### Lecture notes for Part A Probability

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# Review of Prelims Probability: probability spaces, random variables, distributions, independence

#### 1.1 Probability spaces and random variables

We start by reviewing the basic idea of a **probability space** introduced in last year's course. This framework underlies modern probability theory, even though we will seldom need to appeal to it directly in this course.

A **probability space** is a collection  $(\Omega, \mathcal{F}, \mathbb{P})$  with the following structure:

- (i)  $\Omega$  is a set, which we call the **sample space**.
- (ii)  $\mathcal{F}$  is a collection of subsets of  $\Omega$ . An element of  $\mathcal{F}$  is called an **event**.
- (iii) The **probability measure**  $\mathbb{P}$  is a function from  $\mathcal{F}$  to [0,1]. It assigns a **probability** to each event in  $\mathcal{F}$ .

We can think of the probability space as modelling an experiment. The sample space  $\Omega$  represents the set of all possible outcomes of the experiment.

The set  $\mathcal{F}$  of events should satisfy certain natural conditions:

- (1)  $\Omega \in \mathcal{F}$ .
- (2) If  $\mathcal{F}$  contains a set A, then it also contains the complement  $A^c$  (i.e.  $\Omega \setminus A$ ).
- (3) If  $(A_i, i \in \mathcal{I})$  is a finite or countably infinite collection of events in  $\mathcal{F}$ , then their union  $\bigcup_{i \in \mathcal{I}} A_i$  is also in  $\mathcal{F}$ .

By combining (2) and (3), we can also obtain finite or countably infinite intersections, as well as unions.

Finally, the probability measure  $\mathbb{P}$  should satisfy the following conditions (the **probability** axioms):

- (1)  $\mathbb{P}(\Omega) = 1$ .
- (2) If  $(A_i, i \in \mathcal{I})$  is a finite or countably infinite collection of **disjoint** events, then

$$\mathbb{P}\left(\bigcup_{i\in\mathcal{I}}A_i\right) = \sum_{i\in\mathcal{I}}\mathbb{P}(A_i). \tag{1.1}$$

A random variable is a function defined on  $\Omega$ . We will consider real-valued random variables, i.e. functions from  $\Omega$  to  $\mathbb{R}$ .

A random variable represents an **observable** in our experiment; something we can "measure".

Formally, for a function X from  $\Omega$  to  $\mathbb R$  to be a random variable, we require that the subset

$$\{\omega \in \Omega \colon X(\omega) \le x\}$$

of  $\Omega$  is an event in  $\mathcal{F}$ , for every  $x \in \mathbb{R}$ . (Then, by taking complements, unions and intersections, we will in fact have that the set  $\{\omega \in \Omega \colon X(\omega) \in B\}$  is in  $\mathcal{F}$  for a very large class of sets B).

We will usually write X rather than  $X(\omega)$  for the value taken by a random variable. Thus if X is a random variable we can talk about the probability of the event

$$\{X\in B\}=\{\omega\in\Omega\colon X(\omega)\in B\},$$

which we will write as  $\mathbb{P}(X \in B)$ .

Within one experiment, there will be many observables! That is, on the same probability space we can consider many different random variables.

#### Remarks:

- (a) For very simple models, there may be a natural way to set up the sample space  $\Omega$  (e.g. to represent the set of possible outcomes of the throw of a die or a coin). For more complicated models, this quickly becomes less straightforward. In practice, we hardly ever want to consider  $\Omega$  directly; instead we work directly with the "events" and "random variables" (the "observables") in the experiment.
- (b) In contrast, there are settings in probability theory where we care a lot about the collection of events  $\mathcal{F}$ , and its structure. (For example, modelling a process evolving in time, we might have a family of different collections  $\mathcal{F}_t$ ,  $t \geq 0$ , where  $\mathcal{F}_t$  represents the set of events which can be observed by watching the evolution of the process up to time t). However, for the purposes of this course we will hardly ever worry about  $\mathcal{F}$  directly; we will be safe to assume that  $\mathcal{F}$  will always contain any event that we wish to consider.

#### 1.1.1 Examples

Here are some examples of systems (or "experiments") that we might model using a probability space, and, for each one, some examples of random variables that we might want to consider within our model:

- We throw two dice, one red and one blue. Random variables: the score on the red die; the score on the blue die; the sum of the two; the maximum of the two; the indicator function of the event that the blue score exceeds the red score....
- A Geiger counter detecting particles emitted by a radioactive source. Random variables: the time of the kth particle detected, for k = 1, 2, ...; the number of particles detected in the time interval [0, t], for  $t \in [0, \infty)$ ....
- A model for the evolution of a financial market. Random variables: the prices of various stocks at various times; interest rates at various times; exchange rates at various times....
- The growth of a colony of bacteria. Random variables: the number of bacteria present at a given time; the diameter of the colonised region at given times; the number of generations observed in a given time interval....
- A call-centre. The time of arrival of the kth call; the length of service required by the kth caller; the wait-time of the kth caller in the queue before receiving service....

#### 1.2 Probability distributions

We consider the distribution of a random variable X. This can be summarised by the **distribution function** (or **cumulative distribution function**) of X, defined by

$$F(x) = \mathbb{P}(X \le x)$$

for  $x \in \mathbb{R}$ . (Once we know F, we can derive the probabilities  $\mathbb{P}(X \in B)$  for a very wide class of sets B by taking complements, intersections and unions. Formally, the **distribution** of a random variable X is the map  $B \mapsto \mathbb{P}(X \in B)$ , considered on a suitable collection of subsets  $B \subseteq \mathbb{R}$ . In practice, we identify distributions by identifying the cumulative distribution function or any other associated function that uniquely determines a distribution.)

Any distribution function F must obey the following properties:

- (1) F is non-decreasing.
- (2) F is right-continuous.
- (3)  $F(x) \to 0$  as  $x \to -\infty$ .
- (4)  $F(x) \to 1$  as  $x \to \infty$ .

