Probability recall

Course of Machine Learning
Master Degree in Computer Science
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1 Probability

Discrete random variables

A discrete **random variable** X can take values from some finite or countably infinite set $\mathcal{X}$. A **probability mass function** (pmf) associates to each event $X = x$ a probability $p(X = x)$.

Properties

- $0 \leq p(x) \leq 1$ for all $x \in \mathcal{X}$
- $\sum_{x \in \mathcal{X}} p(x) = 1$

Note: we shall denote as x the event $X = x$

Discrete random variables

Joint and conditional probabilities

Given two events x, y, it is possible to define:

- the probability $p(x, y) = p(x \wedge y)$ of their joint occurrence
- the conditional probability $p(x|y)$ of x under the hypothesis that y has occurred

Union of events

Given two events x, y, the probability of x or y is defined as

$$p(x \vee y) = p(x) + p(y) - p(x, y)$$

in particular,

$$p(x \vee y) = p(x) + p(y)$$

The same definitions hold for probability distributions.

Discrete random variables

Product rule

The product rule relates joint and conditional probabilities

$$p(x, y) = p(x|y)p(y) = p(y|x)p(x)$$

where $p(x)$ is the **marginal** probability.

In general,

$$\begin{aligned} p(x_1, \ldots, x_n) &= p(x_2, \ldots, x_n|x_1)p(x_1) \\ &= p(x_3, \ldots, x_n|x_1, x_2)p(x_2|x_1)p(x_1) \\ &= \cdots \\ &= p(x_n|x_1, \ldots, x_{n-1})p(x_{n-1}|x_1 \ldots x_{n-2}) \cdots p(x_2|x_1)p(x_1) \end{aligned}$$

Discrete random variables

Sum rule and marginalization

The sum rule relates the joint probability of two events x, y and the probability of one such events $p(y)$ (or $p(y)$)

$$p(x) = \sum_{y \in \mathcal{Y}} p(x, y) = \sum_{y \in \mathcal{Y}} p(x|y)p(y)$$

Applying the sum rule to derive a marginal probability from a joint probability is usually called **marginalization**

Discrete random variables

Bayes rule

Since

$$\begin{aligned} p(x, y) &= p(x|y)p(y) \\ p(x, y) &= p(y|x)p(x) \\ p(y) &= \sum_{x \in \mathcal{X}} p(x, y) = \sum_{x \in \mathcal{X}} p(y|x)p(x) \end{aligned}$$

it results

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)} = \frac{p(y|x)p(x)}{\sum_{x \in \mathcal{X}} p(y|x)p(x)}$$

Discrete random variables

Terminology

- $p(x)$: **Prior** probability of x (before knowing that y occurred)
- $p(x|y)$: **Posterior** of x (if y has occurred)
- $p(y|x)$: **Likelihood** of y given x
- $p(y)$: **Evidence** of y

Independence

Definition

Two random variables X, Y are **independent** ($X \perp\!\!\!\perp Y$) if their joint probability is equal to the product of their marginals

$$p(x, y) = p(x)p(y)$$

or, equivalently,

$$p(x|y) = p(x) \qquad\qquad p(y|x) = p(y)$$

The condition $p(x|y) = p(x)$, in particular, states that, if two variables are independent, knowing the value of one does not add any knowledge about the other one.

Independence

Conditional independence

Two random variables X, Y are **conditionally independent** w.r.t. a third r.v. Z ($X \perp\!\!\!\perp Y \mid Z$) if

$$p(x, y|z) = p(x|z)p(y|z)$$

Conditional independence does not imply (absolute) independence, and vice versa.

Continuous random variables

A continuous random variable X can take values from a continuous infinite set $\mathcal{X}$. Its probability is defined as **cumulative distribution function** (cdf) $F(x) = p(X \leq x)$.

The probability that X is in an interval $(a, b]$ is then $p(a < X \leq b) = F(b) - F(a)$.

Probability density function

The probability density function (pdf) is defined as $f(x) = \dfrac{dF(x)}{dx}$. As a consequence,

$$p(a < X \leq b) = \int_a^b f(x)dx$$

and

$$p(x < X \leq x + dx) \approx f(x)dx$$

for a sufficiently small dx.

Sum rule and continuous random variables

In the case of continuous random variables, their probability density functions relate as follows.

$$f(x) = \int_{\mathcal{Y}} f(x, y)dy = \int_{y \in \mathcal{Y}} p(x|y)p(y)dy$$

Expectation

Definition

Let x be a discrete random variable with distribution $p(x)$, and let $g : \mathbb{R} \mapsto \mathbb{R}$ be any function: the expectation of $g(x)$ w.r.t. $p(x)$ is

$$E_p[g(x)] = \sum_{x \in V_x} g(x)p(x)$$

If x is a continuous r.v., with probability density $f(x)$, then

$$E_f[g(x)] = \int_{-\infty}^{\infty} g(x)f(x)dx$$

Mean value

Particular case: $g(x) = x$

$$E_p[x] = \sum_{x \in V_x} xp(x) \qquad\qquad E_f[x] = \int_{-\infty}^{\infty} xf(x)dx$$

Elementary properties of expectation

- $E[a] = a$ for each $a \in \mathbb{R}$
- $E[af(x)] = aE[f(x)]$ for each $a \in \mathbb{R}$
- $E[f(x) + g(x)] = E[f(x)] + E[g(x)]$

Variance

Definition

$$Var[X] = E[(x - E[x])^2]$$

We may easily derive:

$$\begin{aligned} E[(x - E[x])^2] &= E[x^2 - 2E[x]x + E[x]^2] \\ &= E[x^2] - 2E[x]E[x] + E[x]^2 \\ &= E[x^2] - E[x]^2 \end{aligned}$$

Some elementary properties:

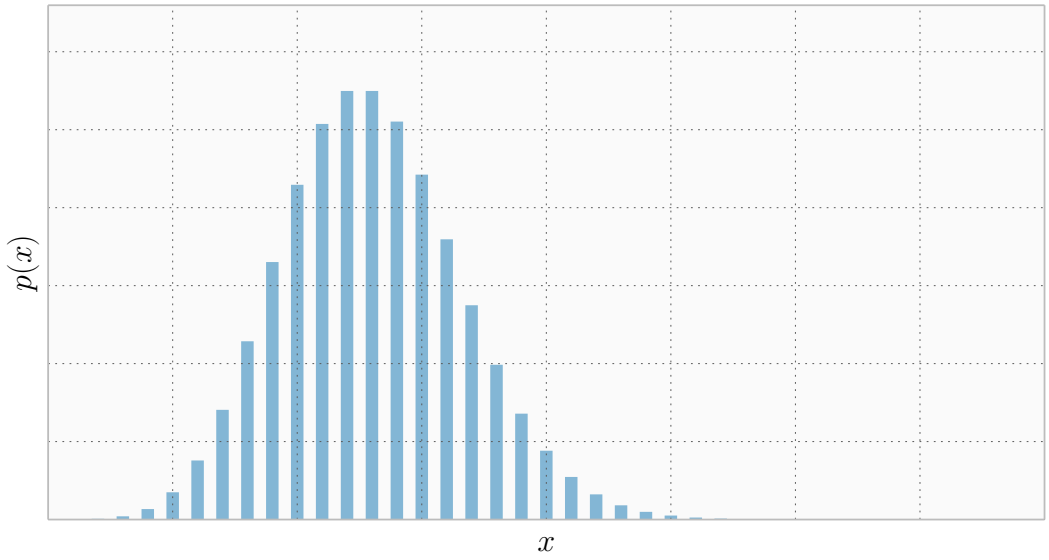
- $Var[a] = 0$ for each $a \in \mathbb{R}$
- $Var[af(x)] = a^2 Var[f(x)]$ for each $a \in \mathbb{R}$

Probability distributions

Probability distribution

Given a discrete random variable $X \in V_X$, the corresponding **probability distribution** is a function $p(x) = P(X = x)$ such that

- $0 \leq p(x) \leq 1$
- $\sum_{x \in V_X} p(x) = 1$
- $\sum_{x \in A} p(x) = P(x \in A)$, with $A \subseteq V_X$

