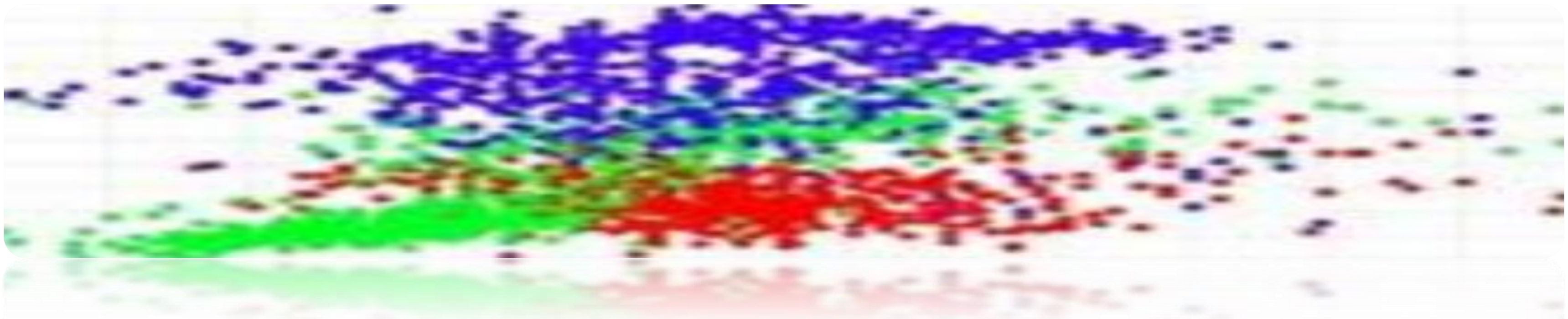


BASICS OF PROBABILITY THEORY

Outline

- Laws of probability
- Random variables
- Probability distributions
- Expectation, variance, covariance
- Maximum likelihood estimation
- Expectation maximization
- Different views on probabilities
- Bayesian inference

Set-theoretic view of probability theory

"As far as the propositions of mathematics refer to reality, they are not certain; and as far as they are certain, they do not refer to reality."

Albert Einstein, 1921

- Probability space
  - (Ω, E, P) with
  - Ω: sample space of elementary events
  - E: event space, i.e. subsets of Ω, closed under $\cap$, $\cup$, and $\neg$, usually $E = 2^{\Omega}$
  - P: $E \rightarrow [0,1]$, probability measure

Properties of P:

1. $P(\emptyset) = 0$ (impossible event)
2. $P(\Omega) = 1$
3. $P(A) + P(\neg A) = 1$
4. $P(A \cup B) = P(A) + P(B) - P(A \cap B)$
5. $P(\bigcup_i A_i) = \sum_i P(A_i)$ for pairwise disjoint A_i

Sample space and events: Examples

- Rolling a die
  - Sample space: {1, 2, 3, 4, 5, 6}
  - Probability of even number: looking for events $A = \{2\}$, $B = \{4\}$, $C = \{6\}$, $P(A \cup B \cup C) = 1/6 + 1/6 + 1/6 = 0.5$

- Tossing two coins
  - Sample space: {HH, HT, TH, TT}
  - Probability of HH or TT: looking for events A = {TT}, B = {HH}, $P(A \cup B) = 0.5$

- In general, when all outcomes in Ω are equally likely, for an $e \in E$ holds:

$$P(e) = \frac{\text{\# outcomes in } e}{\text{\# outcomes in sample space}}$$

Joint, marginal, and conditional probabilities

- Joint and conditional probability
  - $P(A, B) = P(A \cap B) = P(B|A)\,P(A)$ (product rule)
  - Bayes' theorem

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

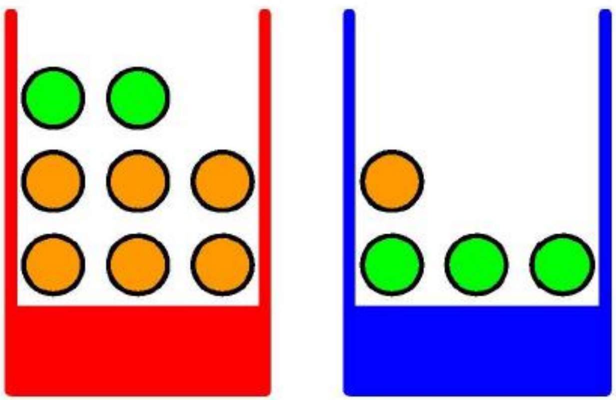
Thomas Bayes

- Total/marginal probability
  - $P(B) = \sum_j P(B \cap A_j)$ for any partitioning of Ω in $A_1, \dots, A_n$ (sum rule)

Joint, marginal, and conditional probabilities: Example

Suppose: P(B = r) = 2/5

Apples and Oranges



Fruit is orange, what is probability that box was blue?

$$P(B = b \mid F = o) = \frac{P(F = o \mid B = b)\, P(B = b)}{P(F = o)}$$

$$P(F = o) = P(F = o \mid B = r)\, P(B = r) + P(F = o \mid B = b)\, P(B = b) = 9/20$$

Example from C. Bishop: PRML

Independent events

- Independence
  - $P(A_1, \ldots, A_n) = P(A_1 \cap \ldots \cap A_n) = P(A_1)\, P(A_2) \ldots P(A_n)$, for independent events $A_1, \ldots, A_n$

- Conditional Independence
  - A is independent of B given $C \Leftrightarrow P(A|B,C) = P(A|C)$
  - If $A_1, \ldots, A_n$ are independent of each other given B then

$$P(A_1 \cap \ldots \cap A_n |B) = \prod_i P(A_i|B)$$

  - If A and B are independent, are they also independent given C?

Example: Which drug works better?