Remark 1.1. Note that two different random variables can have the same distribution! For example, consider the model of two dice mentioned above. If the dice are "fair", then the distribution of the score on the blue die might be the same as the distribution of the score on the red die. However, that does not mean that the two scores are always the same! They are two different "observables" within the same experiment.

If two random variables X and Y have the same distribution, we write  $X \stackrel{d}{=} Y$ .

We single out two important classes of random variables: discrete and continuous.

#### 1.2.1 Discrete random variables

A random variable X is **discrete** if there is a finite or countably infinite set B such that  $\mathbb{P}(X \in B) = 1$ .

We can represent the distribution of a discrete random variable X by its probability mass function

$$p_X(x) = \mathbb{P}(X = x)$$

for  $x \in \mathbb{R}$ . This function is zero except at a finite or countably infinite set of points. We have

- $\sum_{x} p_X(x) = 1$ .
- $\mathbb{P}(X \in A) = \sum_{x \in A} p_X(x)$  for any set  $A \subseteq \mathbb{R}$ .

The points x where  $\mathbb{P}(X=x)>0$  are sometimes called the **atoms** of the distribution of X. In many examples these will be a set of integers such as  $\{0,1,2,\ldots,n\}$  or  $\{0,1,2,\ldots\}$  or  $\{1,2,3,\ldots\}$ .

The cumulative distribution function of X has jumps at the location of the atoms, and is constant on any interval that does not contain an atom.

#### 1.2.2 Continuous random variables

A random variable X is called (absolutely) **continuous** if its distribution function F can be written as an integral. That is, there is a function f such that

$$\mathbb{P}(X \le x) = F(x) = \int_{-\infty}^{x} f(u)du.$$

f is called the **density function** (or **probability density function**) of X.

This certainly implies that F is a continuous function (although note that not all continuous F can be written in this way). In particular,  $\mathbb{P}(X=x)=F(x)-\lim_{y\uparrow x}F(y)=0$  for any x. The density function is not unique; for example, we can change the value of f at any single point without affecting the integral of f. At points where F is differentiable, it is natural to take f(x)=F'(x). For any a< b, we have

$$\mathbb{P}(a \le X \le b) = \int_{a}^{b} f(u)du.$$

#### 1.3 Expectation and variance

Let X be a discrete random variable with probability mass function  $p_X(x) = \mathbb{P}(X = x)$ . The **expectation** (or **mean**) of X, denoted for example by  $\mathbb{E} X$  or  $\mathbb{E}(X)$  or  $\mathbb{E}[X]$ , is defined by

$$\mathbb{E}(X) = \sum_{x} x p_X(x), \tag{1.2}$$

when this sum converges.

If instead X is a continuous random variable with density function f, then its expectation is given by

$$\mathbb{E}(X) = \int_{-\infty}^{\infty} x f(x) dx, \tag{1.3}$$

when this integral converges.

We often want to express the expectation of a function of a random variable X in terms of the density function or the mass function of X. We have

$$\mathbb{E}\,g(X) = \sum_{x} g(x) p_X(x)$$

in the discrete case, and

$$\mathbb{E}\,g(X) = \int_{-\infty}^{\infty} g(x)f(x)dx$$

in the continuous case (again, provided the sum or integral converges).

It is rather unsatisfactory that we have two different definitions of expectation for two different cases, and no definition at all for random variables which are neither continuous nor discrete. In fact it is not difficult to unify the definitions. A very natural way is to consider approximations of a general random variable by discrete random variables. This is analogous to the construction of the integral of a general function by defining the integral of a step function using sums, and then defining the integral of a general function using an approximation by step functions, as seen in the Prelims Analysis course.

This unifies the two definitions above, and extends the definition to all types of random variable, whether discrete, continuous or neither. We will not pursue this here – but we will collect together basic properties of expectation which we will use constantly:

- (1) For any event A, write  $\mathbf{1}_A$  for the indicator function of A. Then  $\mathbb{E} \mathbf{1}_A = \mathbb{P}(A)$ .
- (2) If  $\mathbb{P}(X \geq 0) = 1$ , then  $\mathbb{E} X \geq 0$ .
- (3) (Linearity 1):  $\mathbb{E}(aX) = a \mathbb{E} X$  for any constant a.
- (4) (Linearity 2):  $\mathbb{E}(X+Y) = \mathbb{E}X + \mathbb{E}Y$ .

Formally,  $\mathbb{E}$  is a linear operator on the vector space of random variables  $X \colon \Omega \to \mathbb{R}$  whose expectations exist.

#### 1.3.1 Variance and covariance

The **variance** of a random variable X is defined by

$$\operatorname{var}(X) = \mathbb{E}\left[(X - \mathbb{E}X)^2\right],$$

provided that the expectations exist. This can then alternatively be expressed as

$$var(X) = \mathbb{E}(X^2) - (\mathbb{E}X)^2.$$

The **covariance** of two random variables X and Y is defined by

$$cov(X, Y) = \mathbb{E}[(X - \mathbb{E}X)(Y - \mathbb{E}Y)],$$

if the expectations exist, which can then alternatively be expressed as

$$cov(X, Y) = \mathbb{E}(XY) - (\mathbb{E}X)(\mathbb{E}Y).$$

Note that var(X) = cov(X, X). From the linearity of expectation, we get a bi-linearity property for covariance:

$$cov(aX + b, cY + d) = ac cov(X, Y).$$

As a special case we can obtain

$$var(aX + b) = a^2 var(X).$$

We also have the property

$$var(X + Y) = var(X) + var(Y) + 2cov(X, Y)$$

and more generally

$$var(X_1 + X_2 + \dots + X_n) = \sum_{i=1}^n var(X_i) + 2 \sum_{1 \le i < j \le n} cov(X_i, X_j),$$

always provided that all expectations exist.

