# Advanced Probabilistic Machine Learning

Ralf Herbrich, Rainer Schlosser

## Probability Theory

# Course Setup



- **Goal**: Enabled you to develop machine learning algorithms from scratch
  - 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**: Tuesday, 9:15am – 10:45am (HS2)
  - **Tutorial**: Wednesday: 3:15pm – 4:45pm (HS3)
- **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, October 20)
  - Each assignment has a theory and a practice part
- **Tutorial**: Supporting the material of the lecture and the assignments
  - In the tutorial, Rainer will solve similar exercises to the assignments with you
  - We will answer questions you have with the actual assignments
- **Exam (60 points)**: Counts for 60% of all points; 120 minutes long (**February 24**)

# Course Material

- **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=982
  - **Announcements**: https://moodle.hpi.de/mod/forum/view.php?id=33393
- **GitHub Repository**: Supporting material as well as code samples
  - **Location**: https://github.com/HPI-Artificial-Intelligence-Teaching/pml-wise2025
  - 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



**Foundation**

1. Probability Theory (Unit 1)
2. Linear Algebra (Unit 2)

**Methods**

3. Graphical Models (Unit 3)
4. Exact Inference (Unit 4)
5. Approximate Inference: Expectation Propagation (Unit 5)
6. Approximate Inference: Variational Inference (Unit 6)
7. Approximate Inference: Mixture Models (Unit 7)
8. Approximate Inference: Message Approximation (Unit 8)

**Applications**

8. Text: Topic Models (Unit 9)
9. Images: Conditional Markov Random Fields (Unit 10)
10. Policies: Reinforcement Learning (Unit 11)

# Julia

- 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**

# Overview

1. Probability in Machine Learning
2. Probability Theory
3. Exponential Family Distributions

# Overview

1. **Probability in Machine Learning**
2. Probability Theory
3. Exponential Family Distributions

# 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.

# 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!

# 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 $\mathrm{A} := \{x \mid A(x)\}$ and
    - $\mathrm{A} \subseteq \mathrm{B} \equiv \forall x: A(x) \rightarrow B(x)$ and $\mathrm{A}^c \equiv \forall x: \neg A(x)$
    - $\mathrm{A} \cup \mathrm{B} \equiv \forall x: A(x) \vee B(x)$ and $\mathrm{A} \cap \mathrm{B} \equiv \forall x: A(x) \wedge B(x)$
- **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**: $P(A \cap B) = \underbrace{\frac{P(A \cap B)}{P(B)}}_{P(A|B)} \cdot P(B)$

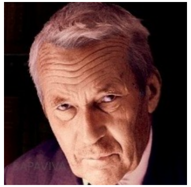
Advanced Probabilistic Machine Learning

*Unit 1 – Probability Theory*

# 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. $P(\bigcup_i A_i) = \sum_i P(A_i)$ *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)**

# The Role of Probability in Machine Learning

HPI Hasso Plattner Institut
Digital Engineering · Universität Potsdam

Objective probability over the repeated draw of training sets $D$

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

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

- **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 $D$?*

$$\boxed{P}(f\,|D)$$

Subjective belief that $f$ is the right predictor given $D$

- **Typical Assumptions**
  1. Independent identically distributed data (IID)
  2. Known conditional dependence of data and predictor
- **Subjectivist view on probability**: Given the certain and known training data $D$, what is the remaining uncertainty over the right predictor for (future) data?