S = Drug succeeds
X = Drug x is used
Y = Drug y is used
W = Patient is woman
M = Patient is man

	Women		Men	
	Drug x	Drug y	Drug x	Drug y
Success	100	5	10	500
Failure	900	95	1	500

Simpson's paradox

$P(S|X,W) = 0.10 \quad P(S|X,M) = 0.91$
$P(S|Y,W) = 0.05 \quad P(S|Y,M) = 0.5$

Drug x works better

$P(S|X) \approx 0.11$
$P(S|Y) \approx 0.46$

Drug y works better

- Observation
  - In above table **being a male is a strong cause for both drug usage and recovery**
  - In such cases, one should evaluate the probabilities on the subgroups separately and report weighted averages

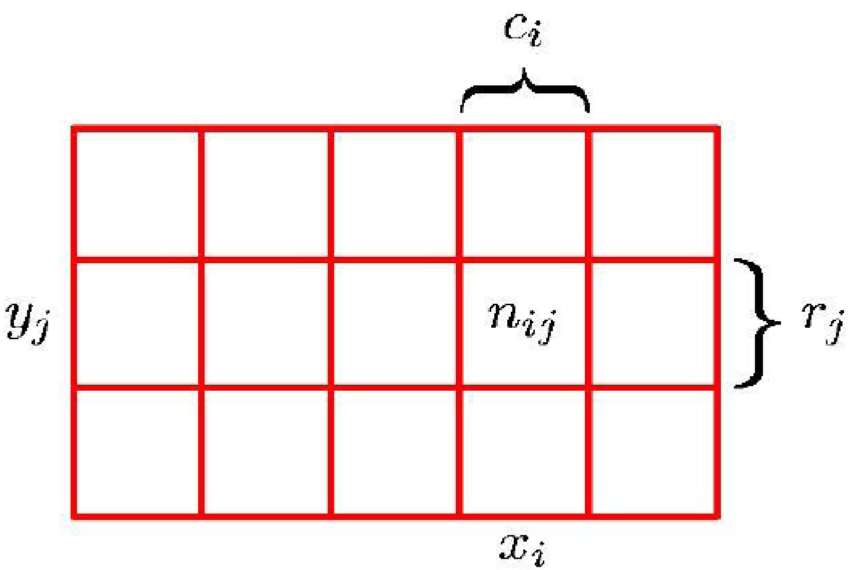
Discrete and continuous random variables

- Random variable on probability space (Ω, E, P)
  - $X\colon \Omega \rightarrow M \subseteq \mathbb{R}$ (numerical representations of outcomes) with $\{e | X(e) \leq x\} \in E$ for all $x \in M$
  - If M is countable X is called discrete, otherwise continuous

- Examples
  - Rolling a die: $X(i) = i$
  - The exact pair of faces when rolling two dice: $X(a, b) = 6(a-1) + b$
  - The sum of faces for two dice: $X(a, b) = a + b$

- Random variables $X_1, \dots, X_2$ are called independent and identically distributed (i.i.d.) if each random variable has the same probability distribution as the others and all are mutually independent

Random variables and probabilities



Example from C. Bishop: PRML

Marginal probability:

$$P(X = x_i) = \frac{c_i}{N}$$

Sum rule:

$$P(X = x_i) = \sum_j P(X = x_i, Y = y_j)$$
$$= \frac{1}{N} \sum_j n_{ij} = \frac{c_i}{N}$$

Joint probability:

$$P(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

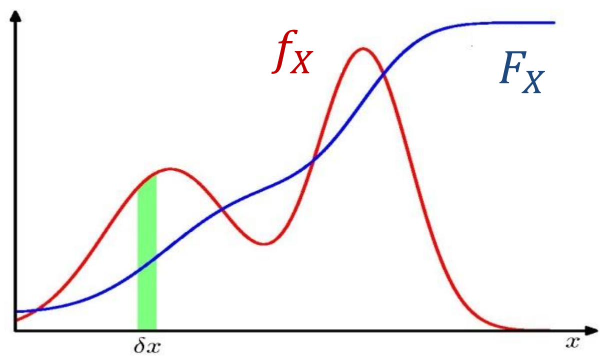
Product rule:

$$P(X = x_i, Y = y_j) = P(Y = y_j | X = x_i) P(X = x_i)$$
$$= \frac{n_{ij}}{c_i} \frac{c_i}{N} = \frac{n_{ij}}{N}$$

Probability theory

- Cumulative distribution function (cdf)
  - $F_X: M \rightarrow [0,1]$ with $F_X(x) = P(X \leq x)$

- Probability density function (pdf)
  - $f_X: M \rightarrow [0,1]$ with $f_X(x) = P(X = x) := P(x \leq X \leq x + \delta x), \delta x \rightarrow 0$



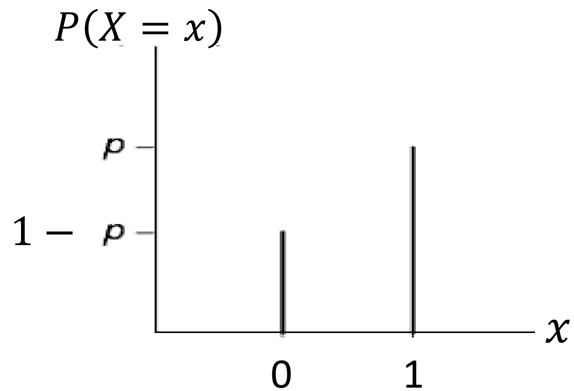
From C. Bishop: Pattern Recognition and Machine Learning

- Quantile function
  - $F^{-1}(q) = \inf\{x | F_X(x) > q\},\ q \in [0,1]$ (for $q = 0.5$, $F^{-1}(q)$ is called **median**)

