Probability and Distribution Refresher

Korbinian Strimmer

8 January 2024

Contents

W	elcom		5		
	Upd	ates	5		
	Lice	nse	5		
Pr	eface		7		
	Abo	ut the author	7		
	Abo	ut the notes	7		
1	Combinatorics				
	1.1	Some basic mathematical notation	9		
	1.2	Number of permutations	9		
	1.3	Multinomial and binomial coefficient	10		
	1.4	De Moivre-Sterling approximation of the factorial	10		
2	Probability 1				
	2.1	Random variables	11		
	2.2	Probability mass and density function	12		
	2.3		12		
	2.4	Families of distributions	13		
	2.5	Expectation of a random variable	14		
	2.6	Jensen's inequality for the expectation	14		
	2.7		14		
	2.8		15		
	2.9	Distribution of sums of random variables	15		
	2.10	Transformation of random variables	15		
	2.11	Random vectors and their mean and variance	16		
	2.12	Correlation matrix	16		
3	Univariate distributions 1				
	3.1	Bernoulli distribution	19		
	3.2	Binomial distribution	20		
	3.3		21		
	3.4	Normal distribution	23		

4 CONTENTS

	3.6	Gamma distribution and special cases	27
4	Mul	tivariate distributions	33
	4.1	Categorical distribution	33
	4.2	Multinomial distribution	34
	4.3	Dirichlet distribution	35
	4.4	Multivariate normal distribution	37
	4.5	Wishart distribution	38
	4.6	Inverse Wishart distribution	39

Welcome

The Probability and Distribution Refresher notes were written by Korbinian Strimmer from 2018–2024. This version is from 8 January 2024.

If you have any questions, comments, or corrections then please email me at korbinian.strimmer@manchester.ac.uk.

Updates

The notes will be updated from time to time. To view the current version visit the online version of the Probability and Distribution Refresher notes.

You may also wish to download the Probability and Distribution Refresher notes as PDF in A4 format for printing (double page layout) or as 6x9 inch PDF for use on tablets (single page layout).

License

These notes are licensed to you under Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International License.

5

6 CONTENTS

Preface

About the author

Hello! My name is Korbinian Strimmer and I am a Professor in Statistics. I am a member of the Statistics group at the Department of Mathematics of the University of Manchester. You can find more information about me on my home page.

About the notes

These supplementary notes aim to provide a quick refresher of some essentials in combinatorics and probability as well as to offer an overview over selected univariate and multivariate distributions.

The notes are supporting information for a number of lecture notes of statistical courses I am or have been teaching at the Department of Mathematics of the University of Manchester.

This includes the current modules:

- MATH27720 Statistics 2: Likelihood and Bayes and
- MATH38161 Multivariate Statistics

as well as the retired module (not offered any more):

• MATH20802 Statistical Methods.

8 CONTENTS

Chapter 1

Combinatorics

1.1 Some basic mathematical notation

Summation:

$$\sum_{i=1}^{n} x_i = x_1 + x_2 + \ldots + x_n$$

Multiplication:

$$\prod_{i=1}^{n} x_i = x_1 \times x_2 \times \ldots \times x_n$$

Indicator function:

$$1_A = \begin{cases} 1 & \text{if } A \text{ is true} \\ 0 & \text{if } A \text{ is not true} \end{cases}$$

1.2 Number of permutations

The number of possible orderings, or permutations, of n distinct items is the number of ways to put n items in n bins with exactly one item in each bin. It is given by the **factorial**

$$n! = \prod_{i=1}^{n} i = 1 \times 2 \times \ldots \times n$$

where n is a positive integer. For n=0 the factorial is defined as

$$0! = 1$$

as there is exactly one permutation of zero objects.

The factorial can also be obtained using the gamma function

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$$

which can be viewed as continuous version of the factorial with $\Gamma(x) = (x - 1)!$ for any positive integer x.

1.3 Multinomial and binomial coefficient

The number of possible permutation of n items of K distinct types, with n_1 of type 1, n_2 of type 2 and so on, equals the number of ways to put n items into K bins with n_1 items in the first bin, n_2 in the second and so on. It is given by the **multinomial** coefficient

$$\binom{n}{n_1,\ldots,n_K} = \frac{n!}{n_1! \times n_2! \times \ldots \times n_K!}$$

with $\sum_{k=1}^{K} n_k = n$ and $K \le n$. Note that it equals the number of permutation of all items divided by the number of permutations of the items in each bin (or of each type).

If all $n_k = 1$ and hence K = n the multinomial coefficient reduces to the factorial.

If there are only two bins / types (K = 2) the multinomial coefficients becomes the **binomial coefficient**

$$\binom{n}{n_1} = \binom{n}{n_1, n - n_1} = \frac{n!}{n_1!(n - n_1)!}$$

which counts the number of ways to choose n_1 elements from a set of n elements.

1.4 De Moivre-Sterling approximation of the factorial

The factorial is frequently approximated by the following formula derived by Abraham de Moivre (1667–1754) and James Stirling (1692-1770)

$$n! \approx \sqrt{2\pi} n^{n + \frac{1}{2}} e^{-n}$$

or equivalently on logarithmic scale

$$\log n! \approx \left(n + \frac{1}{2}\right) \log n - n + \frac{1}{2} \log (2\pi)$$

The approximation is good for small n (but fails for n=0) and becomes more and more accurate with increasing n. For large n the approximation can be simplified to

$$\log n! \approx n \log n - n$$

Chapter 2

Probability

2.1 Random variables

A random variable describes a random experiment. The set of all possible outcomes is the **sample space** or **state space** of the random variable and is denoted by $\Omega = \{\omega_1, \omega_2, \ldots\}$. The outcomes ω_i are the **elementary events**. The sample space Ω can be finite or infinite. Depending on type of outcomes the random variable is **discrete** or **continuous**.

An event $A \subseteq \Omega$ is a subset of Ω and thus itself a set composed of elementary events: $A = \{a_1, a_2, \ldots\}$. This includes as special cases the full set $A = \Omega$, the empty set $A = \emptyset$, and the elementary events $A = \omega_i$. The complementary event A^C is the complement of the set A in the set Ω so that $A^C = \Omega \setminus A = \{\omega_i \in \Omega : \omega_i \notin A\}$.

