Lecture 1: Introduction

Jakub M. Tomczak

Deep learning

VU VRIJE UNIVERSITEIT AMSTERDAM

COURSE ORGANIZATION

DO NOT HESITATE TO CONTACT US!

If you have any question, please contact us:

TAs:

- Dimitrios Alivanistos
- Daniel Daza
- Emile van Krieken
- Anna Kuzina
- Stefan Schouten
- Shuai Wang
- Roderick van der Weerdt
- Taraneh Younesian

Lecturers:

Peter Bloem

Michael Cochez

Jakub Tomczak

LECTURES AND PRACTICAL SESSIONS

During this course we will have:

- 14 lectures (incl. 2 invited lectures)
- 7 days with practical sessions (1 day, 5 time slots)
- 1 meeting for the final exam

LECTURES AND PRACTICAL SESSIONS

Content of the course:

1. From logistic regression to fully-connected networks
2. Convolutional nets, recurrent neural nets
3. Generative modeling: GANs, VAEs, autoregressive models, flows
4. Graph convolutions, self-attention, transformers
5. Reinforcement Learning

LECTURES AND PRACTICAL SESSIONS

Assignments:

1. MLP (Nov 14)
2. Autograd/backpropagation (Nov 28)
3. One of the two (Dec 8):
    a. CNNs
    b. RNNs
4. One of the three (Dec 19):
    a. VAEs & GANs
    b. Graph convolutions
    c. Reinforcement learning

LECTURES AND PRACTICAL SESSIONS

Assignments:

1. Use Python 3 ONLY!
2. Assignments 1 and 2 are implemented INDIVIDUALLY.
3. Assignments 3 and 4 are implemented IN GROUPS OF 3.
4. All methods must be implemented by you unless it's specified otherwise.
5. In the assignments we will use mainly Numpy and PyTorch.
6. THERE IS NO RESIT FOR ASSIGNMENTS.
7. Late submissions: First contact Jakub. Second, -2pts for each day after the deadline.

GRADING

Assignments

- Max. 40 pts (10 pts per assignment)
- Partial grade from the assignments: round(achieved points / 4)

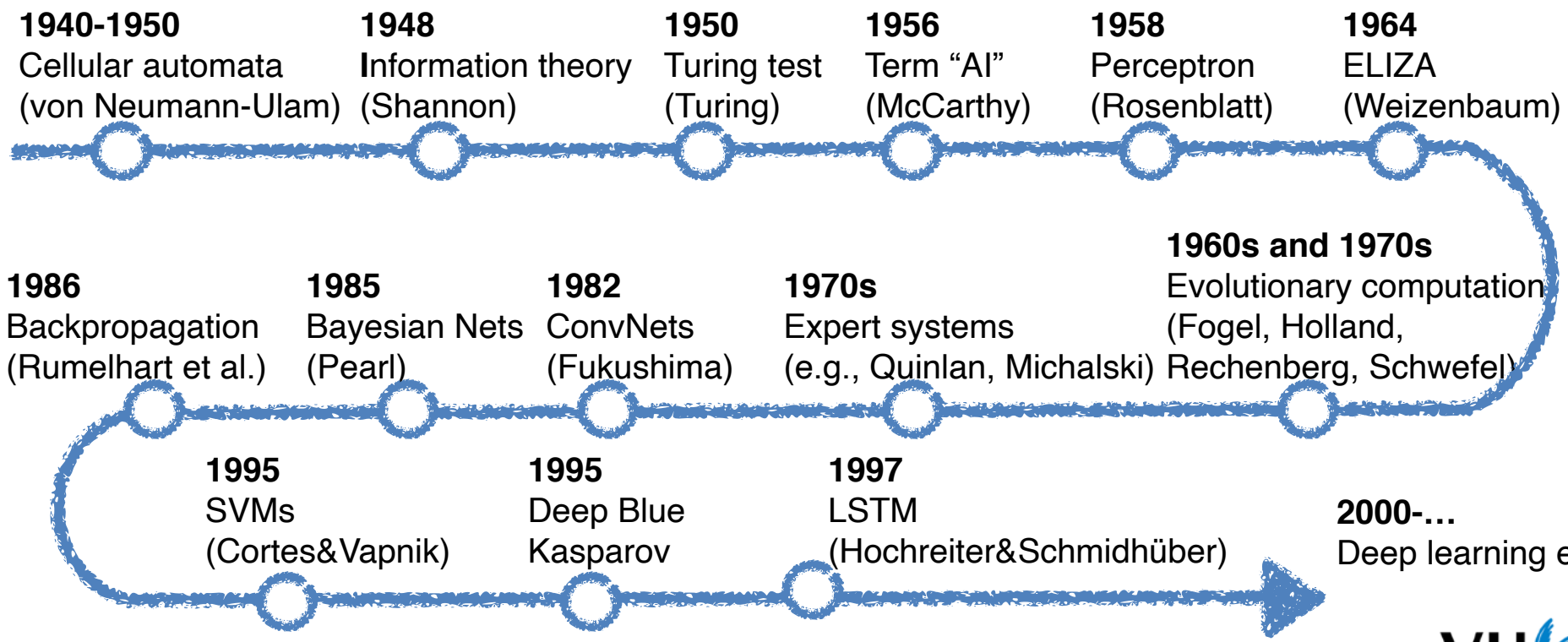
Exam

- Max. 40 pts (40 questions)
- Partial grade: round(achieved points / 4)

Final grade

- At least 5.5 from the assignments and 5.5 from the exam.
- Final grade:
  round(0.5 * partial grade from assignments + 0.5 * partial grade from the exam)

HISTORICAL PERSPECTIVE



WHY AI IS SUCCESSFUL?

Accessible hardware

Powerful hardware

Intuitive programming languages

Specialized packages

COMPONENTS OF AI SYSTEMS

Knowledge representation

How to represent & process data?

Knowledge acquisition (learning objective & algorithms)

How to extract knowledge?

Learning problems

What kind of problems can we formulate?

