

Introduction to Probabilistic Machine Learning

Probability

Rainer Schlosser



Egal was ist, du kannst uns anrufen!

Wir führen unsere Gespräche wertschätzend und unvoreingenommen.
Du bleibst dabei **anonym**.

dienstags, mittwochs, donnerstags und sonntags
von 21 bis 24 Uhr
unter 0331 977 1834 oder im Chat

<https://nightline-potsdam.de>

Weitere Infos:



- **Goal:** Stimulate interest in method development for machine learning algorithms
 - We will pick the pace that helps you to get excited; please interrupt and ask questions!
- **Format:** We have one topic per week with a lecture and tutorial
 - **Lecture:** Monday, 11:00am – 12:30pm (L-E.03)
 - **Tutorial:** Tuesday: 3:15pm – 4:45pm (HS2)
- **Assignment:** Five assignments to solve them (groups of two). They account for 40% of all points (8 points each)
 - Handed out every other week on Monday (starting 2nd week, April 14)
 - Each assignment has a theory and a practice part
- **Tutorial:** Supporting the material of the lecture and the assignments
 - In the tutorial, Rainer and Alex will solve similar exercises to the assignments with you
 - They will answer questions you have with the actual assignments
- **Exam (70 points):** Counts for 60% of all points; 90-120 minutes long (**July 28**)

- **Books:** All our material and communication will happen over Moodle
 - Bishop, C. [Pattern Recognition and Machine Learning](#). Springer. 2006.
 - MacKay, D. [Information Theory, Inference, and Learning Algorithms](#). CUP. 2003
- **Moodle:** Share our lecture slides, tutorials, solutions
 - **Location:** <https://moodle.hpi.de/course/view.php?id=891>
 - **Announcements:** <https://moodle.hpi.de/mod/forum/view.php?id=30842>
- **GitHub Repository:** Supporting material as well as code samples
 - **Location:** <https://github.com/HPI-Artificial-Intelligence-Teaching/pml-sole2025>
 - If you find mistakes, please submit [issues](#) and [pull requests](#)
- **GitHub Classrooms:** Used for all our assignments
 - If you do not have a GitHub account, please create one now
 - Find a team member as assignments are solved in groups of two
 - More details tomorrow in the first tutorial

Course Structure

1. History & Probability Theory (Unit 1)
2. Inference & Decision Theory (Unit 2)
3. Graphical Models: Independence (Unit 3)
4. Graphical Models: Exact Inference (Unit 4)
5. Graphical Models: Approximate Inference (Unit 5)
6. Bayesian Ranking (Unit 6)
7. Linear Basis Function Models (Unit 7)
8. Bayesian Regression (Unit 8)
9. Bayesian Classification (Unit 9)
10. Non-Bayesian Classification (Unit 10)
11. Gaussian Processes (Unit 11)
12. Information Theory (Unit 12)
13. Real-World Applications of Probabilistic Machine Learning (Unit 13)

**Introduction to
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Learning**

Unit 1 - Probability

- 2012 developed by Jeff Bezanson, Alan Edelman, Stefan Karpinski and Viral B. Shah at MIT
- Used for numerical and scientific computing with high performance
 - Execution speed is similar to C and FORTRAN
 - Hierarchical and parameterized type system as well as method overloading („multiple dispatching“) as central concepts
 - Native calls from C-(compiled) code possible (without wrappers)
- Unicode is efficiently supported (e.g., UTF-8)
- Alongside C, C++ and FORTRAN, the only programming language that has entered the “PetaFlop Club”



Jeff Bezanson
(1981–)



Alan Edelman
(1963 –)



Stefan Karpinski
(1981–)



Viral Shah
Introduction to
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Learning

Overview

1. History of Machine Learning
2. Probability in Machine Learning
3. Probability Theory
4. Probability Distributions

**Introduction to
Probabilistic Machine
Learning**

Unit 1 - Probability

Overview

1. **History of Machine Learning**
2. Probability in Machine Learning
3. Probability Theory
4. Probability Distributions

**Introduction to
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Unit 1 - Probability

History of Machine Learning

1950: Turing Test
1957: Perceptrons
1967: Nearest Neighbors
1986: Neural Networks
1995: Support Vector Machines
2000: Graphical Models
2012: Deep Neural Networks