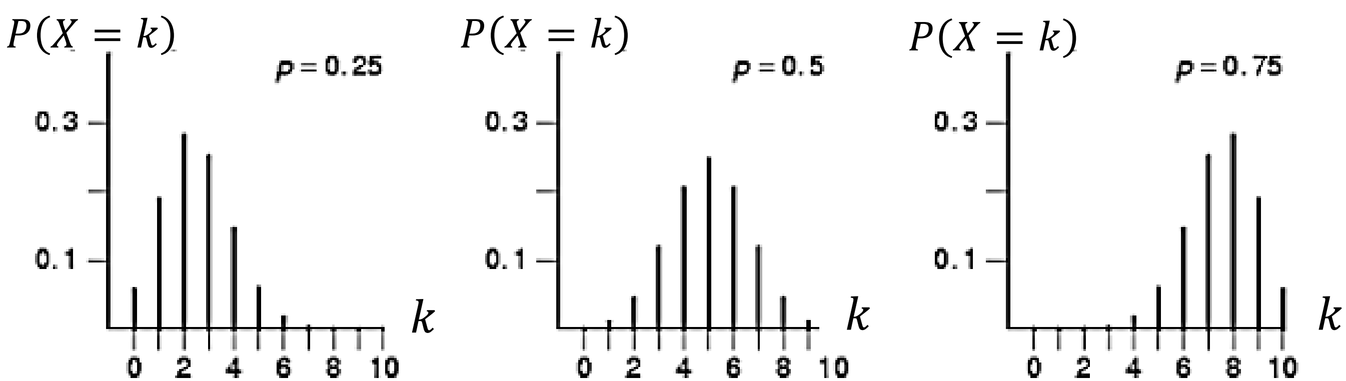
Useful discrete distributions (1)

- **Uniform distribution** over {1, 2, …, m}: $P(X = k) = f_X(k) = \frac{1}{m}$

- **Bernoulli distribution** with parameter p: $P(X = x) = f_X(x) = p^x(1-p)^{1-x}$

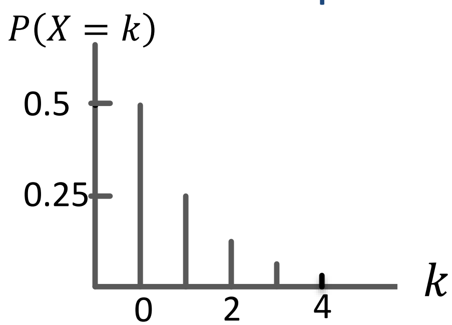


- **Binomial distribution** with parameter p, m: $P(X = k) = f_X(k) = \binom{m}{k} p^k (1-p)^{m-k}$

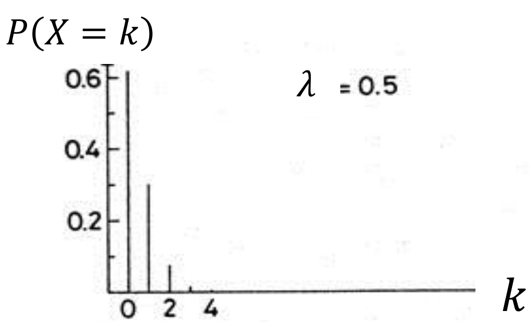


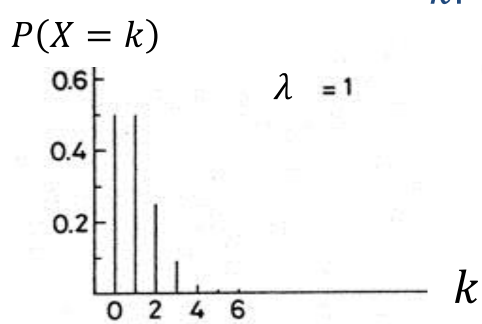
Useful discrete distributions (2)

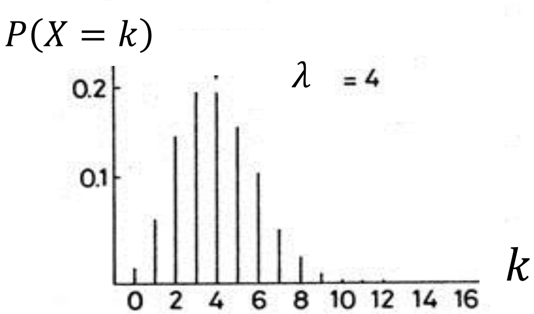
- Geometric distribution with parameter p: $P(X=k)=f_X(k)=(1-p)^k p$

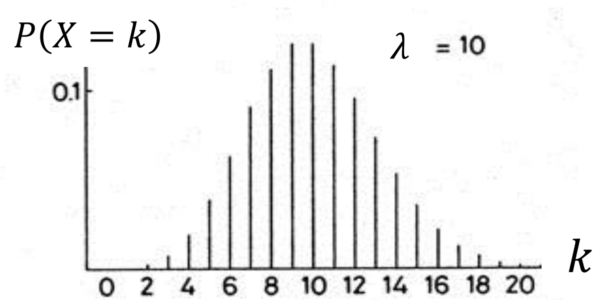


- Poisson distribution: $P(X=k)=f_X(k)=e^{-\lambda}\frac{\lambda^k}{k!}$









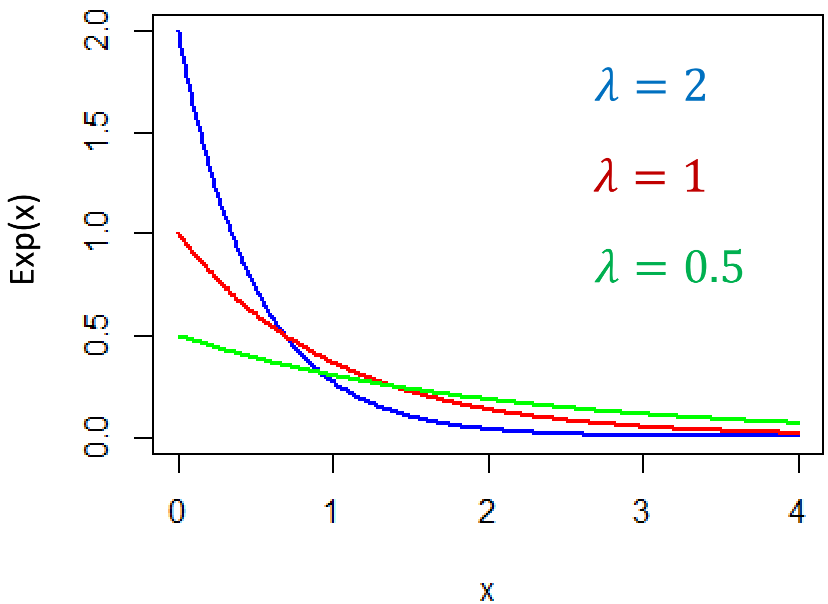
Poisson process

- Counting process
- $P(X=k)$: probability that there will be k increments per time unit
- Parameter λ: expected number of increments per time unit