LEARNING AS OPTIMIZATION

For given **data** $\mathscr{D}$, find the **best data representation** from a given **class of representations** that minimizes given **learning objective (loss)**.

$$\min_{x \in \mathbb{X}} f(x; \mathscr{D})$$

$$\text{s.t. } x \in \mathbb{Y} \subseteq \mathbb{X}$$

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$$\text{s.t. } x \in \mathbb{Y} \subseteq \mathbb{X}$$

Optimization algorithm = learning algorithm.

LEARNING TASKS

Supervised Learning

- We distinguish **inputs** and **outputs**.
- We are interested in **prediction**.
- We minimize a **prediction error.**

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- **No** distinction among variables.
- We look for a **data structure**.
- We minimize a **reconstruction error**, **compression rate**, …

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- An **agent** interacts with an **environment**.
- We want to learn a **policy**.
- Each **action** is **rewarded.**
- We maximize a **total reward**.

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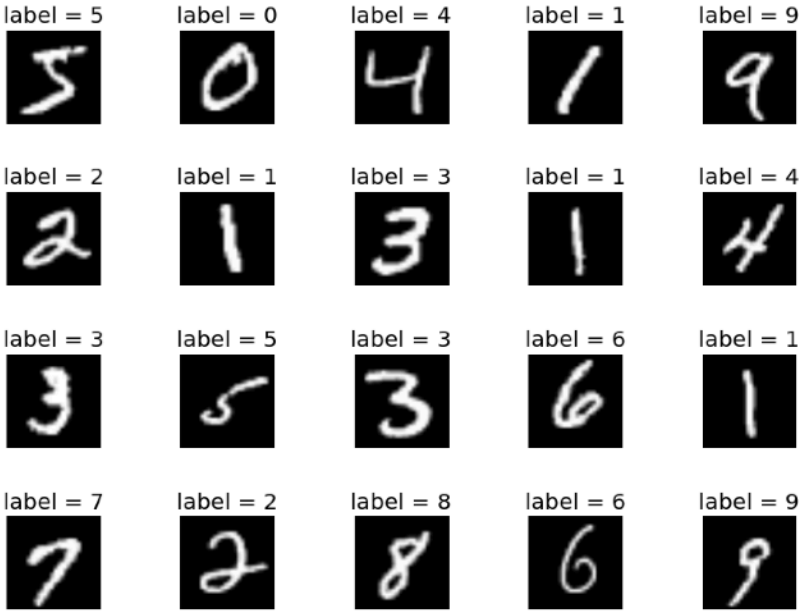
Classification



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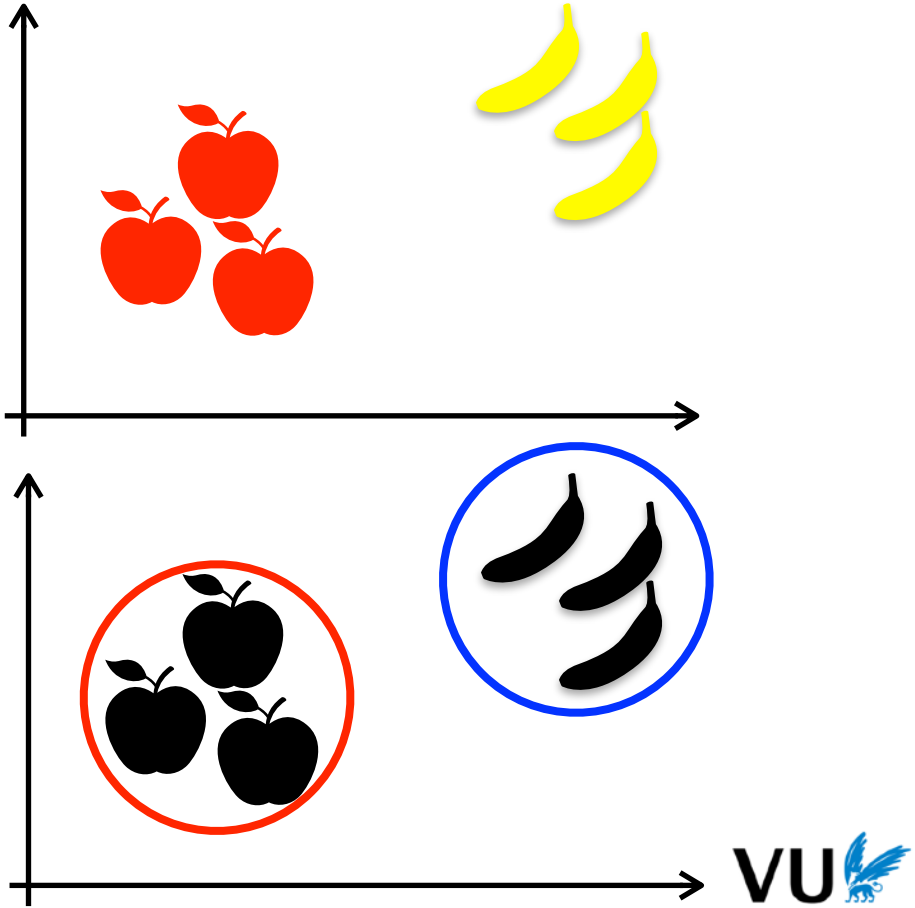

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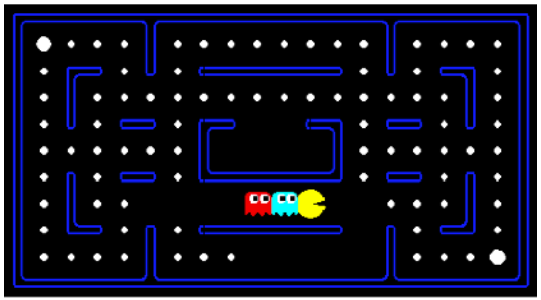