Alan Turing



Frank Rosenblatt



Thomas Cover



Geoffrey Hinton



Vladimir Vapnik



Michael Jordan



Yann LeCun, Geoffrey Hinton, Yoshua Bengio

**Introduction to
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Learning**

Unit 1 - Probability

Machine Learning: Definition

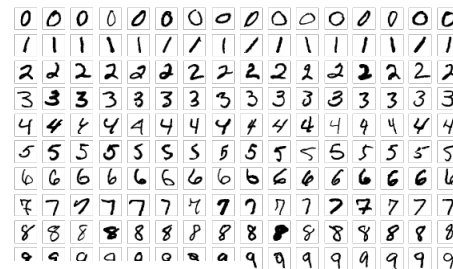
- **Tom Mitchell (1997).** *A computer program is said to **learn** from experience E with respect to some class of tasks T and performance measure P , if its performance at tasks in T , as measured by P , improves with experience E .*
 - **Performance measures** are often called *loss functions*
 - **Experience** is often called *training data*
 - **Task** is also called a *prediction* by a computer program
- **Temporal Definition.** *A computer program is said to **learn** from data D recorded **in the past** if the accuracy of predictions made **in the future** improves over time.*
 - **Accuracy:** Performance measure against which an ML algorithm is judged
 - **Past Data:** Training data
 - **Future Data:** Test data

Machine Learning: Classification

■ Task: Assigning examples to one of K pre-defined classes

□ Examples:

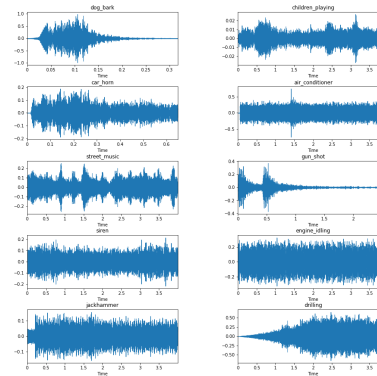
- Digits classification to 10 classes based on pixel images
- Phoneme classification
- Auto-correct models for text input



■ Performance: Cost of misclassifying an example

□ Examples:

- Symmetric loss: $l(\hat{y}, y) = \begin{cases} 1 & \hat{y} \neq y \\ 0 & \text{otherwise} \end{cases}$
- Non-symmetric loss: $l(\hat{y}, y) = C_{\hat{y}, y} \in \mathbb{R}^{K \times K}$



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Unit 1 - Probability

Machine Learning: Regression

■ **Task:** Assigning examples to a real value

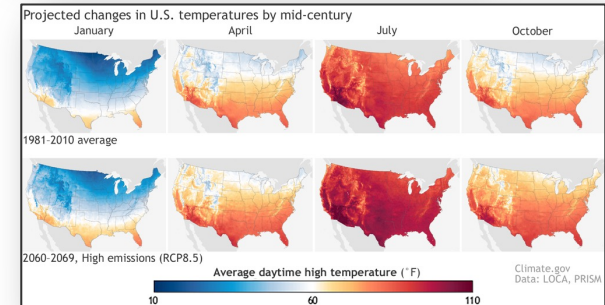
□ **Examples:**

- Price prediction of a good/service (Product Pricing)
- Temperature prediction (Weather Forecast)
- Effect of medication on health metrics (Digital Health)

■ **Performance:** Cost of missing the true target y by $\hat{\Delta} = \hat{y} - y$

□ **Examples:**

- Symmetric loss: $l(\hat{y}, y) = h(|\hat{y} - y|)$ with h being monotonic
- Non-symmetric loss: $l(\hat{y}, y) = h(\hat{y} - y)$



Overview

1. History of Machine Learning
- 2. Probability in Machine Learning**
3. Probability Theory
4. Probability Distributions

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Unit 1 - Probability

What is Probability?

- **Weather forecast:** A meteorologist says

„Tomorrow, it is going to rain in Bangalore with 60%“

- **Two interpretations:**

1. The meteorologist has analyzed all regions which have similar environmental conditions than Bangalore today. His **(objective)** estimate based on past data is that the procedure which predicts rain tomorrow is correct 60% of the time.
2. The meteorologist *believes* that it is more likely that it rains tomorrow in Bangalore (than it is to not rain tomorrow). 60% is the quantification of the **(subjective)** belief of the meteorologist.