Useful continuous distributions (1)

- **Uniform distribution** over [a, b] : $P(X = x) = f_X(x) = \frac{1}{b-a}$ for $a \leq x \leq b$

- **Exponential distribution**: $P(X = x) = f_X(x) = \lambda e^{-\lambda x}$ for $x > 0$



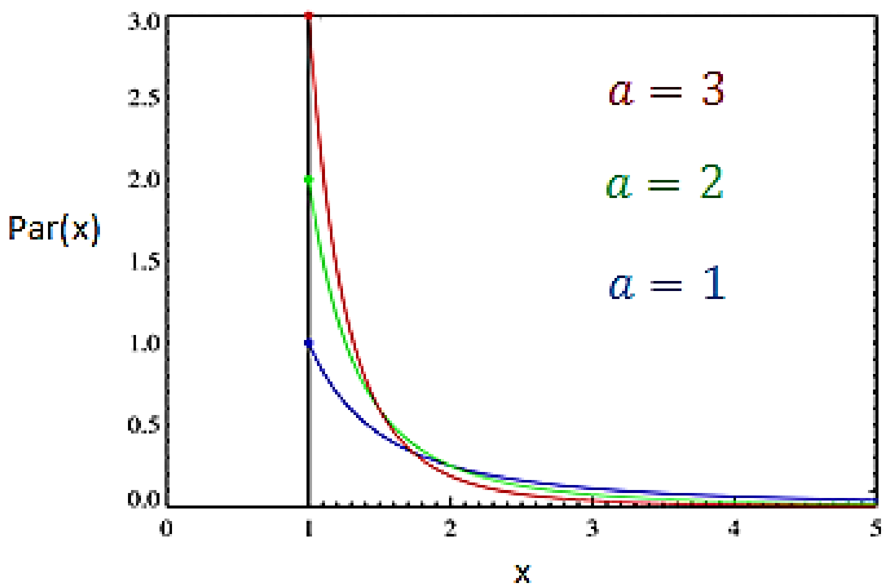
- Describes process in which events occur continuously and independently at constant average rate λ

- Can be used to model
  - Time between two phone calls
  - Modeling of radioactive decay
  - Durability of electronic devices

Useful continuous distributions (2)

- **Pareto distribution** with parameters a, b:

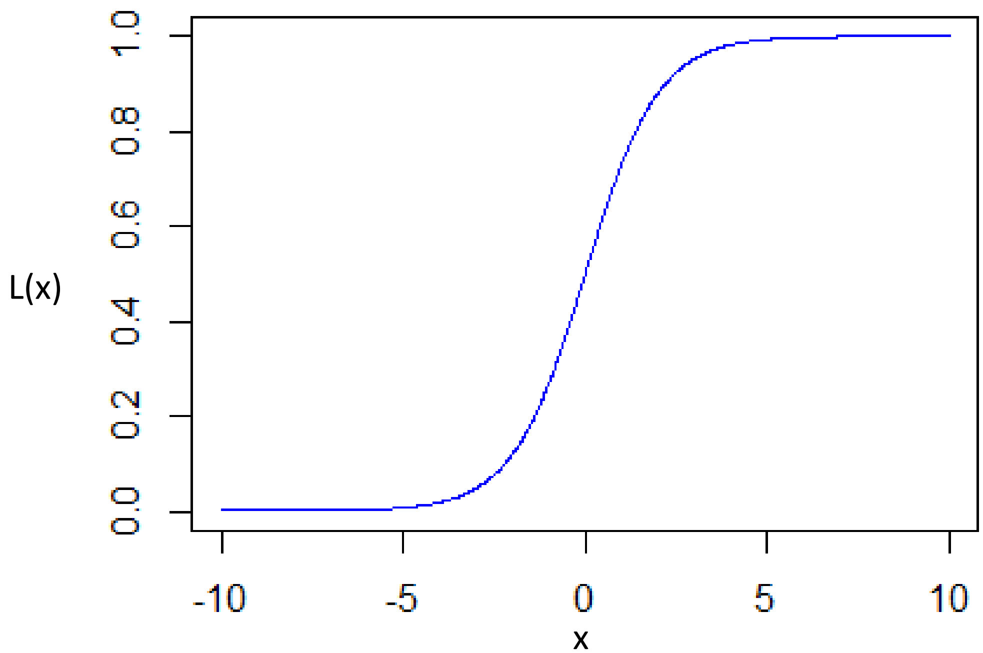
$$P(X = x) = f_X(x) = \frac{a}{b}\left(\frac{b}{x}\right)^{a+1}, \qquad x > b$$



- **Pareto principle**
  - 80% of the effects come from 20% of the causes
  - **Power law distribution**
- Examples of power-law distributions
  - Distribution of populations over cities
  - Distribution of wealth
  - Citations distribution over research papers
  - Degree distribution in web graph (or social graphs)

Useful continuous distributions (3)