The probability of an event A is denoted by Pr(A). Essentially, to obtain this probability we need to count the elementary elements corresponding to A. To do this we assume as axioms of probability that

- $Pr(A) \ge 0$, probabilities are positive,
- $Pr(\Omega) = 1$, the certain event has probability 1, and
- $\Pr(A) = \sum_{a_i \in A} \Pr(a_i)$, the probability of an event equals the sum of its constituting elementary events a_i . This sum is taken over a finite or countable infinite number of elements.

This implies

- $Pr(A) \le 1$, i.e. probabilities all lie in the interval [0,1]
- $Pr(A^C) = 1 Pr(A)$, and
- $Pr(\emptyset) = 0$

Assume now that we have two events A and B. The probability of the event "A and B" is then given by the probability of the set intersection $Pr(A \cap B)$. Likewise

the probability of the event "A or B" is given by the probability of the set union $Pr(A \cup B)$.

From the above it is clear that the definition and theory of probability is closely linked to set theory, and in particular to measure theory. Indeed, viewing probability as a special type of measure allows for an elegant treatment of both discrete and continuous random variables.

2.2 Probability mass and density function

To describe a random variable x with state space Ω we need a way to effectively store the probabilities of the corresponding elementary outcomes $x \in \Omega$. Note that for convenience we use the same symbol to denote the random variable and its elementary outcomes.

For a discrete random variable we define the event $A = \{x : x = a\} = \{a\}$ and get the probability

$$Pr(A) = Pr(x = a) = f(a)$$

directly from the **probability mass function** (PMF), here denoted by lower case f (but we frequently also use p or q). The PMF has the property that $\sum_{x \in \Omega} f(x) = 1$ and that $f(x) \in [0,1]$.

For continuous random variables we need to use a **probability density function** (PDF) instead. We define the event $A = \{x : a < x \le a + da\}$ as an infinitesimal interval and then assign the probability

$$Pr(A) = Pr(a < x \le a + da) = f(a)da.$$

The PDF has the property that $\int_{x \in \Omega} f(x) dx = 1$ but in contrast to a PMF the density $f(x) \ge 0$ may take on values larger than 1.

The set of all x for which f(x) is positive is called the **support** of the PDF/PMF.

2.3 Distribution function and quantile function

As alternative to using PMF/PDFs we may also use a **distribution function** to describe the random variable. This assumes an ordering exist among the elementary events so that we can define the event $A = \{x : x \le a\}$ and compute its probability as

$$F(a) = \Pr(A) = \Pr(x \le a) = \begin{cases} \sum_{x \in A} f(x) & \text{discrete case} \\ \int_{x \in A} f(x) dx & \text{continuous case} \end{cases}$$

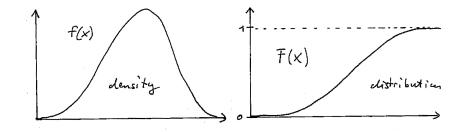
This is also known **cumulative distribution function** (CDF) and is denoted by upper case F (or P and Q). By construction the distribution function is

monotonically non-decreasing and its value ranges from 0 to 1. With its help we can compute the probability of an interval set such as

$$\Pr(a < x \le b) = F(b) - F(a).$$

The inverse of the distribution function y = F(x) is the **quantile function** $x = F^{-1}(y)$. The 50% quantile $F^{-1}\left(\frac{1}{2}\right)$ is called the **median**.

If the random variable x has distribution function F we write $x \sim F$.



2.4 Families of distributions

A distribution F_{θ} with a parameter θ constitutes a **distribution family** collecting all the distributions corresponding to particular instances of the parameter. The parameter θ therefore acts as an index of the distributions contained in the family.

The corresponding density (PDF) or probability mass function (PMF) is written either as $f_{\theta}(x)$, $f(x;\theta)$ or $f(x|\theta)$. The latter form is the most general is it suggests that the parameter θ may potentially also have its own distribution, with a joint density formed by $f(x,\theta) = f(x|\theta)f(\theta)$.

Note that any parameterisation is generally not unique, as a one-to-one transformation of θ will yield another equivalent index to the same distribution family. Typically, for most commonly used distribution families there are several standard parameterisations. Often we use those parameterisations where the parameters can be interpreted easily (e.g. in terms of moments).

If for any pair of different parameter values $\theta_1 \neq \theta_2$ we get distinct distributions with $F_{\theta_1} \neq F_{\theta_2}$ then the distribution family F_{θ} is said to be **identifiable** under the parameter θ .

2.5 Expectation of a random variable

The expected value E(x) of a random variable is defined as the weighted average over all possible outcomes, with the weight given by the PMF / PDF f(x):

$$E_F(x) = \begin{cases} \sum_{x \in \Omega} f(x)x & \text{discrete case} \\ \int_{x \in \Omega} f(x)x dx & \text{continuous case} \end{cases}$$

Note the notation to emphasise that the expectation is taken with regard to the distribution F. The subscript F is usually left out if there are no ambiguities. Furthermore, because the sum or integral may diverge the expectation is not necessarily always defined (in contrast to quantiles).

The expected value of a function of a random variable h(x) is obtained similarly:

$$E_F(h(x)) = \begin{cases} \sum_{x \in \Omega} f(x)h(x) & \text{discrete case} \\ \int_{x \in \Omega} f(x)h(x)dx & \text{continuous case} \end{cases}$$

This is called the "law of the unconscious statistician", or short LOTUS. Again, to highlight that the random variable x has distribution F we write $E_F(h(x))$.

2.6 Jensen's inequality for the expectation

If h(x) is a *convex* function then the following inequality holds:

$$E(h(x)) \ge h(E(x))$$

Recall: a convex function (such as x^2) has the shape of a "valley".

