Statistical Learning II

Lecture 2 - Introduction & supervised learning

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DL3 IASO, Université Paris Dauphine-PSL
17.09.2025

Course Organisation

- 12 classes of 3h, divided in:

  - 1h30 lectures

  - 1h30 exercises & lab (Python)
  (with Leonardo De Filippis)

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- Evaluation: Partiel (25%) + Final (75%)

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Goal: Develop a *mathematical* understanding of *classical* and *modern* machine learning models

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    - LASSO
    - Generalised linear models
    - Kernel methods
    - Principal component analysis (PCA)

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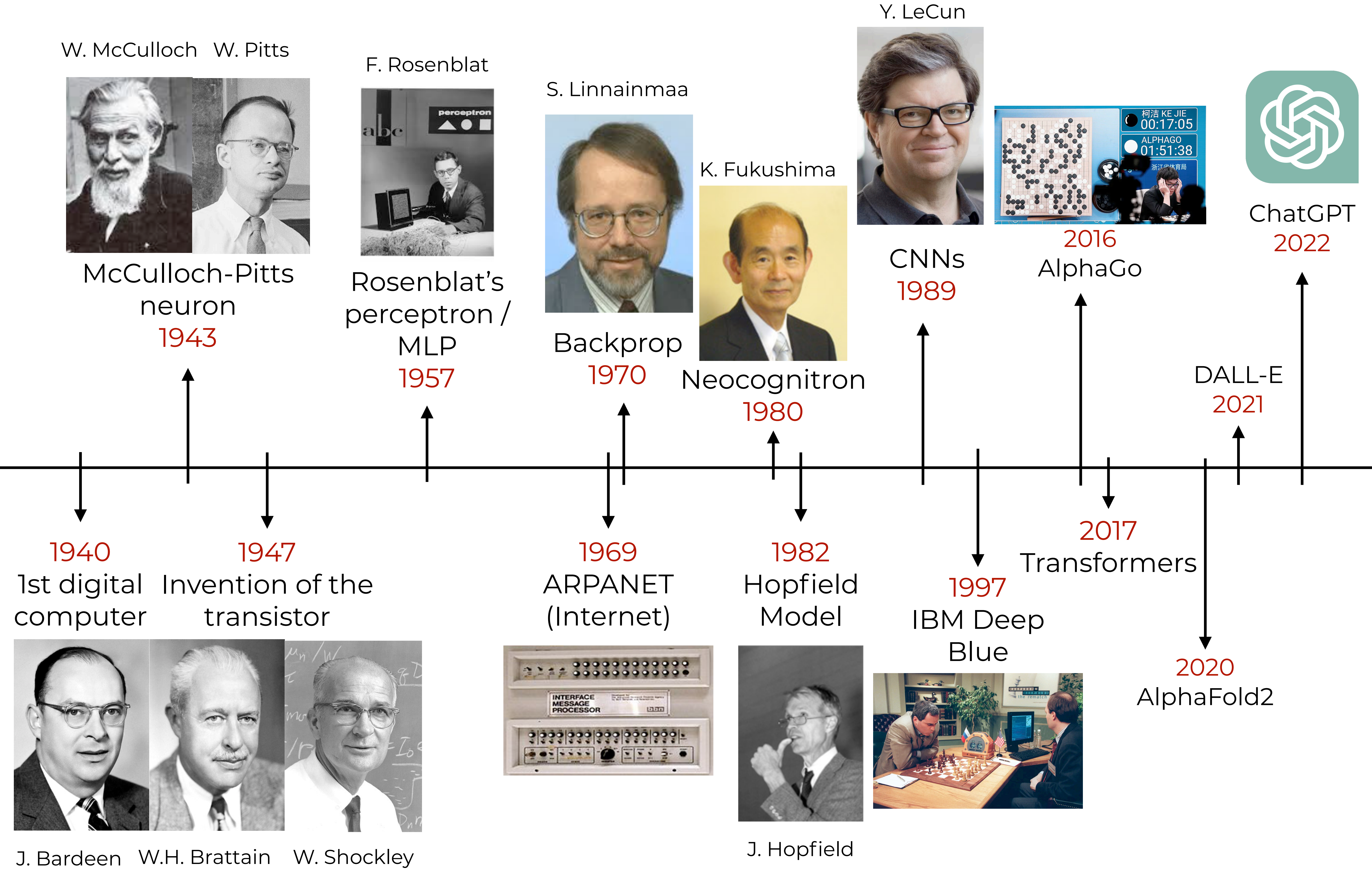
- Classical methods:
    - Ridge regression
    - LASSO
    - Generalised linear models
    - Kernel methods
    - Principal component analysis (PCA)
- Modern methods:
    - Neural networks
    - Diffusion models
    - Your suggestions?

Introduction & Motivation

Or: *why should I care about Statistical Learning?*

A brief history of ML



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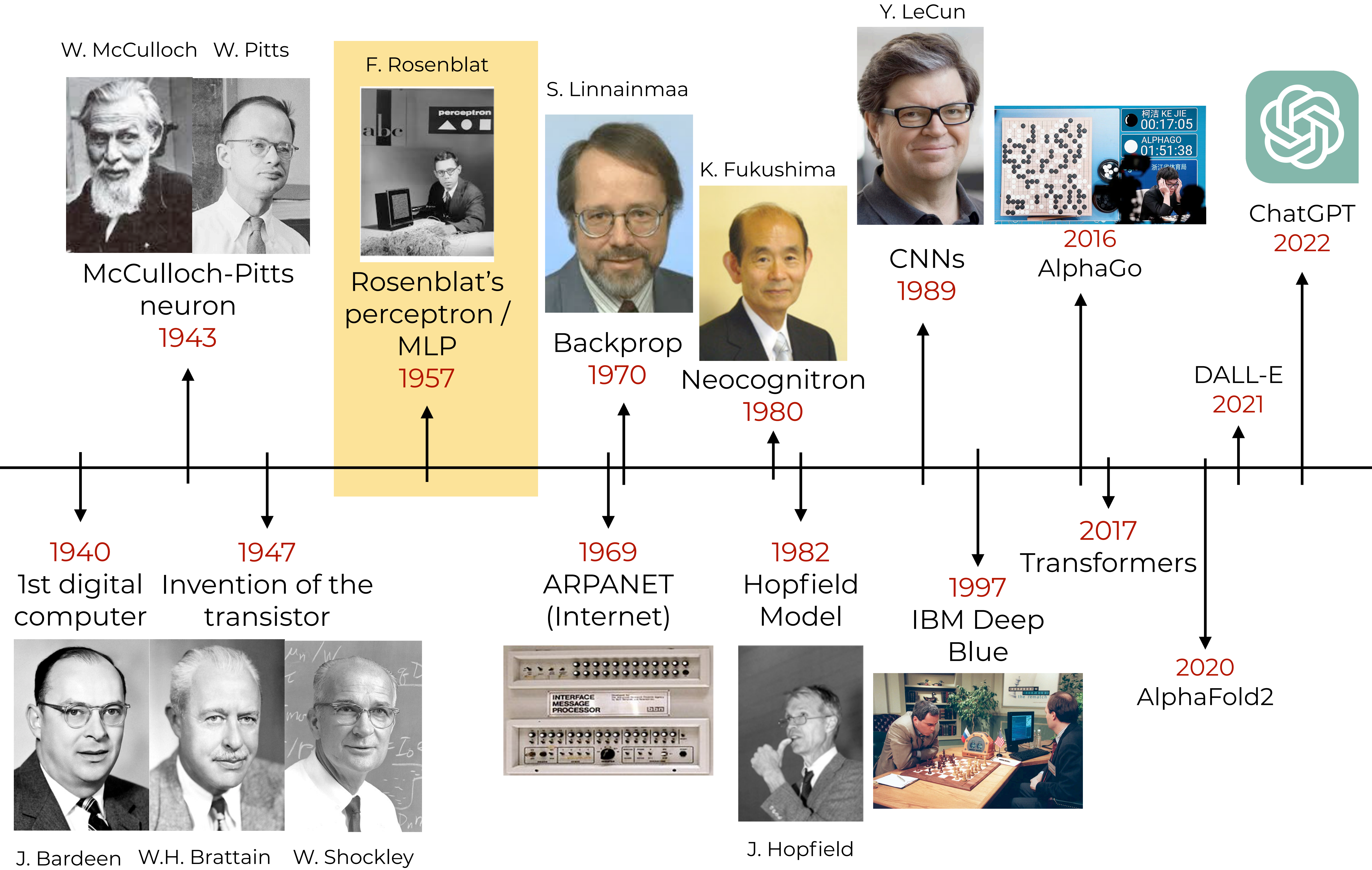