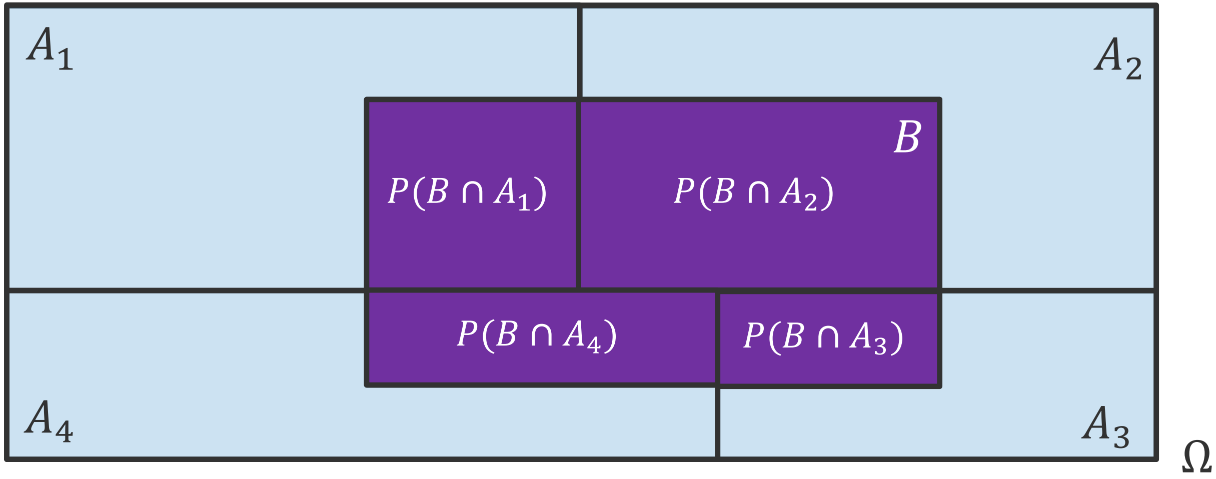
# Overview

# 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 $\Omega$ 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 $P(B) > 0$*

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

law of total probability

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

$$P(A_i \cap B) \cdot \boxed{\frac{P(B)}{P(B)}} = P(A_i \cap B) \cdot \boxed{\frac{P(A_i)}{P(A_i)}}$$

=1 (by definition $P(A_i) > 0$ and $P(B) > 0$)

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

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 $A_i$

$$\underbrace{P(A_i|B)}_{\text{posterior}} \propto \underbrace{P(B|A_i)}_{\text{likelihood}} \cdot \underbrace{P(A_i)}_{\text{prior}}$$

**posterior** **likelihood** **prior**

(Rev) Thomas Bayes
(1701 – 1761)

# Bayes Rule: False-Positive Puzzle

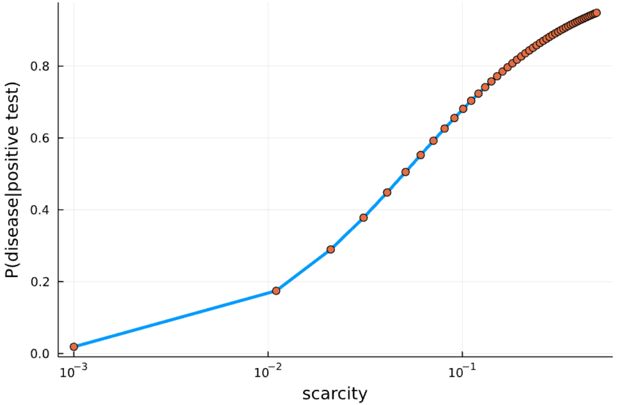
- **Situation**: A test for a rare disease is assumed to be correct 95% of the time (i.e., the probability that the test shows the disease or lack thereof is 95%). It's a rare disease that occurs in 0.1% of the population. If you have a positive test outcome, what is the probability that you have the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

$$A = \text{"Person has the disease"}$$

$$B = \text{"Test result is positive"}$$

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

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




- **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*

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

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

$= P(B \cap A)$

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

- **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!

# 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

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

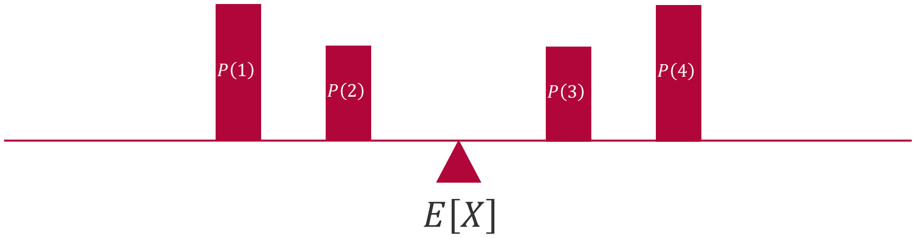
# Probability Theory: Expectation and Variance



- **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* $\mathrm{var}[X]$ *of a random variable* $X$ *is defined by*

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

# Overview

1. Probability in Machine Learning
2. Probability Theory
3. **Exponential Family Distributions**

# Probability Distributions

- Only defined for **random variables**, *not* for events or 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 $\int p(x)\, \mathrm{d}x = 1$
    - 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 $\boldsymbol{\theta} \in \mathbb{R}^d$
  - **Advantages**:
    1. **Storage Efficiency**: Only $d$ real numbers for whole function!
    2. **Compute Efficiency**: Only $O(d)$ computation for rules of probability!
  - **Disadvantages**:
    1. **Real World**: Too restrictive to represent true phenomena in real data
    2. **Bayes' Rule**: Function classes often not closed under Bayes' rule