- Logistic distribution: $P(X \leq x) = F_X(x) = \frac{1}{1+e^{-x}}$

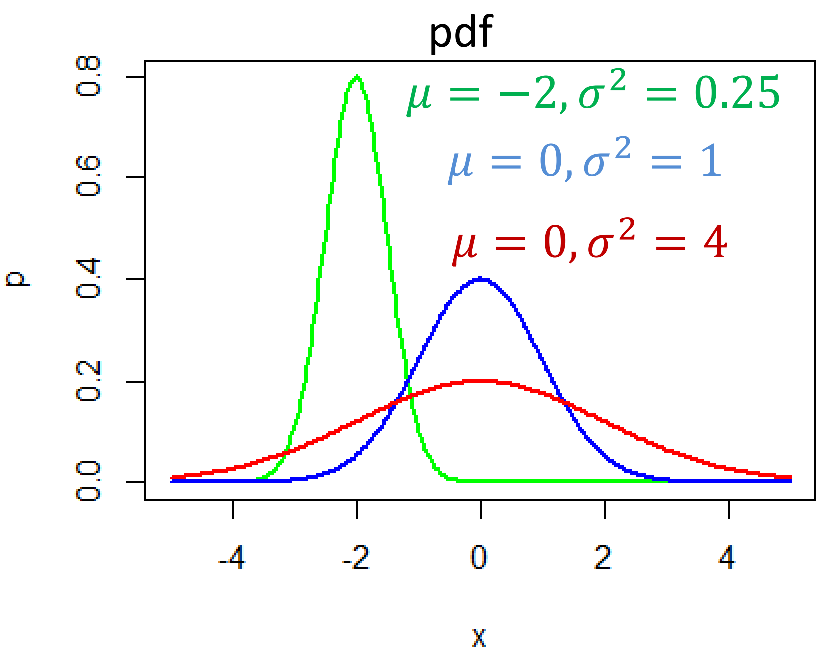


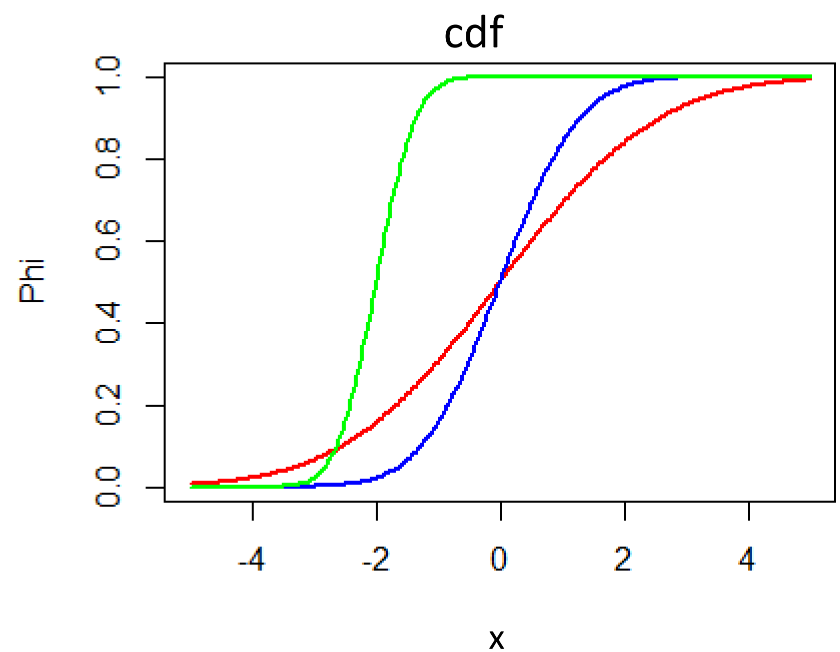
- Applications
  - Classification, e.g., with logistic regression
  - Inference in neural networks
  - In Psychometrics, e.g., modeling the probability of tasks being solved correctly in IQ questionnaires (e.g., in Item-Response Theory)

Useful continuous distributions (4)

- Normal distribution (Gaussian)
  - $X \sim N(\mu, \sigma^2) \Leftrightarrow f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$

    μ: *mean*, σ: *standard deviation*
  - Cumulative distribution of $N(0,1)$: $\Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} e^{\frac{x^2}{2}} dx$





Multivariate distributions

- Let $X_1, \ldots, X_m$ be random variables over the same probability space with domains $dom(X_1), \ldots, dom(X_m)$

- The ***joint distribution*** of $X_1, \ldots, X_m$ has a pdf $f_{X_1,\ldots,X_m}(x_1, \ldots, x_m)$ with

$$\sum_{x_1 \in dom(X_1)} \cdots \sum_{x_m \in dom(X_m)} f_{X_1,\ldots,X_m}(x_1, \ldots, x_m) = 1$$

$$\int_{x_1 \in dom(X_1)} \cdots \int_{x_m \in dom(X_m)} f_{X_1,\ldots,X_m}(x_1, \ldots, x_m)\ dx_1 \ldots dx_m = 1$$

- The ***marginal distribution*** of X_i is $F_{X_1,\ldots,X_m}(x_i) =$

$$\sum_{x_1 \in dom(X_1)} \cdots \sum_{x_{i-1} \in dom(X_{i-1})} \sum_{x_{i+1} \in dom(X_{i+1})} \cdots \sum_{x_m \in dom(X_m)} f_{X_1,\ldots,X_m}(x_1, \ldots, x_m)$$

$$\int_{x_1 \in dom(X_1)} \cdots \int_{x_{i-1} \in dom(X_{i-1})} \int_{x_{i+1} \in dom(X_{i+1})} \cdots \int_{x_m \in dom(X_m)} f_{X_1,\ldots,X_m}(x_1, \ldots, x_m)\ dx_1 \ldots dx_m$$