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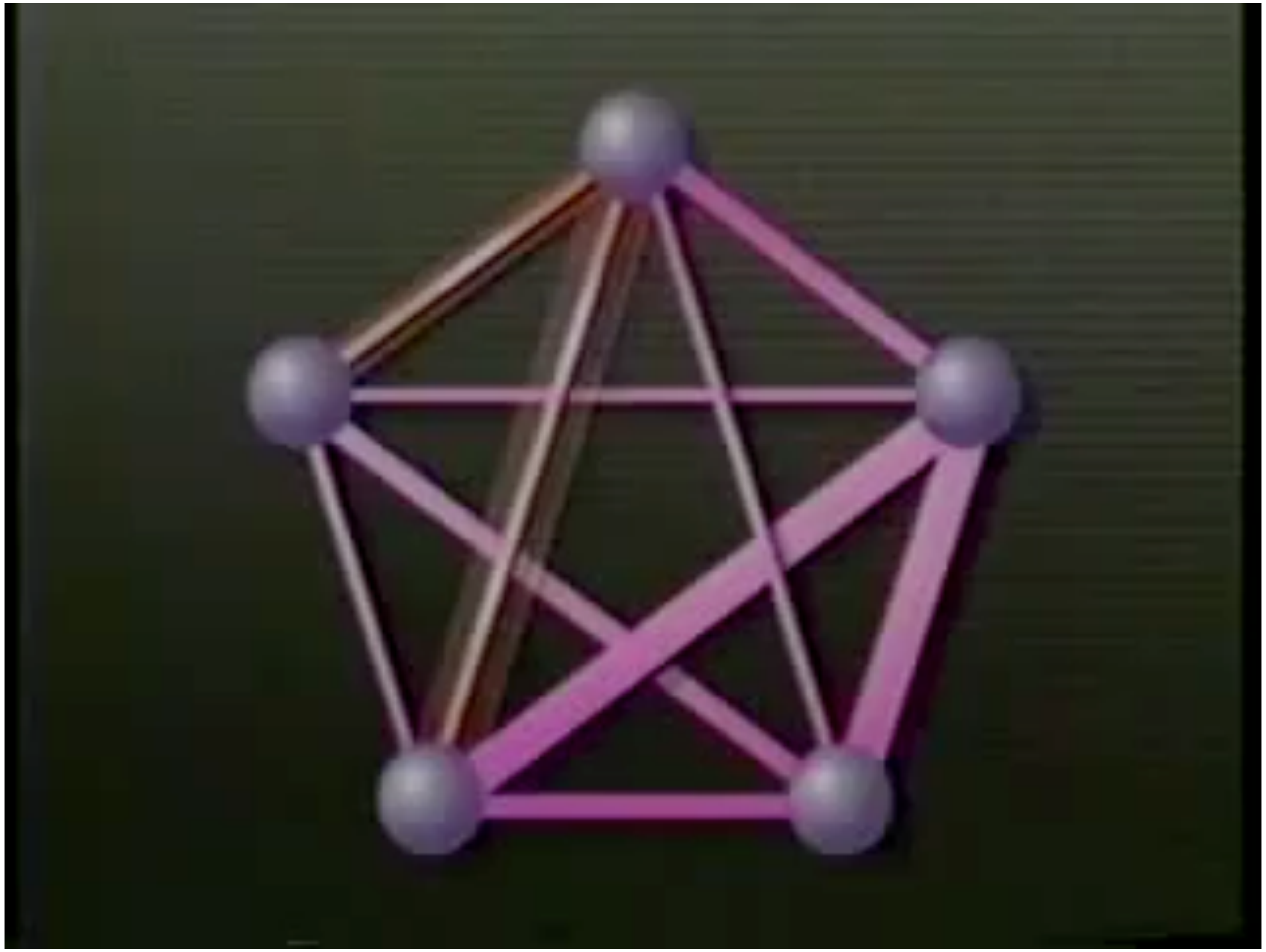

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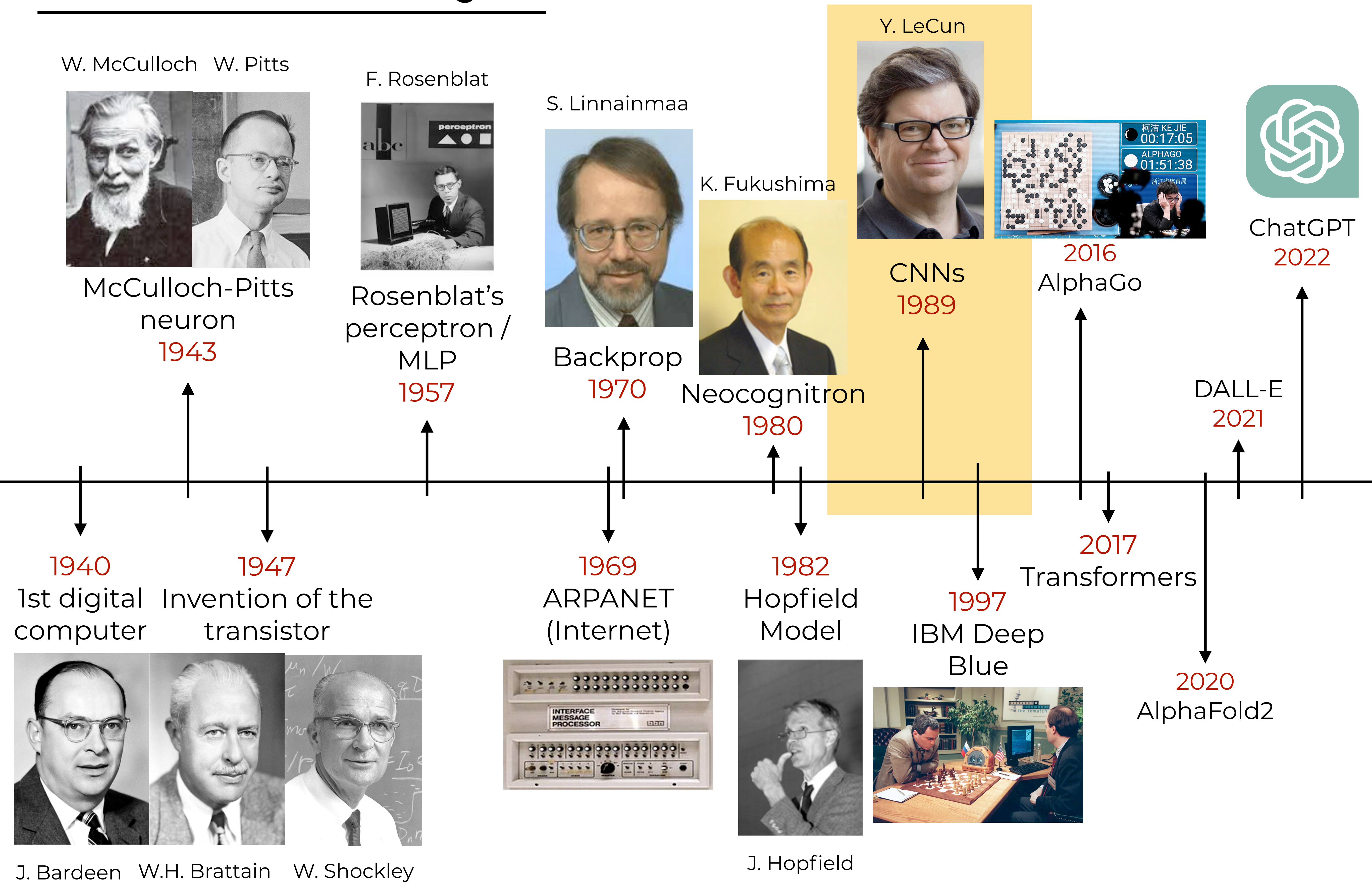

