

Probability recall

Course of Machine Learning
Master Degree in Computer Science
University of Rome "Tor Vergata"
a.a. 2021-2022

Giorgio Gambosi

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,

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

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

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

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,

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

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 ($X \perp\!\!\!\perp Y | Z$) 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 $f(x) = \frac{dF(x)}{dx}$. 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: $g(x) = x$

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

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

$$\text{Var}[X] = E[(x - E[x])^2]$$

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:

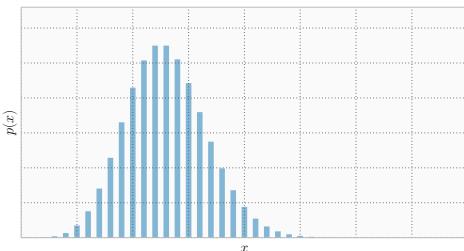
- $\text{Var}[a] = 0$ for each $a \in \mathbb{R}$
- $\text{Var}[af(x)] = a^2\text{Var}[f(x)]$ for each $a \in \mathbb{R}$

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 $A \subseteq V_X$

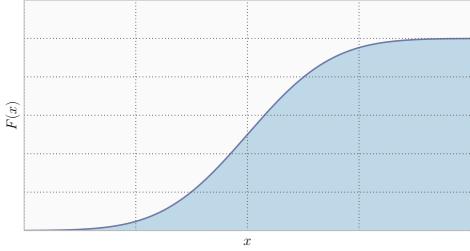


Some definitions

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:

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



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

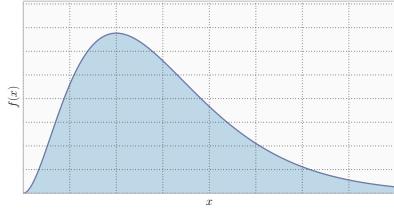
$$f(x) = \frac{dF(x)}{dx}$$

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 $x \sim Bernoulli(p)$, 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

$$E[x] = p \quad \text{Var}[x] = p(1-p)$$

Extension to multiple outcomes

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

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

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

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

Binomial distribution

Definition

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

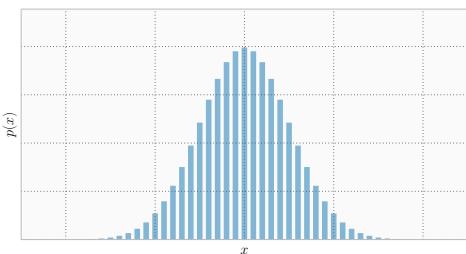
$$p(x) = \binom{n}{x} p^x (1-p)^{n-x} = \frac{n!}{x!(n-x)!} p^x (1-p)^{n-x}$$

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

Mean and variance

$$E[x] = np$$

$$\text{Var}[x] = np(1-p)$$



Poisson distribution

Definition

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

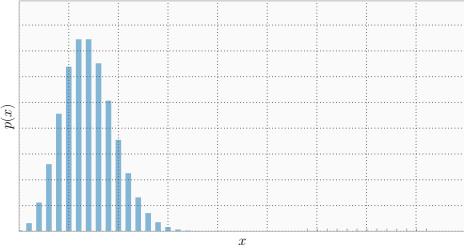
$$p(x) = e^{-\lambda} \frac{\lambda^x}{x!}$$

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

Mean and variance

$$E[x] = \lambda$$

$$\text{Var}[x] = \lambda$$



Normal (gaussian) distribution

Definition

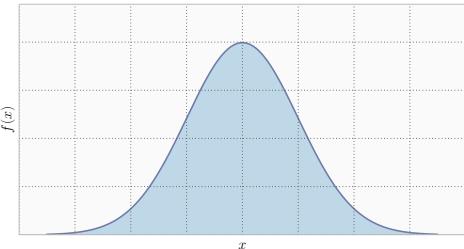
Let $x \in \mathbb{R}$, then $x \sim \text{Normal}(\mu, \sigma^2)$, with $\mu, \sigma \in \mathbb{R}, \sigma \geq 0$, if

