbol $\left._{n}\right)$
- Prediction for new sequence $=\operatorname{argmax}_{\text {label }} P$ (label|sequence)
- Assumption (naive Bayes):

$$
P\left(\text { symbol }_{1}, \ldots, \text { symbol }_{n} \mid \text { label }\right)=\prod_{i=1}^{n} P\left(\text { symbol }_{i} \mid \text { label }\right)
$$

- Fit the model to the data: count!! (simple probabilistic modeling)


## Some Notation: Inputs and Outputs

- Input $x \in X$
- e.g., a news article, a sentence, an image, ...
- Output $y \in y$
- e.g., spam/not spam, a topic, the object in the image (cat? dog?); a segmentation of the image (pedestrian; car; grass; background)
- Input/Output pair: $(x, y) \in X \times y$
- e.g., a news article together with a topic
- e.g., a image together with an object
- e.g., an image partitioned into segmentation regions


## Many Flavours

- Supervised learning: pairs $(x, y)$ are provided at training time (the main focus of this class)
- Examples: perceptron, SVMs, decision trees, nearest neighbor, neural networks, ...
- Caveat: the labels $y$ may be hard or expensive to annotate
- Unsupervised learning: only $x$ is provided; the model needs to figure out what the labels are without any supervision
- Examples: clustering, PCA, ...
- Reinforcement learning: $x$ is provided, and the model can act on the environment to obtain a reward (but doesn't get to know y)
- Example: a robot acting on an environment trying to achieve a goal
- Active learning: the model requests which data points to label next.






## CLASSICAL MACHINE LEARNING



SUPERVISED


"Divide the ties by length"


## UNSUPERVISED


"Make the best outfits from the given clothes"

## Supervised Learning

- We are given a labeled dataset of input/output pairs:

$$
\mathcal{D}=\left\{\left(x_{n}, y_{n}\right)\right\}_{n=1}^{N} \subseteq X \times y
$$

- Goal: learn a predictor $h: X \rightarrow y$ that generalizes well to arbitrary inputs.
- At test time, given $x \in \mathcal{X}$, we predict

$$
\widehat{y}=h(x)
$$

- Hopefully, $\widehat{y} \approx y$ most of the time.

Tasks/problems have different names depending on what $y$ is...

Regression deals with continuous output variables:

- Simple regression: $y=\mathbb{R}$
- e.g., given a news article, how much time a user will spend reading it?
- Multivariate regression: $y=\mathbb{R}^{K}$
- e.g., predict the $\mathrm{X}-\mathrm{Y}$ coordinates in an image where the user will click


## Classification

Tasks/problems have different names depending on what $y$ is...

Classification deals with discrete output variables:

- Binary classification: $y=\{ \pm 1\}$
- e.g., spam detection
- Multi-class classification: $y=\{1,2, \ldots, K\}$
- e.g., topic classification
- Structured classification: $y$ exponentially large and structured
- e.g., machine translation, caption generation, image segmentation


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- Structured classification: $y$ exponentially large and structured
- e.g., machine translation, caption generation, image segmentation
- Later in this course!

Sometimes reductions are convenient:

- logistic regression reduces classification to regression
- one-vs-all reduces multi-class to binary
- greedy search reduces structured classification to multi-class
... but other times it's better to tackle the problem in its native form.

More later!

## Conclusions

- Machine learning allows computer programs to learn from data (observations, interventions, ...) and improve performance with experience
- Can be supervised, unsupervised, self-supervised, reinforced, etc.
- Tasks can be (binary or multi-class) classification, regression, or more nuanced


## Thank you!

## Questions?