DEEP LEARNING

APPLICATION AREAS

Computer Vision

Information Retrieval

Speech Recognition

Natural Language Processing

Recommendation Systems

Drug Discovery

Robotics

…

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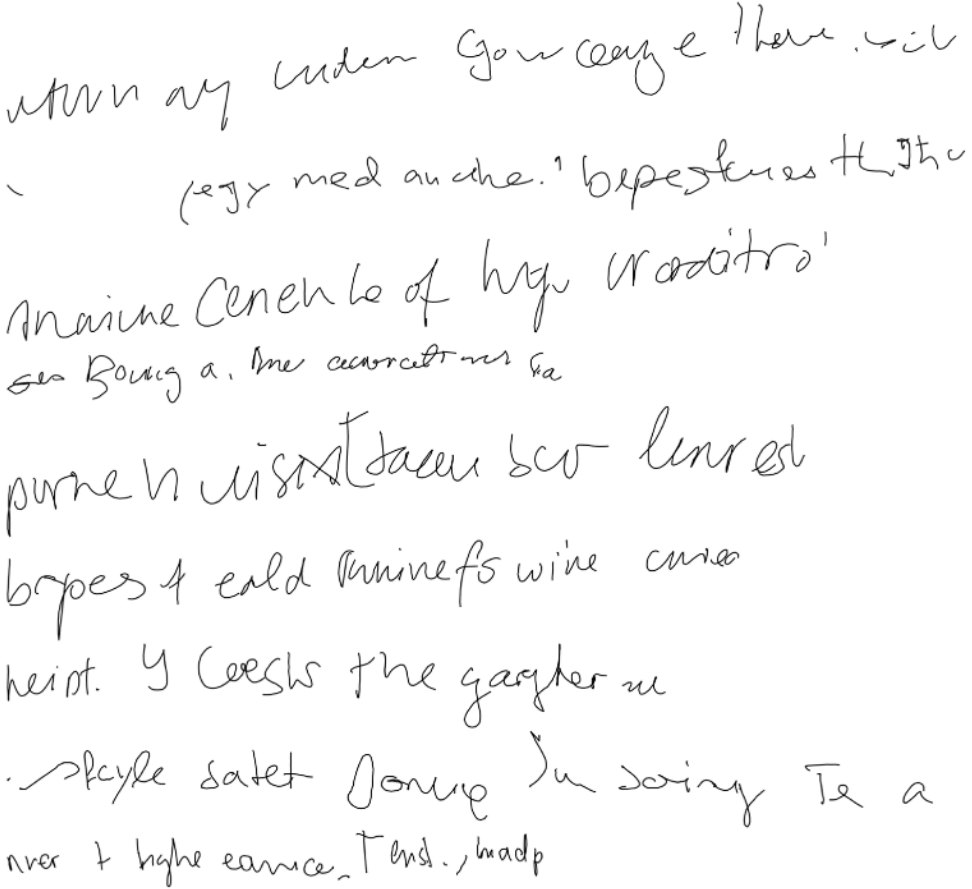
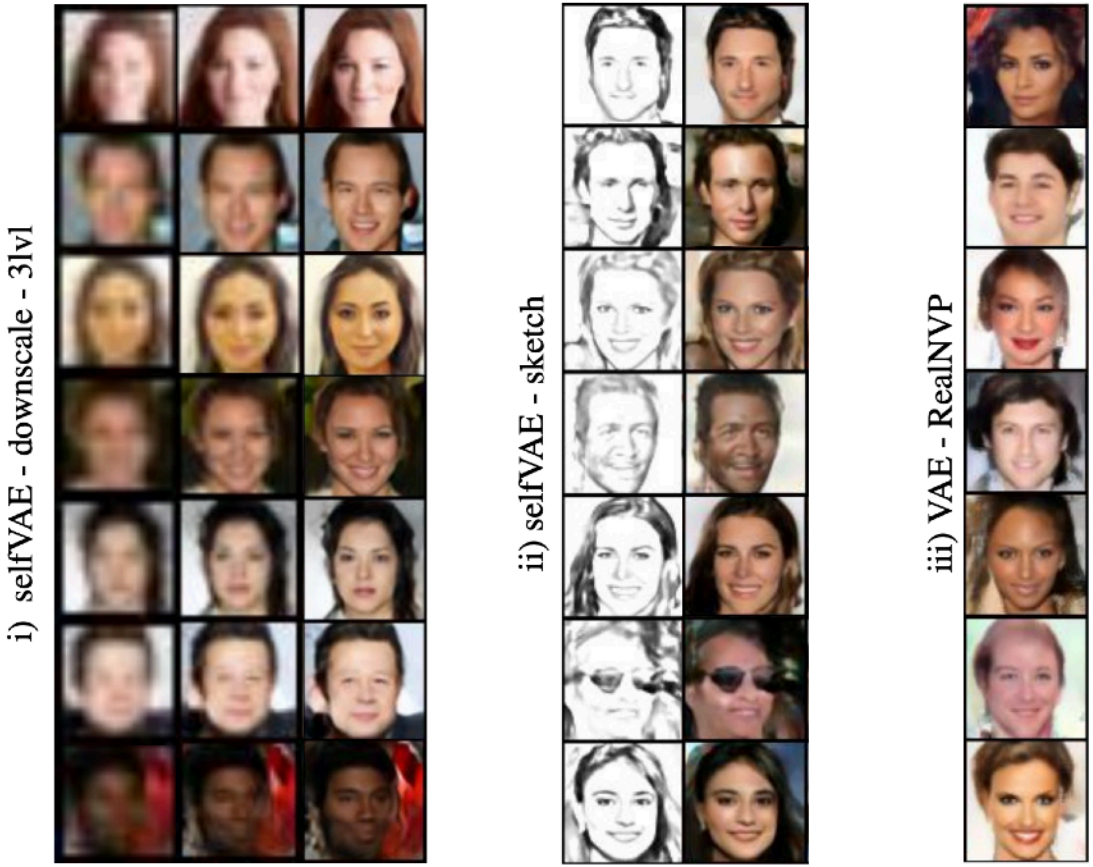
EXAMPLES: HANDWRITING GENERATOR



A. Graves, “Generating Sequences With Recurrent Neural Networks“

EXAMPLES: IMAGE GENERATION



Gatopoulos & Tomczak, “Self-supervised Variational Auto-Encoders“

EXAMPLES: GENERATING IMAGE DESCRIPTIONS

"man in black shirt is playing guitar."

"construction worker in orange safety vest is working on road."

"two young girls are playing with lego toy."

"boy is doing backflip on wakeboard."

"girl in pink dress is jumping in air."

"black and white dog jumps over bar."

"young girl in pink shirt is swinging on swing."

"man in blue wetsuit is surfing on wave."