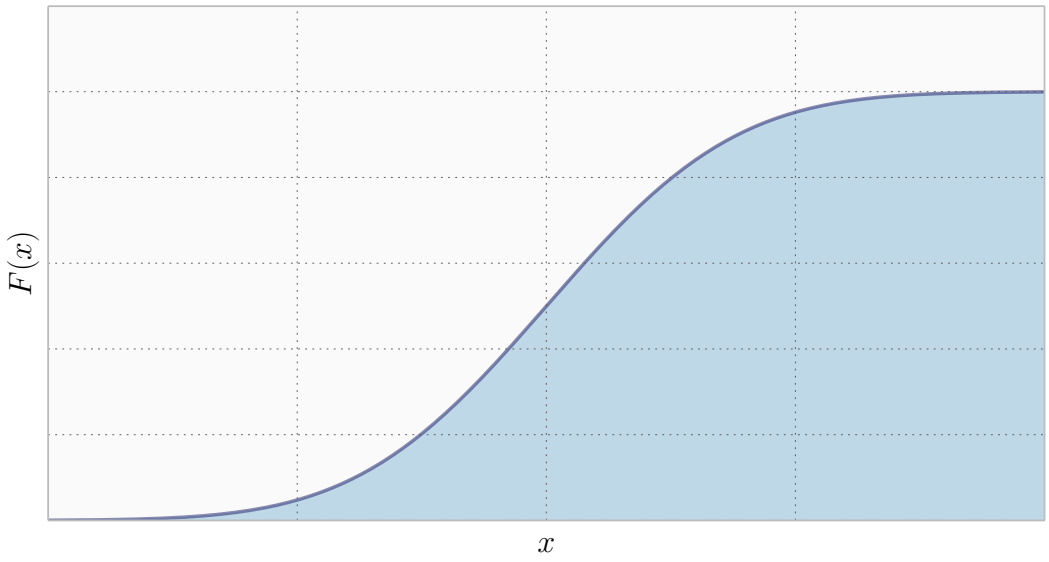


Some definitions

Cumulative distribution

Given a continuous random variable $X \in \mathbb{R}$, the corresponding **cumulative probability distribution** is a function $F(x) = P(X \leq x)$ such that:

- $0 \leq F(x) \leq 1$
- $\lim_{x \to -\infty} F(x) = 0$
- $\lim_{x \to \infty} F(x) = 1$
- $x \leq y \implies F(x) \leq F(y)$



Some definitions

Probability density

Given a continuous random variable $X \in \mathbb{R}$ with derivable cumulative distribution $F(x)$, the probability density is defined as

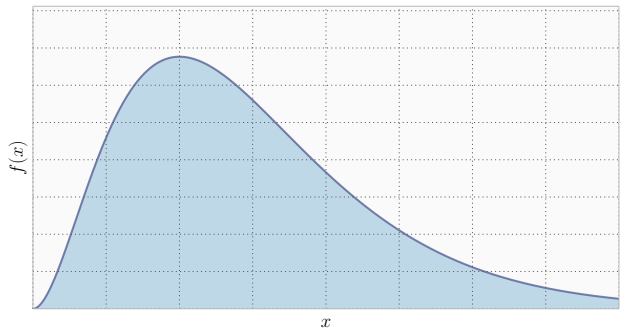
$$f(x) = \frac{dF(x)}{dx}$$

By definition of derivative, for a sufficiently small Δx,

$$Pr(x \leq X \leq x + \Delta x) \approx f(x)\Delta x$$

The following properties hold:

- $f(x) \geq 0$
- $\int_{-\infty}^{\infty} f(x)dx = 1$
- $\int_{x \in A} f(x)dx = P(X \in A)$



Bernoulli distribution

Definition

Let $x \in \{0, 1\}$, then $x \sim \textit{Bernoulli}(p)$, with $0 \leq p \leq 1$, if

$$p(x) = \begin{cases} p & \text{se } x = 1 \\ 1 - p & \text{se } x = 0 \end{cases}$$

or, equivalently,

$$p(x) = p^x (1 - p)^{1-x}$$

Probability that, given a coin with head (H) probability p (and tail probability (T) $1 - p$), a coin toss result into $x \in \{H, T\}$.

Mean and variance

$$E[x] = p \qquad\qquad Var[x] = p(1 - p)$$

Extension to multiple outcomes

Assume k possible outcomes (for example a die toss).

In this case, a generalization of the Bernoulli distribution is considered, usualy named **categorical** distribution.

$$p(x) = \prod_{j=1}^{k} p_j^{x_j}$$

where $(p_1, \ldots, p_k)$ are the probabilites of the different outcomes ($\sum_{j=1}^{k} p_j = 1$) and $x_j = 1$ iff the k-th outcome occurs.

Binomial distribution

Definition

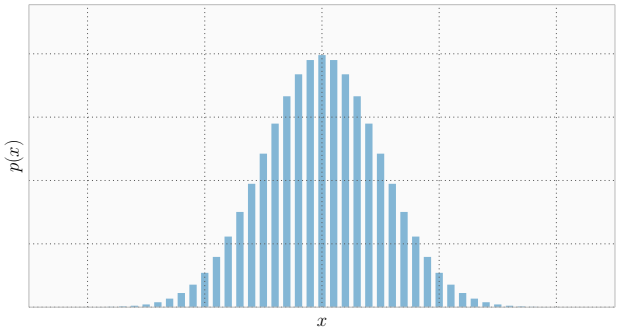
Let $x \in \mathbb{N}$, then $x \sim \textit{Binomial}(n, p)$, with $0 \leq p \leq 1$, if

$$p(x) = \binom{n}{x} p^x (1 - p)^{n-x} = \frac{n!}{x!(n - x)!} p^x (1 - p)^{n-x}$$

Probability that, given a coin with head (H) probability p, a sequence of n independent coin tosses result into x heads.

Mean and variance

$$E[x] = np$$
$$Var[x] = np(1 - p)$$



Poisson distribution

Definition

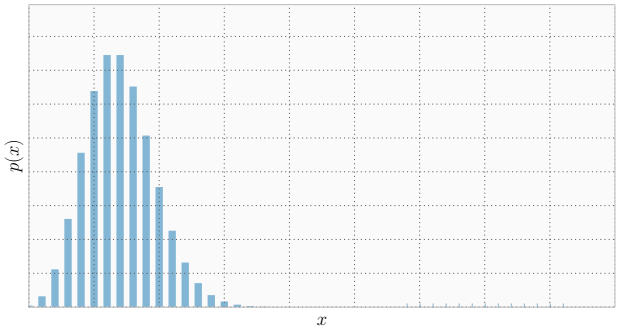
Let $x_i \in \mathbb{N}$, then $x \sim Poisson(\lambda)$, with $\lambda > 0$, if

$$p(x) = e^{-\lambda}\frac{\lambda^x}{x!}$$

Probability that an event with average frequency λ occurs x times in the next time unit.

Mean and variance

$$E[x] = \lambda$$
$$Var[x] = \lambda$$



Normal (gaussian) distribution

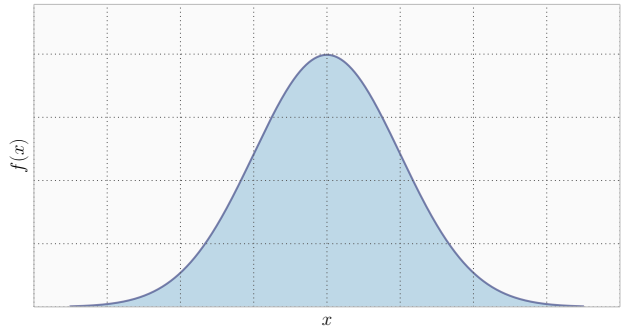
Definition

Let $x \in \mathbb{R}$, then $x \sim Normal(\mu, \sigma^2)$, with $\mu, \sigma \in \mathbb{R}$, $\sigma \geq 0$, if

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma}e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

Mean and variance

$$E[x] = \mu$$
$$Var[x] = \sigma^2$$



Beta distribution

Definition

Let $x \in [0, 1]$, then $x \sim Beta(\alpha, \beta)$, with $\alpha, \beta > 0$, if

$$f(x) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

where

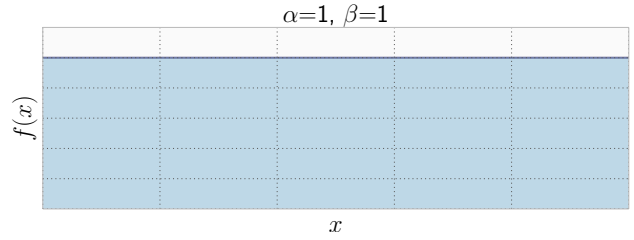
$$\Gamma(x) = \int_0^\infty u^{x-1} e^u du$$