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Unit 1 - Probability

Frequentist vs. Subjectivist Interpretation

■ Frequentist Interpretation

- Probability is a property of the event ("it rains tomorrow in Bangalore")
- Is operationalized by repeated experiments
- Typically used by scientists and engineers

■ Subjective Interpretation

- Probability is an expression of belief of the person that makes a statement
- Is subjective and people-dependent: Two people with identical data can come to different probabilities
- Typically used by philosophers and economists

1. Probability is not a physical measure but a thought model for randomness!
2. The mathematical rules for probability are **identical** for both interpretations!

History of Probability

■ BC:

- Chance games were highly popular in ancient Greece & Rome
- No mathematical analysis of chance (missing algebraic framework)



■ 16th century:

- Girolamo Cardano published first book on methods to calculate the probability of card games and game of dice



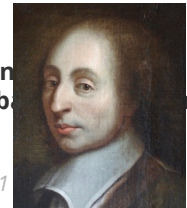
Gerolamo Cardano
(1501 – 1575)

■ 17th century:

- Pierre de Fermat und Blaise Pascal exchange important questions about probability and motivate the first scientific studies of probability



Pierre de Fermat
(1607 – 1665)



Blaise Pascal
(1623 – 1662)

In
Prob
ne
Unit 1

History of Probability (ctd)

■ 18th century:

- Jacob Bernoulli investigates random coin tosses and proves the Law of Large Numbers
- Thomas Bayes investigates conditional probabilities and formulates Bayes' rule (published post-hum)
- Abraham de Moivre introduces the normal distribution as the limit distribution of an infinite sum of Bernoulli random variables (weak form of central limit theorem)



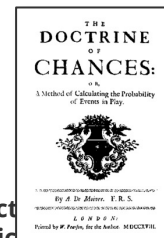
Jacob Bernoulli
(1655 – 1705)



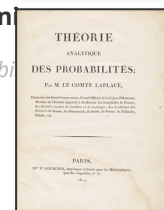
Thomas Bayes
(1701 – 1761)



Abraham de Moivre
(1667 – 1754)



Pierre-Simon Laplace
(1749 – 1827)



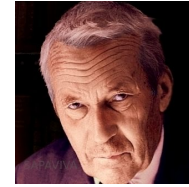
■ 19th century:

- Carl Friedrich Gauss introduces the least-square method and proves that the distribution of independent random variables converges to a normal distribution
- Pierre-Simon Laplace publishes *Théorie analytique des probabilités* where he united probability theory and statistics and introduces hypothesis tests

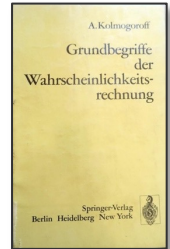
History of Probability (ctd)

■ 20th century:

- Andrey Kolmogorov introduces three axioms that imply the rules of probability theory for relative frequencies (frequentist interpretation)
- Richard Threlkeld Cox introduces three (other) axioms that imply the rules of probability theory for degrees of belief (subjectivist interpretation)



Andrey Kolmogorov
(1903 – 1987)



■ 21st century:

- **1974:** Vladimir Vapnik introduces probability theory as the foundation of the theory of machine learning
- **1980:** Judea Pearl and Phil Dawid introduce graphical models that allow to operationalize probability theory for complex and causal processes
- **2000:** Probability theory and statistics enter every aspect of modern science and artificial intelligence



Richard Threlkeld Cox
(1898 – 1991)



Vladimir Vapnik
(1936 –)



Judea Pearl
(1936 –)



Philip Dawid
(1946 –)