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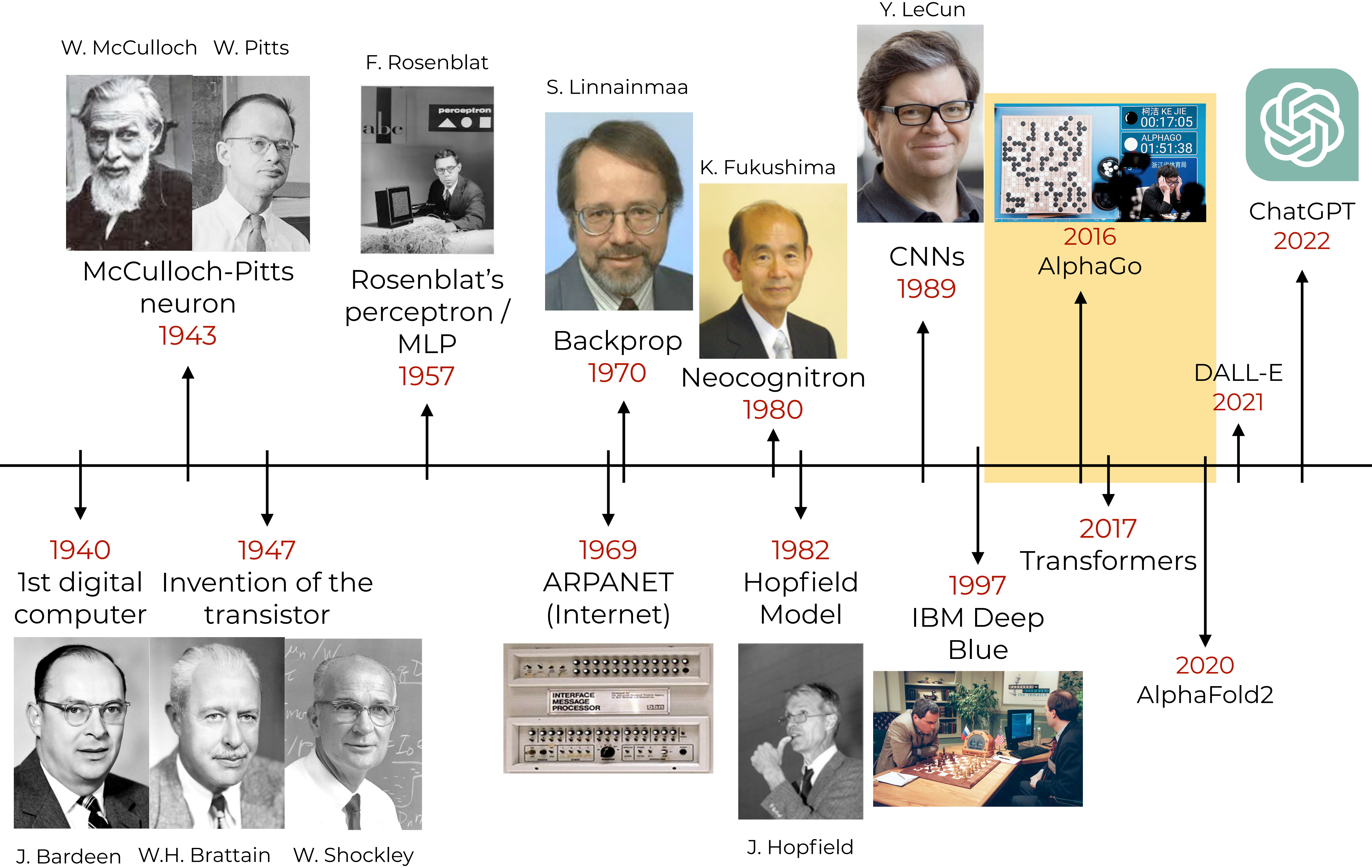

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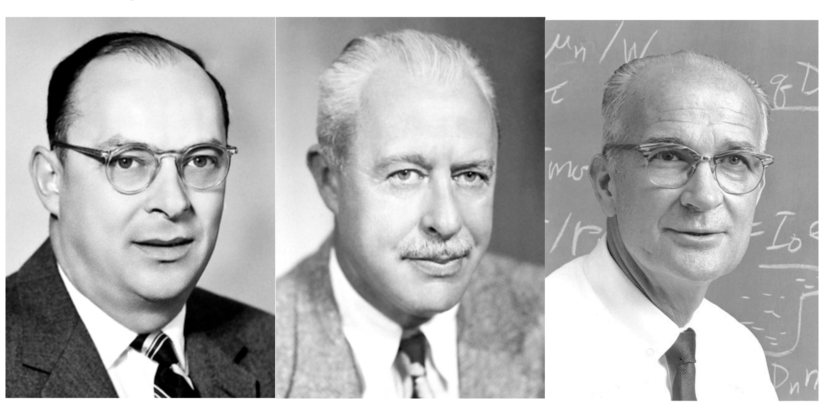
1940
1st digital computer