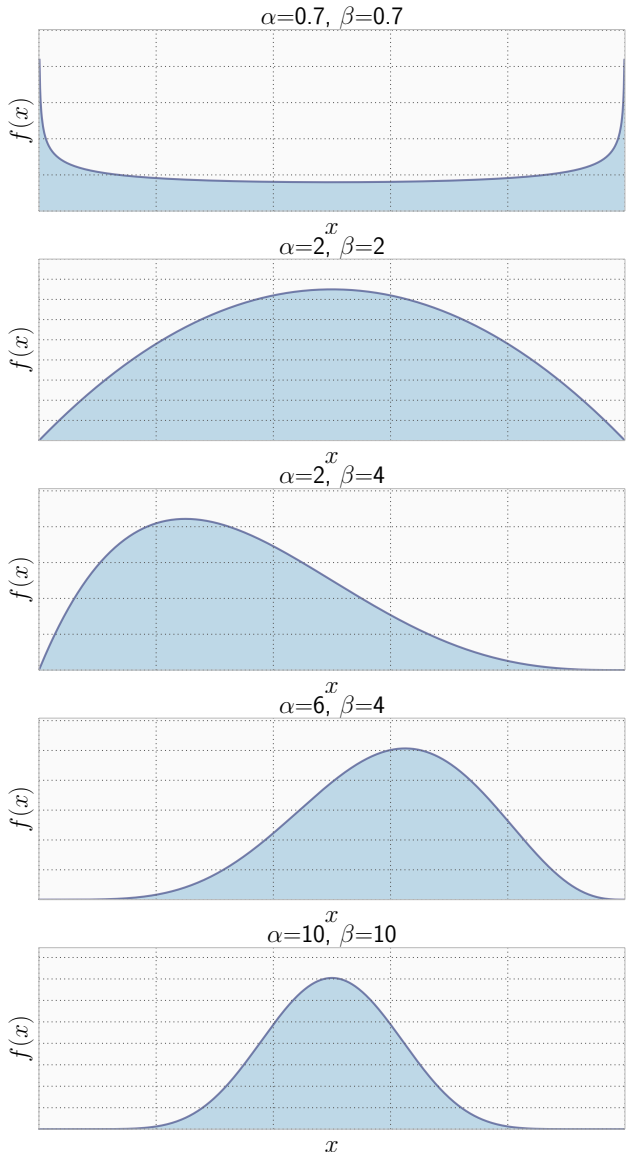
is a generalization of the factorial to the real field $\mathbb{R}$: in particolar, $\Gamma(n) = (n-1)!$ if $n \in \mathbb{N}$

Mean and variance

$$E[x] = \frac{\beta}{\alpha + \beta}$$
$$Var[x] = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$$

Beta distribution





Multivariate distributions

Definition for $k = 2$ discrete variables

Given two discrete r.v. X, Y, their joint distribution is

$$p(x, y) = P(X = x, Y = y)$$

The following properties hold:

1. $0 \leq p(x, y) \leq 1$
2. $\sum_{x \in V_X} \sum_{y \in V_Y} p(x, y) = 1$

Multivariate distributions

Definition for $k = 2$ variables

Given two continuous r.v. X, Y, their cumulative joint distribution is defined as

$$F(x, y) = P(X \leq x, Y \leq y)$$

The following properties hold:

1. $0 \leq F(x,y) \leq 1$
2. $\lim_{x,y\to\infty} F(x,y) = 1$
3. $\lim_{x,y\to-\infty} F(x,y) = 0$

If $F(x,y)$ is derivable everywhere w.r.t. both x and y, **joint probability density** is

$$f(x,y) = \frac{\partial^2 F(x,y)}{\partial x \partial y}$$

The following property derives

$$\int\int_{(x,y)\in A} f(x,y)dxdy = P((X,Y) \in A)$$

Covariance

Definition

$$Cov[X,Y] = E[(X - E[X])(Y - E[Y])]$$

As for the variance, we may derive

$$\begin{aligned} Cov[X,Y] &= E[(X - E[X])(Y - E[Y])] \\ &= E[XY - XE[Y] - YE[X] + E[X]E[Y]] \\ &= E[XY] - E[X]E[Y] - E[Y]E[X] + E[E[X]E[Y]] \\ &= E[XY] - E[X]E[Y] \end{aligned}$$

Moreover, the following properties hold:

1. $Var[X+Y] = Var[X] + Var[Y] + 2Cov[X,Y]$
2. If $X \perp\!\!\!\perp Y$ then $Cov[X,Y] = 0$

Random vectors

Definition

Let $X_1, X_2, \ldots, X_n$ be a set of r.v.: we may then define a random vector as

$$\mathbf{x} = \begin{pmatrix} X_1 \\ \vdots \\ X_2 \end{pmatrix} X_n$$

Expectation and random vectors

Definition

Let $g : \mathbb{R}^n \mapsto \mathbb{R}^m$ be any function. It may be considered as a vector of functions

$$g(\mathbf{x}) = \begin{pmatrix} g_1(\mathbf{x})) \\ \vdots \\ g_m(\mathbf{x})) \end{pmatrix}$$

where $\mathbf{x} \in \mathbb{R}^n$.

The expectation of g is the vector of the expectations of all functions g_i,

$$E[g(\mathbf{x})] = \begin{pmatrix} E[g_1(\mathbf{x})] \\ \vdots \\ E[g_m(\mathbf{x})] \end{pmatrix}$$

Covariance matrix

Definition

Let $\mathbf{x} \in \mathbb{R}^n$ be a random vector: its covariance matrix Σ is a matrix $n \times n$ such that, for each $1 \leq i, j \leq n$, $\Sigma_{ij} = Cov[X_i, X_j] = E[(X_i - \mu_i)(X_j - \mu_j)]$, where $\mu_i = E[X_i]$, $\mu_j = E[X_j]$.

Hence,

$$\begin{aligned} \Sigma &= \begin{bmatrix} Cov[X_1, X_1] & Cov[X_1, X_2] & \cdots & Cov[X_1, X_n] \\ Cov[X_2, X_1] & Cov[X_2, X_2] & \cdots & Cov[X_2, X_n] \\ \vdots & \vdots & \ddots & \vdots \\ Cov[X_n, X_1] & Cov[X_n, X_2] & \cdots & Cov[X_n, X_n] \end{bmatrix} \\ &= \begin{bmatrix} Var[X_1] & \cdots & Cov[X_1, X_n] \\ \vdots & \ddots & \vdots \\ Cov[X_n, X_1] & \cdots & Var[X_n] \end{bmatrix} \end{aligned}$$

Covariance matrix

By definition of covariance,

$$\begin{aligned} \Sigma &= \begin{bmatrix} E[X_1^2] - E[X_1]^2 & \cdots & E[X_1 X_n] - E[X_1]E[X_n] \\ \vdots & \ddots & \vdots \\ E[X_n X_1] - E[X_n]E[X_1] & \cdots & E[X_n^2] - E[X_n]E[X_n] \end{bmatrix} \\ &= E[\mathbf{X}\mathbf{X}^T] - \boldsymbol{\mu}\boldsymbol{\mu}^T \end{aligned}$$

where $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)^T$ is the vector of expectations of the random variables $X_1, \ldots, X_n$.

Properties

The covariance matrix is necessarily:

- semidefinite positive: that is, $\mathbf{z}^T \Sigma \mathbf{z} \geq 0$ for any $\mathbf{z} \in \mathbb{R}^n$
- symmetric: $Cov[X_i, X_j] = Cov[X_j, X_i]$ for $1 \leq i, j \leq n$

Correlation

For any pair of r.v. X, Y, the **Pearson correlation coefficient** is defined as

$$\rho_{X,Y} = \frac{Cov[X, Y]}{\sqrt{Var[X]Var[Y]}}$$

Note that, if $Y = aX + b$ for some pair a, b, then

$$Cov[X, Y] = E[(X - \mu)(aX + b - a\mu - b)] = E[a(X - \mu)^2] = aVar[X]$$

and, since

$$Var[Y] = (aX - a\mu)^2 = a^2 Var[X]$$

it results $\rho_{X,Y} = 1$. As a corollary, $\rho_{X,X} = 1$.

Observe that if X and Y are independent, $p(X,Y) = p(X)p(Y)$: as a consequence, $Cov[X,Y] = 0$ and $\rho_{X,Y} = 0$. That is, independent variables have null covariance and correlation.