2.7 Probability as expectation

Probability itself can also be understood as an expectation. For an event A we can define a corresponding indicator function $1_{x \in A}$ for an elementary element x to be part of A. From the above it then follows

$$E(1_{x\in A})=\Pr(A)\,,$$

Interestingly, one can develop the whole theory of probability from this perspective. ¹

2.8 Moments and variance of a random variable

The moments of a random variable are defined as follows:

- Zeroth moment: $E(x^0) = 1$ by construction of PDF and PMF,
- First moment: $E(x^1) = E(x) = \mu$, the mean,
- Second moment: $E(x^2)$
- The variance is the second moment centred about the mean μ :

$$Var(x) = E((x - \mu)^2) = \sigma^2$$

15

• The variance can also be computed by $Var(x) = E(x^2) - E(x)^2$. This provides an example of Jensen's inequality, with $E(x^2) = E(x)^2 + Var(x) \ge E(x)^2$.

A distribution does not necessarily need to have any finite first or higher moments. An example is the Cauchy distribution that does not have a mean or variance (or any other higher moment).

2.9 Distribution of sums of random variables

The sum of two normal random variables is also normal (with the appropriate mean and variance).

The **central limit theorem**, first postulated by Abraham de Moivre (1667–1754), asserts that in many cases the distribution of the sum of identically distributed random variables converges to a normal distribution, even if the individual random variables are not normal.

For example, as a result the binomial distribution (as sum of Bernoulli random variables) can be approximated by a normal distribution.

2.10 Transformation of random variables

Linear transformation of random variables: if a and b are constants and x is a random variable, then the random variable y = a + bx has mean E(y) = a + bE(x) and variance $Var(y) = b^2Var(x)$.

For a general invertible coordinate transformation y = h(x) = y(x) the backtransformation is $x = h^{-1}(y) = x(y)$.

The transformation of the infinitesimal volume element is $dy = \left| \frac{dy}{dx} \right| dx$.

The transformation of the density is $f_y(y) = \left| \frac{dx}{dy} \right| f_x(x(y))$.

Note that
$$\left| \frac{dx}{dy} \right| = \left| \frac{dy}{dx} \right|^{-1}$$
.

 $^{^1\}mbox{Whittle, P. 2000.}$ Probability via Expectation (3rd ed.). Springer. https://doi.org/10.1007/978-1-4612-0509-8

Instead of scalar random variables one often also considers random vectors and also random matrices.

For a random vector $\mathbf{x} = (x_1, x_2, ..., x_d)^T$ the mean $\mathbf{E}(\mathbf{x}) = \boldsymbol{\mu}$ is simply comprised of the means of its components, i.e. $\boldsymbol{\mu} = (\mu_1, ..., \mu_d)^T$. Thus, the mean of a random vector of dimension is a vector of the same length.

The variance of a random vector of length d, however, is not a vector but a matrix of size $d \times d$. This matrix is called the **covariance matrix**:

$$\operatorname{Var}(x) = \underbrace{\Sigma}_{d \times d} = (\sigma_{ij}) = \begin{pmatrix} \sigma_{11} & \dots & \sigma_{1d} \\ \vdots & \ddots & \vdots \\ \sigma_{d1} & \dots & \sigma_{dd} \end{pmatrix}$$
$$= \operatorname{E}\left(\underbrace{(x - \mu)(x - \mu)^{T}}_{d \times 1}\right)$$
$$= \operatorname{E}(xx^{T}) - \mu\mu^{T}$$

The entries of the covariance matrix $\sigma_{ij} = \text{Cov}(x_i, x_j)$ describe the covariance between the random variables x_i and x_j . The covariance matrix is symmetric, hence $\sigma_{ij} = \sigma_{ji}$. The diagonal entries $\sigma_{ii} = \text{Cov}(x_i, x_i) = \text{Var}(x_i) = \sigma_i^2$ correspond to the variances of the components of x. The covariance matrix is by construction **positive semi-definite**, i.e. the eigenvalues of Σ are all positive or equal to zero.

However, wherever possible one will aim to use models with non-singular covariance matrices, with all eigenvalues positive, so that the covariance matrix is invertible.

For univariate x and scalar constant a the variance of ax equals $Var(ax) = a^2Var(x)$. For a random vector x of dimension d and constant matrix A of dimension $m \times d$ this generalises to $Var(Ax) = AVar(x)A^T$.

2.12 Correlation matrix

A covariance matrix can be factorised into the product

$$\mathbf{\Sigma} = \mathbf{V}^{\frac{1}{2}} \mathbf{P} \mathbf{V}^{\frac{1}{2}}$$

where \boldsymbol{V} is a diagonal matrix containing the variances

$$\boldsymbol{V} = \begin{pmatrix} \sigma_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{dd} \end{pmatrix}$$

and the matrix *P* ("upper case rho") is the symmetric **correlation matrix**

$$\boldsymbol{P} = (\rho_{ij}) = \begin{pmatrix} 1 & \dots & \rho_{1d} \\ \vdots & \ddots & \vdots \\ \rho_{d1} & \dots & 1 \end{pmatrix} = \boldsymbol{V}^{-\frac{1}{2}} \boldsymbol{\Sigma} \boldsymbol{V}^{-\frac{1}{2}}$$

Thus, the correlation between x_i and x_i is defined as

2.12. CORRELATION MATRIX

$$\rho_{ij} = \operatorname{Cor}(x_i, x_j) = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$$

Chapter 3

Univariate distributions

3.1 Bernoulli distribution

The **Bernoulli distribution** $\mathrm{Ber}(\theta)$ is the simplest of all distribution families. It is named after Jacob Bernoulli (1655-1705) who also discovered the law of large numbers.

It describes a discrete binary random variable with two states x = 0 ("failure") and x = 1 ("success"), where the parameter $\theta \in [0,1]$ is the probability of "success". Often the Bernoulli distribution is also referred to as "coin tossing" model with the two outcomes "heads" and "tails".

Correspondingly, the probability mass function of $Ber(\theta)$ is

$$p(x = 0|\theta) = \Pr(\text{"failure"}|\theta) = 1 - \theta$$

and

$$p(x = 1|\theta) = \Pr(\text{"success"}|\theta) = \theta$$

A compact way to write the PMF of the Bernoulli distribution is

$$p(x|\theta) = \theta^x (1-\theta)^{1-x}$$

The log PMF is

$$\log p(x|\theta) = x \log \theta + (1-x) \log(1-\theta)$$

If a random variable *x* follows the Bernoulli distribution we write

$$x \sim \text{Ber}(\theta)$$
.