1943
W. McCulloch W. Pitts

McCulloch-Pitts neuron
1943

1947
Invention of the transistor



J. Bardeen W.H. Brattain W. Shockley

F. Rosenblat

Rosenblat's perceptron / MLP
1957

1969
ARPANET (Internet)

S. Linnainmaa

Backprop
1970

K. Fukushima

Neocognitron
1980

1982
Hopfield Model

J. Hopfield

Y. LeCun

CNNs
1989

1997
IBM Deep Blue

2016
AlphaGo

2017
Transformers

2020
AlphaFold2

DALL-E
2021

ChatGPT
2022

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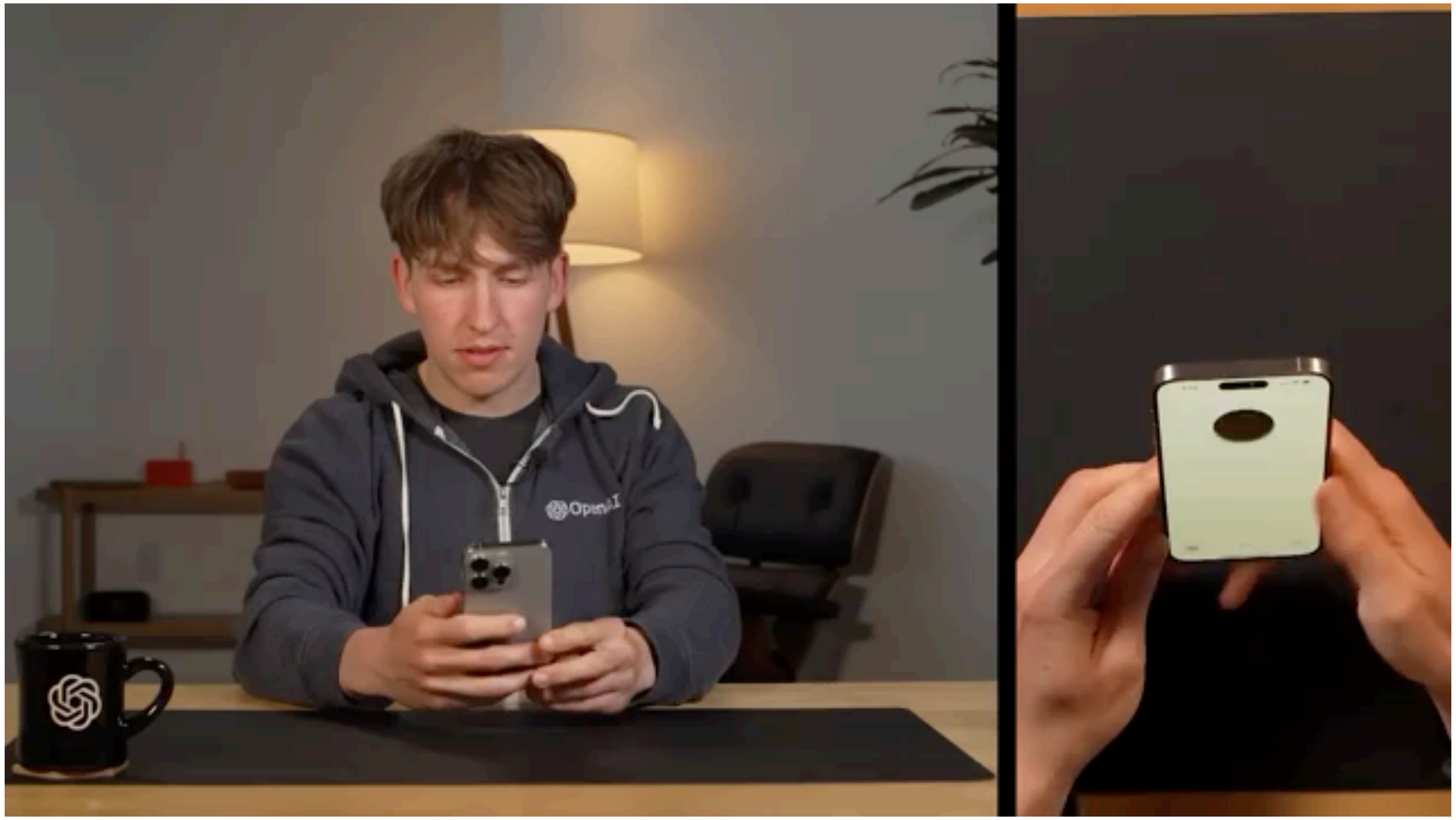


What about the maths?

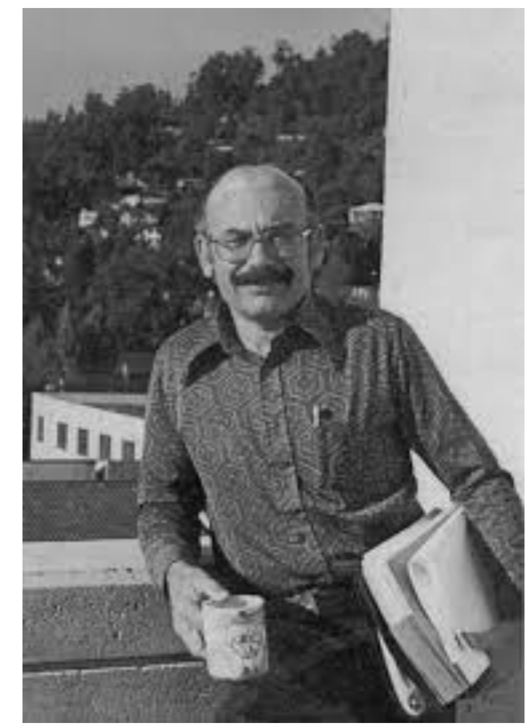
Yet, on the mathematical side...

Leo Breiman
Statistics Department, University of California, Berkeley, CA 94305;
e-mail: leo@stat.berkeley.edu

Reflections After Refereeing Papers for NIPS

For instance, there are many important questions regarding neural networks which are largely unanswered. There seem to be conflicting stories regarding the following issues:

- Why don't heavily parameterized neural networks overfit the data?
- What is the effective number of parameters?
- Why doesn't backpropagation head for a poor local minima?
- When should one stop the backpropagation and use the current parameters?



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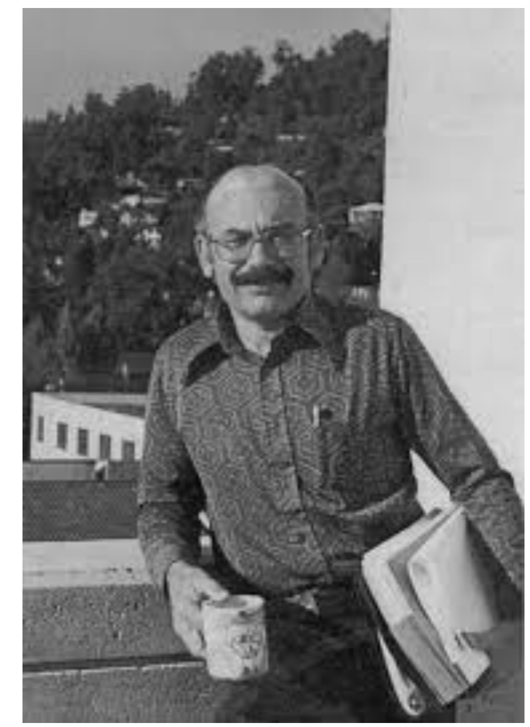

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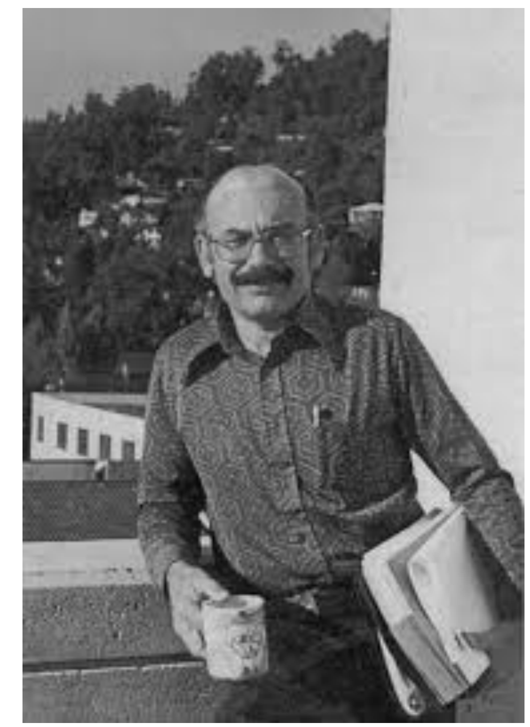

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But why should I care?