The contrary is not true: null correlation does not imply indepedence: see for example X uniform in $[-1,1]$ and $Y = X^2$.

Correlation matrix

The **correlation matrix** of $(X_1, \ldots, X_n)^T$ is defined as

$$\begin{aligned}\Sigma &= \begin{bmatrix} \rho_{X_1,X_1} & \rho_{X_1,X_2} & \cdots & \rho_{X_1,X_n} \\ \vdots & \ddots & \vdots & \\ \rho_{X_n,X_1} & \rho_{X_n,X_2} & \cdots & \rho_{X_n,X_n} \end{bmatrix} \\ &= \begin{bmatrix} 1 & \rho_{X_1,X_2} & \cdots & \rho_{X_1,X_n} \\ \vdots & \ddots & \vdots & \\ \rho_{X_n,X_1} & \rho_{X_n,X_2} & \cdots & 1 \end{bmatrix}\end{aligned}$$

Multinomial distribution

Definition

Let $x_i \in \mathbb{N}$ for $i = 1, \ldots, k$, then $(x_1, \ldots, x_k) \sim Mult(n, p_1, \ldots, p_k)$ with $0 \leq p \leq 1$, if

$$p(x_1, \ldots, x_k) = \frac{n!}{x_1! \ldots x_k!} \prod_{i=1}^{k} p_i^{x_i} \qquad \text{con} \sum_{i=1}^{k} x_i = n$$

Generalization of the binomial distribution to $k \geq 2$ possible toss results $t_1, \ldots, t_k$ with probabilities $p_1, \ldots, p_k$ ($\sum_{i=1}^{k} p_i = 1$).

Probability that in a sequence of n independent tosses $p_1, \ldots, p_k$, exactly x_i tosses have result t_i ($i = 1, \ldots, k$).

Mean and variance

$$E[x_i] = np_i \qquad Var[x_i] = np_i(1 - p_i) \qquad i = 1, \ldots, k$$

Dirichlet distribution

Definition

Let $x_i \in [0,1]$ for $i = 1, \ldots, k$, then $(x_1, \ldots, x_k) \sim Dirichlet(\alpha_1, \alpha_2, \ldots, \alpha_k)$ if

$$f(x_1, \ldots, x_k) = \frac{\Gamma(\sum_{i=1}^{k} \alpha_i)}{\prod_{i=1}^{k} \Gamma(\alpha_i)} \prod_{i=1}^{k} x_i^{\alpha_i - 1} = \frac{1}{\Delta(\alpha_1, \ldots, \alpha_k)} \prod_{i=1}^{k} x_i^{\alpha_i - 1}$$

with $\sum_{i=1}^{k} x_i = 1$.

Generalization of the Beta distribution to the multinomial case $k \geq 2$.

A random variable $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_K)$ with Dirichlet distribution takes values on the $K - 1$ dimensional simplex (set of points $\mathbf{x} \in \mathbb{R}^K$ such that $x_i \geq 0$ for $i = 1, \ldots, K$ and $\sum_{i=1}^{K} x_i = 1$)

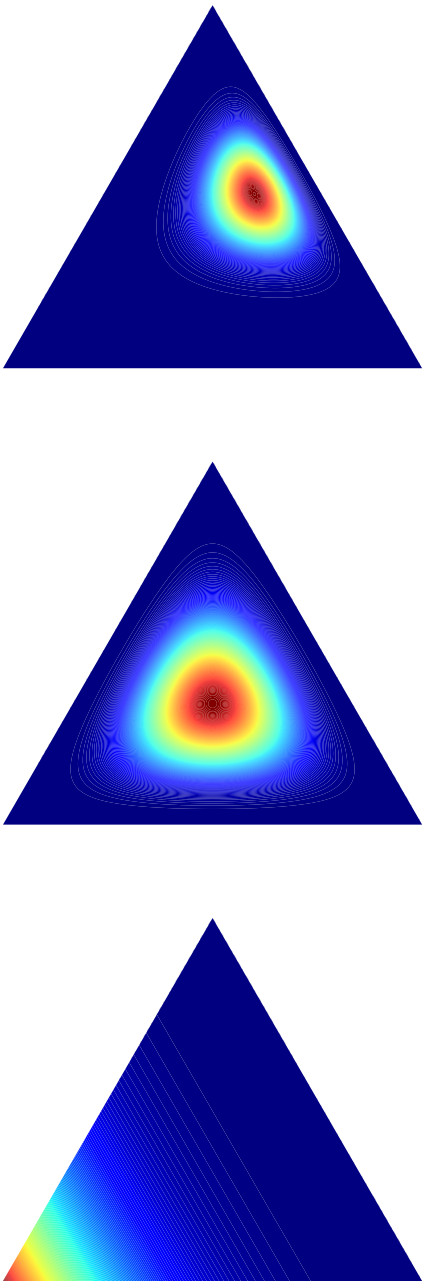
Mean and variance

$$E[x_i] = \frac{\alpha_i}{\alpha_0} \qquad Var[x_i] = \frac{\alpha_i(\alpha_0 - \alpha_i)}{\alpha_0^2(\alpha_0 + 1)} \qquad i = 1, \ldots, k$$

with $\alpha_0 = \sum_{j=1}^{k} \alpha_j$

Dirichlet distribution

Examples of Dirichlet distributions with $k = 3$



Dirichlet distribution

Symmetric Dirichlet distribution

Particular case, where $\alpha_i = \alpha$ for $i = 1, \ldots, K$

$$p(\phi_1, \ldots, \phi_K | \alpha, K) = \text{Dir}(\boldsymbol{\phi} | \alpha, K) = \frac{\Gamma(K\alpha)}{\Gamma(\alpha)^K} \prod_{i=1}^{K} \phi_i^{\alpha-1} = \frac{1}{\Delta_K(\alpha)} \prod_{i=1}^{K} \phi_i^{\alpha-1}$$

Mean and variance

In this case,

$$E[x_i] = \frac{1}{K} \qquad Var[x_i] = \frac{K-1}{K^2(\alpha+1)} \qquad i = 1, \ldots, K$$

2 The normal distribution

Gaussian distribution

- Properties
  - Analytically tractable
  - Completely specified by the first two moments
  - A number of processes are asintotically gaussian (theorem of the Central Limit)
  - Linear transformation of gaussians result in a gaussian

Univariate gaussian

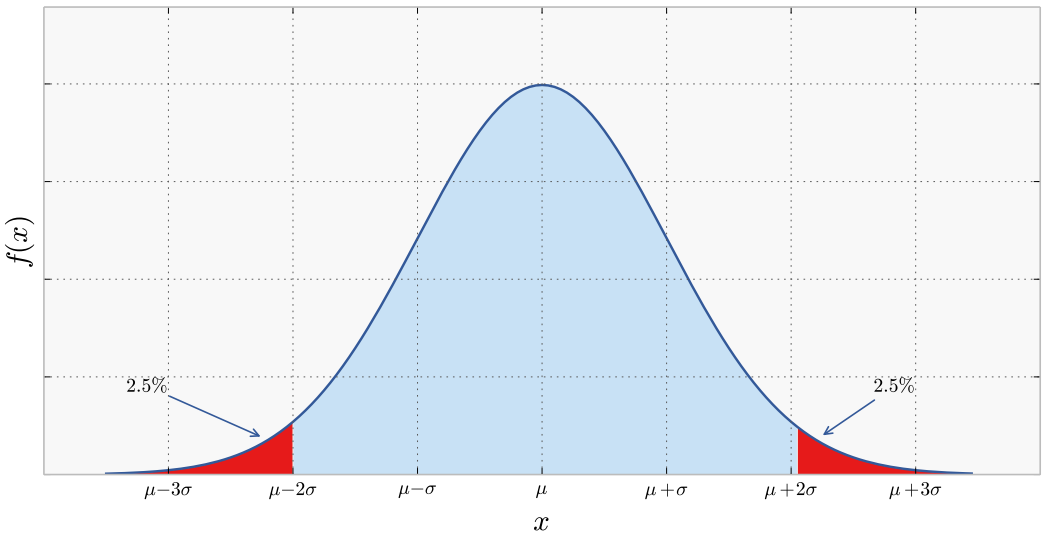
For $x \in \mathbb{R}$:

$$\begin{aligned} p(x) &= \mathcal{N}(\mu, \sigma^2) \\ &= \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \end{aligned}$$

with

$$\mu = E[x] = \int_{-\infty}^{\infty} x p(x) dx$$
$$\sigma^2 = E[(x-\mu)^2] = \int_{-\infty}^{\infty} (x-\mu)^2 p(x) dx$$

Univariate gaussian



A univariate gaussian distribution has about 95% of its probability in the interval $|x - \mu| \geq 2\sigma$.