The expected value is $E(x) = \theta$ and the variance is $Var(x) = \theta(1 - \theta)$.

3.2 Binomial distribution

Closely related to the Bernoulli distribution is the **binomial distribution** $Bin(n, \theta)$ which results from repeating a Bernoulli experiment n times and counting the number of successes among the n trials (without keeping track of the ordering of the experiments). Thus, if x_1, \ldots, x_n are n independent $Ber(\theta)$ random variables then $y = \sum_{i=1}^{n} x_i$ is distributed as $Bin(n, \theta)$.

If a random variable y follows the binomial distribution we write

$$y \sim Bin(n, \theta)$$

The corresponding probability mass function is:

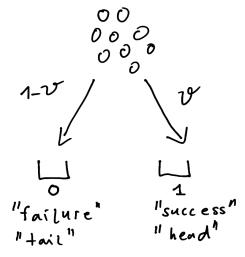
$$p(y|n,\theta) = \binom{n}{y} \theta^y (1-\theta)^{n-y}$$

with support $y \in \{0, 1, 2, ..., n\}$. The binomial coefficient $\binom{n}{y}$ is needed to account for the multiplicity of ways (orderings of samples) in which we can observe y successes.

The expected value is $E(y) = n\theta$ and the variance is $Var(y) = n\theta(1 - \theta)$.

If we standardise the support of the binomial variable to the unit interval with $\frac{y}{n} \in \{0, \frac{1}{n}, ..., 1\}$ then the mean is $E\left(\frac{y}{n}\right) = \theta$ and the variance is $Var\left(\frac{y}{n}\right) = \frac{\theta(1-\theta)}{n}$.

The binomial distribution may be illustrated by an urn model distributing n balls into 2 bins:



For n = 1 the binomial distribution reduces to the Bernoulli distribution.

In R the PMF of the binomial distribution is given by dbinom(), the cumulative distribution function is pbinom() and the quantile function is qbinom(). The binomial coefficient itself is computed by choose().

3.3 Beta distribution

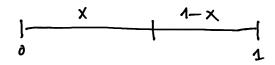
3.3.1 Standard parameterisation

A beta-distributed random variable is denoted by

$$x \sim \text{Beta}(\alpha, \beta)$$

where the support is $x \in [0, 1]$ and $\alpha > 0$ and $\beta > 0$ are two shape parameters.

The beta random variable can be visualised as breaking a unit stick of length one into two pieces of length x and 1-x:



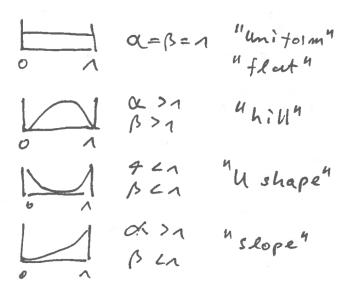
The density of the beta distribution Beta(α , β) is

$$p(x|\alpha,\beta) = \frac{1}{B(\alpha,\beta)} x^{\alpha-1} (1-x)^{\beta-1}$$

This depends on the beta function defined as

$$B(z_1, z_1) = \frac{\Gamma(z_1)\Gamma(z_2)}{\Gamma(z_1 + z_2)}$$

The beta distribution is very flexible and can assume a number of different shapes, depending on the value of α and β . For example, for $\alpha = \beta = 1$ it becomes the uniform distribution over the unit interval:



In R the PDF of the beta distribution is given by dbeta(), the cumulative distribution function is pbeta() and the quantile function is qbeta().

3.3.2 Mean parameterisation

Instead of employing α and β as parameters another useful reparameterisation Beta(μ , k) of the beta distribution is in terms of a mean parameter $\mu \in [0,1]$ and a concentration parameter k > 0. These are given by

 $k = \alpha + \beta$

and

$$\mu = \frac{\alpha}{\alpha + \beta}$$

The original parameters can be recovered by $\alpha = \mu k$ and $\beta = (1 - \mu)k$.

The mean and variance of the beta distribution expressed in terms of μ and k are

$$E(x) = \mu$$

and

$$Var(x) = \frac{\mu(1-\mu)}{k+1}$$

With increasing concentration parameter k the variance decreases and thus the probability mass becomes more concentrated around the mean.

The uniform distribution (with $\alpha = \beta = 1$) corresponds to $\mu = 1/2$ and k = 2.

Finally, note that the mean and variance of the continuous beta distribution closely match those of the unit-standardised discrete binomial distribution above.

3.4 Normal distribution

The **normal distribution** is the most important continuous probability distribution. It is also called **Gaussian distribution** named after Carl Friedrich Gauss (1777–1855).

The univariate normal distribution $N(\mu, \sigma^2)$ has two parameters μ (location) and σ^2 (scale) and support $x \in]-\infty, \infty[$.

$$x \sim N(\mu, \sigma^2)$$

with mean

$$E(x) = \mu$$

and variance

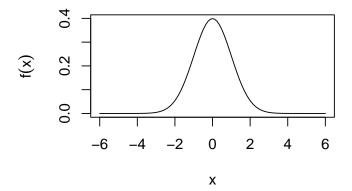
$$Var(x) = \sigma^2$$

Probability density function (PDF):

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

The standard normal distribution is N(0, 1) with mean 0 and variance 1.

Plot of the PDF of the standard normal:

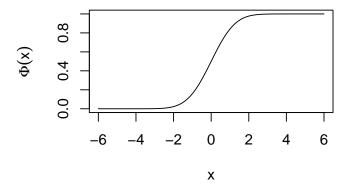


The cumulative distribution function (CDF) of the standard normal N(0,1) is

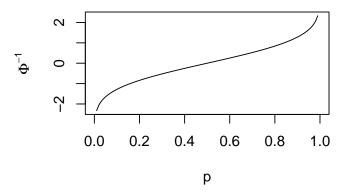
$$\Phi(x) = \int_{-\infty}^{x} p(x'|\mu = 0, \sigma^2 = 1)dx'$$

There is no analytic expression for $\Phi(x)$.

Plot of the CDF of the standard normal:



The inverse $\Phi^{-1}(p)$ is called the quantile function of the standard normal.



In R the normal PDF is given by dnorm(), the cumulative distribution function is pnorm() and the quantile function is qnorm().