Rules of Probability

- **Mathematical Definition.** A number $P(A) \in [0,1]$ assigned to an event or statement A that indicates how likely A is to occur.
- **Set Theory.** We model events and statements via set theory and assume
 - A countably infinite total set $\Omega \supseteq A$
 - If $A(x)$ is a 1st order logic statement, then $A := \{x \mid A(x)\}$ and
 - $A \subseteq B \equiv \forall x: A(x) \rightarrow B(x)$ and $A^c \equiv \forall x: \neg A(x)$
 - $A \cup B \equiv \forall x: A(x) \vee B(x)$ and $A \cap B \equiv \forall x: A(x) \wedge B(x)$
- **Rules:** For all $A, B \subseteq \Omega$
 - **Monotonicity:** If $A \subseteq B$ then $P(A) \leq P(B)$
 - **Complement Rule:** $P(A^c) = 1 - P(A)$
 - **Sum Rule:** $P(A \cup B) = P(A) + P(B) - P(A \cap B)$
 - **Product Rule:** $P(A \cap B) = \underbrace{\frac{P(A \cap B)}{P(B)}}_{P(A|B)} \cdot P(B)$

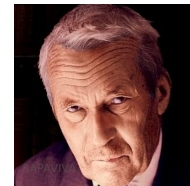
Frequentist vs. Subjective Probabilities

- **Kolmogorov (1933):** *The rules of probability for **sets** follow from the following 3 axioms*

1. $P(A) \geq 0$ for all $A \subseteq \Omega$
2. $P(\Omega) = 1$
3. $P(\cup_i A_i) = \sum_i P(A_i)$ if for all $i \neq j: A_i \cap A_j = \emptyset$

- **Cox (1944):** *The rules of probability for **logic** follow from the following 3 axioms*

1. $P(A) \in [0,1]$ for all logical statements A
2. $P(A)$ is independent of how the statement is represented
3. If $P(A|C') > P(A|C)$ and $P(B|A \wedge C') = P(B|A \wedge C)$ then
$$P(A \wedge B|C') \geq P(A \wedge B|C)$$



Andrey Kolmogorov
(1903 – 1987)



Richard Threlkeld Cox
(1898 – 1991)

Introduction to
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Learning

Unit 1 - Probability

The Role of Probability in Machine Learning

- **Theory:** *How likely is it, that the accuracy of a predictor $\mathcal{A}(D)$ learned from training data D is small?*

$$P(\text{Accuracy}(\mathcal{A}(D)) < \varepsilon) \leq \delta$$

- **Typical Assumptions**

1. Independent identically distributed data (IID)
2. Accuracy is an expected performance measure on the next test example

- **Frequentist view on probability:**
Over N applications of the learning algorithm and draws of random training data D , for how many is the learned predictor accurate?

- **Practice:** *What can we say about the plausibility of a single predictor f in light of training data D ?*

$$P(f|D)$$

- **Typical Assumptions**

- Independent identically distributed data (IID)
- Known conditional dependence of data and predictor

- **Subjectivist view on probability:**
Given the certain and known training data, what is the remaining uncertainty over the right predictor for (future) data?

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Unit 1 - Probability

Overview

1. History of Machine Learning
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- 3. Probability Theory**
4. Probability Distributions

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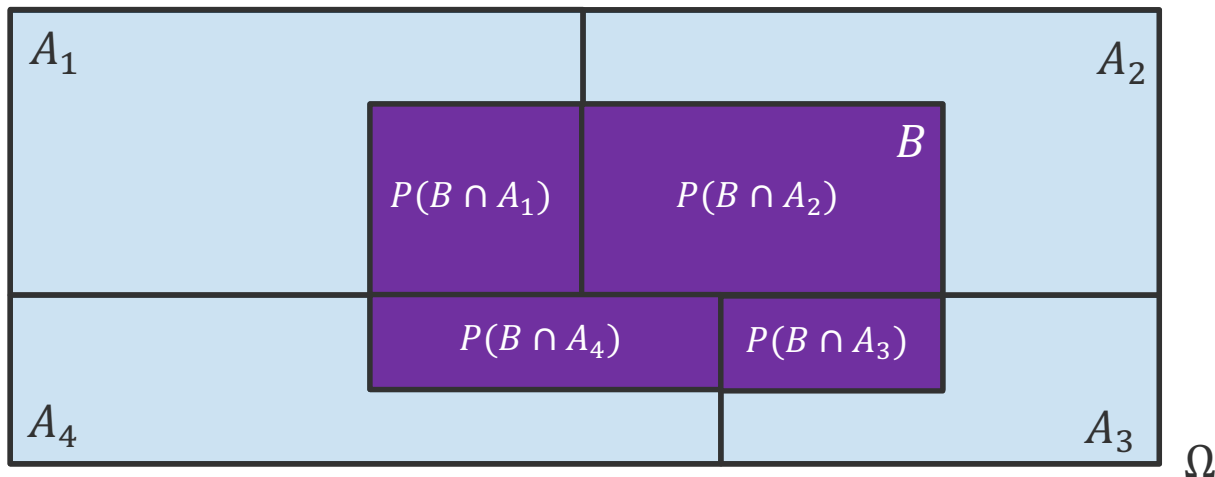
Unit 1 - Probability