Multivariate gaussian

For $\mathbf{x} \in \mathbb{R}^d$:

$$\begin{aligned} p(\mathbf{x}) &= \mathcal{N}(\boldsymbol{\mu}, \Sigma) \\ &= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})} \end{aligned}$$

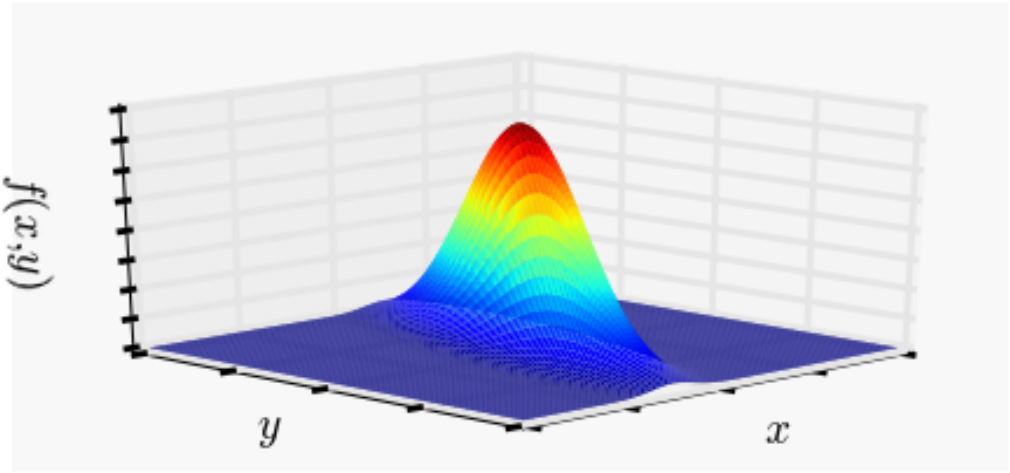
where

$$\boldsymbol{\mu} = E[\mathbf{x}] = \int \mathbf{x} p(\mathbf{x}) d\mathbf{x}$$

$$\Sigma = E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T] = \int (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T p(\mathbf{x}) d\mathbf{x}$$

Multivariate gaussian

- $\boldsymbol{\mu}$: expectation (vector of size d)
- Σ: matrix $d \times d$ of covariance. $\sigma_{ij} = E[(X_i - \mu_i)(X_j - \mu_j)]$



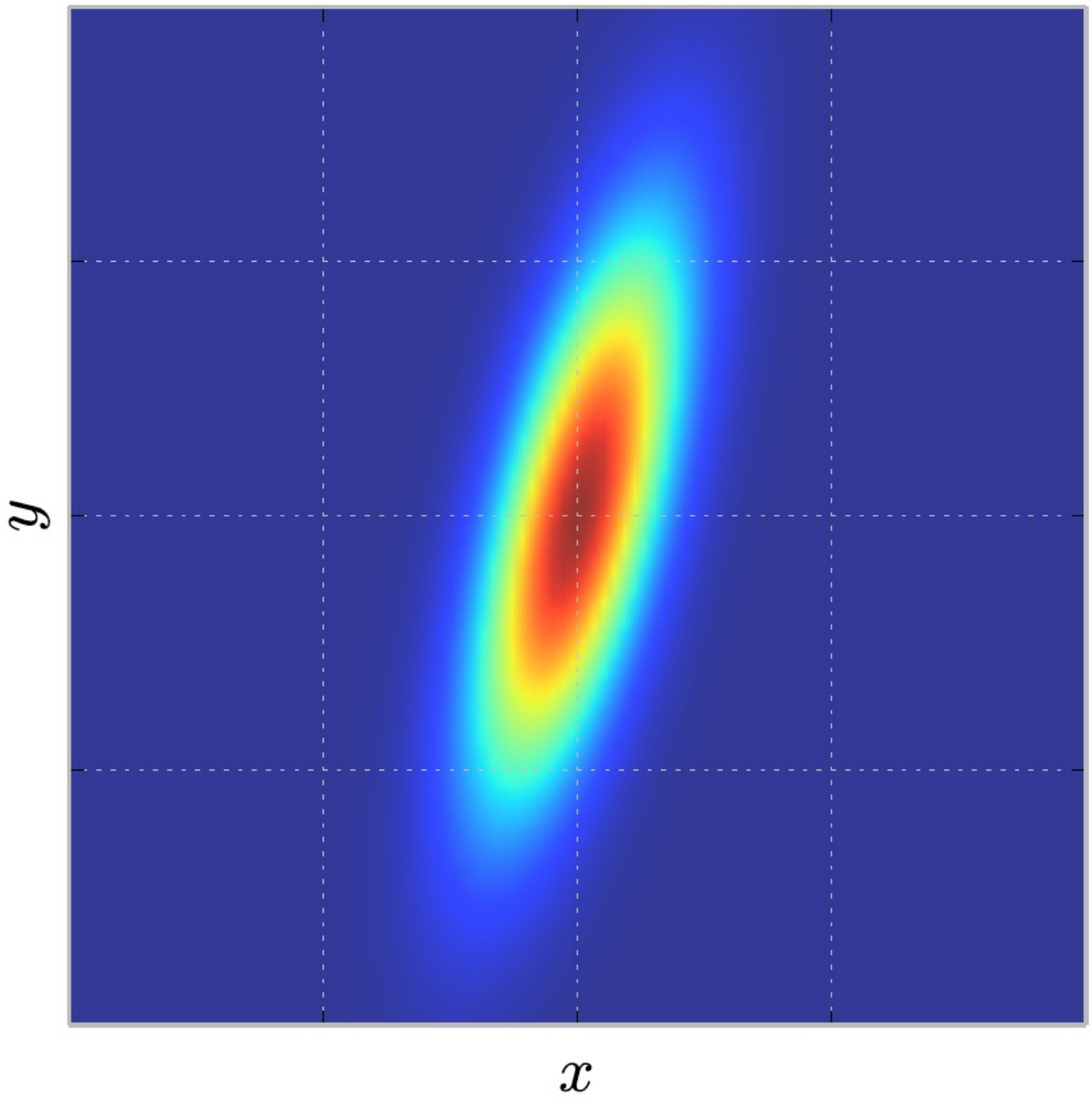
Multivariate gaussian

Mahalanobis distance

- Probability is a function of $\mathbf{x}$ through the quadratic form

$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

- Δ is the Mahalanobis distance from $\boldsymbol{\mu}$ to $\mathbf{x}$: it reduces to the euclidean distance if $\Sigma = \mathbf{I}$.
- Constant probability on the curves (ellipsis) at constant Δ.



Diagonal covariance matrix

Assume a diagonal covariance matrix:

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

then, $|\Sigma| = \sigma_1^2 \sigma_n^2 \dots \sigma_n^2$ and

$$\Sigma^{-1} = \begin{bmatrix} \frac{1}{\sigma_1^2} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sigma_2^2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sigma_n^2} \end{bmatrix}$$

Diagonal covariance matrix

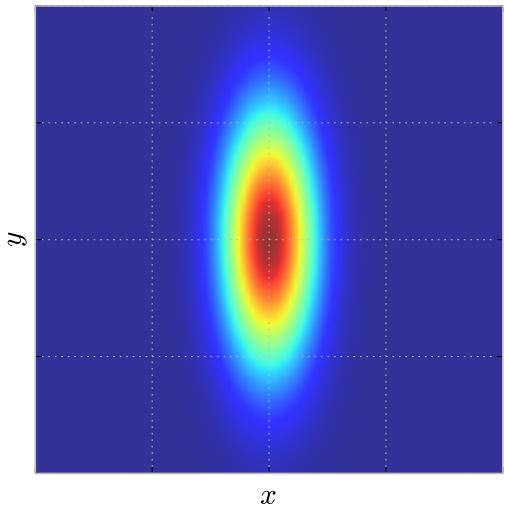
Easy to verify that

$$(\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) = \sum_{i=1}^{n} \frac{(x_i - \mu_i)^2}{\sigma_i^2}$$

and

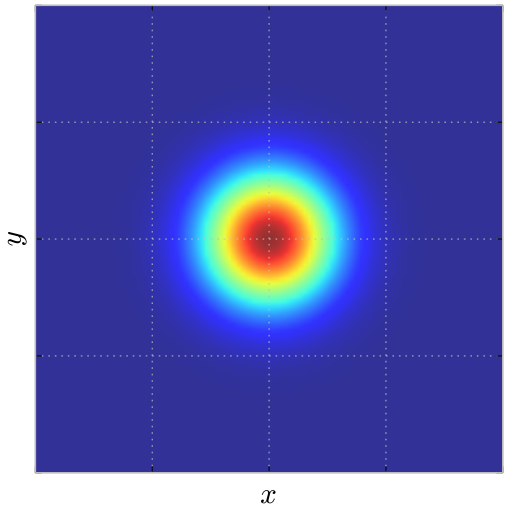
$$f(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{1}{2}\frac{(x_i - \mu_i)^2}{\sigma_i^2}\right)$$

The multivariate distribution turns out to be the product of d univariate gaussians, one for each coordinate x_i.