#### 1.4 Independence

Events A and B are **independent** if

$$\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(B).$$

More generally, a family of events  $(A_i, i \in \mathcal{I})$ , possibly infinite, even uncountable, is called independent if for all finite subsets J of  $\mathcal{I}$ ,

$$\mathbb{P}\left(\bigcap_{i\in J} A_i\right) = \prod_{i\in J} \mathbb{P}(A_i).$$

Remark 1.2. Remember that this is a stronger condition than pairwise independence! Even for three events, it is possible that  $A_1$ ,  $A_2$  are independent,  $A_2$ ,  $A_3$  are independent and  $A_1$ ,  $A_3$  are independent but that  $A_1$ ,  $A_2$ ,  $A_3$  are **not** independent.

Random variables  $X_1, X_2, \ldots, X_n$  are independent if events  $\{X_1 \in B_1\}, \{X_2 \in B_2\}, \ldots, \{X_n \in B_n\}$  are independent for all  $B_1, B_2, \ldots, B_n \subset \mathbb{R}$ .

In fact, it turns out to be enough to check that for all  $x_1, x_2, \ldots, x_n$ ,

$$\mathbb{P}(X_1 \le x_1, X_2 \le x_2, \dots, X_n \le x_n) = \mathbb{P}(X_1 \le x_1) \mathbb{P}(X_2 \le x_2) \cdots \mathbb{P}(X_n \le x_n)$$
$$= F_{X_1}(x_1) F_{X_2}(x_2) \cdots F_{X_n}(x_n).$$

If the random variables are all discrete, another equivalent condition is that

$$\mathbb{P}(X_1 = x_1, X_2 = x_2, \dots, X_n = x_n) = \mathbb{P}(X_1 = x_1)\mathbb{P}(X_2 = x_2) \cdots \mathbb{P}(X_n = x_n).$$

A sequence of random variables  $X_i$ ,  $i \geq 1$ , is independent if for all  $n \geq 2$ , the random variables  $X_1, X_2, \ldots, X_n$  are independent.

When X and Y are independent random variables whose expectations exist, we have  $\mathbb{E}(XY) = \mathbb{E}(X)\mathbb{E}(Y)$ , or equivalently cov(X,Y) = 0. That is, X and Y are uncorrelated. The converse is *not* true; uncorrelated does not imply independent!

Various of the properties above can be summarised by the phrase "independence means multiply".

#### 1.5 Examples of probability distributions

We review some of the families of probability distributions which are of particular importance in applications and in theory.

#### 1.5.1 Continuous distributions

#### Uniform distribution

X has the uniform distribution on an interval [a, b] if its probability density function is given by

$$f(x) = \begin{cases} \frac{1}{b-a}, & \text{if } a \le x \le b, \\ 0, & \text{otherwise.} \end{cases}$$

We write  $X \sim U[a, b]$ .

#### **Exponential distribution**

X has exponential distribution with parameter (or rate)  $\lambda$  if its distribution function is given by

$$F(x) = \begin{cases} 0, & x < 0, \\ 1 - e^{-\lambda x}, & x \ge 0. \end{cases}$$

Its density function is

$$f(x) = \begin{cases} 0 & x < 0, \\ \lambda e^{-\lambda x} & x \ge 0. \end{cases}$$

We write  $X \sim \text{Exp}(\lambda)$ . We have  $\mathbb{E} X = 1/\lambda$  and  $\text{var} X = 1/\lambda^2$ . If  $X \sim \text{Exp}(\lambda)$  and a > 0, then  $aX \sim \text{Exp}(\lambda/a)$ . An important property of the distribution is the **memoryless property**:  $\mathbb{P}(X > x + t \mid X > t)$  does not depend on t.

#### Normal distribution

X has the normal (or Gaussian) distribution with mean  $\mu$  and variance  $\sigma^2$  if its density function is given by

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right).$$

We write  $X \sim N(\mu, \sigma^2)$ . The standard normal distribution is N(0, 1).

If  $X \sim N(\mu, \sigma^2)$  then  $aX + b \sim N(a\mu + b, a^2\sigma^2)$ . In particular,  $(X - \mu)/\sigma$  has standard normal distribution.

If  $X \sim N(\mu_X, \sigma_X^2)$  and  $Y \sim N(\mu_Y, \sigma_Y^2)$  are independent,  $X + Y \sim N(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2)$ .

The normal distribution has an extremely important role in probability theory, exemplified by the fact that it appears as the limit in the Central Limit Theorem.

We write  $\Phi$  for the distribution function of the standard normal distribution:

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) dz.$$

#### Gamma distribution

The family of gamma distributions generalises the family of exponential distributions. The gamma distribution with  $rate \lambda$  and shape r has density

$$f(x) = \begin{cases} \frac{\lambda^r}{\Gamma(r)} x^{r-1} e^{-\lambda x} & x \ge 0, \\ 0 & x < 0. \end{cases}$$

Here  $\Gamma(r)$  is the gamma function, defined by  $\Gamma(r) = \int_0^\infty z^{r-1} e^{-z} dz$ . It is the analytic continuation of the factorial function, in that  $\Gamma(r) = (r-1)!$  when r is an integer.

A gamma distribution with shape r = 1 is an exponential distribution.

If  $X \sim \text{Gamma}(r_X, \lambda)$  and  $Y \sim \text{Gamma}(r_Y, \lambda)$  are independent, then we have  $X + Y \sim \text{Gamma}(r_X + r_Y, \lambda)$ . As a special case, if  $X_1, X_2, \ldots, X_n$  are i.i.d. with  $\text{Exp}(\lambda)$  distribution, then  $X_1 + X_2 + \cdots + X_n$  has  $\text{Gamma}(n, \lambda)$  distribution.

#### 1.5.2 Discrete distributions

#### Discrete uniform distribution

X has the discrete uniform distribution on a set B of size n (for example the set  $\{1, 2, \dots, n\}$ ) if

$$p_X(x) = \begin{cases} 1/n, & x \in B \\ 0, & x \notin B \end{cases}.$$

#### Bernoulli distribution

X has Bernoulli distribution with parameter p if

$$p_X(1) = p, \ p_X(0) = 1 - p$$

(and so of course  $p_X(x) = 0$  for other values of x).

We have  $\mathbb{E} X = p$  and var X = p(1-p).