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

Mean and variance

$$E[x] = \mu$$

$$\text{Var}[x] = \sigma^2$$



Beta distribution

Definition

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

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

where

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

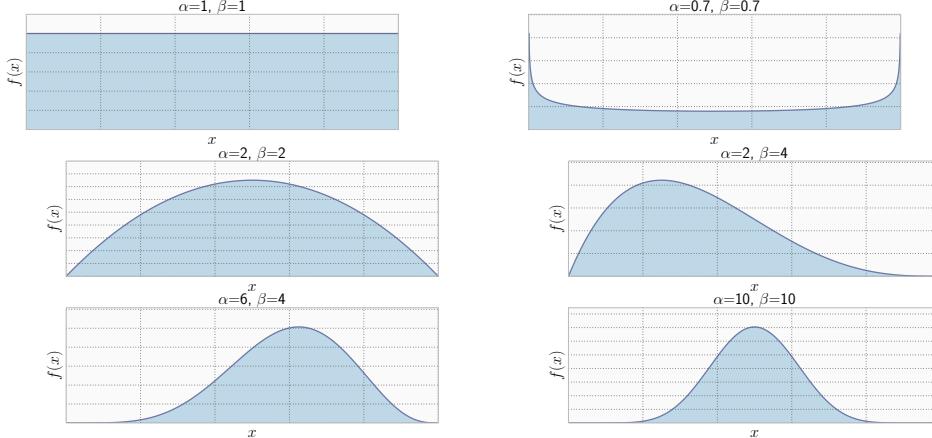
is a generalization of the factorial to the real field \mathbb{R} : in particular, $\Gamma(n) = (n-1)!$ if $n \in \mathbb{N}$

Mean and variance

$$E[x] = \frac{\beta}{\alpha + \beta}$$

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

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

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

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

Covariance

Definition

$$\text{Cov}[X, Y] = E[(X - E[X])(Y - E[Y])]$$

As for the variance, we may derive

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

Moreover, the following properties hold:

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

Random vectors

Definition

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

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

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 $1 \leq i, j \leq n$, $\Sigma_{ij} = \text{Cov}[X_i, X_j] = E[(X_i - \mu_i)(X_j - \mu_j)]$, where $\mu_i = E[X_i]$, $\mu_j = E[X_j]$.

Hence,

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

Covariance matrix

By definition of covariance,

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

where $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n)^T$ is the vector of expectations of the random variables X_1, \dots, 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: $\text{Cov}[X_i, X_j] = \text{Cov}[X_j, X_i]$ for $1 \leq i, j \leq n$

Correlation

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

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

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

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

and, since

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

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, $\text{Cov}[X, Y] = 0$ and $\rho_{X,Y} = 0$. That is, independent variables have null covariance and correlation.

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

Correlation matrix

The correlation matrix of $(X_1, \dots, X_n)^T$ 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 $x_i \in \mathbf{N}$ for $i = 1, \dots, k$, then $(x_1, \dots, x_k) \sim Mult(n, p_1, \dots, p_k)$ with $0 \leq p \leq 1$, if

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

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

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

Mean and variance

$$E[x_i] = np_i \quad \text{Var}[x_i] = np_i(1 - p_i) \quad i = 1, \dots, k$$

Dirichlet distribution

Definition

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

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

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

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

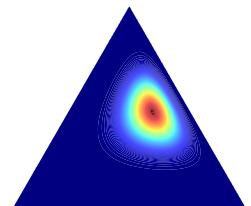
A random variable $\phi = (\phi_1, \dots, \phi_K)$ with Dirichlet distribution takes values on the $K - 1$ dimensional simplex (set of points $\mathbf{x} \in \mathbf{R}^K$ such that $x_i \geq 0$ for $i = 1, \dots, K$ and $\sum_{i=1}^K x_i = 1$)

Mean and variance

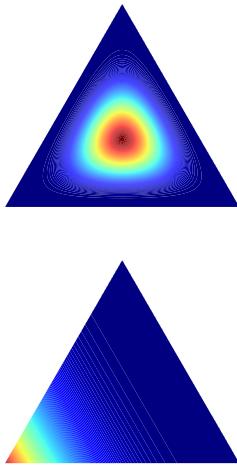
$$E[x_i] = \frac{\alpha_i}{\alpha_0} \quad \text{Var}[x_i] = \frac{\alpha_i(\alpha_0 - \alpha_i)}{\alpha_0^2(\alpha_0 + 1)} \quad i = 1, \dots, k$$