3.5 Gamma distribution and special cases

The gamma distribution is widely used in statistics, and also appears in various parameterisations and under some other names, such as univariate Wishart and scaled chi-squared distribution

3.5.1 Standard parameterisation

The gamma distribution $Gam(\alpha, \theta)$ is a continuous distribution with two parameters $\alpha > 0$ (shape) and $\theta > 0$ (scale):

$$x \sim \text{Gam}(\alpha, \theta)$$

and support $x \in [0, \infty[$ with mean

$$E(x) = \alpha \theta$$

and variance

$$Var(x) = \alpha \theta^2$$

The gamma distribution is also often used with a rate parameter $\beta = 1/\theta$ (so one needs to pay attention which parameterisation is used).

The probability density function (PDF) is:

$$p(x|\alpha,\theta) = \frac{1}{\Gamma(\alpha)\theta^{\alpha}} x^{\alpha-1} e^{-x/\theta}$$

The density of the gamma distribution is available in the R function dgamma(). The cumulative density function is pgamma() and the quantile function is qgamma().

3.5.2 Wishart parameterisation and scaled chi-squared distribution

The gamma distribution is often used with a different set of parameters $k = 2\alpha$ and $s^2 = \theta/2$ (hence conversely $\alpha = k/2$ and $\theta = 2s^2$). In this form it is known as **univariate or one-dimensional Wishart distribution**

$$W_1\left(s^2,k\right)$$

named after John Wishart (1898–1954). In the Wishart parameterisation the mean is

$$E(x) = ks^2$$

and the variance

$$Var(x) = 2ks^4$$

Another name for the one-dimensional Wishart distribution with exactly the same parameterisation is scaled chi-squared distribution denoted as

$$s^2\chi_k^2$$

Finally, we also often employ the Wishart distribution in mean parameterisation

$$W_1\left(s^2 = \frac{\mu}{k}, k\right)$$

with parameters $\mu = ks^2$ and k (and thus $\theta = 2\mu/k$). In this parameterisation the mean is

$$E(x) = \mu$$

and the variance

$$Var(x) = \frac{2\mu^2}{k}$$

3.5.3 Construction as sum of squared normals

A gamma distributed variable can be constructed as follows. Assume *k* independent normal random variables with mean 0 and variance s^2 :

$$z_1, z_2, \ldots, z_k \sim N(0, s^2)$$

Then the sum of the squares

$$x = \sum_{i=1}^{k} z_i^2$$

follows

$$x \sim s^2 \chi_k^2$$

$$= W_1 \left(s^2, k \right)$$

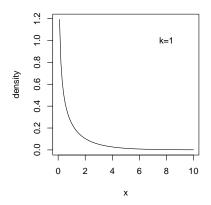
$$= \operatorname{Gam} \left(\alpha = \frac{k}{2}, \theta = 2s^2 \right)$$

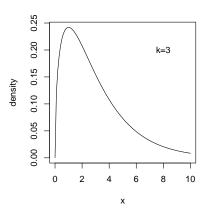
3.5.4 Chi-squared distribution

The **chi-squared distribution** χ^2_{k} is a special one-parameter restriction of the gamma resp. Wishart distribution obtained when setting $s^2 = 1$ or, equivalently, $\theta = 2$ or $\mu = k$.

It has mean E(x) = k and variance Var(x) = 2k. The chi-squared distribution χ_k^2 equals $Gam(\alpha = k/2, \theta = 2) = W_1(1, k)$.

Here is a plot of the density of the chi-squared distribution for degrees of freedom k = 1 and k = 3:





27

In R the density of the chi-squared distribution is given by dchisq(). The cumulative density function is pchisq() and the quantile function is qchisq().

Exponential distribution 3.5.5

The **exponential distribution** $Exp(\theta)$ with scale parameter θ is another special one-parameter restriction of the gamma distribution with shape parameter set to $\alpha = 1$ (or equivalently k = 2).

It thus equals $Gam(\alpha = 1, \theta) = W_1(s^2 = \theta/2, k = 2)$. It has mean θ and variance

Just like the gamma distribution the exponential distribution is also often specified using a rate parameter $\beta = 1/\theta$ instead of a scale parameter θ .

In R the command dexp() returns the density of the exponential distribution, pexp() is the corresponding cumulative density function and qexp() is the quantile function.

Inverse gamma distribution

Also know as inverse univariate Wishart distribution.

3.6.1 Standard parameterisation

A random variable x following an **inverse gamma distribution** is denoted by

$$x \sim \text{Inv-Gam}(\alpha, \beta)$$

with two parameters $\alpha > 0$ (shape parameter) and $\beta > 0$ (scale parameter) and support x > 0.

The inverse of *x* is then gamma distributed

$$\frac{1}{x} \sim \text{Gam}(\alpha, \theta = \beta^{-1})$$

where α is the shared shape parameter and θ the scale parameter of the gamma distribution.

The inverse gamma distribution Inv-Gam(α , β) has density

$$p(x|\alpha,\beta) = \frac{\beta^{\alpha}}{\Gamma(\alpha)} (1/x)^{\alpha+1} e^{-\beta/x}$$

The mean of the inverse gamma distribution is

$$E(x) = \frac{\beta}{\alpha - 1}$$

and the variance

$$Var(x) = \frac{\beta^2}{(\alpha - 1)^2(\alpha - 2)}$$

Thus, for the mean to exist we have the restriction $\alpha > 1$ and for the variance to exist $\alpha > 2$.

In the R extraDistr package the density of the inverse gamma distribution is given by extraDistr::dinvgamma(), the function extraDistr::pinvgamma() returns the corresponding cumulative density and extraDistr::qinvgamma() is the quantile function.

3.6.2 Wishart parameterisation

The inverse gamma distribution is frequently used with a different set of parameters $\psi=2\beta$ (scale parameter) and $\nu=2\alpha$ (shape parameter), or conversely $\alpha=\nu/2$ and $\beta=\psi/2$. In this form it is called **one-dimensional inverse Wishart distribution**

$$W_1^{-1}(\psi, \nu)$$

with mean given by

$$E(x) = \frac{\psi}{\nu - 2}$$

for $\nu > 2$ and variance

$$Var(x) = \frac{2\psi^2}{(\nu - 2)^2(\nu - 4)}$$

for $\nu > 4$.