If A is an event with  $\mathbb{P}(A) = p$ , then its indicator function  $\mathbf{1}_A$  has Bernoulli distribution with parameter p.

#### Binomial distribution

If  $X_1, X_2, \ldots, X_n$  are i.i.d. Bernoulli random variables with the same parameter p, then their sum  $X_1 + \cdots + X_n$  has Binomial distribution with parameters n and p.

Equivalently, if  $A_1, \ldots, A_n$  are independent events, each with probability p, then the total number of those events which occur has Binomial(n, p) distribution.

If  $X \sim \text{Binomial}(n, p)$  then

$$p_X(k) = \binom{n}{k} p^k (1-p)^{n-k}$$
 for  $k \in \{0, 1, \dots, n\}$ .

 $\mathbb{E} X = np \text{ and } \text{var} X = np(1-p).$ 

#### Geometric distribution

Let  $p \in (0,1)$  and let X have mass function

$$p_X(k) = (1-p)^{k-1}p$$
 for  $k \in \{1, 2, 3, \dots\}$ .

Let Y = X - 1; then Y has mass function

$$p_Y(k) = (1-p)^k p$$
 for  $k \in \{0, 1, 2, \dots\}$ .

The terminology is not consistent; either X or Y might be said to have a geometric distribution with parameter p. (Or even sometimes with parameter 1-p).

If we have a sequence of independent trials, with probability p of success at each trial, then X could represent the number of trials needed for the first success to occur, while Y could represent the number of failures needed before the first success occurs.

We have

$$\mathbb{P}(X > k) = \mathbb{P}(Y \ge k) = (1 - p)^k$$
 for  $k = 0, 1, 2, \dots$ 

The geometric distribution can be thought of as a discrete analogue of the exponential distribution. It too has a memoryless property; for  $k, m \in \{0, 1, 2, ...\}$ , the conditional probability  $\mathbb{P}(X > k + m \mid X > k)$  does not depend on k.

#### Poisson distribution

X has Poisson distribution with mean  $\lambda$  if

$$\mathbb{P}(X=r) = \frac{e^{-\lambda}\lambda^r}{r!} \quad \text{for } r = 0, 1, 2, \dots$$

 $\mathbb{E} X = \lambda \text{ and } \text{var} X = \lambda.$ 

If  $X \sim \text{Poisson}(\lambda)$  and  $Y \sim \text{Poisson}(\mu)$  are independent, then  $X + Y \sim \text{Poisson}(\lambda + \mu)$ .

The Poisson distribution arises in many applications; it is a good model for the total number of events occurring when there are a large number of possible events which each occur with small probability.

# Convergence of random variables, and limit theorems

#### 2.1 Modes of convergence for random variables

Let X and Y be random variables. What might we mean by saying "X and Y are close"?

- (1) We might be describing a particular realisation. For example, we made an observation of X and Y, and on this occasion  $|X Y| < \epsilon$ .
- (2) We might be making a statement about the joint distribution of X and Y, for example

$$\mathbb{P}(|X - Y| < \epsilon) > 1 - \epsilon$$

or

$$\mathbb{E}\left(|X - Y|\right) < \epsilon.$$

(3) We might be comparing the distribution of X with the distribution of Y, for example

$$|F_X(x) - F_Y(x)| < \epsilon \text{ for all } x.$$

Correspondingly, there are several different things we might mean when we say that a sequence of random variables converges to a limit.

Let  $X_1, X_2, \ldots$  and X be random variables.

Note that  $\{X_n \to X \text{ as } n \to \infty\}$  is an **event**. More formally we could write

$$\{\omega \in \Omega \colon X_n(\omega) \to X(\omega) \text{ as } n \to \infty\}$$

to emphasise the dependence on  $\omega$ ; the event might hold for some  $\omega$  but not for others.

**Definition.**  $X_n \to X$  almost surely (or "with probability 1") if

$$\boxed{\mathbb{P}(X_n \to X \text{ as } n \to \infty) = 1.}$$
(2.1)

We often abbreviate to " $X_n \to X$  a.s.".

**Definition.**  $X_n \to X$  in probability (written  $X_n \xrightarrow{P} X$ ) if for every  $\epsilon > 0$ ,

$$\boxed{\mathbb{P}(|X_n - X| < \epsilon) \to 1 \text{ as } n \to \infty.}$$
(2.2)

Let  $F_1, F_2, \ldots$  and F be the distribution functions of  $X_1, X_2, \ldots$  and X respectively.

**Definition.**  $X_n \to X$  in distribution (or weakly), written  $X_n \stackrel{d}{\to} X$ , if, for every x such that F is continuous at x,

$$F_n(x) \to F(x) \text{ as } n \to \infty.$$
 (2.3)

We will see later that these formulations are in decreasing order of strength.

#### 2.2 Convergence in distribution

Notice that in the definition of convergence in distribution in (2.3), the random variables involved appear only through their distributions. Hence we do not even need all the random variables to be defined on the same probability space. This is really a definition about convergence of distributions, not about convergence of random variables. The joint distribution of the random variables does not need to be defined. This is in contrast to the definitions of almost sure convergence in (2.1) and of convergence in probability in (2.2), where we genuinely do need all the random variables to be defined on the same space.

As a result, we might sometimes vary the notation by writing a distribution rather than a random variable on the right-hand side; e.g. " $X_n \stackrel{d}{\to} N(0,1)$ " if the limit in distribution is the standard normal, or " $X_n \stackrel{d}{\to} U[0,1]$ " if the limit in distribution is the uniform distribution on [0,1].

In many cases the limit will be deterministic; e.g. if the limit is a distribution which puts all its mass at the value 0, then we will write  $X_n \stackrel{d}{\to} 0$ .

In (2.3), why did we ask for the limit to hold only for x which are continuity points of F, rather than at all x? The first couple of examples (which are almost trivial) make this clear.

**Example 2.1.** Let  $X_n$  have the uniform distribution on the interval [-1/n, 1/n]. Then  $F_n(x) \to 0$  for all x < 0, and  $F_n(x) \to 1$  for all x > 0.