Karpathy & Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions"

THREE CORE COMPONENTS OF DEEP LEARNING

- The INTERNET
- Unlabeled data
- ImageNet database

14,197,122 images

IMAGENET

- Parallel computing
- GPU, FPGA
- Deep learning frameworks

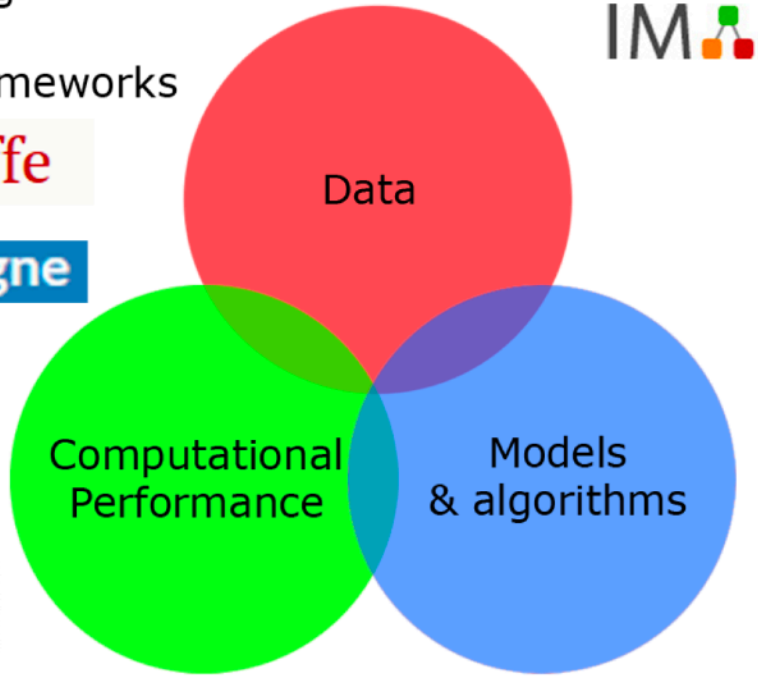
theano Caffe

TensorFlow Lasagne

torch

PYTORCH

cuDNN



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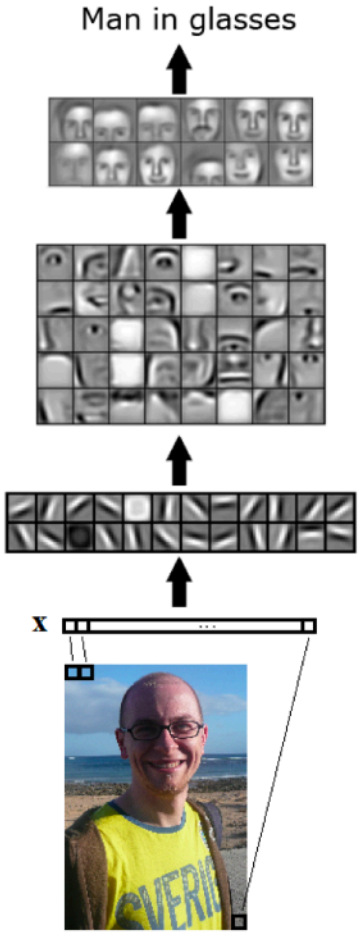
AUTOMATIC FEATURE EXTRACTION / REPRESENTATION LEARNING

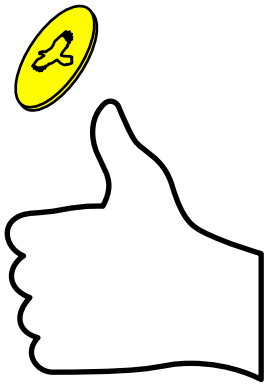
- A **representation** = a set of (abstract) features.
- Deep learning automatically extract feature.
- A hidden layer = an abstraction level.
- Good-quality features should be:
  - ? **Informative** (e.g., discriminative);
  - **Robust** to small perturbations;
  - ? **Invariant**/**Equivariant** to transformations.
- **Representation Learning** = optimization algo.



PROBABILISTIC LEARNING

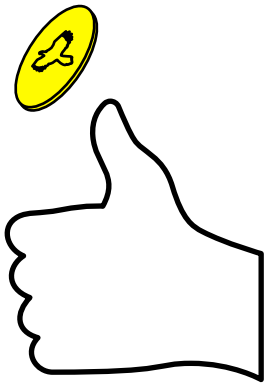
TOSS A COIN… 🎶

- $c \in \{0,1\}$ - a **random variable** (a result of tossing a coin)



TOSS A COIN… 🎶

- $c \in \{0,1\}$ - a **random variable** (a result of tossing a coin)
- $x = p(c = 1)$ - **probability** of observing *head*
- $1 - x = p(c = 0)$ - probability of observing *tail*
- $p(c \mid x) = x^c \ (1 - x)^{1-c}$ - **Bernoulli distribution**



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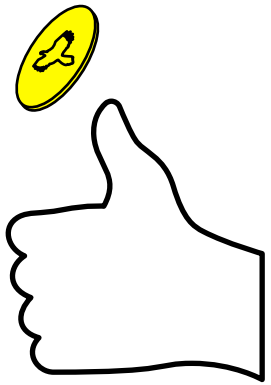

Quick check:

$$p(c = 0 \mid x) = x^0 \ (1 - x)^{1-0} = 1 - x$$

$$p(c = 1 \mid x) = x^1 \ (1 - x)^{1-1} = x$$

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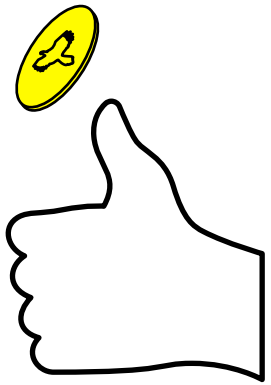
- $\mathcal{D} = \{c_1, c_2, \ldots, c_N\}$ - *iid* observations (**data**)



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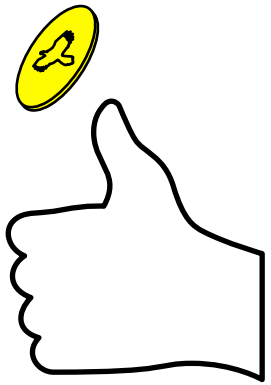