Probability Theory: Law of Total Probability

- **Total Probability Theorem.** Let $A_1, A_2, \dots, A_n \subseteq \Omega$ be disjoint events that form a partition of the sample space Ω and $P(A_i) > 0$ for all A_i . Then, for any event $B \subseteq \Omega$

$$P(B) = \sum_{i=1}^n P(B \cap A_i) = \sum_{i=1}^n P(B|A_i) \cdot P(A_i)$$

- **Geometric Proof**



Probability Theory: Bayes Rule

- **Bayes' Theorem.** Let A_1, A_2, \dots, A_n be disjoint events that form a partition of the sample space S and $P(A_i) > 0$ for all A_i . Then, for any event B with $P(B) > 0$

$$P(A_i|B) = \frac{P(B|A_i)P(A_i)}{P(B)} = \frac{P(B|A_i)P(A_i)}{\sum_{j=1}^n P(B|A_j) \cdot P(A_j)}$$

law of total probability

- **Proof.** Follows from the definition of conditional probability and “multiply-by-1”

$$P(A_i \cap B) \cdot \frac{P(B)}{P(B)} = P(A_i \cap B) \cdot \frac{P(A_i)}{P(A_i)} = 1 \text{ (by definition } P(A_i) > 0 \text{ and } P(B) > 0)$$

$$P(A_i|B) \cdot P(B) = P(B|A_i) \cdot P(A_i) \text{ by definition of conditional probability}$$

$$P(A_i|B) = \frac{P(B|A_i)P(A_i)}{P(B)}$$

- **Simplified view** when looking at the probabilities as functions of A_i

$$P(A_i|B) \propto P(B|A_i) \cdot P(A_i)$$

posterior likelihood prior



(Rev) Thomas Bayes
(1701 – 1761)

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Unit 1 - Probability

Bayes Rule: False-Positive Puzzle

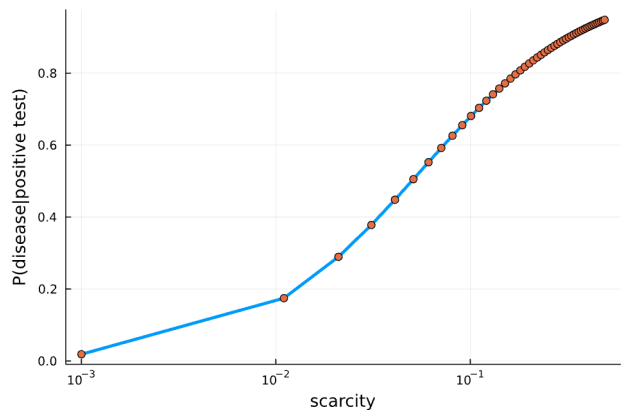
- **Situation:** A test for a rare disease is assumed to be correct 95% of the time (i.e., the probability that the test shows the disease or lack thereof is 95%). It's a rare disease that occurs in 0.1% of the population. If you have a positive test outcome, what is the probability that you have the disease?
- **Solution:**

A = "Person has the disease"

B = "Test result is positive"

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B|A) \cdot P(A) + P(B|\neg A) \cdot P(\neg A)}$$

$$P(A|B) = \frac{0.95 \cdot 0.001}{0.95 \cdot 0.001 + 0.05 \cdot 0.999} \approx 0.0187$$



Unit 1 - Probability

- **Counterintuitive:** According to *The Economist* (February 20, 1999), 80% of leading American hospital staff guessed the probability to be 95%!