So we have  $X_n \stackrel{d}{\to} 0$ , i.e. the distribution of  $X_n$  converges to that of a deterministic random variable which is equal to 0 with probability 1. Such a random variable has distribution function given by F(x) = 0 for x < 0 and F(x) = 1 for  $x \ge 0$ .

Note that  $F_n(0) = 1/2$  for all n, while F(0) = 1. So convergence does not hold at the point 0 itself (but this is OK, since 0 is not a continuity point of F).

**Example 2.2.** Let  $X_n$  be a deterministic random variable taking the value 1/n with probability 1. Let X be a deterministic random variable taking the value 0 with probability 1 (as above). Then once again,  $X_n \stackrel{d}{\to} X$ , (even though  $\mathbb{P}(X_n \leq 0) = 0$  for all n while  $\mathbb{P}(X \leq 0) = 1$ ).

There are many situations in which a sequence of discrete random variables converges to a continuous limit. Here is one example, showing that a geometric distribution with a small parameter is well approximated by an exponential distribution: **Example 2.3.** Let  $X_n$  have geometric distribution on the positive integers, with parameter  $p_n$ , i.e.  $\mathbb{P}(X_n = k) = (1 - p_n)^{k-1}p_n$  for  $k = 1, 2, \ldots$  Show that if  $p_n \to 0$  as  $n \to \infty$ , then  $p_n X_n$  converges in distribution to the exponential distribution with mean 1.

**Solution:** We have  $\mathbb{P}(X_n > k) = (1 - p_n)^k$  for  $k = 0, 1, 2, \ldots$  For  $k \geq 0$ , we have

$$\mathbb{P}(p_n X_n > x) = \mathbb{P}\left(X_n > \frac{x}{p_n}\right) = \mathbb{P}\left(X_n > \left\lfloor \frac{x}{p_n} \right\rfloor\right) = (1 - p_n)^{\lfloor x/p_n \rfloor} \to e^{-x} \text{ as } n \to \infty$$

because  $p_n \to 0$ ; here we use the fact that  $(1 - \epsilon)^{x/\epsilon} \to e^{-x}$  as  $\epsilon \to 0$ , and also that  $|x/p_n| - x/p_n$  is bounded.

Hence if  $F_n$  is the distribution function of  $p_n X_n$ , then  $1 - F_n(x) \to e^{-x}$  as  $n \to \infty$ . So  $F_n(x) \to 1 - e^{-x}$  for all x > 0, while  $F_n(x) = 0$  for all  $x \le 0$  and all n.

So indeed  $F_n(x) \to F(x)$  for all x, where F is the distribution function of a random variable with Exp(1) distribution.

There are several more examples on the problem sheets.

#### 2.3 Comparison of different modes of convergence

**Theorem 2.4.** The following implications hold:

$$X_n \to X \ almost \ surely \Rightarrow X_n \to X \ in \ probability \Rightarrow X_n \to X \ in \ distribution$$

The reverse implications do not hold in general.

Before starting the proof we note a useful fact, which is a simple consequence of the countable additivity axiom for unions of disjoint sets (1.1).

**Lemma 2.5.** Let  $A_n, n \ge 1$ , be an increasing sequence of events; that is,  $A_1 \subseteq A_2 \subseteq A_3 \subseteq \dots$ . Then

$$\lim_{n \to \infty} \mathbb{P}(A_n) = \mathbb{P}\left(\bigcup_{n \ge 1} A_n\right). \tag{2.4}$$

*Proof.* Because the sequence  $A_n$  is increasing, it is easy to rewrite the union as a disjoint union:

$$\mathbb{P}\left(\bigcup_{n\geq 1} A_n\right) = \mathbb{P}\left(A_1 \cup \bigcup_{n\geq 1} (A_{n+1} \setminus A_n)\right) \\
= \mathbb{P}(A_1) + \sum_{i=1}^{\infty} \mathbb{P}\left(A_{i+1} \setminus A_i\right) \quad \text{(using countable additivity)} \\
= \mathbb{P}(A_1) + \lim_{n\to\infty} \sum_{i=1}^{n-1} \mathbb{P}\left(A_{i+1} \setminus A_i\right) \\
= \lim_{n\to\infty} \left(\mathbb{P}(A_1) + \sum_{i=1}^{n-1} \mathbb{P}\left(A_{i+1} \setminus A_i\right)\right) \\
= \lim_{n\to\infty} \mathbb{P}\left(A_1 \cup \bigcup_{1\leq i\leq n-1} (A_{i+1} \setminus A_i)\right) \\
= \lim_{n\to\infty} \mathbb{P}(A_n).$$

Proof of Theorem 2.4.

(1) First we will show that convergence in probability implies convergence in distribution. Let  $F_n$  be the distribution function of  $X_n$ , and F the distribution function of X. Fix any x such that F is continuous at x, and fix any  $\epsilon > 0$ .

Observe that if  $X_n \leq x$ , then either  $X \leq x + \epsilon$  or  $|X_n - X| > \epsilon$ . Hence

$$F_n(x) = \mathbb{P}(X_n \le x)$$

$$\le \mathbb{P}(X \le x + \epsilon \text{ or } |X_n - X| > \epsilon)$$

$$\le \mathbb{P}(X \le x + \epsilon) + \mathbb{P}(|X_n - X| > \epsilon)$$

$$\to F(x + \epsilon) \text{ as } n \to \infty,$$

using the convergence in probability. So  $F_n(x) < F(x + \epsilon) + \epsilon$  for all large enough n.

Similarly by looking at  $1 - F_n(x) = \mathbb{P}(X_n > x)$ , we can obtain that  $F_n(x) > F(x - \epsilon) - \epsilon$  for all large enough n.

Since  $\epsilon > 0$  is arbitrary, and since F is continuous at x, this implies that  $F_n(x) \to F(x)$  as  $n \to \infty$ .