EXAMPLE:

$\mathscr{D} = \{0,0,1,1,0,1,1\}$

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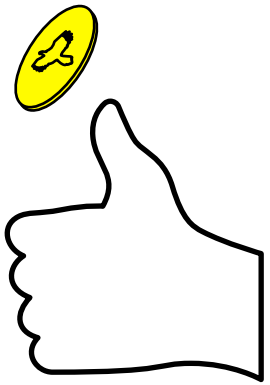
- The **likelihood function**:

$$p(\mathcal{D} \mid x) = \prod_{n=1}^{N} p(c_n \mid x)$$



TOSS A COIN… 🎶

The optimization problem:

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Find such $x \in [0,1]$ that minimizes the **negative log-likelihood function**:

$$\min_{x \in [0,1]} -\log p(\mathcal{D} \mid x)$$

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Remarks:

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TOSS A COIN… 🎶

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Remarks:

1) Why **negative**? Because: $\max \; f(x) = \min \; \{-f(x)\}$.

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Remarks:

1) Why **negative**? Because: $\max\ f(x) = \min\ \{-f(x)\}$.

2) Why **logarithm**? Because: $\log \prod = \sum \log$ and optimum is the same.

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TOSS A COIN… 🎶

$$\log p(\mathscr{D} \mid x) = \log \prod_{n=1}^{N} p(c_n \mid x)$$

the log-likelihood

TOSS A COIN… 🎶

$$\log p(\mathcal{D}\,|\,x) = \log \prod_{n=1}^{N} p(c_n\,|\,x)$$

$$= \sum_{n=1}^{N} \log p(c_n\,|\,x)$$

the log-likelihood

$$\log \prod = \sum \log$$

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$$= \sum_{n=1}^{N} \log x^{c_n}\,(1-x)^{1-c_n}$$

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Bernoulli distribution

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$$= \sum_{n=1}^{N} \Big(c_n \log x + (1-c_n)\log(1-x) \Big)$$

the log-likelihood

$$\log \prod = \sum \log$$

Bernoulli distribution

$$\log a^b = b \log a$$

$$\log ab = \log a + \log b$$

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(Finding $x^\star$) Calculate derivative wrt x and set to 0:

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$$\frac{\mathrm{d}}{\mathrm{d}x}\sum_{n=1}^{N}\Big(c_n \log x + (1-c_n)\log(1-x)\Big) = 0$$

$$\sum_{n=1}^{N}\left(\frac{c_n}{x} - \frac{(1-c_n)}{(1-x)}\right) = 0$$

$\frac{\mathrm{d}}{\mathrm{d}x} f(x) = 0$ gives optimum

and

$$\frac{\mathrm{d}}{\mathrm{d}x}\log x = \frac{1}{x}$$

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$$\sum_{n=1}^{N} c_n - x\sum_{n=1}^{N} c_n - Nx + x\sum_{n=1}^{N} c_n = 0 \quad \Rightarrow \quad \boxed{x = \frac{1}{N}\sum_{n=1}^{N} c_n}$$

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EXAMPLE:

$\mathcal{D} = \{0,0,1,1,0,1,1\}$

$x^\star = 4/7$

PROBABILISTIC LEARNING (LIKELIHOOD-BASED)

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1) Determine $p(y \mid x)$.

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4) Find the best solution by minimizing $-\log p(\mathscr{D} \mid x)$.

PROBABILISTIC LEARNING (LIKELIHOOD-BASED)

1) Determine $p(y \mid x)$. e.g., Bernoulli, Gaussian…

2) Determine $p(\mathcal{D} \mid x)$. e.g., *iid* or sequential

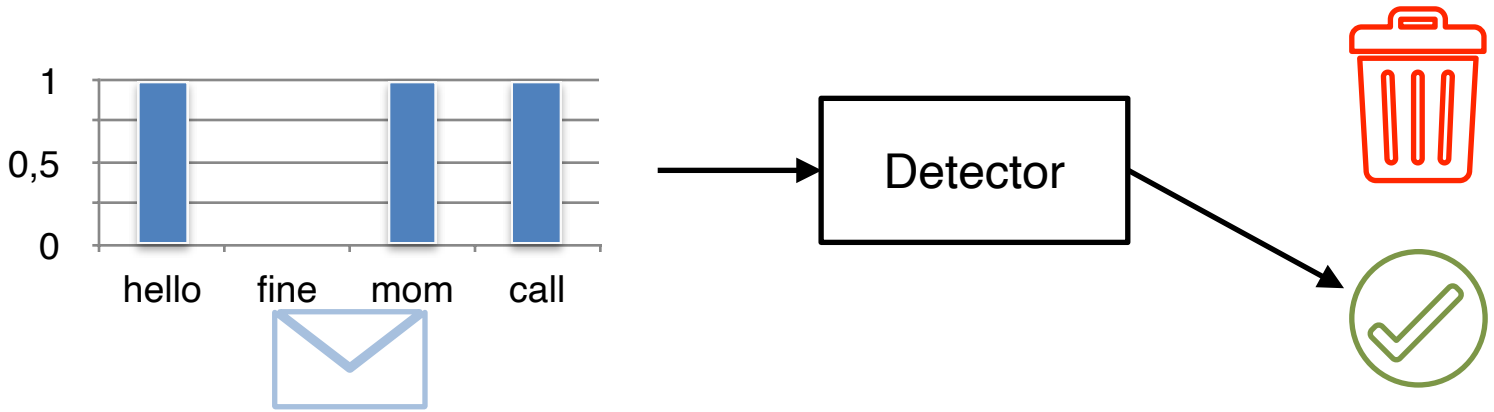
3) Check constraints. e.g., only values between [0, 1]

4) Find the best solution by minimizing $-\log p(\mathcal{D} \mid x)$. e.g., using gradient-descent

LOGISTIC REGRESSION

SPAM DETECTION

- Example: Spam detection
  - $x \in \{0,1\}^D$ - whether a *d*th word occurs in an e-mail ($x = 1$) or not
  - $y \in \{0,1\}$ - whether an e-mail is a spam ($y = 1$) or not
  - Goal: provide probability of a spam OR classify messages.