# Efficient Bayes' Rule

- **Bayes' rule** over random variables $X$ and $Y$

$$p(x|y) = \frac{p(y|x) \cdot p(x)}{p(y)} = \underbrace{\frac{1}{p(y)} \cdot \left[\int p(y|x)\,\mathrm{d}x\right]}_{\text{Normalization constant independent of } x} \cdot \underbrace{\left[\frac{p(y|x)}{\int p(y|x)\,\mathrm{d}x}\right]}_{\text{Probability distribution } p_y(\cdot) \text{ over } x} \cdot \underbrace{p(x)}_{\text{Probability distribution } p(\cdot) \text{ over } x}$$

- **Idea**: If $p(y|x)$ and $p(x)$ are exponentials of a linear function of transformation of $x$ then (up to normalization), the product becomes a linear operation!

$$p(y|x) \propto \exp\left(\boldsymbol{\theta}_y^{\mathrm{T}} \cdot \boldsymbol{T}(x)\right)$$

$$p(x) \propto \exp\left(\boldsymbol{\theta}^{\mathrm{T}} \cdot \boldsymbol{T}(x)\right)$$

$$\Rightarrow \quad p(x|y) \propto \exp\left(\underbrace{\left[\boldsymbol{\theta}_y + \boldsymbol{\theta}\right]^{\mathrm{T}}}_{\text{Product in distribution becomes addition!}} \cdot \boldsymbol{T}(x)\right)$$

# Exponential Family

- **Exponential Family Distribution**. *A distribution* $p(\cdot\,|\boldsymbol{\theta})$ *over a random variable* $X$ *is called an* exponential family distribution *if it can be expressed as follows:*

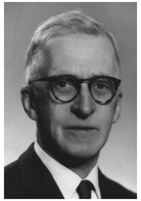
$$p(x|\boldsymbol{\theta}) = \exp\left(\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{T}(x) - A(\boldsymbol{\theta})\right)$$

*where* $\boldsymbol{\theta}$ *is called the* natural parameters *of the distribution,* $\boldsymbol{T}(\cdot)$ *is called the* sufficient statistics *and* $A(\boldsymbol{\theta})$ *is the* log-normalization *given by*

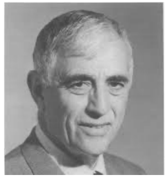
$$A(\boldsymbol{\theta}) = \log\left(\int \exp\left(\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{T}(x)\right)\, \mathrm{d}x\right)$$

- Every discrete probability distribution over the outcome $x \in \{1, \dots, K\}$ is an exponential family distribution with

$$\boldsymbol{\theta} = \begin{bmatrix} \log\left(p(1)\right) \\ \vdots \\ \log\left(p(x-1)\right) \\ \log\left(p(x)\right) \\ \log\left(p(x+1)\right) \\ \vdots \\ \log\left(p(K)\right) \end{bmatrix} \qquad \boldsymbol{T}(x) = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$


Edwin J. G. Pitman
(1897 – 1993)


Georges Darmois
(1888 - 1960)


Bernhard O. Koopman
(1900 – 1981)

# Exponential Family Distributions: Categorical Distribution

HPI Hasso Plattner Institut
Digital Engineering · Universität Potsdam

- **Categorical Distribution**. *Given* $\boldsymbol{\eta} \in \mathbb{R}^K$ *or a probability vector* $\boldsymbol{\pi} \in [0,1]^K$ *such that* $\sum_{k=1}^{K} \pi_k = 1$ *, a discrete random variable* $X$ *over the first* $K$ *unit vectors is said to have a categorical distribution if the density is given by*

$$\mathcal{C}(\boldsymbol{x}; \boldsymbol{\eta}) = \frac{\exp\left(\boldsymbol{\eta}^{\mathrm{T}} \boldsymbol{x}\right)}{\sum_{k=1}^{K} \exp(\eta_k)} \qquad \mathrm{Cat}(\boldsymbol{x}; \boldsymbol{\pi}) = \boldsymbol{\pi}^{\mathrm{T}} \boldsymbol{x}$$