Identity covariance matrix

The distribution is the product of d "copies" of the same univariate gaussian, one copy for each coordinate x_i.



Spectral properties of Σ

Σ is real and symmetric: then,

1. all its eigenvalues λ_i are in $\mathbb{R}$
2. there exists a corresponding set of orthonormal eigenvectors i (i.e. such that ($i^T j = 1$ if $i = j$ and 0 otherwise)

Multivariate gaussian

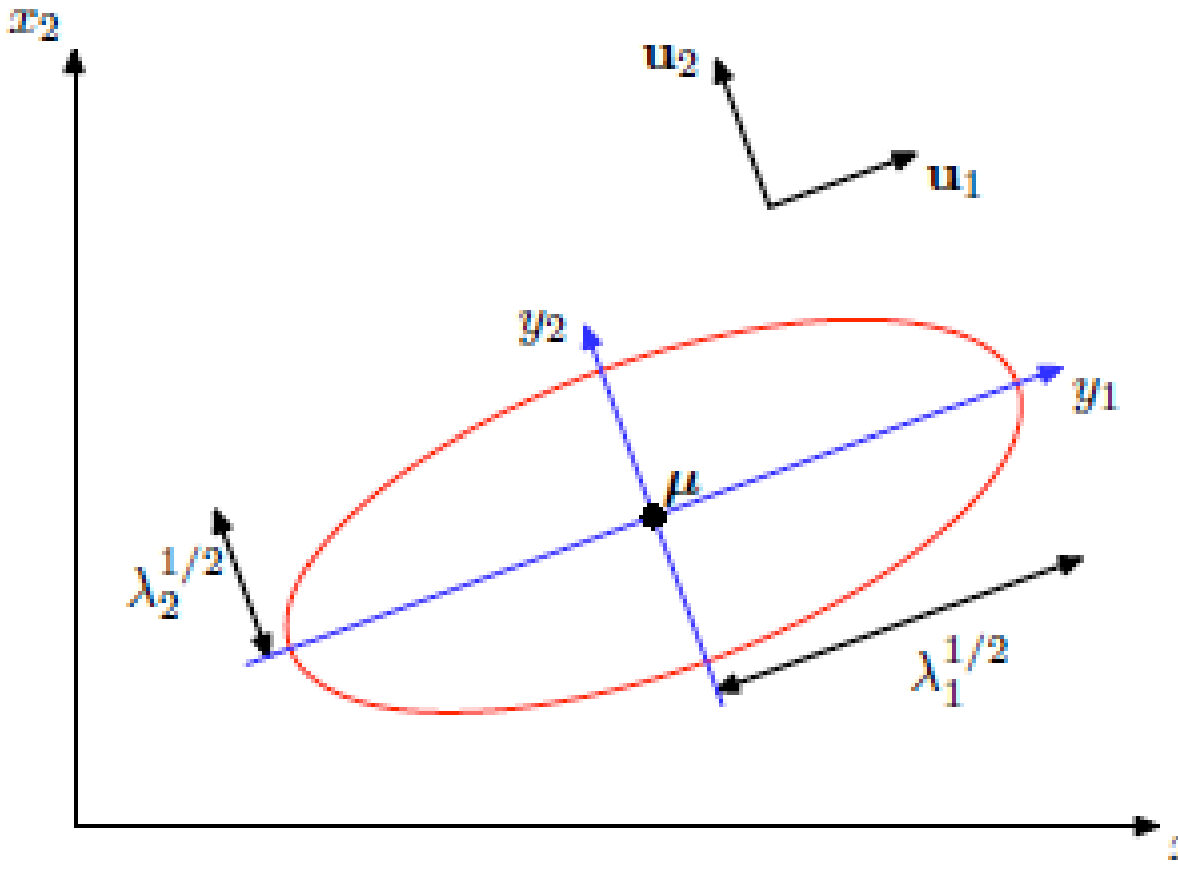
Density as a function of eigenvalues and eigenvectors

Let $y_i = i^T(\mathbf{x} - \boldsymbol{\mu})$ the projection of the vector $\mathbf{x} - \boldsymbol{\mu}$ along the direction of the i-th eigenvector: then

$$f(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\lambda_i}} \exp\left(-\frac{1}{2}\frac{y_i^2}{\lambda_i}\right)$$

Multivariate gaussian

y_i is the scalar product of $\mathbf{x} - \boldsymbol{\mu}$ and the i-th eigenvector i, that is the length of the projection of $\mathbf{x} - \boldsymbol{\mu}$ along the direction of the eigenvector. Since eigenvectors are orthonormal, they are the basis of a new space, and for each vector $\mathbf{x} = (x_1, \ldots, x_d)$, the values $(y_1, \ldots, y_d)$ are the coordinates of $\mathbf{x}$ in the eigenvector space.



Eigenvectors of Σ correspond to the axes of the distribution; each eigenvalue is a scale factor along the axis of the corresponding eigenvector.

Linear transformations

Let $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{A} \in \mathbb{R}^{d \times k}$, $\mathbf{y} = \mathbf{A}^T\mathbf{x} \in \mathbb{R}^k$: then, if $\mathbf{x}$ is normally distributed, so is $\mathbf{y}$.

In particular, if the distribution of $\mathbf{x}$ has mean $\boldsymbol{\mu}$ and covariance matrix Σ, the distribution of $\mathbf{y}$ has mean $\mathbf{A}^T\boldsymbol{\mu}$ and covariance matrix $\mathbf{A}^T\Sigma\mathbf{A}$.

$$\mathrm{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma) \implies \mathrm{y} \sim \mathcal{N}(\mathrm{A}^T\boldsymbol{\mu}, \mathrm{A}^T\Sigma\mathrm{A})$$

Marginal and conditional of a joint gaussian

Let $\mathbf{x}_1 \in \mathbb{R}^h$, $\mathbf{x}_2 \in \mathbb{R}^k$ be such that $\left[\begin{array}{c} \mathbf{x}_1 \\ \hline \mathbf{x}_2 \end{array}\right] \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$ and let

- $\boldsymbol{\mu} = \left[\begin{array}{c} \boldsymbol{\mu}_1 \\ \hline \boldsymbol{\mu}_2 \end{array}\right]$ with $\boldsymbol{\mu}_1 \in \mathbb{R}^h, \boldsymbol{\mu}_2 \in \mathbb{R}^k$
- $\Sigma = \left[\begin{array}{c|c} \Sigma_{11} & \Sigma_{12} \\ \hline \Sigma_{21} & \Sigma_{22} \end{array}\right]$ with $\Sigma_{11} \in \mathbb{R}^{h \times h}$, $\Sigma_{12} \in \mathbb{R}^{h \times k}$, $\Sigma_{21} \in \mathbb{R}^{k \times h}$, $\Sigma_{22} \in \mathbb{R}^{k \times k}$

then

- the marginal distribution of $\mathbf{x}_1$ is $\mathbf{x}_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \Sigma_{11})$

- the conditional distribution of $\mathbf{x}_1$ given $\mathbf{x}_2$ is $\mathbf{x}_1|\mathbf{x}_2 \sim \mathcal{N}(\boldsymbol{\mu}_{1|2}, \Sigma_{1|2})$ with

$$\boldsymbol{\mu}_{1|2} = \boldsymbol{\mu}_1 - \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$$
$$\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$$

Bayes' formula and gaussians

Let $\mathbf{x}, \mathbf{y}$ be such that

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma_1) \qquad \text{and} \qquad \mathbf{y}|\mathbf{x} \sim \mathcal{N}(\mathbf{A}\mathbf{x} + \mathbf{b}, \Sigma_2)$$