Some good reasons to care

- Reliability and Liability

  If a model does something unexpected, who is responsible?

  Crucial in sensitive applications, e.g. medicine, law, self-driving cars/planes…

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- And in the worst case, understanding the maths will make you a better engineer / data scientist.

Our expectations

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- Get acquainted with the most popular machine learning algorithms

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<u>Your expectations:</u> Let’s make a quick survey!

https://forms.gle/nhTyc3pHHiKgTJg9A

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Let $(\boldsymbol{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$, $i = 1, \ldots, n$,
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???

Supervised Learning

Inputs / covariates $x \in \mathcal{X}$

x_1

x_2

x_3

y_1
Not grumpy

y_2
Grumpy

y_3
???

Outputs / Labels / response $y \in \mathcal{Y}$

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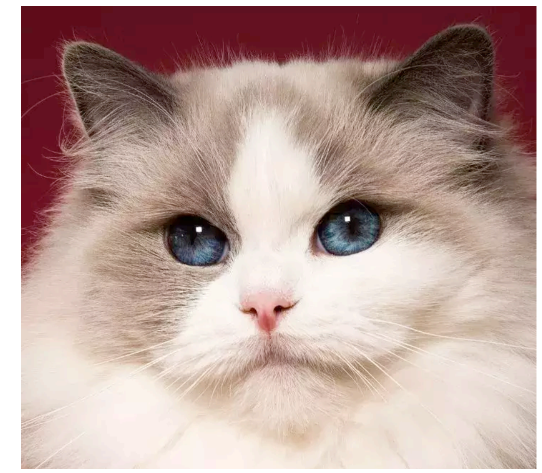
Inputs / covariates $x \in \mathcal{X}$

x_1

x_2



x_3

y_1
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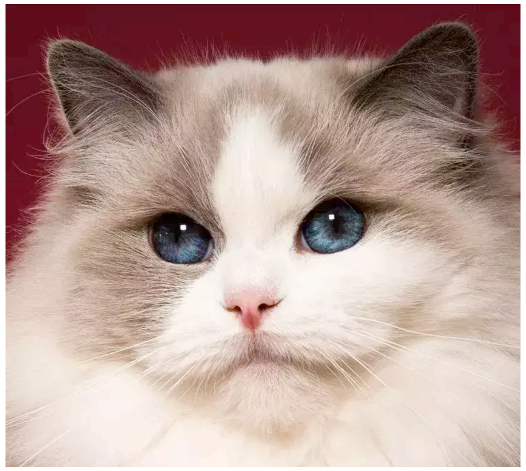

x_1 x_2 x_3

$f : \mathscr{X} \to \mathscr{Y}$

y_1 Not grumpy

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y_3 ???

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It is very common to consider a one-hot encoding $\mathscr{Y} = \{0,1\}^k$ in classification.

Supervised Learning

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Examples of classification:

- Grumpy vs. Non-grumpy cats

$\mathscr{X} = \{\text{photos of cats}\}$, $\mathscr{Y} = \{\text{grumpy}, \text{not grumpy}\}$

- E-mail spam detection

$\mathscr{X} = \{\text{your inbox}\}$, $\mathscr{Y} = \{\text{spam}, \text{not spam}\}$

- Medical diagnosis

$\mathscr{X} = \{\text{medical data}\}$, $\mathscr{Y} = \{\text{diseases}\}$

- Sentiment analysis

$\mathscr{X} = \{\text{text}\}$, $\mathscr{Y} = \{\text{positive}, \text{negative}, \text{neutral}\}$

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Examples of regression:

- Temperature prediction
$\mathscr{X} = \mathbb{R}^3, \mathscr{Y} = \mathbb{R}$

- Stock price prediction
$\mathscr{X} = \{\text{list of stocks}\}, \mathscr{Y} = \mathbb{R}_+$

- Life expectancy
$\mathscr{X} = \{\text{medical data}\}, \mathscr{Y} = \mathbb{R}_+$

- Any price, cost, income, etc. prediction.

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$$f : \mathscr{X} \to \mathscr{Y}$$

For classification, it is common to define instead:

$$f : \mathscr{X} \to [0,1]^{|\mathscr{Y}|}$$

Where $f(x)$ is a vector of class probabilities. In this case, final prediction is given by:

$$\hat{y} = \underset{k \in |\mathscr{Y}|}{\operatorname{argmax}} f(x)$$

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Two key words: correctly and learn.

Loss function

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$$\ell : \mathscr{Y} \times \mathscr{Y} \to \mathbb{R}_+$$

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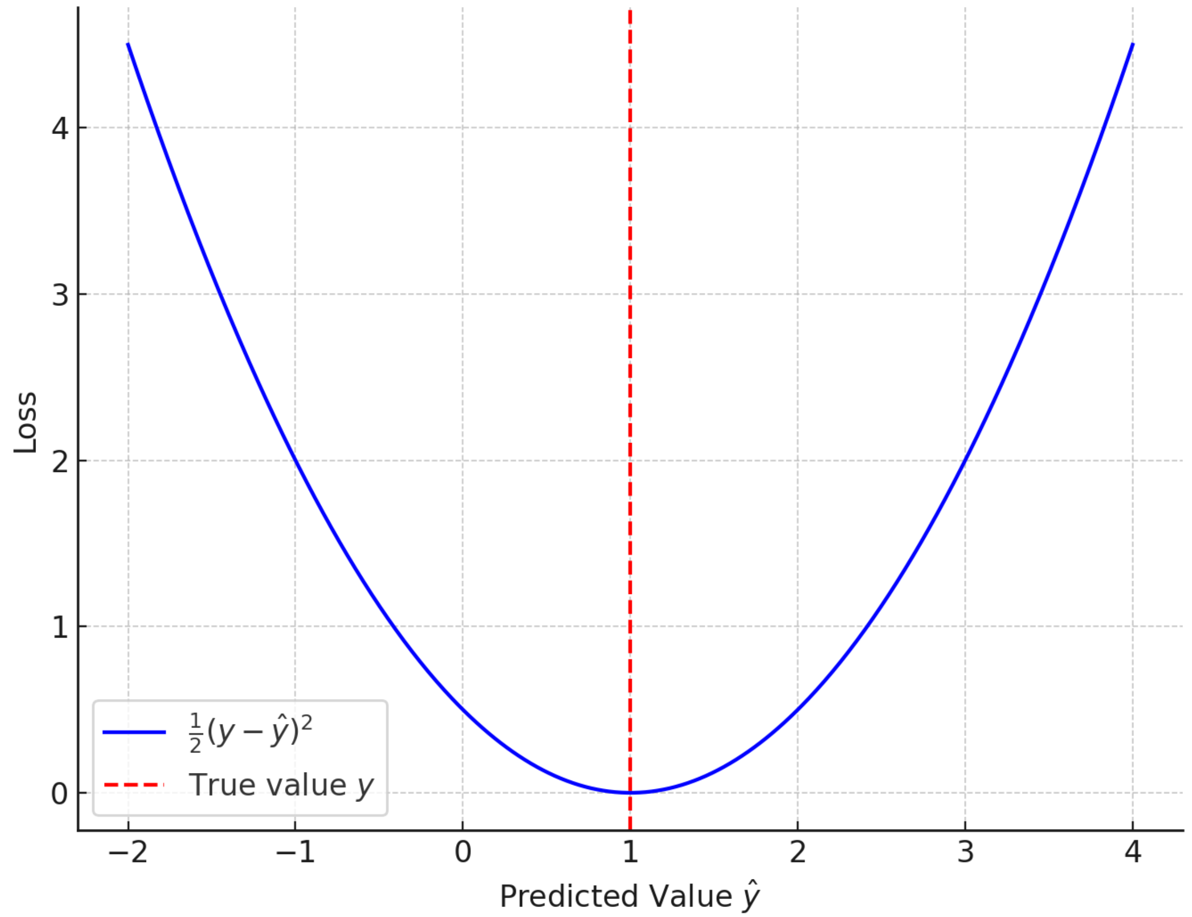
For classification this will also depend on the encoding.