- (2) For convergence in distribution, we do not need the random variables to be defined on the same probability space. But even if they are, convergence in distribution does not imply convergence in probability. For example, suppose that X and Y are random variables with the same distribution but with  $\mathbb{P}(X=Y) < 1$ . Then the sequence  $X, X, X, \ldots$  converges to Y in distribution, but not in probability.
- (3) Now we will show that almost sure convergence implies convergence in probability. Fix  $\epsilon > 0$  and for  $N \in \mathbb{N}$ , define the event  $A_N$  by

$$A_N = \{|X_n - X| < \epsilon \text{ for all } n \ge N\}.$$

Suppose that  $X_n \to X$  almost surely. If the event  $\{X_n \to X\}$  occurs, then the event  $A_N$  must occur for some N, so we have  $\mathbb{P}(\bigcup A_N) = 1$ .  $A_N$  is an increasing sequence of events, so (2.4) then gives  $\lim_{N\to\infty} \mathbb{P}(A_N) = 1$ .

But  $A_N$  implies  $|X_N - X| < \epsilon$ , giving  $\mathbb{P}(|X_N - X| < \epsilon) \to 1$ . Since  $\epsilon$  is arbitrary, this means that  $X_n \to X$  in probability, as desired.

(4) Finally we want to show that convergence in probability does not imply almost sure convergence.

Consider a sequence of independent random variables  $X_n$  where  $\mathbb{P}(X_n = 1) = 1/n$  and  $\mathbb{P}(X_n = 0) = (n-1)/n$ .

We have  $X_n \to 0$  in probability as  $n \to \infty$  because for any  $\epsilon > 0$ ,  $\mathbb{P}(|X_n - 0| < \epsilon) \ge \mathbb{P}(X = 0) \to 1$ .

Since  $X_n$  only take the values 0 and 1, the event  $\{X_n \to 0\}$  is the same as the event  $\{X_n = 0 \text{ eventually}\}$ . This is  $\bigcup_{N>1} B_N$  where  $B_N = \{X_n = 0 \text{ for all } n \geq N\}$ .

But for any N and K,

$$\mathbb{P}(B_N) \le \mathbb{P}(X_n = 0 \text{ for all } n = N, \dots, N + K) = \frac{N-1}{N} \frac{N}{N+1} \frac{N+1}{N+2} \cdots \frac{N+K-1}{N+K}$$
$$= \frac{N-1}{N+K}.$$

As  $K \ge 1$  is arbitrary, we obtain that  $\mathbb{P}(B_N) = 0$ . Hence also by Lemma 2.5,  $\mathbb{P}(\bigcup_{N \ge 1} B_N) = 0$ , and so  $\mathbb{P}(X_n \to 0) = 0$ . Hence it is not the case that  $X_n$  converges to 0 almost surely.  $\square$ 

Although convergence in distribution is weaker than convergence in probability, there is a partial converse, for the case when the limit is deterministic:

**Theorem 2.6.** Let  $X_1, X_2, ...$  be a sequence of random variables defined on the same probability space. If  $X_n \to c$  in distribution where c is some constant, then also  $X_n \to c$  in probability.

*Proof.* Exercise (see problem sheet).  $\Box$ 

#### 2.4 Review: Weak law of large numbers

This was covered at the end of last year's course (without explicitly introducing the notion of convergence in probability).

Let  $S_n = X_1 + X_2 + \cdots + X_n$ , where  $X_i$  are i.i.d. with mean  $\mu$ . The law of large numbers tells us that, roughly speaking,  $S_n$  behaves to first order like  $n\mu$  as  $n \to \infty$ . The weak law phrases this in terms of convergence in probability. (Later we will see a stronger result in terms of almost sure convergence).

**Theorem** (Weak Law of Large Numbers). Let  $X_1, X_2, ...$  be i.i.d. random variables with finite mean  $\mu$ . Let  $S_n = X_1 + X_2 + \cdots + X_n$ . Then

$$\frac{S_n}{n} \stackrel{P}{\to} \mu \text{ as } n \to \infty.$$

That is, for all  $\epsilon > 0$ ,

$$\mathbb{P}\left(\left|\frac{S_n}{n} - \mu\right| < \epsilon\right) \to 1 \text{ as } n \to \infty.$$
 (2.5)

Given Theorem 2.6, we could equivalently write  $\frac{S_n}{n} \stackrel{d}{\to} \mu$ .

We will give an extremely simple proof of the weak law of large numbers, under an additional condition (that the  $X_i$  have finite variance). To do this, we need some results which give probability bounds on the tail of a distribution in terms of its mean and variance.

**Theorem** (Markov's inequality). Let X be random variable taking non-negative values (i.e.  $\mathbb{P}(X \geq 0) = 1$ ). Then for any z > 0,

$$\mathbb{P}(X \ge z) \le \frac{\mathbb{E}X}{z}.\tag{2.6}$$

*Proof.* We consider a random variable  $X_z = z\mathbf{1}\{X \geq z\}$ . So  $X_z$  takes the value 0 whenever X is in [0,z) and the value z whenever X is in  $[z,\infty)$ . So  $X \geq X_z$  always (here we use the fact that X is non-negative).

Then 
$$\mathbb{E} X \geq \mathbb{E} X_z = z \mathbb{E} \mathbf{1} \{X \geq z\} = z \mathbb{P}(X \geq z)$$
. Rearranging gives the result.

**Theorem** (Chebyshev's inequality). Let Y be a random variable with finite mean and variance. Then for any  $\epsilon > 0$ ,

$$\mathbb{P}(|Y - \mathbb{E} Y| \ge \epsilon) \le \frac{\operatorname{var}(Y)}{\epsilon^2}.$$

Proof.

$$\begin{split} \mathbb{P}\big(|Y - \mathbb{E}\,Y| \ge \epsilon\big) &= \mathbb{P}\big([Y - \mathbb{E}\,Y]^2 \ge \epsilon^2\big) \\ &\le \frac{\mathbb{E}\,\big([Y - \mathbb{E}\,Y]^2\big)}{\epsilon^2} \end{split}$$

(by applying Markov's inequality (2.6) with  $X = [Y - \mathbb{E}Y]^2$  and  $z = \epsilon^2$ )

$$=\frac{\operatorname{var}(Y)}{\epsilon^2}.$$

Proof of the weak law of large numbers in the case of random variables with finite variance. Let  $X_i$  be i.i.d. with mean  $\mu$  and variance  $\sigma^2$ . Recall  $S_n = X_1 + \cdots + X_n$ . We want to show that  $S_n/n \stackrel{P}{\to} \mu$  as  $n \to \infty$ .