That is, the marginal distribution of $\mathbf{x}$ (the prior) is a gaussian and the conditional distribution of $\mathbf{y}$ w.r.t. $\mathbf{x}$ (the likelihood) is also a gaussian with (conditional) mean given by a linear combination on $\mathbf{x}$. Then, both the the conditional distribution of $\mathbf{x}$ w.r.t. $\mathbf{y}$ (the posterior) and the marginal distribution of y (the evidence) are gaussian.

$$\mathbf{y} \sim \mathcal{N}(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \Sigma_2 + \mathbf{A}\Sigma_1\mathbf{A}^T)$$
$$\mathbf{x}|\mathbf{y} \sim \mathcal{N}(\hat{\boldsymbol{\mu}}, \hat{\Sigma})$$

where

$$\hat{\boldsymbol{\mu}} = (\Sigma_1^{-1} + \mathbf{A}^T\Sigma_2^{-1}\mathbf{A})^{-1}(\mathbf{A}^T\Sigma_2^{-1}(\mathbf{y} - \mathbf{b}) + \Sigma_1^{-1}\boldsymbol{\mu})$$
$$\hat{\Sigma} = (\Sigma_1^{-1} + \mathbf{A}^T\Sigma_2^{-1}\mathbf{A})^{-1}$$

3 Bayesian statistics

Bayesian statistics

Classical (frequentist) statistics

- Interpretation of probability as frequence of an event over a sufficiently long sequence of reproducible experiments.
- Parameters seen as constants to determine

Bayesian statistics

- Interpretation of probability as degree of belief that an event may occur.
- Parameters seen as random variables

Bayes' rule

Cornerstone of bayesian statistics is Bayes' rule

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

Given two random variables X, Θ, it relates the conditional probabilities $p(X = x|\Theta = \theta)$ and $p(\Theta = \theta|X = x)$.

Bayesian inference

Given an observed dataset $\mathbf{X}$ and a family of probability distributions $p(x|\Theta)$ with parameter Θ (a probabilistic model), we wish to find the parameter value which best allows to describe $\mathbf{X}$ through the model.

In the bayesian framework, we deal with the distribution probability $p(\Theta)$ of the parameter Θ considered here as a random variable. Bayes' rule states that

$$p(\Theta|\mathbf{X}) = \frac{p(\mathbf{X}|\Theta)p(\Theta)}{p(\mathbf{X})}$$

Bayesian inference

Interpretation

- $p(\Theta)$ stands as the knowledge available about Θ **before** $\mathbf{X}$ is observed (a.k.a. **prior distribution**)
- $p(\Theta|\mathbf{X})$ stands as the knowledge available about Θ **after** $\mathbf{X}$ is observed (a.k.a. **posterior distribution**)
- $p(\mathbf{X}|\Theta)$ measures how much the observed data are coherent to the model, assuming a certain value Θ of the parameter (a.k.a. **likelihood**)
- $p(\mathbf{X}) = \sum_{\Theta'} p(\mathbf{X}|\Theta')p(\Theta')$ is the probability that $\mathbf{X}$ is observed, considered as a mean w.r.t. all possible values of Θ (a.k.a. **evidence**)

Conjugate distributions

Definition

Given a likelihood function $p(y|x)$, a (prior) distribution $p(x)$ is **conjugate** to $p(y|x)$ if the posterior distribution $p(x|y)$ is of the same type as $p(x)$.

Consequence

If we look at $p(x)$ as our knowledge of the random variable x before knowing y and with $p(x|y)$ our knowledge once y is known, the new knowledge can be expressed as the old one.

Examples of conjugate distributions: beta-bernoulli

The Beta distribution is conjugate to the Bernoulli distribution. In fact, given $x \in [0, 1]$ and $y \in \{0, 1\}$, if

$$p(\phi|\alpha, \beta) = \text{Beta}(\phi|\alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}\phi^{\alpha-1}(1-\phi)^{\beta-1}$$
$$p(x|\phi) = \phi^x(1-\phi)^{1-x}$$

then

$$p(\phi|x) = \frac{1}{Z}\phi^{\alpha-1}(1-\phi)^{\beta-1}\phi^x(1-\phi)^{1-x} = \text{Beta}(x|\alpha + x - 1, \beta - x)$$

where Z is the normalization coefficient

$$Z = \int_0^1 \phi^{\alpha+x-1}(1-\phi)^{\beta-x}d\phi = \frac{\Gamma(\alpha + \beta + 1)}{\Gamma(\alpha + x)\Gamma(\beta - x + 1)}$$

Examples of conjugate distributions: beta-binomial

The Beta distribution is also conjugate to the Binomial distribution. In fact, given $x \in [0, 1]$ and $y \in \{0, 1\}$, if

$$p(\phi|\alpha, \beta) = \text{Beta}(\phi|\alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}\phi^{\alpha-1}(1-\phi)^{\beta-1}$$
$$p(k|\phi, N) = \binom{N}{k}\phi^k(1-\phi)^{N-k} = \frac{N!}{(N-k)!k!}\phi^N(1-\phi)^{N-k}$$

then

$$p(\phi|k, N, \alpha, \beta) = \frac{1}{Z}\phi^{\alpha-1}(1-\phi)^{\beta-1}\phi^k(1-\phi)^{N-k} = \text{Beta}(\phi|\alpha + k - 1, \beta + N - k - 1)$$

with the normalization coefficient

$$Z = \int_0^1 \phi^{\alpha+k-1}(1-\phi)^{\beta+N-k-1}d\phi = \frac{\Gamma(\alpha + \beta + N)}{\Gamma(\alpha + k)\Gamma(\beta + N - k)}$$

Multivariate distributions

Multinomial

Generalization of the binomial

$$p(n_1, \ldots, n_K|\phi_1, \ldots, \phi_K, n) = \frac{n!}{\prod_{i=1}^K n_i!}\prod_{i=1}^K \phi_i^{n_i} \qquad \sum_{i=1}^k n_i = n, \sum_{i=1}^k \phi_i = 1$$

the case $n = 1$ is a generalization of the Bernoulli distribution

$$p(x_1, \ldots, x_K|\phi_1, \ldots, \phi_K) = \prod_{i=1}^K \phi_i^{x_i} \qquad \forall i : x_i \in \{0, 1\}, \sum_{i=1}^K x_i = 1, \sum_{i=1}^K \phi_i = 1$$

Likelihood of a multinomial

$$p(\mathbf{X}|\phi_1, \ldots, \phi_K) \propto \prod_{i=1}^N \prod_{j=1}^K \phi_j^{x_{ij}} = \prod_{j=1}^K \phi_j^{N_j}$$

Conjugate of the multinomial

Dirichlet distribution

The conjugate of the multinomial is the Dirichlet distribution, generalization of the Beta to the case $K > 2$

$$p(\phi_1, \ldots, \phi_K|\alpha_1, \ldots, \alpha_K) = \text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha}) = \frac{\Gamma(\sum_{i=1}^K \alpha_i)}{\prod_{i=1}^K \Gamma(\alpha_i)}\prod_{i=1}^K \phi_i^{\alpha_i-1}$$
$$= \frac{1}{Z}\prod_{i=1}^K \phi_i^{\alpha_i-1}$$

with $\alpha_i > 0$ for $i = 1, \ldots, K$

Random variables and Dirichlet distribution

A random variable $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_K)$ with Dirichlet distribution takes values on the $K-1$ dimensional simplex (set of points $\mathbf{x} \in \mathbb{R}^K$ such that $x_i \geq 0$ for $i = 1, \ldots, K$ and $\sum_{i=1}^K x_i = 1$)

Examples of conjugate distributions: dirichlet-multinomial

Assume $\boldsymbol{\phi} \sim \text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha})$ and $z \sim \text{Mult}(z|\boldsymbol{\phi})$. Then,

$$p(\boldsymbol{\phi}|z, \boldsymbol{\alpha}) = \frac{p(z|\boldsymbol{\phi})p(\boldsymbol{\phi}|\boldsymbol{\alpha})}{p(z|\boldsymbol{\alpha})} = \frac{1}{Z}\prod_{i=1}^K \phi_i^{z_i}\prod_{i=1}^K \phi_i^{\alpha_i - 1}$$
$$= \frac{1}{Z}\prod_{i=1}^K \phi_i^{\alpha_i + z_i - 1} = \text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha}')$$

where $\boldsymbol{\alpha}' = (\alpha_1 + z_1, \ldots, \alpha_K + z_K)$

Text modeling

Unigram model

Collection $\mathbf{W}$ of N term occurrences: N observations of a same random variable, with multinomial distribution over a dictionary $\mathbf{V}$ of size V.