Regression losses

Examples in regression:

- Square loss: $\ell(y, z) = \frac{1}{2}(y - z)^2$



Regression losses

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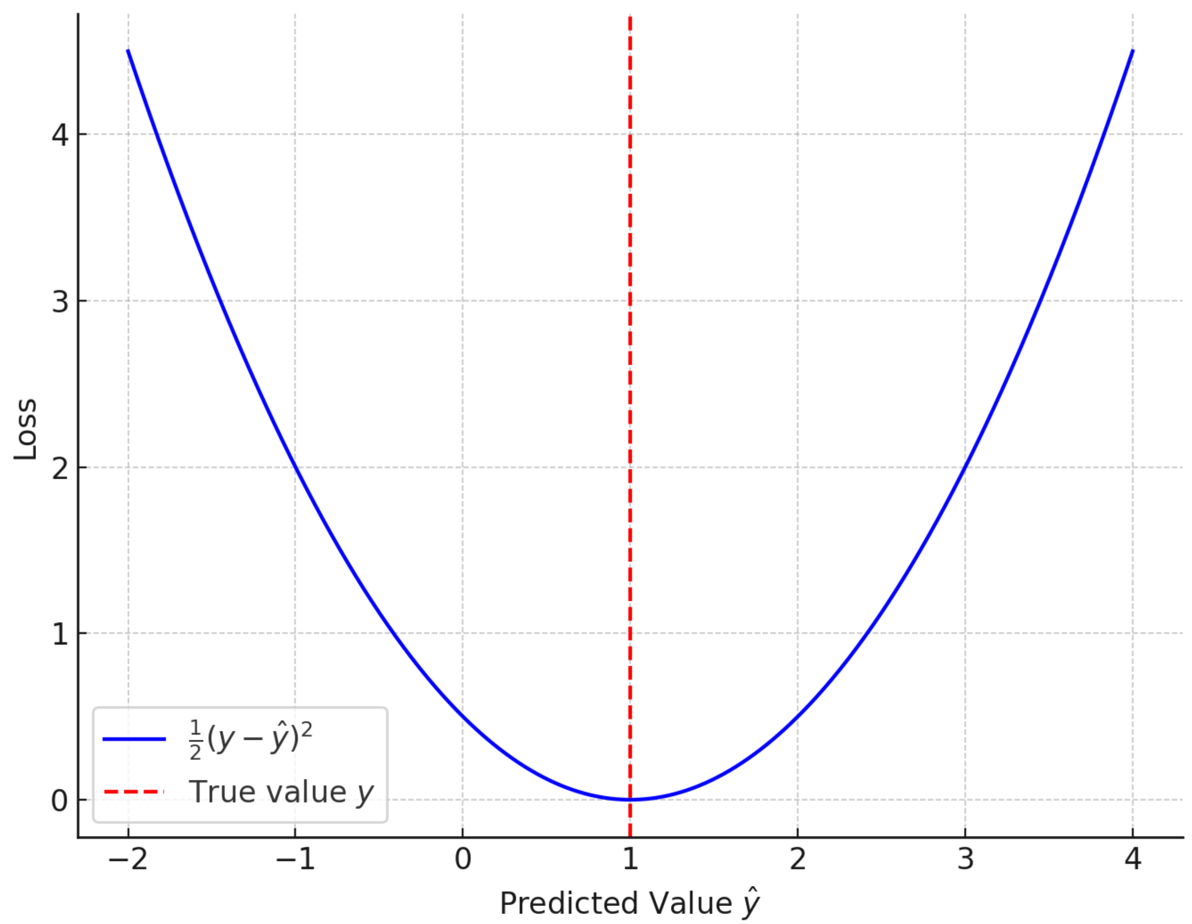
The square loss is sensitive to outliers

Exercise: show this.