The inverse univariate Wishart and univariate Wishart distributions are linked. If a random variable *x* is inverse Wishart distributed

$$x \sim \mathrm{W}_1^{-1}(\psi, \nu)$$

then the inverse of *x* is Wishart distributed with inverted scale parameter:

$$\frac{1}{x} \sim W_1(s^2 = \psi^{-1}, k = \nu)$$

where k is the shape parameter and s^2 the scale parameter of the Wishart distribution.

Instead of ψ and ν we may also equivalently use $\kappa = \nu - 2$ and $\mu = \psi/(\nu - 2)$ as parameters for the inverse Wishart distribution, so that

$$W_1^{-1}(\psi=\kappa\mu,\nu=\kappa+2)$$

has mean

$$E(x) = \mu$$

with $\kappa > 0$ and the variance is

$$Var(x) = \frac{2\mu^2}{\kappa - 2}$$

with $\kappa > 2$. This **mean parameterisation** is useful when employing the inverse gamma distribution as prior and posterior.

Finally, with $W_1^{-1}(\psi = \nu \tau^2, \nu)$, where $\tau^2 = \mu \frac{\kappa}{\kappa + 2} = \frac{\psi}{\nu}$ is a biased mean parameter, we get the **scaled inverse chi-squared distribution** $\tau^2 \text{Inv-} \chi_{\nu}^2$ with

$$E(x) = \tau^2 \frac{v}{v - 2}$$

for v > 2 and

$$Var(x) = \frac{2\tau^4}{\nu - 4} \frac{\nu^2}{(\nu - 2)^2}$$

for $\nu > 4$.

3.7 Location-scale t-distribution and special cases

3.7.1 Location-scale *t*-distribution

The location-scale t-distribution $\operatorname{lst}(\mu, \tau^2, \nu)$ is a generalisation of the normal distribution. It has an additional parameter $\nu > 0$ (degrees of freedom) that controls the probability mass in the tails. For small values of ν the distribution is heavy-tailed — indeed so heavy that for $\nu \le 1$ even the mean is not defined and for $\nu \le 2$ the variance is undefined.

The probability density of $lst(\mu, \tau^2, \nu)$ is

$$p(x|\mu,\tau^2,\nu) = \frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\pi\nu\tau^2}\Gamma(\frac{\nu}{2})} \left(1 + \frac{(x-\mu)^2}{\nu\tau^2}\right)^{-(\nu+1)/2}$$

with support $x \in]-\infty, \infty[$. The mean is (for $\nu > 1$)

$$E(x) = \mu$$

and the variance (for v > 2)

$$Var(x) = \tau^2 \frac{v}{v - 2}$$

For $\nu \to \infty$ the location-scale *t*-distribution lst(μ , τ^2 , ν) becomes the normal distribution $N(\mu, \tau^2)$.

In the R extraDistr package the command extraDistr::dlst() returns the density of the location-scale *t*-distribution, extraDistr::plst() is the corresponding cumulative density function and extraDistr::qlst() is the quantile function.

3.7.2 Location-scale t-distribution as compound distribution

Suppose that

$$x|s^2 \sim N(\mu, s^2)$$

with corresponding density $p(x|s^2)$ and mean $E(x|s^2) = \mu$ and variance $Var(x|s^2) = s^2$.

Now let the variance s^2 be distributed as inverse gamma / inverse Wishart

$$s^2 \sim W^{-1}(\psi = \kappa \sigma^2, \nu = \kappa + 2) = W^{-1}(\psi = \tau^2 \nu, \nu)$$

with corresponding density $p(s^2)$ and mean $E(s^2) = \sigma^2 = \tau^2 v/(v-2)$. Note we use here both the mean parameterisation (σ^2 , κ) and the inverse chi-squared parameterisation (τ^2, ν) .

The joint density for x and s^2 is $p(x, s^2) = p(x|s^2)p(s^2)$. We are interested in the marginal density for x:

$$p(x) = \int p(x, s^2)ds^2 = \int p(s^2)p(x|s^2)ds^2$$

This is a compound distribution of a normal with fixed mean μ and variance s^2 varying according the inverse gamma distribution. Calculating the integral results in the location-scale *t*-distribution with parameters

$$x \sim \operatorname{lst}\left(\mu, \sigma^2 \frac{\kappa}{\kappa + 2}, \kappa + 2\right) = \operatorname{lst}\left(\mu, \tau^2, \nu\right)$$

with mean

$$E(x) = \mu$$

and variance

$$Var(x) = \sigma^2 = \tau^2 \frac{\nu}{\nu - 2}$$

31

From the law of total expectation and variance we can also directly verify that

$$E(x) = E(E(x|s^2)) = \mu$$

and

$$Var(x) = E(Var(x|s^2)) + Var(E(x|s^2)) = E(s^2) = \sigma^2 = \tau^2 \frac{\nu}{\nu - 2}$$

Student's *t*-distribution

For $\mu = 0$ and $\tau^2 = 1$ the location-scale *t*-distribution becomes the Student's *t*-distribution t_{ν} with mean 0 (for $\nu > 1$) and variance $\frac{\nu}{\nu-2}$ (for $\nu > 2$).

It can thus be viewed as a generalisation of the standard normal distribution N(0,1).

If $y \sim t_v$ then $x = \mu + \tau y$ is distributed as $x \sim \text{lst}(\mu, \tau^2, \nu)$.

For $\nu \to \infty$ the *t*-distribution becomes equal to N(0,1).

In R the command dt() returns the density of the *t*-distribution, pt() is the corresponding cumulative density function and qt() is the quantile function.

Cauchy and standard Cauchy distribution

For v = 1 the location-scale *t*-distribution becomes the Cauchy distribution Cau(μ , τ) with density $p(x|\mu,\tau) = \frac{\tau}{\tau(\tau^2 + (x-\mu)^2)}$.

For v = 1 the *t*-distribution becomes the standard Cauchy distribution Cau(0, 1) with density $p(x) = \frac{1}{\pi(1+x^2)}$.