- **Properties**:

$$E[X_i] = \frac{\exp(\eta_i)}{\sum_{k=1}^{K} \exp(\eta_k)} = \pi_i \qquad \boldsymbol{T}(\boldsymbol{x}) = \begin{bmatrix} x_1 \\ \vdots \\ x_K \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \log(\pi_1) \\ \vdots \\ \log(\pi_K) \end{bmatrix}$$

$$\mathrm{var}[X_i] = \pi_i \cdot (1 - \pi_i)$$

- **Conversions**:

$$\mathcal{C}(\boldsymbol{x}; \boldsymbol{\eta}) = \mathrm{Cat}\left(\boldsymbol{x}; \frac{1}{\sum_{k=1}^{K} \exp(\eta_k)} \cdot \begin{bmatrix} \exp(\eta_1) \\ \vdots \\ \exp(\eta_K) \end{bmatrix}\right) \qquad \mathrm{Cat}(\boldsymbol{x}; \boldsymbol{\pi}) = \mathcal{C}\left(\boldsymbol{x}; \begin{bmatrix} \log(\pi_1) \\ \vdots \\ \log(\pi_K) \end{bmatrix}\right)$$

- **Importance**. The categorical distribution plays a key role in selection processes and classification and is also known as the *generalized Bernoulli distribution*.


**Jacob Bernoulli (1655 – 1705)**

# Categorical Distribution: Efficient Products & Divisions

- **Theorem (Multiplication).** *Given two categorical distributions $\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_1)$ and $\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_2)$*

Correction factor

$$\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_1)\cdot\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_2)=\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_1+\boldsymbol{\eta}_2)\cdot\frac{\sum_{k=1}^{K}\exp\left(\eta_{1,k}+\eta_{2,k}\right)}{\left[\sum_{k=1}^{K}\exp\left(\eta_{1,k}\right)\right]\cdot\left[\sum_{k=1}^{K}\exp\left(\eta_{2,k}\right)\right]}$$

Additive updates!

- **Theorem (Division).** *Given two categorical distributions $\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_1)$ and $\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_2)$*

Correction factor

$$\frac{\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_1)}{\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_2)}=\mathcal{C}(\boldsymbol{x};\boldsymbol{\eta}_1-\boldsymbol{\eta}_2)\cdot\frac{\left[\sum_{k=1}^{K}\exp\left(\eta_{1,k}-\eta_{2,k}\right)\right]\cdot\left[\sum_{k=1}^{K}\exp\left(\eta_{2,k}\right)\right]}{\left[\sum_{k=1}^{K}\exp\left(\eta_{1,k}\right)\right]}$$

Subtractive updates!

# Exponential Family Distributions: Dirichlet Distribution

- **Dirichlet Distribution**. *Given $\boldsymbol{\alpha} \in \mathbb{R}^K$ with $\alpha_k > 0$, a continuous random variable $\boldsymbol{X} \in [0,1]^K$ over the $K-1$ dimensional simplex (that is, $\sum_{k=1}^K X_k = 1$) is said to have a Dirichlet distribution if the density is given by*

$$\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}) = \frac{1}{\mathcal{B}(\boldsymbol{\alpha})} \cdot \prod_{k=1}^{K} x_k^{\alpha_k - 1} \qquad \mathcal{B}(\boldsymbol{\alpha}) = \frac{\prod_{k=1}^K \Gamma(\alpha_k)}{\Gamma(\prod_{k=1}^K \alpha_k)}$$

- **Properties**:

$$E[X_i] = \frac{\alpha_i}{\sum_{k=1}^K \alpha_k}$$

$$E[\log(X_i)] = \psi(\alpha_i) - \psi\left(\sum_{k=1}^{K} \alpha_k\right) \qquad \psi(z) = \frac{\mathrm{d}}{\mathrm{d}z}\log\big(\Gamma(z)\big)$$

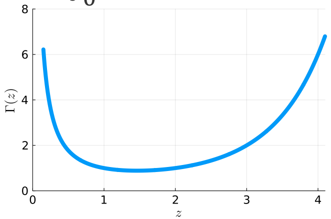
- **Natural Parameters and Sufficient Statistics**:

$$\boldsymbol{T}(\boldsymbol{x}) = \begin{bmatrix} \log(x_1) \\ \vdots \\ \log(x_K) \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \alpha_1 - 1 \\ \vdots \\ \alpha_K - 1 \end{bmatrix}$$

- **Importance**. The product of a Dirichlet $\mathrm{Dir}(\boldsymbol{\pi};\boldsymbol{\alpha})$ and a categorical $\mathrm{Cat}(\boldsymbol{x};\boldsymbol{\pi})$ is again a Dirichlet distribution $\mathrm{Dir}(\boldsymbol{\pi};\boldsymbol{\alpha}+\boldsymbol{x})$!