Regression losses

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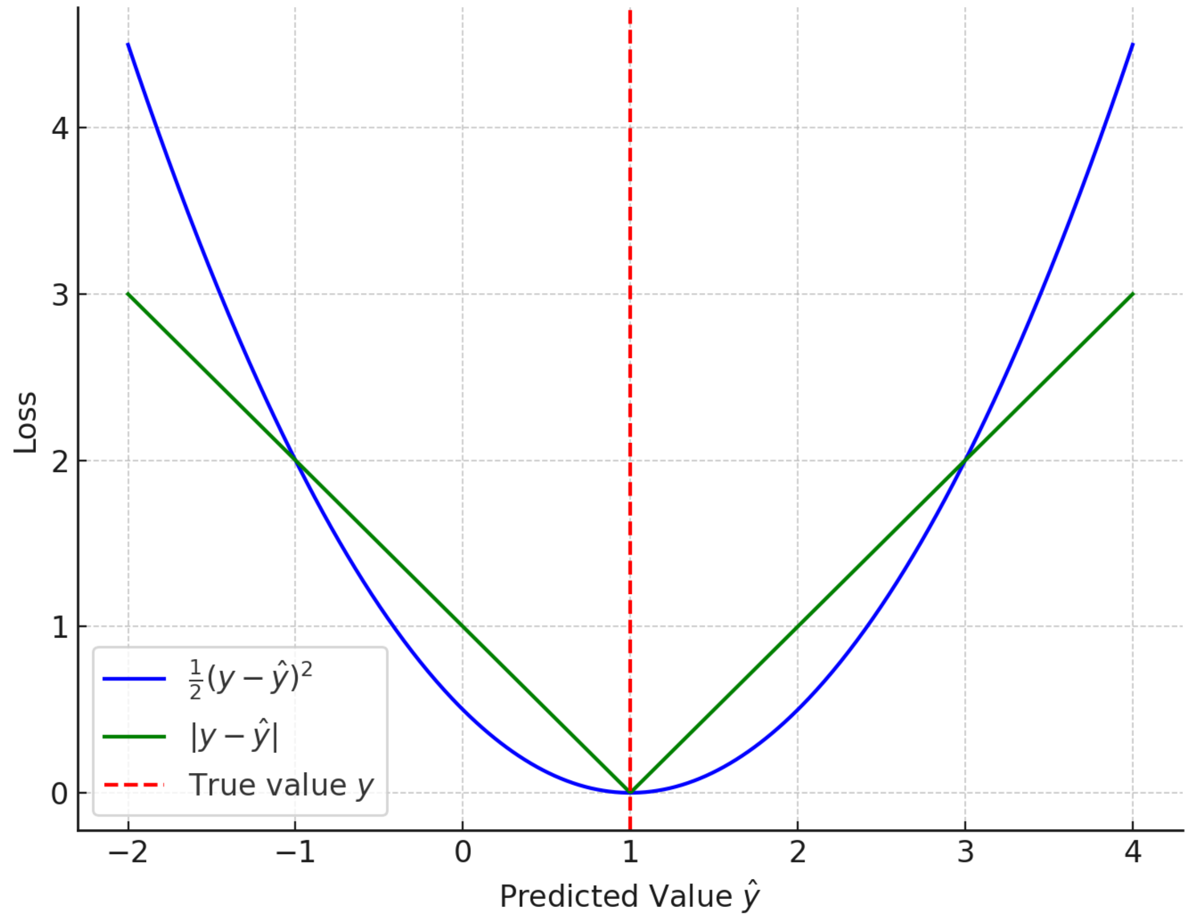
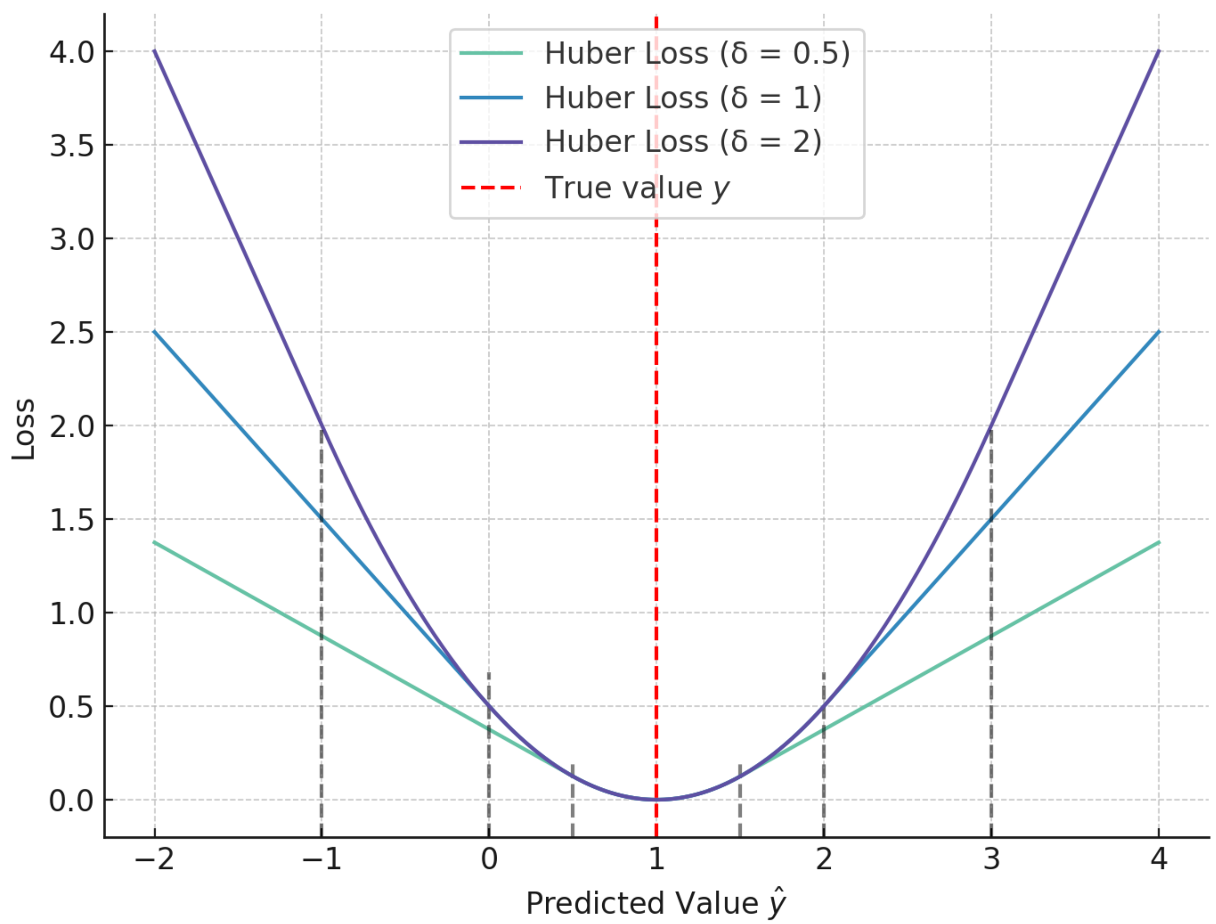
- Absolute loss: $\ell(y, z) = |y - z|$



Regression losses

Examples in regression:

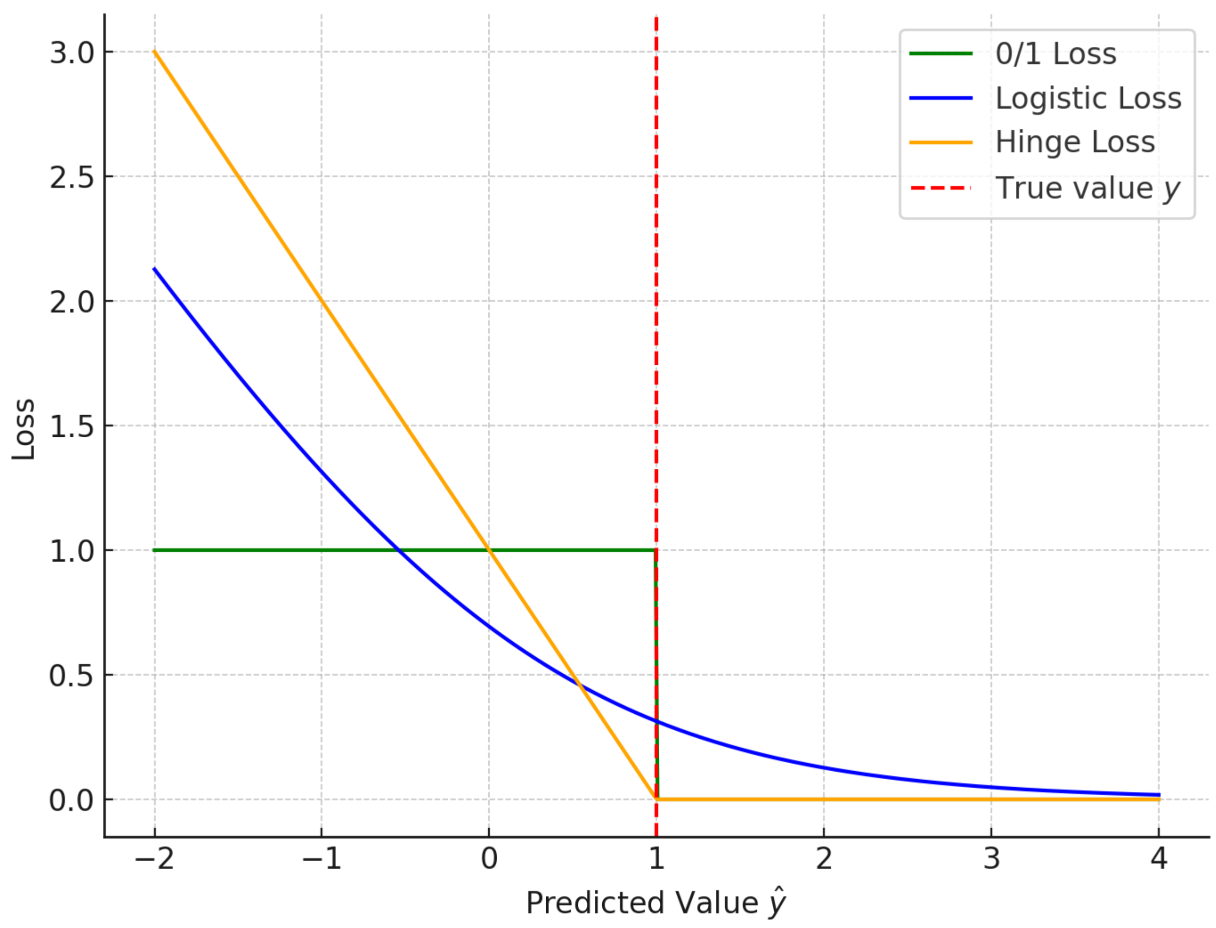
- Huber loss: $\ell_\delta(y,z) = \begin{cases} \frac{1}{2}(y-z)^2 & \text{if } ||y-z| \leq \delta \\ \delta(|y-z| - \frac{1}{2}\delta) & \text{if } |y-z| > \delta \end{cases}$