We have  $\mathbb{E}(S_n/n) = \mu$ , and (using the independence of the  $X_i$ ),

$$\operatorname{var}\left(\frac{S_n}{n}\right) = \frac{\operatorname{var}(S_n)}{n^2}$$

$$= \frac{\operatorname{var}X_1 + \dots + \operatorname{var}X_n}{n^2}$$

$$= \frac{n\sigma^2}{n^2}$$

$$= \frac{\sigma^2}{n}.$$

Fix any  $\epsilon > 0$ . Using Chebyshev's inequality applied to the random variable  $S_n/n$ , we have

$$\mathbb{P}\left(\left|\frac{S_n}{n} - \mu\right| \ge \epsilon\right) \le \frac{\operatorname{var}\left(\frac{S_n}{n}\right)}{\epsilon^2}$$

$$= \frac{\sigma^2}{n\epsilon^2}$$

$$\to 0 \text{ as } n \to \infty.$$

So indeed (2.5) holds, as required.

Remark. Observe that we could relax considerably the assumptions in the weak law of large numbers, and still get the same result using almost the same proof. We never used at all the assumption that the  $X_i$  all had the same distribution. We could also relax the assumption that the  $X_i$  are independent, as long as the variance of  $S_n$  grows more slowly than  $n^2$ . For example, if we have an upper bound on the variance of each  $X_i$ , and a bound which is  $o(n^2)$  on the sum  $\sum_{1 \le i < j \le n} \text{cov}(X_i, X_j)$ , then exactly the same idea applies to show that  $(S_n - \mathbb{E} S_n)/n$  converges to 0 in probability.

#### 2.5 Strong law of large numbers

In the weak law of large numbers, we proved convergence in distribution of the average of i.i.d. random variables to the mean. The strong law says more: the convergence occurs with probability 1.

**Theorem** (Strong Law of Large Numbers). Let  $X_1, X_2, ...$  be i.i.d. with mean  $\mu$ . Let  $S_n = X_1 + \cdots + X_n$ . Then

 $\frac{S_n}{n} \to \mu \text{ almost surely as } n \to \infty.$ 

#### 2.5.1 Proof of the strong law of large numbers (non-examinable)

A proof of the strong law of large numbers in full generality is somewhat involved. A nice proof uses martingales and is part of next year's course on Probability, Measure and Martingales.

However, if we assume an extra condition, namely that the distribution has a finite fourth moment, then a relatively straightforward proof is possible. [NB the proof is not examinable.]

Proof of Strong Law of Large Numbers, under the additional condition  $\mathbb{E} X_n^4 < \infty$ . Let us centre the  $X_n$ , writing  $W_n = X_n - \mu$ .

Then  $\mathbb{E} W_n = 0$ , and we have  $\mathbb{E} X_n^4 < \infty \Rightarrow \mathbb{E} W_n^4 < \infty$  (exercise).

Note also that

$$(\mathbb{E} W_n^2)^2 = \mathbb{E} (W_n^4) - \operatorname{var}(W_n^2) \le \mathbb{E} (W_n^4).$$

We will consider  $\mathbb{E}\left[(S_n - n\mu)^4\right]$ . Expanding the fourth power and using linearity of expectation, we obtain

$$\begin{split} \mathbb{E} \left[ (S_n - n\mu)^4 \right] &= \mathbb{E} \left[ (W_1 + W_2 + \dots + W_n)^4 \right] \\ &= \sum_{1 \leq i \leq n} \mathbb{E} \, W_i^4 + 4 \sum_{\substack{1 \leq i,j \leq n \\ i \neq j}} \mathbb{E} \, W_i^3 W_j + 3 \sum_{\substack{1 \leq i,j \leq n \\ i \neq j}} \mathbb{E} \, W_i^2 W_j^2 \\ &+ 6 \sum_{\substack{1 \leq i,j,k \leq n \\ i,j,k \text{ distinct}}} \mathbb{E} \, W_i^2 W_j W_k + \sum_{\substack{1 \leq i,j,k,l \leq n \\ i,j,k,l \text{ distinct}}} \mathbb{E} \, W_i W_j W_k W_l. \end{split}$$

(The exact constants in front of the sums are not too important!) Using independence and  $\mathbb{E} W_i = 0$ , most of these terms vanish. For example,  $\mathbb{E} W_i^3 W_j = \mathbb{E} W_i^3 \mathbb{E} W_j = 0$ . We are left with only

$$\mathbb{E}\left[ (S_n - n\mu)^4 \right] = n\mathbb{E} W_1^4 + 3n(n-1) \left( \mathbb{E} [W_1^2] \right)^2 < 3n^2\mathbb{E} W_1^4.$$

From this we have

$$\mathbb{E}\left[\sum_{n=1}^{\infty} \left(\frac{S_n}{n} - \mu\right)^4\right] = \sum_{n=1}^{\infty} \mathbb{E}\left[\left(\frac{S_n}{n} - \mu\right)^4\right] = \sum_{n=1}^{\infty} \frac{1}{n^4} \mathbb{E}\left[\left(S_n - n\mu\right)^4\right]$$
$$\leq \sum_{n=1}^{\infty} \frac{3\mathbb{E}W_1^4}{n^2} < \infty.$$

But if Z is a random variable with  $\mathbb{E} Z < \infty$ , then certainly  $\mathbb{P}(Z < \infty) = 1$ . Applying this with  $Z = \left(\frac{S_n}{n} - \mu\right)^4$ , we get

$$\mathbb{P}\left(\sum_{n=1}^{\infty} \left(\frac{S_n}{n} - \mu\right)^4 < \infty\right) = 1.$$