**Peter Gustav Dirichlet**
**(1805 – 1859)**

$$\Gamma(z) = \int_0^\infty t^{z-1} \cdot \exp(-t)\,\mathrm{d}t$$




$$\forall z > 0: \quad \Gamma(z+1) = z \cdot \Gamma(z)$$

# Dirichlet Distribution: Efficient Products & Divisions

- **Theorem (Multiplication).** *Given two Dirichlet distributions* $\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_1)$ *and* $\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_2)$

$$\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_1)\cdot\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_2)=\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2-\mathbf{1})\cdot\frac{\mathcal{B}(\boldsymbol{\alpha}_1+\boldsymbol{\alpha}_2-\mathbf{1})}{\mathcal{B}(\boldsymbol{\alpha}_1)\cdot\mathcal{B}(\boldsymbol{\alpha}_2)}$$

Correction factor

Additive updates!

- **Theorem (Division).** *Given two Dirichlet distributions* $\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_1)$ *and* $\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_2)$

$$\frac{\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_1)}{\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_2)}=\mathrm{Dir}(\boldsymbol{x};\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2+\mathbf{1})\cdot\frac{\mathcal{B}(\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2+\mathbf{1})\cdot\mathcal{B}(\boldsymbol{\alpha}_2)}{\mathcal{B}(\boldsymbol{\alpha}_1)}$$

Correction factor

Subtractive updates!

# Exponential Family Distributions: 1D Gaussian

- **1D Gaussian Distribution**. *A continuous random variable $X$ is said to have a one-dimensional Gaussian distribution if the density is given by*

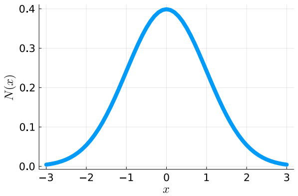
$$\mathcal{N}(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- **Properties**:

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

- **Importance**. The 1D Gaussian 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)**



# 1D Gaussian Distribution: Representations

- **Scale-Location Parameters**

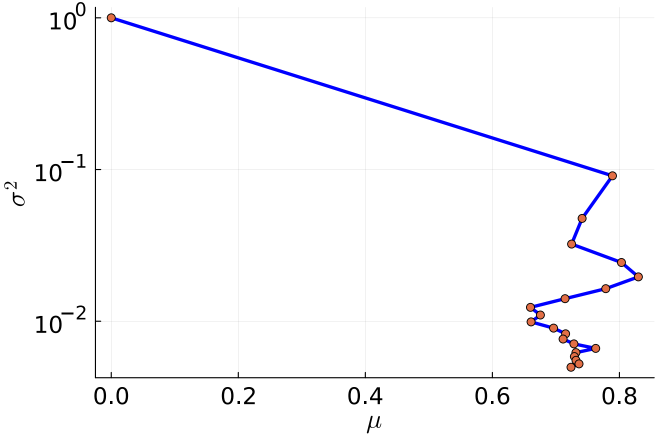
$$\mathcal{N}(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- **Conversions**

$$\mathcal{N}(x;\mu,\sigma^2) = \mathcal{G}\left(x;\frac{\mu}{\sigma^2},\frac{1}{\sigma^2}\right)$$

Two divisions only!

- **Posterior Inference**




- **Natural Parameters**

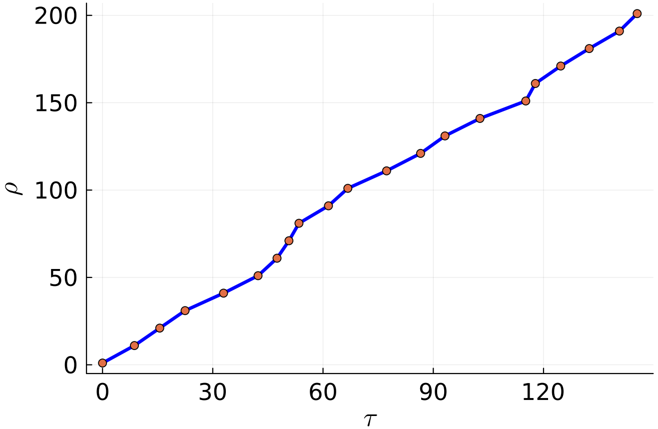
$$\mathcal{G}(x;\tau,\rho) = \sqrt{\frac{\rho}{2\pi}} \cdot \exp\left(-\frac{\tau^2}{2\rho}\right) \cdot \exp\left(\tau \cdot x - \rho \cdot \frac{x^2}{2}\right)$$