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 $i = 1, \dots, K$

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

Mean and variance

In this case,

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

2 The normal distribution

Gaussian distribution

- Properties

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

Univariate gaussian

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

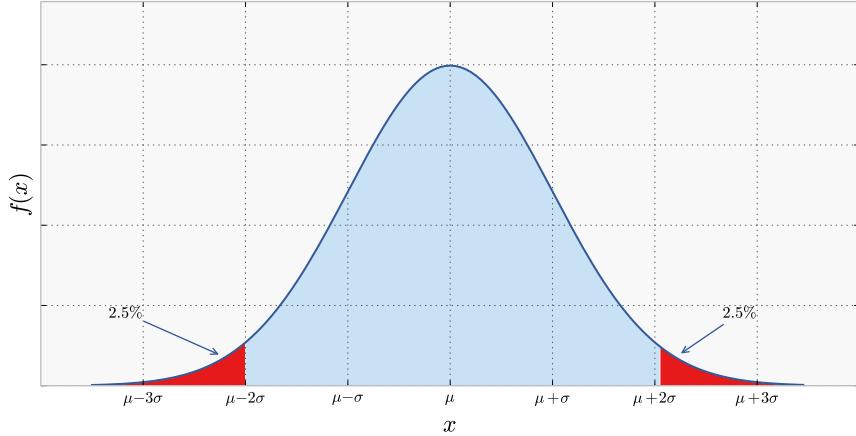
$$\begin{aligned} p(x) &= \mathcal{N}(\mu, \sigma^2) \\ &= \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \end{aligned}$$

with

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

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

Univariate gaussian



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

Multivariate gaussian

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

$$p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \Sigma)$$

$$= \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} e^{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})}$$

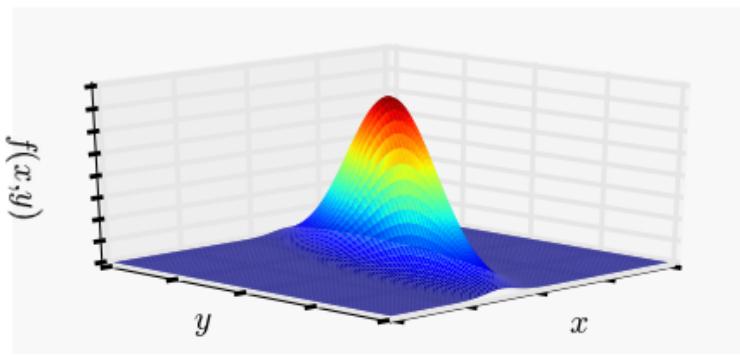
where

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

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

Multivariate gaussian

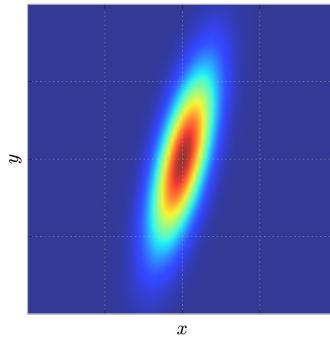
- $\boldsymbol{\mu}$: expectation (vector of size d)
- Σ : matrix $d \times d$ of covariance. $\sigma_{ij} = E[(X_i - \mu_i)(X_j - \mu_j)]$



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 .



Multivariate gaussian

In general,

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = (\mathbf{x}^T \mathbf{A} \mathbf{x})^T = \mathbf{x}^T \mathbf{A}^T \mathbf{x}$$

this implies that

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} + \frac{1}{2} \mathbf{x}^T \mathbf{A}^T \mathbf{x} = \mathbf{x}^T \left(\frac{1}{2} \mathbf{A} + \frac{1}{2} \mathbf{A}^T \right) \mathbf{x}$$

- $\mathbf{A} + \mathbf{A}^T$ is necessarily symmetric, as a consequence, Σ is symmetric
- as a consequence, its inverse Σ^{-1} does exist.

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, $|\Sigma| = \sigma_1^2 \sigma_2^2 \dots \sigma_n^2$ 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

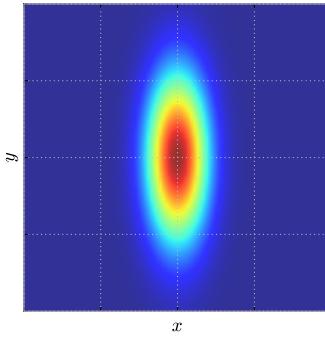
Easy to verify that

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

and

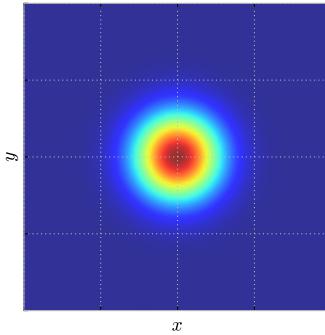
$$f(\mathbf{x} | \boldsymbol{\mu}, \Sigma) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_i)^2}{\sigma_i^2}\right)$$