Useful multivariate distributions

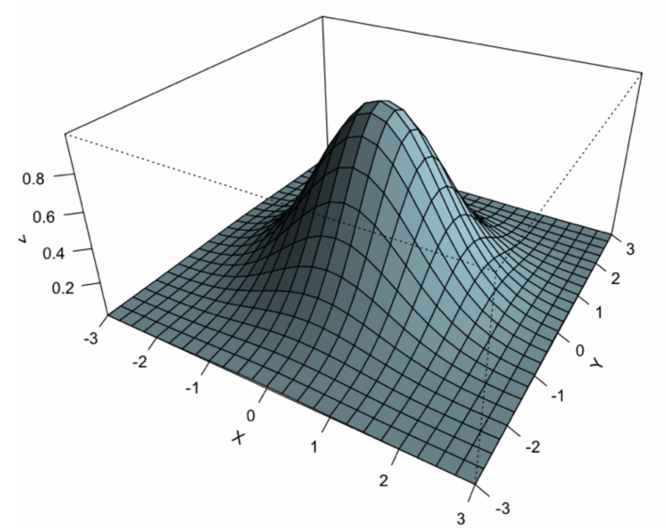
- **Multinomial distribution** with parameters n, m (rolling n m-sided dice)

  $$P(X_1 = k_1 \dots X_m = k_m) = f_{X_1,\dots,X_m}(k_1, \dots, k_m) = \frac{n!}{k_1! \dots k_m!} {p_1}^{k_1} \dots {p_m}^{k_m}$$

  with $k_1 + \cdots + k_m = n$ and $p_1 + \ \dots + \ p_m = 1$

- **Multivariate Gaussian** with parameters $\vec{\mu}, \Sigma$ where $\Sigma_{ij} := Cov(X_i, X_j)$

  $$f_{X_1,\dots,X_m}(\vec{x}) = \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} e^{-\frac{1}{2}(\vec{x}-\vec{\mu})^T \Sigma^{-1} (\vec{x}-\vec{\mu})}$$



Expectation of random variables

- For discrete variable X: $E(X) = \sum_x x \, f_X(x)$ is the expectation of X
- For continuous variable X: $E(X) = \int_{-\infty}^{\infty} x \, f_X(x) \, dx$
- Properties
  - $E(X_i + X_j) = E(X_i) + E(X_j)$
  - $E(X_i X_j) = E(X_i)E(X_j)$ for independent, identically distributed (i.i.d.) variables X_i, X_j
  - $E(aX + b) = aE(X) + b$ for constants a, b

Variance, standard deviation, and covariance

- Variance
  - $Var(X) = E[(X - E[X])^2] = E[X^2] - E[X]^2$
  - Properties
    - $Var\left(X_i + X_j\right) = Var(X_i) + Var(X_j)$ for i.i.d. variables X_i, X_j
    - $Var(aX + b) = a^2 Var(x)$ for constants a, b

- Standard deviation
  - $StDev(X) = \sqrt{Var(X)}$

- Covariance
  - $Cov\left(X_i, X_j\right) = E[(X_i - E[X_i])\ (X_j - E[X_j])]$
  - $Var(X) = Cov(X, X)$
  - In general: $Var(X + Y) = Var(X) + Var(Y) + Cov(X, Y)$

Maximum likelihood estimation (MLE)

- Suppose that after tossing a coin n times, we have seen k times head
- Let p be the unknown probability of the coin showing head
- Is it possible to estimate p?

- We know that observation corresponds to Binomial distribution, hence:

$$L(p; k, n) = P(k, n|p) = \binom{n}{k} p^k (1-p)^{n-k}$$

- Maximizing $L(p; k, n)$ is equivalent to maximizing $\log L(p; k, n)$
- $\log L(p; k, n)$ is called ***log-likelihood function***

$$\log L(p; k, n) = \log \binom{n}{k} + k \log p + (n-k) \log(1-p)$$

$$\frac{\partial \log L}{\partial p} = \frac{k}{p} - \frac{(n-k)}{(1-p)} = 0 \Rightarrow p = \frac{k}{n}$$

MLE example

- Assume $x_1, \ldots, x_n$ originate from a Gaussian with unknown μ and σ^2

$$L(\mu, \sigma; x_1, \ldots, x_n) = \left(\frac{1}{\sqrt{2\pi\sigma}}\right)^n \prod_{i=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

$$\simeq n \cdot ln\left(\frac{1}{\sqrt{2\pi\sigma}}\right) + \sum_i - \frac{(x_i - \mu)^2}{2\sigma^2}$$

$$\frac{\partial \log L}{\partial \mu} = \frac{1}{2\sigma^2} \sum_{i=1}^{n} 2(x_i - \mu) = 0$$

$$\frac{\partial \log L}{\partial \sigma} = -\frac{n}{\sigma} + \frac{1}{\sigma^3} \sum_{i=1}^{n} (x_i - \mu)^2 = 0$$

$$\Rightarrow \hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)^2$$

MLE generalization

- Let $x_1, \ldots, x_n$ be a random sample from a distribution $f(\boldsymbol{\theta}, x)$
- $x_1, \ldots, x_n$ can be viewed as the values of i.i.d. random variables $X_1, \ldots, X_n$

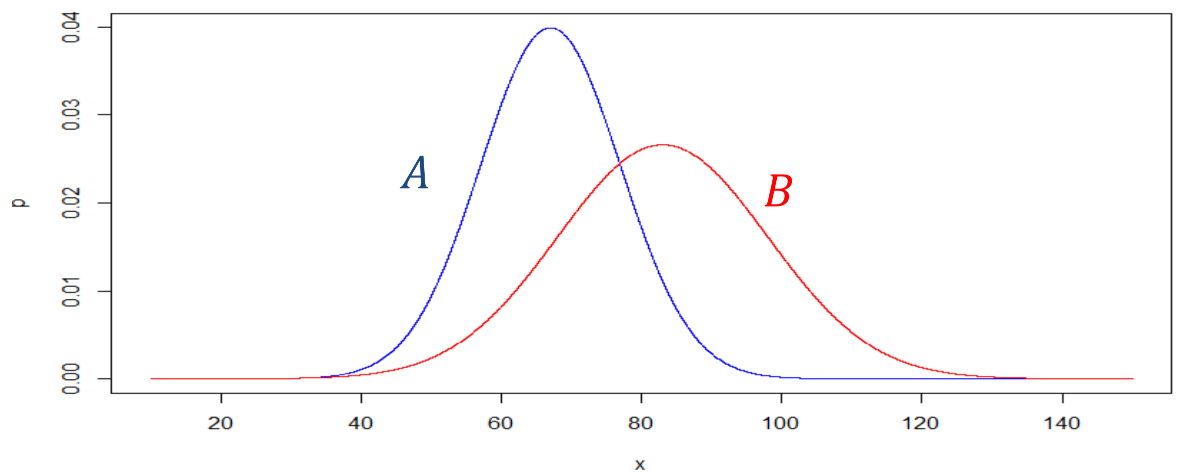
- $L(\boldsymbol{\theta}; x_1, \ldots, x_n) = P[x_1, \ldots, x_n \text{ originate from } f(\boldsymbol{\theta}, x)]$
- Maximizing $L(\boldsymbol{\theta}; x_1, \ldots, x_n)$ is equivalent to maximizing $\log L(\boldsymbol{\theta}; x_1, \ldots, x_n)$, i.e., the log-likelihood function: $\log P(x_1, \ldots, x_n | \boldsymbol{\theta})$.