- **Conversions**

$$\mathcal{G}(x;\tau,\rho) = \mathcal{N}\left(x;\frac{\tau}{\rho},\frac{1}{\rho}\right)$$

$$\boldsymbol{T}(x) = \begin{bmatrix} x \\ -\frac{x^2}{2} \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \tau \\ \rho \end{bmatrix}$$

- **Posterior Inference**



# 1D Gaussian Distribution: Efficient Products & Divisions

- **Theorem (Multiplication).** *Given two one-dimensional Gaussian distributions* $\mathcal{G}(x;\tau_1,\rho_1)$ *and* $\mathcal{G}(x;\tau_2,\rho_2)$ *we have*

$$\mathcal{G}(x;\tau_1,\rho_1)\cdot\mathcal{G}(x;\tau_2,\rho_2)=\mathcal{G}(x;\underbrace{\tau_1+\tau_2}_{\text{Additive updates!}},\underbrace{\rho_1+\rho_2}_{\text{Additive updates!}})\cdot\underbrace{\mathcal{N}(\mu_1;\mu_2,\sigma_1^2+\sigma_2^2)}_{\text{Gaussian density}}$$

- **Theorem (Division).** *Given two one-dimensional Gaussian distributions* $\mathcal{G}(x;\tau_1,\rho_1)$ *and* $\mathcal{G}(x;\tau_2,\rho_2)$ *where* $\rho_1>\rho_2$ *we have*

$$\frac{\mathcal{G}(x;\tau_1,\rho_1)}{\mathcal{G}(x;\tau_2,\rho_2)}=\frac{\mathcal{G}(x;\tau_1-\tau_2,\rho_1-\rho_2)}{\underbrace{\mathcal{N}(\mu_1;\mu_2,\sigma_2^2-\sigma_1^2)}_{\text{Gaussian density}}}\cdot\underbrace{\frac{\sigma_2^2}{\sigma_2^2-\sigma_1^2}}_{\text{Correction factor}}$$

Subtractive updates!

# Limit 1D Gaussian Distributions: Dirac Delta and Uniform

- **Dirac Delta**. The Dirac delta function $\delta(\cdot)$ is defined as the limit $\sigma^2 \to 0$

$$\delta(x) = \lim_{\sigma^2 \to 0} \mathcal{N}(x; 0, \sigma^2)$$

- **Gaussian Uniform**. The Gaussian uniform $\mathcal{U}(\cdot)$ is defined as the limit $\sigma^2 \to \infty$

$$\mathcal{U}(x) = \lim_{\sigma^2 \to +\infty} \mathcal{N}(x; 0, \sigma^2)$$

- **Theorem (Convolution of Normal with Dirac)**. *For any $\mu \in \mathbb{R}$ and $\sigma^2 \in \mathbb{R}^+$*

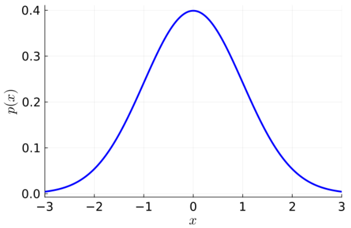
$$\int_{-\infty}^{+\infty} \delta(x) \cdot \mathcal{N}(x; \mu, \sigma^2)\, \mathrm{d}x = \boxed{\mathcal{N}(0; \mu, \sigma^2)}$$

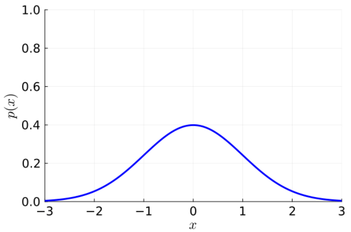
Gaussian density at $x = 0$

- **Theorem (Product of Normal with Uniform)**. *For any $\mu \in \mathbb{R}$ and $\sigma^2 \in \mathbb{R}^+$*

$$\frac{\mathcal{U}(x) \cdot \mathcal{N}(x; \mu, \sigma^2)}{\int_{-\infty}^{+\infty} \mathcal{U}(\tilde{x}) \cdot \mathcal{N}(\tilde{x}; \mu, \sigma^2)\, \mathrm{d}\tilde{x}} = \boxed{\mathcal{N}(x; \mu, \sigma^2)}$$