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 \mathbf{u}_i (i.e. such that $(\mathbf{u}_i^T \mathbf{u}_j = 1$ if $i = j$ and 0 otherwise)

Let us define the $d \times d$ matrix \mathbf{U} whose columns correspond to the orthonormal eigenvectors

$$\mathbf{U} = \begin{pmatrix} & & \\ \mathbf{u}_1 & \cdots & \mathbf{u}_2 \\ & & \end{pmatrix} \mathbf{u}_d$$

and the diagonal $d \times d$ matrix Λ with eigenvalues on the diagonal

$$\Lambda = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \lambda_3 & \\ & & & 0 \\ 0 & & & & \ddots & \\ & & & & & \lambda_d \end{bmatrix}$$

Multivariate gaussian

Decomposition of Σ

By the definition of \mathbf{U} and Λ , and since $\Sigma \mathbf{u}_i = \mathbf{u}_i \lambda_i$ for all $i = 1, \dots, d$, we may write

$$\Sigma \mathbf{U} = \mathbf{U} \Lambda$$

Since the eigenvectors u_i are orthonormal, $\mathbf{U}^{-1} = \mathbf{U}^T$ by the properties of orthonormal matrices: as a consequence ,

$$\Sigma = \mathbf{U} \Lambda \mathbf{U}^{-1} = \mathbf{U} \Lambda \mathbf{U}^T = \sum_{i=1}^d \lambda_i \mathbf{u}_i \mathbf{u}_i^T$$

Then, its inverse matrix is a diagonal matrix itself

$$\Sigma^{-1} = \sum_{i=1}^d \frac{1}{\lambda_i} \mathbf{u}_i \mathbf{u}_i^T$$

Multivariate gaussian

Density as a function of eigenvalues and eigenvectors

As shown before,

$$\begin{aligned} \Delta^2 &= (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) = (\mathbf{x} - \boldsymbol{\mu})^T \sum_{i=1}^d \frac{1}{\lambda_i} \mathbf{u}_i \mathbf{u}_i^T (\mathbf{x} - \boldsymbol{\mu}) \\ &= \sum_{i=1}^d \frac{1}{\lambda_i} (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{u}_i \mathbf{u}_i^T (\mathbf{x} - \boldsymbol{\mu}) = \sum_{i=1}^d \frac{1}{\lambda_i} (\mathbf{u}_i^T (\mathbf{x} - \boldsymbol{\mu}))^T \mathbf{u}_i^T (\mathbf{x} - \boldsymbol{\mu}) \\ &= \sum_{i=1}^d \frac{(\mathbf{u}_i^T (\mathbf{x} - \boldsymbol{\mu}))^2}{\lambda_i} \end{aligned}$$

Let $y_i = \mathbf{u}_i^T (\mathbf{x} - \boldsymbol{\mu})$: then

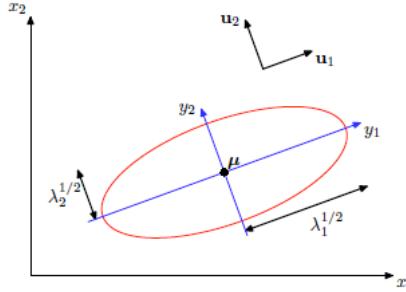
$$(\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) = \sum_{i=1}^n \frac{y_i^2}{\lambda_i}$$

and

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

Multivariate gaussian

y_i is the scalar product of $\mathbf{x} - \mu$ and the i -th eigenvector \mathbf{u}_i , that is the length of the projection of $\mathbf{x} - \mu$ along the direction of the eigenvector. Since eigenvectors are orthonormal, they are the basis of a new space, and for each vector $\mathbf{x} = (x_1, \dots, x_d)$, the values (y_1, \dots, 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 μ and covariance matrix Σ , the distribution of \mathbf{y} has mean $\mathbf{A}^T \mu$ and covariance matrix $\mathbf{A}^T \Sigma \mathbf{A}$.