Probability Theory: Independence

- **Independence.** We say that the events A_1, A_2, \dots, A_n are independent if

$$P\left(\bigcap_{i \in I} A_i\right) = \prod_{i \in I} P(A_i), \quad \text{for all subsets } I \text{ of } \{1, \dots, n\}$$

- **Intuition.** Knowledge of an event A with $P(A) > 0$ does not provide information about the probability of an independent event B

$$P(B|A) = P(B) \Leftrightarrow P(B|A) \cdot P(A) = P(B) \cdot P(A)$$

$$= P(B \cap A)$$

- **Important modelling assumption** (often implicitly) used in machine learning when making assumptions about training and test data generation: knowing one training example provides no information about the probability of any other training example (realistic?!)
- **Counterintuitive geometry:** If A and B are disjoint, they are **not** independent!

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Unit 1 - Probability

Probability Theory: Random Variable

- **Random Variable.** *A random variable is a real-valued function of the outcome of the experiment. A function of a random variable defines another random variable.*
 - **Examples:**
 - Tossing a coin N times, the **number** of heads
 - Given an image, the **pixel intensity** of the top-left pixel (in 8-bit)
- **Probability Mass Function.** *The probability mass function $p(x)$ assigns each value x the probability that the random variable takes the value x .*
 - **Example:** Coin toss: If $N = 2$ then

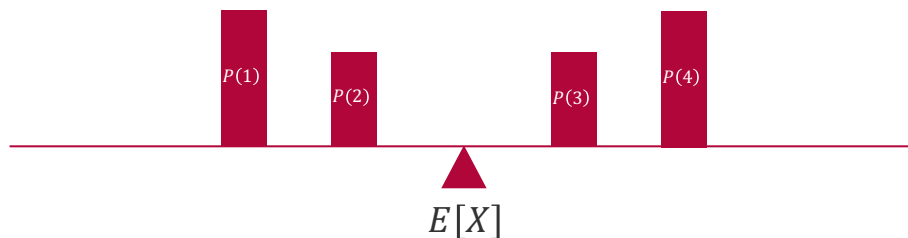
$$\begin{aligned}p(0) &= P(\text{tail, tail}) \\p(1) &= P(\text{head, tail}) + P(\text{tail, head}) \\p(2) &= P(\text{head, head})\end{aligned}$$

Probability Theory: Expectation and Variance

- **Expected Value.** The expected value $E[X]$ (also called expectation) of a random variable X is defined by

$$E[X] := \sum_x x \cdot p(x)$$

- **Intuition.** Center of gravity when placing the weight $p(x)$ at position x on a straight line



- **Variance.** The variance $\text{var}[X]$ of a random variable X is defined by

$$\text{var}[X] := \sum_x (x - E[X])^2 \cdot p(x) = E[(X - E[X])^2]$$

Overview

1. History of Machine Learning
2. Probability in Machine Learning
3. Probability Theory
4. **Probability Distributions**

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Unit 1 - Probability

Probability Distributions

- Only defined for **random variables**, *not* for events of logic statements!
 - **Discrete random variables:** $p: \mathbb{Z} \mapsto [0,1]$ and $\sum_x p(x) = 1$
 - **Continuous random variables:** $p: \mathbb{R} \mapsto \mathbb{R}^+$ and $\int p(x)dx = 1$
 - Note that, by definition, they are only a **model** for real data!
- In computational statistics some classes of probability distributions have emerged whose distributions can be fully described with a small number of parameters $\theta \in \mathbb{R}^d$
 - **Advantages:**
 1. **Storage Efficiency:** Only d real numbers for whole function!
 2. **Compute Efficiency:** Only $O(d)$ computation for rules of probability!
 - **Disadvantages:**
 1. Too restrictive to represent true phenomena in real data
 2. Function classes often not closed under Bayes' rule

Bayes' Rule for Random Variables

$$p(\theta|x) = \frac{p(x|\theta) \cdot p(\theta)}{p(x)}$$

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Probability Distributions: Bernoulli

- **Bernoulli Distribution.** A random variable which only takes the values 0 and 1 is said to have a Bernoulli distribution parameterized by the probability π of the outcome 1

$$p_X(k) = \begin{cases} \pi & \text{if } k = 1 \\ 1 - \pi & \text{if } k = 0 \end{cases}$$