LOGISTIC REGRESSION

- $x \in \mathbb{R}^D$, $y \in \{0,1\}$, $\theta \in \mathbb{R}^D$
- We model y by using the Bernoulli distribution:

$$p(y \mid x, \theta) = \text{Bern}(y \mid \text{sigm}(\theta^\top x))$$

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where:

linear dependency: $\theta^\top x = \sum_{d=1}^{D} \theta_d x_d$

sigmoid function: $\text{sigm}(s) = \frac{1}{1 + \exp(-s)}$

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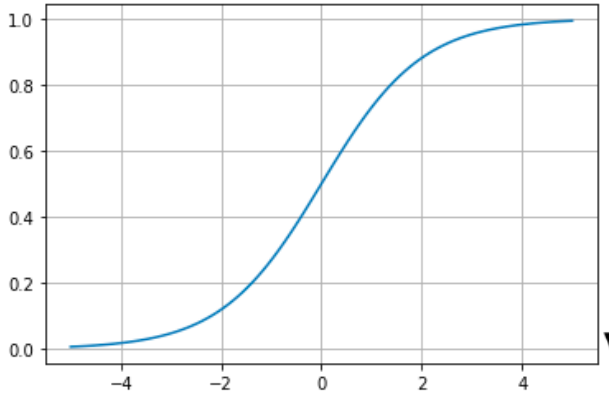
Sigmoid can model probabilities!



LOGISTIC REGRESSION

- Properties of the sigmoid function:
  - $\text{sigm}(s) \in [0,1]$
  - $\frac{\mathrm{d}}{\mathrm{d}s}\text{sigm}(s) = \text{sigm}(s)\ (1 - \text{sigm}(s))$
  - $\text{sigm}(-s) = 1 - \text{sigm}(s)$
- In our model we have:

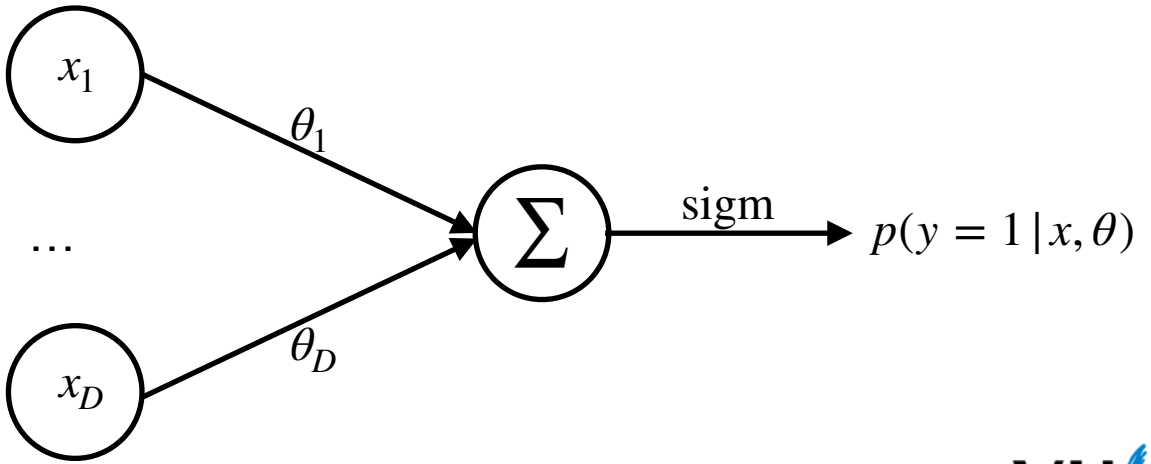
$$p(y = 1 \,|\, x, \theta) = \text{sigm}(\theta^\top x)$$

$$p(y = 0 \,|\, x, \theta) = 1 - \text{sigm}(\theta^\top x)$$

LOGISTIC REGRESSION

- $p(y \mid x, \theta) = \text{Bern}(y \mid \text{sigm}(\theta^\top x))$

where: $\theta^\top x = \sum_{d=1}^{D} \theta_d x_d$



LOGISTIC REGRESSION: GRADIENT-DESCENT

$$\nabla_\theta - \log p(\mathscr{D}_y \mid \mathscr{D}_x, \theta) = \nabla_\theta - \sum_i \log p(y_i \mid x_i, \theta)$$

LOGISTIC REGRESSION: GRADIENT-DESCENT

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$$
\begin{aligned}
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&= - \sum_i \left(y_i\, x_i - \operatorname{sigm}(\theta^\top x_i)\, x_i \right) \\
&= \sum_i \left(\operatorname{sigm}(\theta^\top x_i) - y_i \right) x_i
\end{aligned}
$$

LOGISTIC REGRESSION: GRADIENT-DESCENT

- The update rule:

$$\theta := \theta - \alpha \sum_{i=1}^{N} \left(\text{sigm}(\theta^\top x_i) - y_i \right) x_i$$

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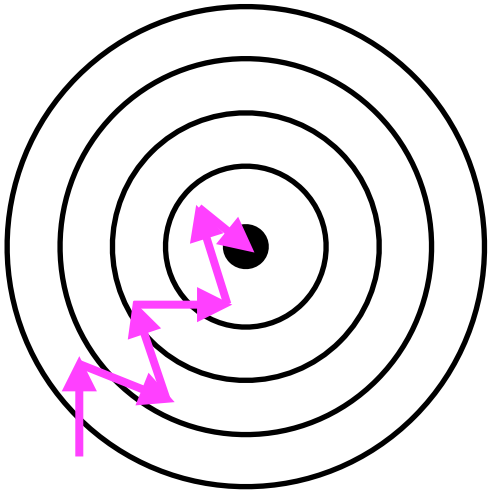
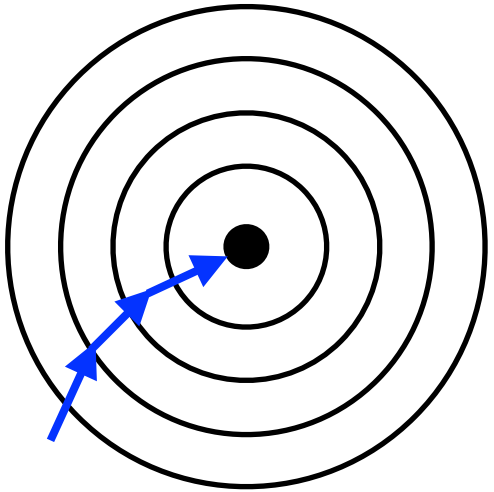
or even:

$$\theta := \theta - \alpha \left(\text{sigm}(\theta^\top x_j) - y_j \right) x_j$$