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

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 $\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma)$ and let

- $\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$ with $\mu_1 \in \mathbb{R}^h$, $\mu_2 \in \mathbb{R}^k$
- $\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$ 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 $\mathbf{x}_1 \sim \mathcal{N}(\mu_1, \Sigma_{11})$
- the conditional distribution of \mathbf{x}_1 given \mathbf{x}_2 is $\mathbf{x}_1 | \mathbf{x}_2 \sim \mathcal{N}(\mu_{1|2}, \Sigma_{1|2})$ with

$$\mu_{1|2} = \mu_1 - \Sigma_{12} \Sigma_{22}^{-1} (\mathbf{x}_2 - \mu_2)$$

$$\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$$

Bayes' formula and gaussians

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

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

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 conditional distribution of \mathbf{x} w.r.t. \mathbf{y} (the posterior) and the marginal distribution of y (the evidence) are gaussian.

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

$$\mathbf{x} | \mathbf{y} \sim \mathcal{N}(\hat{\mu}, \hat{\Sigma})$$

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 frequency 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

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

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

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

Likelihood of a multinomial

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

Conjugate of the multinomial

Dirichlet distribution

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

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

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

Random variables and Dirichlet distribution

A random variable $\phi = (\phi_1, \dots, \phi_K)$ 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 $i = 1, \dots, K$ and $\sum_{i=1}^K x_i = 1$)

Examples of conjugate distributions: dirichlet-multinomial

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

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

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

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 .

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

Parameter model

Use of a Dirichlet distribution, conjugate to the multinomial

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

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)

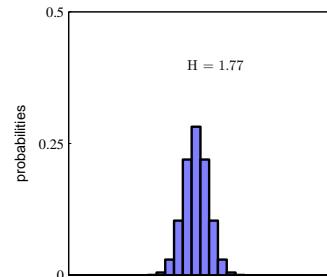
this results into $h(x) = -\log_2 p(x)$ (usually base 2)

Entropy

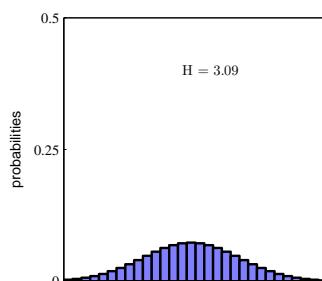
A sender transmits the value of X to a receiver: the expected amount of information transmitted (w.r.t. $p(x)$) is the **entropy** of X

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

- 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, \dots, 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 if X is known.

KL divergence

Assume the distribution $p(x)$ of X is unknown, and we have modeled it 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

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

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

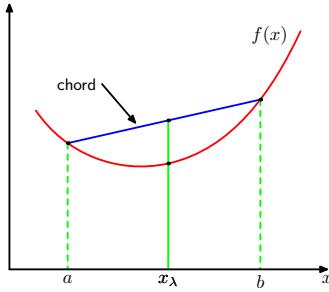
- $KL(p||p) = 0$
- $KL(p||q) \neq KL(q||p)$: the function is not symmetric, it is not a distance (it would be $d(x, y) = d(y, x)$)

Convexity

A function is convex (in an interval $[a, b]$) if, for all $0 \leq \lambda \leq 1$, the following inequality holds

$$f(\lambda a + (1 - \lambda)b) \leq \lambda f(a) + (1 - \lambda)f(b)$$

- $\lambda a + (1 - \lambda)b$ is a point $x \in [a, b]$ and $f(\lambda a + (1 - \lambda)b)$ is the corresponding value of the function
- $\lambda f(a) + (1 - \lambda)f(b) = f(x)$ is the value at $\lambda a + (1 - \lambda)b$ of the chord from $(a, f(a))$ to $(b, f(b))$.



Jensen's inequality and KL divergence

- If $f(x)$ is a convex function, the *Jensen's inequality* holds for any set of points x_1, \dots, x_M

$$f\left(\sum_{i=1}^M \lambda_i x_i\right) \leq \sum_{i=1}^M \lambda_i f(x_i)$$

where $\lambda_i \geq 0$ for all i and $\sum_{i=1}^M \lambda_i = 1$.

- In particular, if $\lambda_i = p(x_i)$,

$$f(E[x]) \leq E[f(x)]$$

- if x is a continuous variable, this results into

$$f\left(\int x p(x) dx\right) \leq \int f(x) p(x) dx$$

- applying the inequality to $KL(p||q)$, since the logarithm is convex,

$$KL(p||q) = - \int p(x) \ln \frac{q(x)}{p(x)} dx \geq - \ln \int q(x) dx = 0$$

thus proving the KL is always non-negative.

Applying KL divergence

- $\mathbf{x} = (x_1, \dots, x_n)$, 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 $I(X, Y) = H(Y) - H(Y|X)$