Chapter 4

Multivariate distributions

4.1 Categorical distribution

The **categorical distribution** is a generalisation of the Bernoulli distribution from two classes to *K* classes.

The categorical distribution $Cat(\pi)$ describes a discrete random variable with K states ("categories", "classes", "bins") where the parameter vector $\pi = (\pi_1, \dots, \pi_K)^T$ specifies the probability of each of class so that $Pr(\text{"class k"}) = \pi_k$. The parameters satisfy $\pi_k \in [0,1]$ and $\sum_{k=1}^K \pi_k = 1$, hence there are K-1 independent parameters in a categorical distribution (and not K).

There are two main ways to numerically represent "class k":

- i) by "integer encoding", i.e. by the corresponding integer k.
- ii) by "one hot encoding", i.e. by an indicator vector $\mathbf{x} = (x_1, \dots, x_K)^T = (0, 0, \dots, 1, \dots, 0)^T$ containing zeros everywhere except for the element $x_k = 1$ at position k. Thus all $x_k \in \{0, 1\}$ and $\sum_{k=1}^K x_k = 1$.

In the following we use "one hot encoding". Therefore sampling from a categorical distribution with parameters $\boldsymbol{\pi}$

$$x \sim \operatorname{Cat}(\pi)$$

yields a random index vector x.

The corresponding probability mass function (PMF) can be written conveniently in terms of x_k as

$$p(x|\pi) = \prod_{k=1}^{K} \pi_k^{x_k} = \{\pi_k \text{ if } x_k = 1\}$$

and the log PMF as

$$\log p(x|\pi) = \sum_{k=1}^{K} x_k \log \pi_k = \{\log \pi_k \quad \text{if } x_k = 1\}$$

In order to be more explicit that the categorical distribution has K-1 and not K parameters we rewrite the log-density with $\pi_K = 1 - \sum_{k=1}^{K-1} \pi_k$ and $x_K = 1 - \sum_{k=1}^{K-1} x_k$ as

$$\log p(x|\pi) = \sum_{k=1}^{K-1} x_k \log \pi_k + x_K \log \pi_K$$

$$= \sum_{k=1}^{K-1} x_k \log \pi_k + \left(1 - \sum_{k=1}^{K-1} x_k\right) \log \left(1 - \sum_{k=1}^{K-1} \pi_k\right)$$

Note that there is no particular reason to choose π_K as dependent of the probabilities of the other classes, in its place any other of the π_k may be selected.

The expected value is $E(x) = \pi$, in component notation $E(x_k) = \pi_k$. The covariance matrix is $Var(x) = Diag(\pi) - \pi \pi^T$, which in component notation is $Var(x_i) = \pi_i(1 - \pi_i)$ and $Cov(x_i, x_j) = -\pi_i \pi_j$.

The form of the categorical covariance matrix follows directly from the definition of the variance $Var(x) = E(xx^T) - E(x)E(x)^T$ and noting that $x_i^2 = x_i$ and $x_ix_j = 0$ if $i \neq j$. Furthermore, the categorical covariance matrix is singular by construction, as the K random variables x_1, \ldots, x_K are dependent through the constraint $\sum_{k=1}^K x_k = 1$.

For K=2 the categorical distribution reduces to the Bernoulli Ber(θ) distribution, with $\pi_1=\theta$ and $\pi_2=1-\theta$.

4.2 Multinomial distribution

The **multinomial distribution** $\operatorname{Mult}(n,\pi)$ arises from repeated categorical sampling, in the same fashion as the binomial distribution arises from repeated Bernoulli sampling. Thus, if x_1, \ldots, x_n are n independent $\operatorname{Cat}(\pi)$ random categorical variables then $y = \sum_{i=1}^n x_i$ is distributed as $\operatorname{Mult}(n,\pi)$.

The corresponding PMF describes the probability of a pattern y_1, \ldots, y_K of samples distributed across K classes (with $n = \sum_{k=1}^{K} y_k$):

$$p(\boldsymbol{y}|n,\theta) = \binom{n}{y_1,\ldots,y_n} \prod_{k=1}^K \pi_k^{y_k}$$

where $\binom{n}{y_1, \dots, y_n}$ is the multinomial coefficient.

The expected value is

$$E(y) = n\pi$$

which in component notation is $E(y_k) = n\pi_k$. The covariance matrix is

$$Var(\mathbf{y}) = n(Diag(\boldsymbol{\pi}) - \boldsymbol{\pi}\boldsymbol{\pi}^T)$$

which in component notation is $Var(x_i) = n\pi_i(1 - \pi_i)$ and $Cov(x_i, x_j) = -n\pi_i\pi_j$. Standardised to unit interval we get:

$$\frac{y_i}{n} \in \left\{0, \frac{1}{n}, \frac{2}{n}, \dots, 1\right\}$$

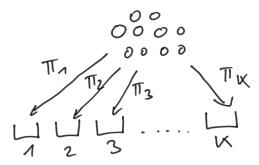
$$E\left(\frac{y}{n}\right) = \pi$$

$$\operatorname{Var}\left(\frac{y}{n}\right) = \frac{\operatorname{Diag}(\pi) - \pi\pi^T}{n}$$

$$\operatorname{Var}\left(\frac{y_i}{n}\right) = \frac{\pi_i(1 - \pi_i)}{n}$$

$$\operatorname{Cov}\left(\frac{y_i}{n}, \frac{y_j}{n}\right) = -\frac{\pi_i\pi_j}{n}$$

The multinomial distribution may be illustrated by an urn model distributing n balls into K bins:



For n = 1 the multinomial distribution reduces to the categorical distribution.

For K = 2 the multinomial distribution reduces to the Binomial distribution.

4.3 Dirichlet distribution

4.3.1 Standard parameterisation

The Dirichlet distribution is the multivariate generalisation of the beta distribution.

A Dirichlet distributed random vector is denoted by

$$x \sim \text{Dir}(\alpha)$$

with parameter $\alpha = (\alpha_1, ..., \alpha_K)^T > 0$ and $K \ge 2$ and where the support of x is the K-1 dimensional simplex with $x_i \in [0,1]$ and $\sum_{i=1}^K x_i = 1$.