- **Machine Learning:** Distribution that is used for modelling classes of objects
- **Properties:**

$$E[X] = \pi$$

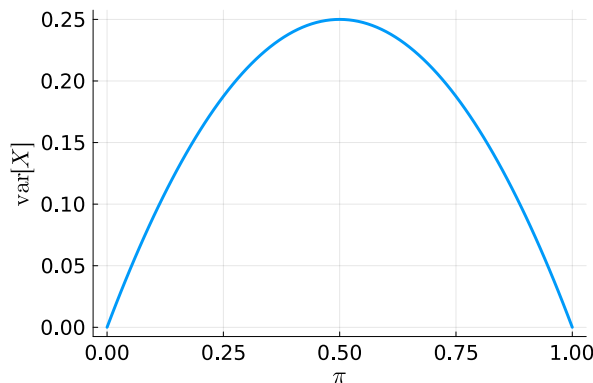
$$\text{var}[X] = \pi \cdot (1 - \pi)$$

- In **machine learning**, the parameter π is often **parameterized** by a function of the inputs x

$$\text{sigmoid}(f(x)) := \frac{\exp(f(x))}{1 + \exp(f(x))}$$



Jacob Bernoulli
(1655 – 1705)

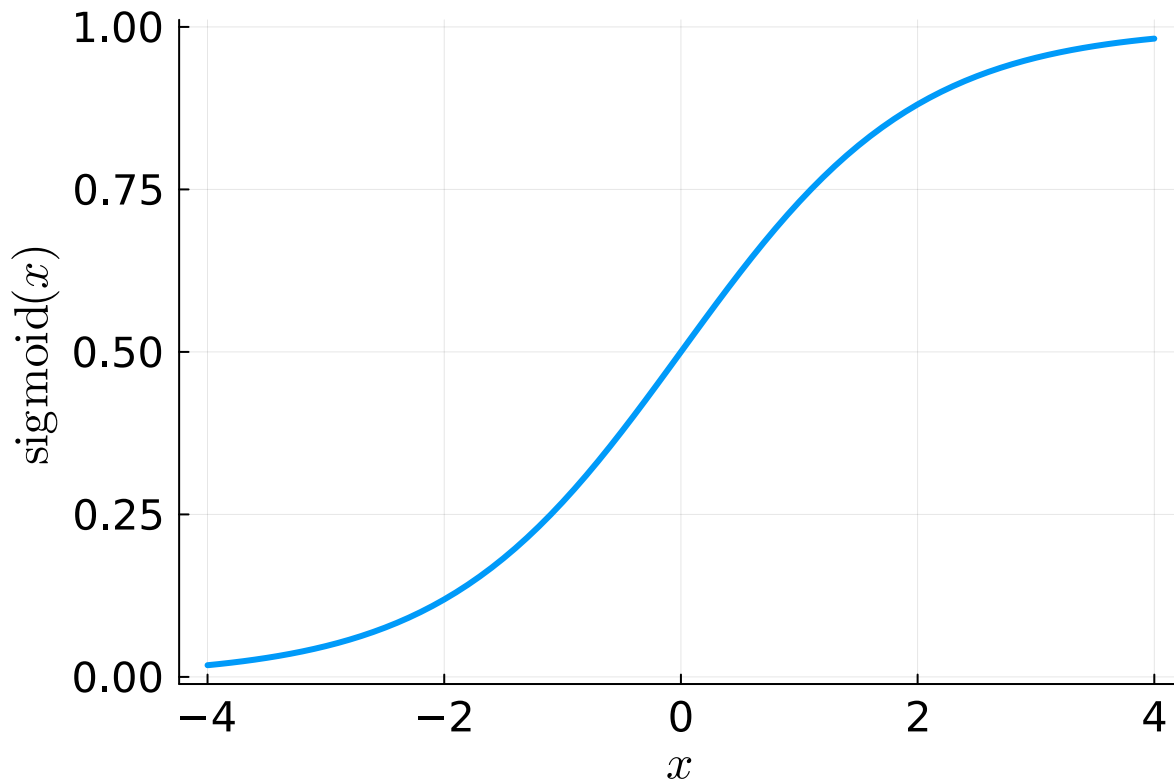


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Probability Distributions: Logistic Function $\text{sigmoid}(x)$

$$\text{sigmoid}(x) := 1 - \text{sigmoid}(-x)$$



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Probability Distributions: Binomial Distribution