- If $\frac{\partial \log L}{\partial p}$ is analytically intractable, use iterative numerical methods, e.g. Expectation Maximization (EM)

Mixture models

- **Example: Gaussian Mixture Model (GMM)**

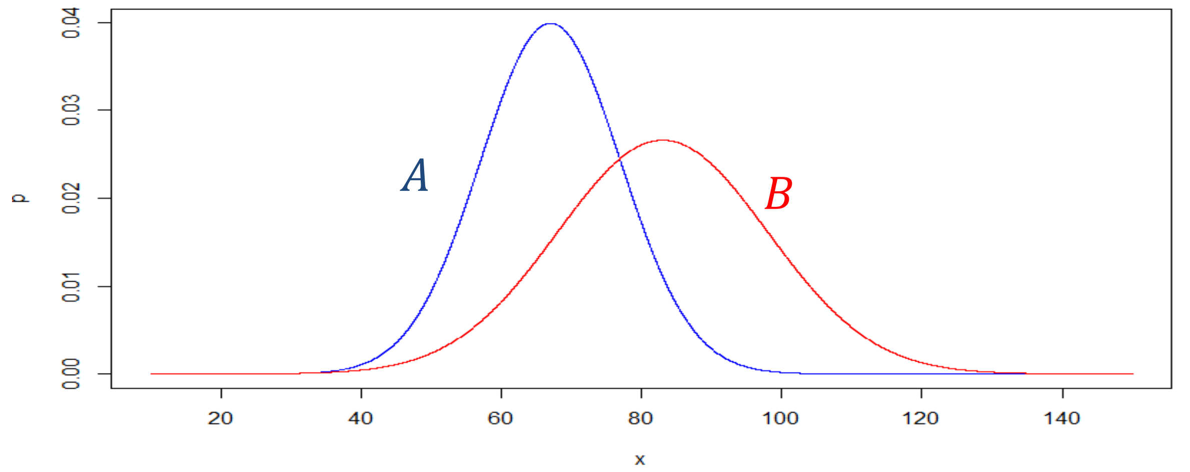
  Suppose $x_1, \ldots, x_n$ are random samples from a mixture of Gaussians $M(A, B)$ with $A(\mu_A, {\sigma_A}^2)$ and $B(\mu_B, {\sigma_B}^2)$, with unknown means and variances (e.g., weights of women and men)



$$L(\mu_A, \sigma_A, \mu_B, \sigma_B, p_A, p_B; x_1, \ldots, x_n) = \prod_i (p_A\, P(x_i|A) + p_B\, P(x_i|B))$$

with $p_A + p_B = 1$ and $P(x_i|A) = A(\mu_A, {\sigma_A}^2, x_i) = \frac{1}{\sqrt{2\pi {\sigma_A}^2}} e^{\frac{(x_i - \mu_A)^2}{2{\sigma_A}^2}}$

Expectation maximization (EM)



$$L(\mu_A, \sigma_A, \mu_B, \sigma_B, p_A, p_B; x_1, \dots, x_n) = \prod_i (p_A\, P(x_i|A) + p_B\, P(x_i|B))$$

1. **Expectation step:** Estimate the expected membership value of each point x_i given the current estimations of $\mu_A, \sigma_A, \mu_B, \sigma_B, p_A, p_B$

2. **Maximization step:** Use the expected membership values to re-estimate the parameters, and continue with Step 1 until convergence of $\log L(\mu_A, \sigma_A, \mu_B, \sigma_B, p_A, p_B; x_1, \dots, x_n)$

EM algorithm for mixture models

$$L(\mu_A, \sigma_A, \mu_B, \sigma_B, p_A, p_B; x_1, \dots, x_n) = \prod_i (p_A\, P(x_i|A) + p_B\, P(x_i|B))$$

1. Initialize the parameters $\mu_A, \sigma_A, \mu_B, \sigma_B, p_A, p_B$ to some random values (constraint: $p_A + p_B = 1$)

2. E-step: For each x_i compute expected membership values $P(A|x_i), P(B|x_i)$

3. M-step: Re-estimate the parameters

4. Iterate steps 2 and 3 until convergence (i.e., until changes of log likelihood are negligible)

Exact EM calculations for the GMM example

$$L(\mu_A, \sigma_A, \mu_B, \sigma_B, p_A, p_B; x_1, \ldots, x_n) = \prod_i (p_A\, P(x_i|A) + p_B\, P(x_i|B))$$

- Start with random parameters
- Maximize log-likelihood (i.e., target function) by iterating following steps:
  1. Compute membership weights

$$w_{Ai} = P(A|x_i) = \frac{P(x_i|A)\ P(A)}{P(x_i|A)\, P(A) + P(x_i|B)\, P(B)} = \frac{P(x_i|A)\ p_A}{P(x_i|A)\, p_A + P(x_i|B)\, p_B}$$