The Dirichlet random variable can be visualised as breaking a unit stick of length one in K pieces of length x_1 to x_K :

The density of the Dirichlet distribution $Dir(\alpha)$ is

$$p(\mathbf{x}|\boldsymbol{\alpha}) = \frac{1}{B(\boldsymbol{\alpha})} \prod_{k=1}^{K} x_k^{\alpha_k - 1}$$

This depends on the beta function with multivariate argument defined as

$$B(z) = \frac{\prod_{k=1}^{K} \Gamma(z_k)}{\Gamma\left(\sum_{k=1}^{K} z_k\right)}$$

For K = 2 the Dirichlet distribution reduces to the beta distribution.

4.3.2 Mean parameterisation

Instead of employing α as parameter vector another useful reparameterisation $Dir(\pi, k)$ of the Dirichlet distribution is in terms of a mean parameter π , with $\pi_i \in [0,1]$ and $\sum_{i=1}^K \pi_i = 1$, and a concentration parameter k > 0. These are given

$$k = \sum_{i=1}^{K} \alpha_i$$

and

$$\pi = \frac{\alpha}{k}$$

The original parameters can be recovered by $\alpha = \pi k$.

The mean and variance of the Dirichlet distribution expressed in terms of π and k are

$$E(x) = \pi$$

and

$$Var(x) = \frac{Diag(\pi) - \pi \pi^{T}}{k+1}$$

which in component notation is

4.4. MULTIVARIATE NORMAL DISTRIBUTION

$$Var(x_i) = \frac{\pi_i(1 - \pi_i)}{k + 1}$$

and

$$Cov(x_i, x_j) = -\frac{\pi_i \pi_j}{k+1}$$

Finally, note that the mean and variance of the continuous Dirichlet distribution closely match those of the unit-standardised discrete multinomial distribution above.

Multivariate normal distribution

The univariate normal distribution for a random scalar x generalises to the multivariate normal distribution for a random vector $\mathbf{x} = (x_1, x_2, ..., x_d)^T$.

If x follows a multivariate normal distribution we write

$$x \sim N_d(\mu, \Sigma)$$

where μ is the mean (location) parameter and Σ the variance (scale) parameter. The corresponding density is

$$p(x|\mu, \Sigma) = \det(2\pi\Sigma)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\underbrace{(x-\mu)^T}_{1\times d}\underbrace{\Sigma^{-1}}_{d\times d}\underbrace{(x-\mu)}_{d\times 1}\right)$$

As $\det(2\pi\Sigma)^{-\frac{1}{2}} = \det(2\pi I_d)^{-\frac{1}{2}} \det(\Sigma)^{-\frac{1}{2}} = (2\pi)^{-d/2} \det(\Sigma)^{-\frac{1}{2}}$ the density can also be written as

$$p(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = (2\pi)^{-\frac{d}{2}} \det(\boldsymbol{\Sigma})^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}-\boldsymbol{\mu})\right)$$

with explicit occurrence of the dimension d.

The expectation of x is $E(x) = \mu$ and the variance is $Var(x) = \Sigma$.

For d=1 the random vector $\mathbf{x}=\mathbf{x}$ is a scalar and $\mathbf{\mu}=\mathbf{\mu}$ and $\mathbf{\Sigma}=\sigma^2$ and the multivariate normal density reduces to the univariate normal density.

4.6. INVERSE WISHART DISTRIBUTION

4.5 Wishart distribution

The Wishart distribution is a multivariate generalisation of the gamma distribution.

Recall that the gamma distribution can be motivated as the distribution of sums of squared normal random variables. Likewise, the Wishart distribution can be understood as the sum of squared multivariate normal variables:

$$z_1, z_2, \ldots, z_k \stackrel{\text{iid}}{\sim} N_d(0, S)$$

with $S = (s_{ij})$ the specified covariance matrix. The random variable

$$\underbrace{X}_{d \times d} = \sum_{i=1}^{k} \underbrace{z_i z_i^T}_{d \times d}$$

is a random *matrix* and is distributed as

$$X \sim W_d(S, k)$$

with mean

$$E(X) = kS$$

and variances

$$Var(x_{ij}) = k \left(s_{ij}^2 + s_{ii} s_{jj} \right)$$

We often also employ the Wishart distribution in mean parameterisation

$$W_d\left(S = \frac{M}{k}, k\right)$$

with parameters M = kS and k. In this parameterisation the mean is

$$E(X) = M = (\mu_{ii})$$

and variances are

$$Var(x_{ij}) = \frac{\mu_{ij}^2 + \mu_{ii}\mu_{jj}}{k}$$

If *S* or *M* is a scalar rather than a matrix then the multivariate Wishart distribution reduces to the univariate Wishart aka gamma distribution.

4.6 Inverse Wishart distribution

The inverse Wishart distribution is a multivariate generalisation of the inverse gamma distribution and is linked to the Wishart distribution.

A random matrix *X* following an **inverse Wishart distribution** is denoted by

$$X \sim W_d^{-1}(\Psi, \nu)$$

where Ψ is the scale parameter and ν the shape parameter. The corresponding mean is given by

$$E(X) = \frac{\Psi}{\nu - d - 1}$$

and the variances are

$$Var(x_{ij}) = \frac{(\nu - d + 1)\psi_{ij}^2 + (\nu - d - 1)\psi_{ii}\psi_{jj}}{(\nu - d)(\nu - d - 1)^2(\nu - d - 3)}$$

The inverse of *X* is then Wishart distributed:

$$X^{-1} \sim W_d \left(S = \Psi^{-1}, k = \nu \right)$$

Instead of Ψ and ν we may use the mean parameterisation with parameters $\kappa = \nu - d - 1$ and $M = \Psi/(\nu - d - 1)$:

$$X \sim W_d^{-1} (\Psi = \kappa M, \nu = \kappa + d + 1)$$

with mean

$$E(X) = M$$

and variances

$$Var(x_{ij}) = \frac{(\kappa + 2)\mu_{ij}^2 + \kappa \mu_{ii}\mu_{jj}}{(\kappa + 1)(\kappa - 2)}$$

If Ψ or M is a scalar rather than a matrix then the multivariate inverse Wishart distribution reduces to the univariate inverse Wishart aka inverse gamma distribution.