- **Binomial Distribution.** *The sum of n independent Bernoulli random variables with the same success probability π has a Binomial distribution with*

$$\forall k \in \{0, 1, \dots, n\}: \quad p_X(k) = \binom{n}{k} \pi^k (1 - \pi)^{n-k}$$

- **Rarely** used in Machine Learning practice but in Machine Learning theory (for modelling the distribution of the *number* of prediction errors)

- **Properties:**

$$E[X] = n \cdot \pi$$
$$\text{var}[X] = n \cdot \pi \cdot (1 - \pi)$$



Jacob Bernoulli
(1655 – 1705)

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Probability Distributions: Normal

- **Normal Distribution.** A continuous random variable X is said to have a standard normal distribution if the density is given by

$$p(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$

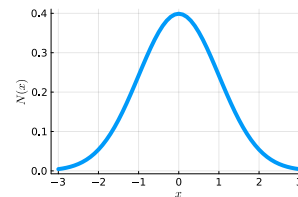
- **Properties:**

$$E[X] = \mu$$
$$\text{var}[X] = \sigma^2$$

- **Importance.** The Normal distribution plays a fundamental role in ML!
 - **Data Modelling:** The limit distribution for the sum of a large number of independent and identically distributed random variables.
 - **Machine Learning:** The most common belief distribution for the parameters of prediction functions!
 - **Information Theory:** The distribution function with the most uncertainty ("entropy") when fixing mean and variance of the random variable.



Carl Friedrich Gauss
(1777 - 1855)



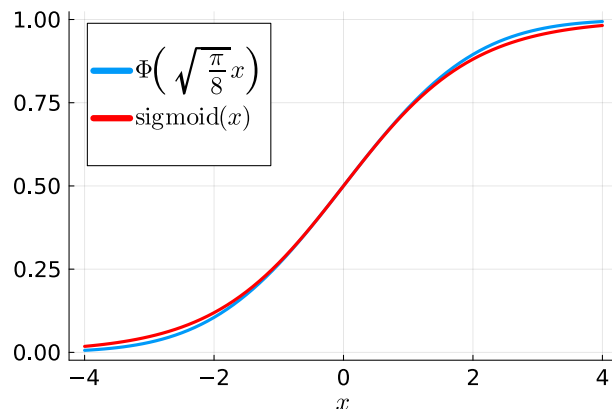
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Probability Distribution: Normal (ctd)

- **Cumulative Density Function (CDF).** The Normal CDF is defined by

$$\Phi(x; \mu, \sigma^2) := \int_{-\infty}^x \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(t - \mu)^2}{2\sigma^2}\right) dt$$



Milton Abramowitz
(1915 – 1958)



Irene Stegun
(1919 – 2008)

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Unit 1 - Probability

- Approximation using the Erf function: $\Phi(x) = \frac{1 + \text{Erf}(x/\sqrt{2})}{2}$ (Erf function is implemented in many math libraries)

- **Numerical Recipes.** $\text{Erf}(x) \approx 1 - t \cdot \exp(-x^2 + \sum_{i=0}^9 a_i t^i)$, $t = \left(1 + \frac{1}{2}|x|\right)^{-1}$

■ History of Machine Learning

- Machine learning is a 70-year-old field of research
- Key step in artificial intelligence improving on a task based on data

■ Probability in Machine Learning

- Probability is not a physical quantity but a mathematical model of uncertainty
- Two different axiomatic justifications of the same math: one for data and one for parameters!

■ Probability Theory

- Two key rules of probability theory: (1) Total probability rule and (2) Bayes' rule
- Independence is a concept of probability; it does not require random variables!
- A random variable is a real-valued function of the outcome of the experiment

■ Probability Distributions

- The Bernoulli distribution with a sigmoid link function is key for classification learning
- The normal distribution is centrally important in probabilistic machine learning

See you next week!