  2. Compute parameters

$$p_A = \frac{1}{n} \sum_i w_{Ai}$$

$$p_B = \frac{1}{n} \sum_i w_{Bi}$$

$$\mu_A = \frac{w_{A1} x_1 + \ldots + w_{An} x_n}{w_{A1} + \ldots + w_{An}}$$

$$\mu_B = \frac{w_{B1} x_1 + \ldots + w_{Bn} x_n}{w_{B1} + \ldots + w_{Bn}}$$

$$\sigma_A{}^2 = \frac{w_{A1}(x_1 - \mu_A)^2 + \ \ldots + w_{An}(x_n - \mu_A)^2}{w_{A1} + \ldots + w_{An}}$$

$$\sigma_B{}^2 = \frac{w_{B1}(x_1 - \mu_B)^2 + \ \ldots + w_{Bn}(x_n - \mu_B)^2}{w_{B1} + \ldots + w_{Bn}}$$

EM generalization

- For observed data points $x_1, \dots, x_n$ and hidden values $z_1, \dots, z_m$ and model parameters $\boldsymbol{\theta}$, estimate the maximum likelihood of

$$L(\boldsymbol{\theta}; \mathbf{x}) = \sum_{\mathbf{z}} P(\mathbf{x}, \mathbf{z} | \boldsymbol{\theta})$$

Expectation step:

- Estimate the expected value of $\mathbf{z}$ under the current parameters $\boldsymbol{\theta}^{(t)}$ and the observed data points $\mathbf{x}$
- Estimate the expected value of $\log P(\mathbf{x}, \mathbf{z} | \boldsymbol{\theta}^{(t)})$ with the current value of $\mathbf{z}$

Maximization step:

- Use the just computed estimation of $\mathbf{z}$ to find $\boldsymbol{\theta}^{(t+1)}$ that maximizes $\log P(\mathbf{x}, \mathbf{z} | \boldsymbol{\theta}^{(t+1)})$

- Note: EM monotonically approaches local maximum

Different views: The frequentists' view

- Probability of an event should be assessed objectively
  - I.e., measure the probability of the event as the relative occurrence frequency of that event based on a large number of trials

- Examples
  - Fraction of heads when tossing a coin n times
  - Relative frequency with which the face 6 shows up when rolling a die n times
  - Relative frequency with which a drug shows certain adverse reaction when tested on n subjects

- Shortcomings
  - Can be only applied to frequently repeatable events
  - The higher the frequency of an event, the more "meaningful" the probability estimate

Different views: The Bayesian view

- **Prior beliefs / probabilities** are used to quantify the uncertainty about the occurrence of events
  - I.e., prior beliefs are used to quantify the uncertainty of parameters of a statistical model

- Prior beliefs are updated based on new observations and allow the adaptation of the parameters to the new data

- With increasing number of observations, prior beliefs become less and less relevant (i.e., uncertainty is reduced)

- Drawback: Reasoning and inference has to include the prior beliefs

Bayesian inference

- By applying Bayes' theorem: $P(\boldsymbol{\theta}|x_1, \ldots, x_n) = \frac{P(x_1,\ldots, x_n|\boldsymbol{\theta})\, P(\boldsymbol{\theta})}{P(x_1,\ldots, x_n)}$

Evidence

$$P(\boldsymbol{\theta}|x_1, \ldots, x_n) \propto P(x_1, \ldots, x_n|\boldsymbol{\theta})\, P(\boldsymbol{\theta})$$

Posterior distribution of parameters

Likelihood of parameters in light of data

Prior probability distribution for parameters

Iterative substitution as more and more data points are observed

Typically with exponential family distributions with pdfs of the form:

$$P(\boldsymbol{x};\ \boldsymbol{\theta}) = h(\boldsymbol{x})g(\boldsymbol{\theta})\exp\{\boldsymbol{\theta}^T \boldsymbol{u}(\boldsymbol{x})\}$$

Important property: closure under multiplication

Bayesian inference: Example

- $P(\boldsymbol{\theta}|x_1, \dots, x_n) \propto P(x_1, \dots, x_n|\boldsymbol{\theta})\, P(\boldsymbol{\theta})$

- Why exponential family distributions?
- For algebraic convenience!

- Example

  Suppose $P(k_1, k_2|\theta) = \binom{k_1+k_2}{k_1} \theta^{k_1}(1-\theta)^{k_2}$ (binomially distributed data)

  Assume $P(\theta) = \frac{\theta^{a-1}(1-\theta)^{b-1}}{B(a,b)}$ (θ is Beta distributed with hyper-parameters a, b: counts reflecting belief formation)

$$P(\theta|k_1, k_2) = \frac{\binom{k_1+k_2}{k_1} \theta^{k_1+a-1}(1-\theta)^{k_2+b-1} \frac{1}{B(a,b)}}{\int_{\theta=0}^{1} \left(\binom{k_1+x_2}{k_1} \theta^{k_1+a-1}(1-\theta)^{k_2+b-1} \frac{1}{B(a,b)} \right) d\theta}$$

$$= \frac{\theta^{k_1+a-1}(1-\theta)^{k_2+b-1}}{B(k_1+a, k_2+b)}$$

Posterior of parameters has same form as the prior

Bayesian inference: Conjugate priors

- $P(\boldsymbol{\theta})$ is called a conjugate prior of $P(x_1, \ldots, x_n|\boldsymbol{\theta})$ if the posterior, $P(\boldsymbol{\theta}|x_1, \ldots, x_n)$, is in the same pdf family as the prior.

- Examples

Likelihood function	Conjugate prior
Bernoulli	Beta
Binomial	Beta
Poisson	Gamma
Multinomial	Dirichlet
Gaussian	Gaussian

Cox's theorem

- *Any belief system satisfying the following conditions can be described by the laws of probability*
  - *The belief in the occurrence of an event is dependent on information about the event (**dependency**)*
  - *The belief in the occurrence of an event can be represented by a real number (**numerical comparability**)*
  - *The belief in the occurrence of an event changes sensibly with observations (**common sense**)*
  - *If the belief in the occurrence of an event can be derived in many ways, all the results must be equal (**consistency**)*