LOGISTIC REGRESSION: SGD VS. GD



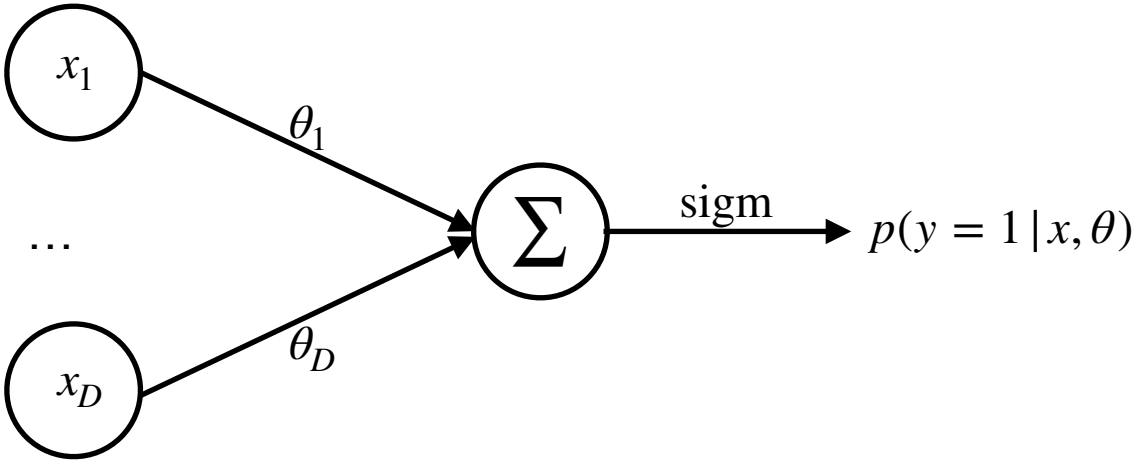
Stochastic Gradient Descent



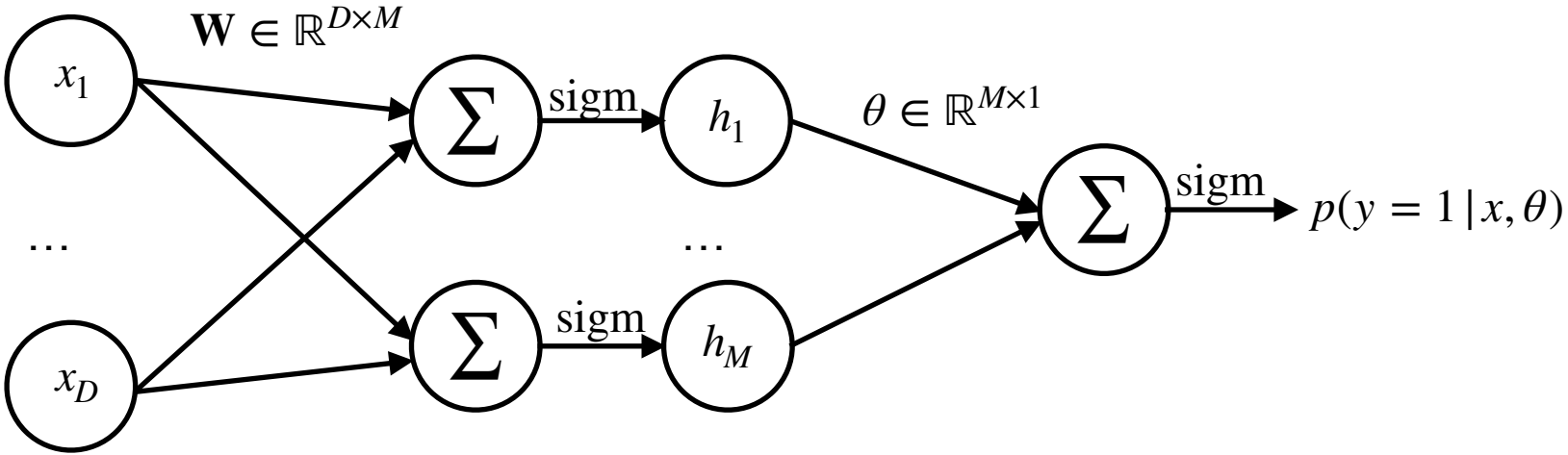
Gradient Descent

FULLY-CONNECTED NEURAL NETWORKS

WHAT IF WE STACK MULTIPLE LOGISTIC REGRESSORS



STACKING LOGISTIC REGRESSORS



weights: $\mathbf{W} \in \mathbb{R}^{D \times M}$, $\theta \in \mathbb{R}^{M \times 1}$

FULLY CONNECTED NEURAL NETWORKS (FCN)

- Stacking logistic regressions models the probability as follows:

$$p(y = 1 \,|\, x, \mathbf{W}, \theta) = \text{sigm}\Big(\theta^\top \underbrace{\text{sigm}(\mathbf{W}x)}_{h}\Big)$$

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- We can stack even more:

$$p(y = 1 \,|\, x, \{\mathbf{W}_i\}, \theta) = \text{sigm}\Big(\theta^\top \text{sigm}\big(\cdots \mathbf{W}_2 \text{sigm}(\mathbf{W}_1 x)\big)\Big)$$