Equivalent to multiplying with 1




**Advanced Probabilistic Machine Learning**

*Unit 1 – Probability Theory*

# Exponential Family Distributions: Gamma Distribution

- **Gamma Distribution**. *Given $\beta > -1$ and $\lambda > 0$, a positive continuous random variable $X$ is said to have a Dirichlet distribution if the density is given by*

$$\mathrm{Gam}(x;\beta,\lambda) = \frac{\lambda^{\beta+1}}{\Gamma(\beta+1)} \cdot x^{\beta} \cdot \exp(-\lambda x) \cdot \mathbb{I}(x > 0)$$

- **Properties**:

$$E[X] = \frac{\beta+1}{\lambda}$$

$$E[\log(X)] = \psi(\beta+1) - \log(\lambda) \qquad \psi(z) = \frac{\mathrm{d}}{\mathrm{d}z}\log\big(\Gamma(z)\big)$$

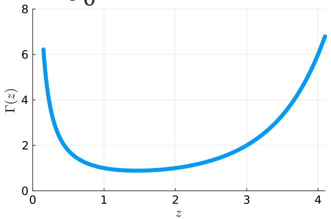
- **Natural Parameters and Sufficient Statistics**:

$$\boldsymbol{T}(x) = \begin{bmatrix} \log(x) \\ -x \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \beta \\ \lambda \end{bmatrix}$$

- **Importance**. The product of a Gamma distribution $\mathrm{Gam}(\rho;\beta,\lambda)$ and a Normal distribution $\mathcal{N}(x;\mu,\rho^{-1})$ is again a Gamma distribution $\mathrm{Gam}\left(\rho;\beta+\frac{1}{2},\lambda+\frac{(x-\mu)^2}{2}\right)$!

**Karl Pearson**
**(1857 – 1936)**

$$\Gamma(z) = \int_0^\infty t^{z-1} \cdot \exp(-t)\,\mathrm{d}t$$




$$\forall z > 0: \quad \Gamma(z+1) = z \cdot \Gamma(z)$$

# Gamma Distribution: Efficient Products & Divisions

- **Theorem (Multiplication).** *Given two Gamma distributions* $\mathrm{Gam}(x;\beta_1,\lambda_1)$ *and* $\mathrm{Gam}(x;\beta_2,\lambda_2)$

$$\mathrm{Gam}(x;\beta_1,\lambda_1)\cdot\mathrm{Gam}(x;\beta_2,\lambda_2)=\mathrm{Gam}(x;\boxed{\beta_1+\beta_2,\lambda_1+\lambda_2})\cdot\boxed{\frac{\mathrm{Gam}(1;\beta_1,\lambda_1)\cdot\mathrm{Gam}(1;\beta_2,\lambda_2)}{\mathrm{Gam}(1;\beta_1+\beta_2,\lambda_1+\lambda_2)}}$$

Correction factor

Additive updates!

- **Theorem (Division).** *Given two Gamma distributions* $\mathrm{Gam}(x;\beta_1,\lambda_1)$ *and* $\mathrm{Gam}(x;\beta_2,\lambda_2)$

$$\frac{\mathrm{Gam}(x;\beta_1,\lambda_1)}{\mathrm{Gam}(x;\beta_2,\lambda_2)}=\mathrm{Gam}(x;\boxed{\beta_1-\beta_2,\lambda_1-\lambda_2})\cdot\boxed{\frac{\mathrm{Gam}(1;\beta_1,\lambda_1)}{\mathrm{Gam}(1;\beta_1-\beta_2,\lambda_1-\lambda_2)\cdot\mathrm{Gam}(1;\beta_2,\lambda_2)}}$$

Correction factor

Subtractive updates!

# Summary

- **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
- **Exponential Family Distributions**
  - Density is proportional to an exponential of a *fixed* $d$-dimensional linear mapping of the random variable (*sufficient statistic*) and a (*natural*) *parameter* vector
  - Taking products and divisions of densities is an $\mathcal{O}(d)$ operation!
  - Key distributions are categorical, Dirichlet, Gaussian and Gamma distributions

See you next week!