$$p(\mathbf{W}|\boldsymbol{\phi}) = L(\boldsymbol{\phi}|\mathbf{W}) = \prod_{i=1}^V \phi_i^{N_i} \qquad \sum_{i=1}^V \phi_i = 1, \sum_{i=1}^V N_i = N$$

Parameter model

Use of a Dirichlet distribution, conjugate to the multinomial

$$p(\boldsymbol{\phi}|\boldsymbol{\alpha}) = \text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha})$$
$$p(\boldsymbol{\phi}|\mathbf{W}, \boldsymbol{\alpha}) = \text{Dir}(\boldsymbol{\phi}|\boldsymbol{\alpha} + \mathbf{N})$$

Information theory

Let X be a discrete random variable:

- define a measure $h(x)$ of the information (surprise) of observing $X = x$
- requirements:
  - likely events provide low surprise, while rare events provide high surprise: $h(x)$ is inversely proportional to $p(x)$
  - X, Y independent: the event $X = x, Y = y$ has probability $p(x)p(y)$. Its surprise is the sum of the surprise for $X = x$ and for $Y = y$, that is, $h(x, y) = h(x) + h(y)$ (information is additive)

  this results into $h(x) = -\log x$ (usually base 2)

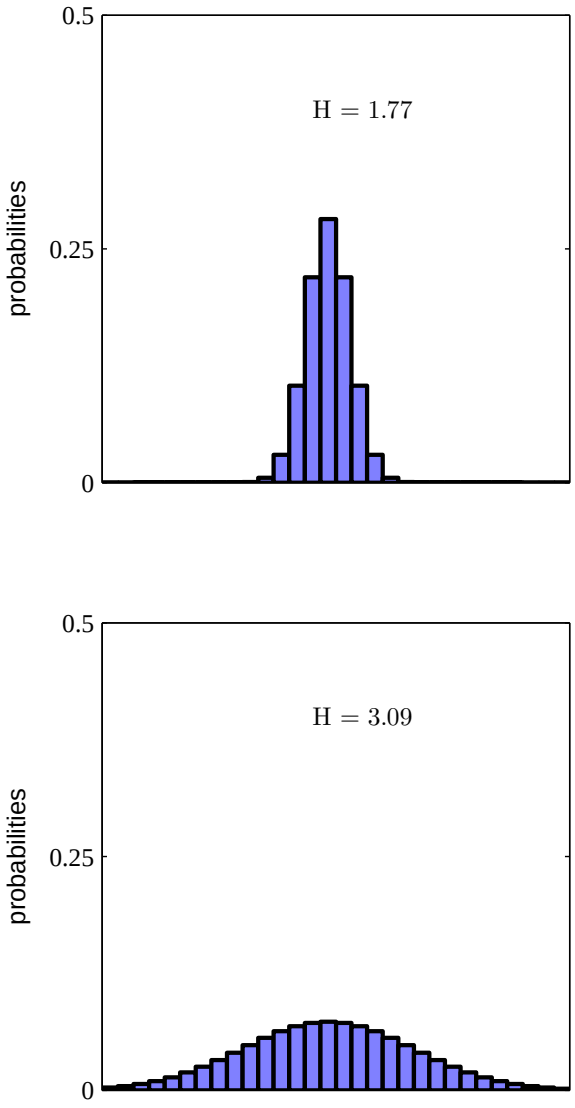
Entropy

A sender transmits the value of X to a receiver: the expected amount of information transmitted (w.r.t. $p(x)$) is the entropy of X

$$H(x) = -\sum_x p(x) \log_2 p(x)$$

- lower entropy results from more sharply peaked distributions
- the uniform distribution provides the highest entropy

Entropy is a measure of disorder.



Entropy, some properties

- $p(x) \in [0, 1]$ implies $p(x) \log_2 p(x) \leq 0$ and $H(X) \geq 0$
- $H(X) = 0$ if there exists x such that $p(x) = 1$

Maximum entropy

Given a fixed number k of outcomes, the distribution $p_1, \ldots, p_k$ with maximum entropy is derived by maximizing $H(X)$ under the constraint $\sum_{i=1}^{k} p_i = 1$. By using Lagrange multipliers, this amounts to maximizing

$$-\sum_{i=1}^{k} p_i \log_2 p_i + \lambda \left(\sum_{i=1}^{k} p_i - 1 \right)$$

Setting the derivative of each p_i to 0,

$$0 = -\log_2 p_i - \log_2 e + \lambda$$

results into $p_i = 2^{\lambda} - e$ for each i, that is into the uniform distribution $p_i = \frac{1}{k}$ and $H(X) = \log_2 k$

Entropy, some properties

$H(X)$ is a lower bound on the expected number of bits needed to encode the values of X

- trivial approach: code of length $\log_2 k$ (assuming uniform distribution of values for X)
- for non-uniform distributions, better coding schemes by associating shorter codes to likely values of X

Conditional entropy

Let X, Y be discrete r.v. : for a pair of values x, y the additional information needed to specify y if x is known is $-\ln p(y|x)$.

The expected additional information needed to specify the value of Y if we assume the value of X is known is the **conditional entropy** of Y given X

$$H(Y|X) = -\sum_{x} \sum_{y} p(x, y) \ln p(y|x)$$

Clearly, since $\ln p(y|x) = \ln p(x, y) - \ln p(x)$

$$H(X, Y) = H(Y|X) + H(X)$$

that is, the information needed to describe (on the average) the values of X and Y is the sum of the information needed to describe the value of X plus that needed to describe the value of Y is X is known.

KL divergence

Assume the distribution $p(x)$ of X is unknown, and we have modeled is as an approximation $q(x)$.

If we use $q(x)$ to encode values of X we need an average length $-\sum_x p(x) \ln q(x)$, while the minimum (known $p(x)$) is $-\sum_x p(x) \ln p(x)$.

The additional amount of information needed, due to the approximation of $p(x)$ through $q(x)$ is the **Kullback-Leibler divergence**

$$\begin{aligned} KL(p||q) &= -\sum_{x} p(x) \ln q(x) + \sum p(x) \ln p(x) \\ &= -\sum_{x} p(x) \ln \frac{q(x)}{p(x)} \end{aligned}$$

$KL(p||q)$ measures the difference between the distributions p and q.

- $KL(p||p) = 0$
- $KL(p||q) \neq KL(q||p)$: the function is not symmetric, it is not a distance (it would be $d(x, y) = d(y, x)$)

Applying KL divergence

- $\mathbf{x} = (x_1, \ldots, x_n)$, dataset generated by a unknown distribution $p(x)$
- we want to infer the parameters of a probabilistic model $q_\theta(x|\theta)$
- approach: minimize

$$\begin{aligned} KL(p||q_\theta) &= -\sum_x p(x) \ln \frac{q(x|\theta)}{p(x)} \\ &\approx -\frac{1}{n}\sum_{i=1}^{n} \ln \frac{q(x_i|\theta)}{p(x_i)} \\ &= \frac{1}{n}\sum_{i=1}^{n} (\ln p(x_i) - \ln q(x_i|\theta)) \end{aligned}$$

First term is independent of θ, while the second one is the negative log-likelihood of $\mathbf{x}$. The value of θ which minimizes $KL(p||q_\theta)$ also maximizes the log-likelihood.

Mutual information

- Measure of the independence between X and Y

$$I(X,Y) = KL(p(X,Y)||p(X),p(Y)) = -\sum_x \sum_y p(x,y) \ln \frac{p(x)p(y)}{p(x,y)}$$

additional encoding length if independence is assumed

- We have:

$$\begin{aligned} I(X,Y) &= -\sum_x \sum_y p(x,y) \ln \frac{p(x)p(y)}{p(x,y)} \\ &= -\sum_x \sum_y p(x,y) \ln \frac{p(x)p(y)}{p(x|y)p(y)} \\ &= -\sum_x \sum_y p(x,y) \ln \frac{p(x)}{p(x|y)} \\ &= -\sum_x \sum_y p(x,y) \ln p(x) + \sum_x \sum_y p(x,y) \ln p(x|y) = H(X) - H(X|Y) \end{aligned}$$

- Similarly, it derives $I(X,Y) = H(Y) - H(Y|X)$