FCN: COMPONENTS

- A **linear layer**: $a = \mathbf{W}x$ (or with explicit bias: $a = \mathbf{W}x + b$)
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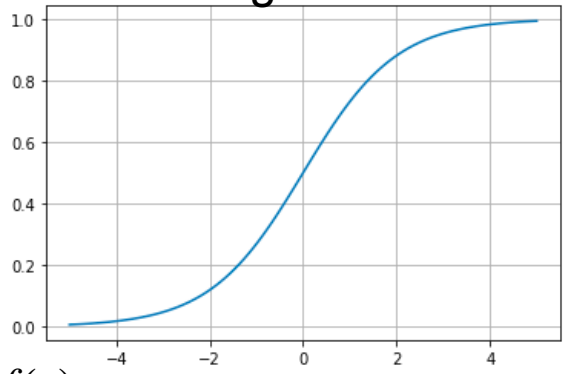
- with a **non-linearity**: $h = f(\mathbf{W}x)$
- Typical non-linearities:
  - **sigmoid**: $\text{sigm}(x) = \left(1 + \exp(-x)\right)^{-1}$
  - **tanh**: $\tanh(x) = 2\text{sigm}(x) - 1$
  - **ReLU**: $\text{relu}(x) = \max\{0, x\}$
  - **softmax**: $\text{softmax}(x) = \exp(x_i) \Big/ \sum \exp(x_j)$

LINEAR LAYERS

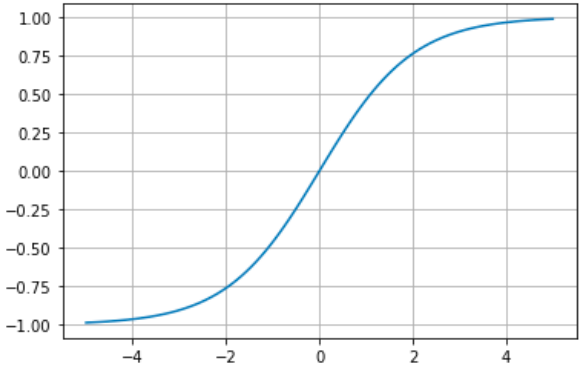
- A **linear layer**: $a = \mathbf{W}x$
- Initialization of $\mathbf{W} \in \mathbb{R}^{D \times M}$:
  - Gaussian: $\mathbf{W} \sim \mathcal{N}(0, \sigma^2)$
  - Xavier (for tanh): $\mathbf{W} \sim \mathcal{N}(0, \sqrt{1/D})$
  - He (for ReLU): $\mathbf{W} \sim \mathcal{N}(0, \sqrt{2/D})$

ACTIVATION FUNCTIONS

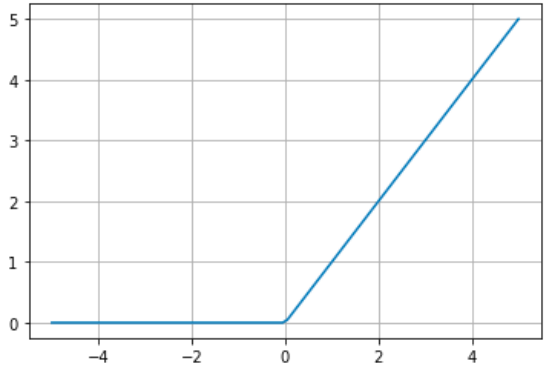
sigmoid



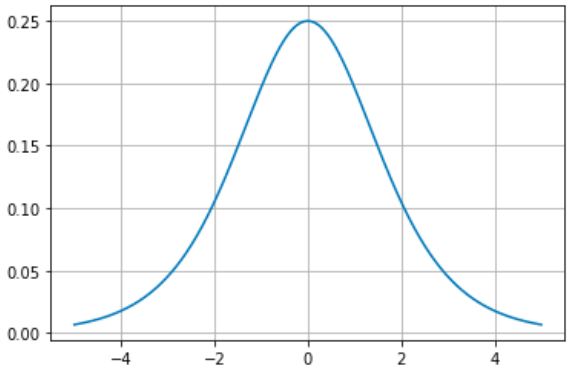
tanh

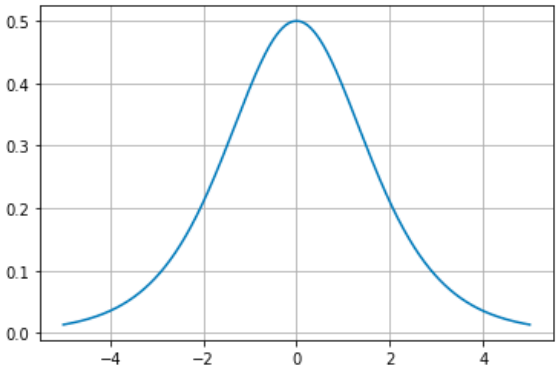


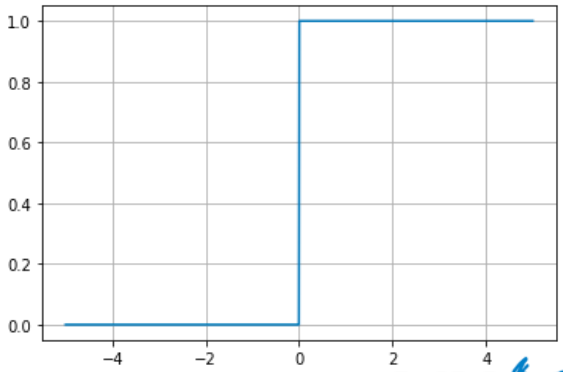
ReLU



$\nabla f(x)$







HOW TO DEAL WITH MULTIPLE CLASSES?

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- How to deal with *K* classes?
- **Softmax** function:

$$p(y = i \mid x, \theta) = \frac{\exp(\theta_i^\top x)}{\sum_{k=1}^{K} \exp(\theta_k^\top x)}$$

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Negative log-likelihood

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Full derivation:
Homework 🤓
Or wait till the next lecture!

VANISHING GRADIENT PROBLEM

- The sigmoid function is a good choice to model probabilities, however, it is bad as a non-linearity for hidden layers.
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If $\mathrm{sigm}(x) \approx 1$, then:

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For instance:

$$\frac{\mathrm{d}\ell}{\mathrm{d}u} = \frac{\mathrm{d}\ell}{\mathrm{d}f_1} \cdot 0 \cdot \frac{\mathrm{d}f_2}{\mathrm{d}u} = 0$$

Thank you!

VU VRIJE UNIVERSITEIT AMSTERDAM

EXTRA READING

Bishop, “Pattern Recognition and Machine Learning”

Murphy, “Machine Learning: A Probabilistic Perspective”

Courville, Goodfellow, Bengio,“Deep Learning”

Kruse et al., “Computational Intelligence: A Methodological Introduction”, Springer