Classification losses

Examples in binary classification $\mathcal{Y} = \{-1, +1\}$:

- 0/1 loss: $\ell(y, z) = \delta_{yz}$ (or $\ell(y,z) = \theta(y - z) = \begin{cases} 1 & \text{if } y - z \le 0 \\ 0 & \text{otherwise} \end{cases}$)
- Logistic loss: $\ell(y, z) = \log(1 + e^{-yz})$
- Hinge loss: $\ell(y, z) = \max(0, 1 - yz)$



Empirical risk

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Given a loss function $\ell : \mathscr{Y} \times \mathscr{Y} \to \mathbb{R}_+$, and a predictor $f : \mathscr{X} \to \mathscr{Y}$ define the empirical risk:

$$\hat{\mathscr{R}}_n(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(x_i))$$

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Also known as the training loss. This quantifies how well we fit the data. But is this a good notion of learning?

$$f(x) = \begin{cases} y_i & \text{if } x \in \mathcal{D} \\ 0 & \text{otherwise} \end{cases} \quad \Rightarrow \quad \hat{\mathcal{R}}_n = 0$$

Probabilistic framework

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- The "i.i.d." assumption might not always hold. (Sampling bias, distribution shift, etc.)

- Under this assumption, $\hat{\mathscr{R}}_n$ is a random function.

Population risk

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$$\mathcal{R}(f) = \mathbb{E}\left[\ell(y, f(x))\right]$$

Also known as the generalisation or test error.

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$\mathcal{R}$ is a deterministic function of the predictor f

Validation set

In practice, the statistician almost never has access to the data distribution.

A common procedure to estimate $\mathscr{R}$ consists of splitting the training data in training and validation set $\mathscr{D} = \mathscr{D}_{\mathrm{T}} \cup \mathscr{D}_{\mathrm{V}}$.

Train on $\mathscr{D}_{\mathrm{T}}$, test on $\mathscr{D}_{\mathrm{V}}$.

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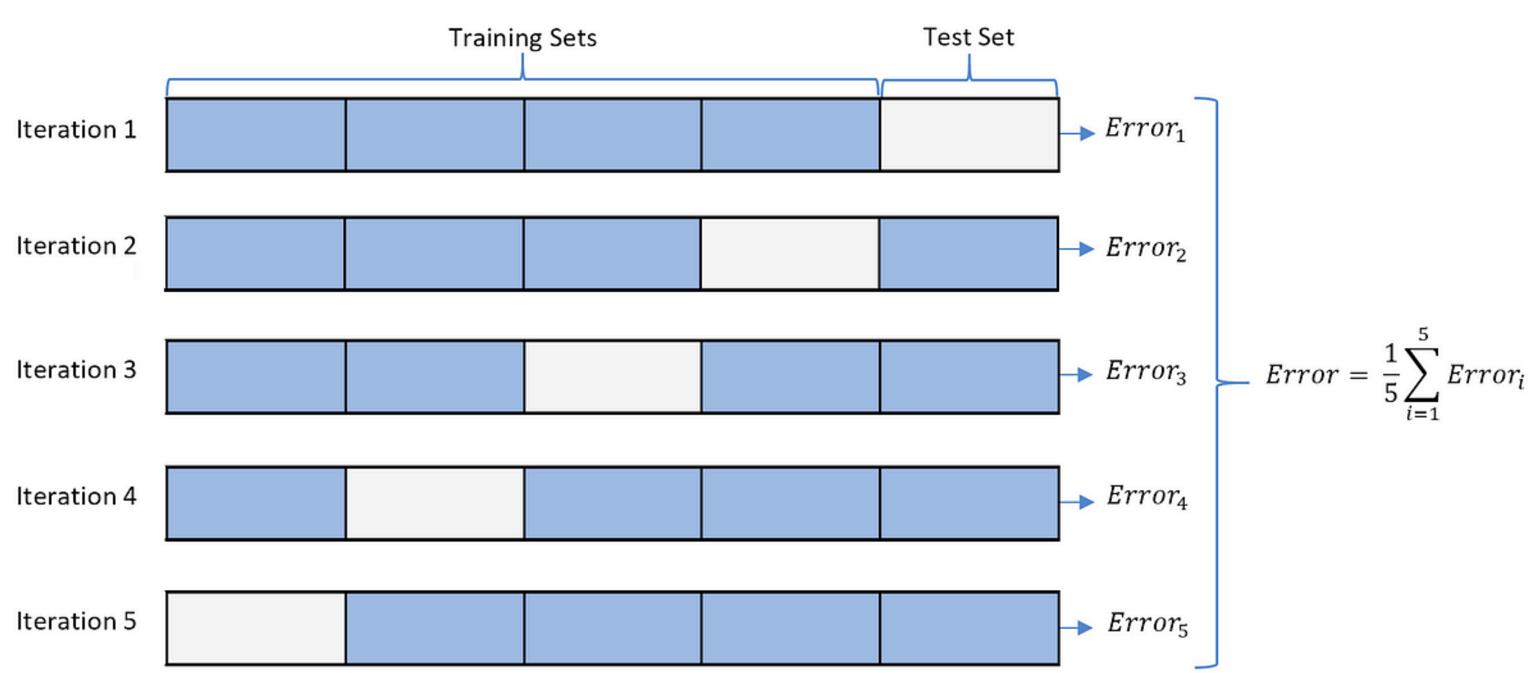
To reduce error, often one repeats this procedure k times, averaging over the result. This is known as k fold cross-validation.



Conditional risk

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$$\begin{aligned}\mathscr{R}(f) &= \mathbb{E}_{(X,Y)\sim p}[\ell(Y, f(X))] \\ &= \mathbb{E}_{X\sim p_x}\left[\mathbb{E}[\ell(Y, f(x)) \,|\, X = x]\right]\end{aligned}$$

The internal expectation is over the conditional distribution $Y | X = x$

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$$\mathcal{R}(f) = \mathbb{E}_{(X,Y)\sim p}[\ell(Y, f(X))]$$

$$= \mathbb{E}_{X\sim p_x}\left[r(z \mid X)\right] \qquad z = f(x) \in \mathcal{Y}$$

Where we have defined:

$$\boxed{r(z \mid x) = \mathbb{E}[\ell(Y, z) \mid X = x]}$$

"Conditional risk"

Bayes risk

The Bayes predictor is the best achievable predictor:

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- The Bayes predictor $f_\star$ might not be unique.
- Typically we have $\mathscr{R}_\star \neq 0$.   Examples in the TD