Finally, if  $\sum (a_n - \mu)^4$  is finite, then certainly  $a_n \to \mu$  as  $n \to \infty$ . So we can conclude that

$$\mathbb{P}\left(\frac{S_n}{n} \to \mu \text{ as } n \to \infty\right) = 1,$$

as required.  $\Box$ 

#### 2.6 Central limit theorem: statement and examples

#### 2.6.1 Central limit theorem

The weak law of large numbers tells us that the distribution of  $S_n/n$  concentrates around  $\mu$  as n becomes large. The **central limit theorem** (CLT) goes much further, telling us that (if the random variables  $X_i$  have finite variance) the "fluctuations" of  $S_n$  around  $n\mu$  are of order  $\sqrt{n}$ . Moreover, the behaviour of these fluctuations is *universal*; whatever the distribution of the  $X_i$ , if we scale  $S_n - n\mu$  by  $\sqrt{n}$ , we obtain a normal distribution as the limit as  $n \to \infty$ .

**Theorem** (Central Limit Theorem). Let  $X_1, X_2, \ldots$  be i.i.d. random variables with mean  $\mu$  and variance  $\sigma^2 \in (0, \infty)$ . Let  $S_n = X_1 + X_2 + \cdots + X_n$ . Then

$$\frac{S_n - n\mu}{\sigma\sqrt{n}} \xrightarrow{d} N(0,1) \text{ as } n \to \infty.$$
 (2.7)

We will prove the CLT later using generating functions.

Remark 2.7. We can summarise the CLT in three stages:

- (1) The distribution of  $S_n$  concentrates around  $n\mu$ ;
- (2) The fluctuations of  $S_n$  around  $n\mu$  are of order  $\sqrt{n}$ ;
- (3) The asymptotic distribution of these fluctuations is normal.

These are somehow in increasing order of refinement. Some students take in the third of these, but not the first two; they remember that the RHS in (2.7) is a normal distribution, but are hazy about what is going on on the LHS. This is a bit perverse; without knowing the scale of the fluctuations, or what they fluctuate around, knowing their distribution is not so useful!

Remark 2.8. The CLT can be formulated in other ways: in the setting of the theorem,

• 
$$\mathbb{P}\left(a \leq \frac{S_n - n\mu}{\sigma\sqrt{n}} \leq b\right) \to \mathbb{P}\left(a \leq Z \leq b\right)$$
, as  $n \to \infty$ , for  $Z \sim N(0, 1)$ , and for all  $a \leq b$ ,

• and 
$$\frac{S_n - n\mu}{\sqrt{n}} \stackrel{d}{\to} N(0, \sigma^2)$$
, as  $n \to \infty$ .

For the first, apply the definition of convergence in distribution to the difference of the cdf at b and at a. For the second, note that  $\sigma Z \sim N(0, \sigma^2)$ .

#### 2.6.2 Example: tail probabilities

**Example 2.9.** An insurance company sells 10,000 similar car insurance policies. They estimate that the amount paid out in claims on a typical policy has mean £240 and standard deviation £800. Estimate how much they need to put aside in reserves to be 99% sure that the reserve will exceed the total amount claimed.

**Solution:** Let  $\mu = £240$ ,  $\sigma = £800$ , n = 10,000, and note  $\Phi^{-1}(0.99) = 2.326$  where  $\Phi$  is the distribution function of the standard normal.

Let  $S_n$  be the total amount claimed. For large n, the Central Limit Theorem tells us that

$$\mathbb{P}\left(\frac{S_n - n\mu}{\sigma\sqrt{n}} < \Phi^{-1}(0.99)\right) \approx 0.99,$$

i.e.

$$\mathbb{P}\left(S_n < \Phi^{-1}(0.99)\sigma\sqrt{n} + n\mu\right) \approx 0.99.$$

So the amount needed in reserves is approximately  $\Phi^{-1}(0.99)\sigma\sqrt{n} + n\mu$ , which in this case is £2,586,080.

Notice that the reserve required per customer is about £258.61, which is £18.61 higher than  $\mu$ . We can see from the calculation above that this surplus is proportional to  $n^{-1/2}$ . If we had 100 customers rather than 10,000, we would need a surplus 10 times bigger, while with 1,000,000 customers it would be 10 times smaller.

The fact that the amount per customer needed to cover the fluctuations around the mean is decreasing in the number of customers is an example of **risk pooling**.

Of course, the example of identical customers is a bit simplistic, but the effect of risk pooling that we observe is a very real one. Our analysis also assumed that the different customers are independent – is that realistic? For car insurance, it is not such a bad assumption. Similarly for life insurance. In the case of property insurance, it could be a very bad assumption (for example, floods can damage many properties simultaneously). In that situation, the effect of risk pooling is a lot smaller (which explains why obtaining insurance for a property subject to a risk of flooding can be problematic, even if the risk is not that great).

#### 2.6.3 Example: CLT versus Poisson approximation

**Example 2.10** (Binomial distribution: CLT and Poisson approximation). Let  $p \in (0,1)$  and let  $Y_n$  have Binomial(n,p) distribution. Then we can write  $Y_n = X_1 + \cdots + X_n$  where the  $X_i$  are i.i.d. Bernoulli(p) random variables. (We can think of the  $X_i$  as indicator functions of independent events, all with the same probability, e.g. arising from random sampling).

The  $X_i$  each have mean p and variance p(1-p). So we can apply the CLT to obtain

$$\frac{Y_n - np}{\sqrt{n}} \stackrel{d}{\to} N(0, p(1-p))$$
 as  $n \to \infty$ .

Now instead of considering fixed p, consider random variables  $W_n$  with Binomial $(n, p_n)$  distribution, where  $p_n \to 0$  as  $n \to \infty$ . Now a very different limit applies, describing a situation in which we have a very large number of trials but each one has a very small probability of success. Let  $\lambda_n = np_n$ , the mean of  $W_n$ . Suppose that  $\lambda_n$  converges to a limit

 $\lambda$  as  $n \to \infty$ , so that the expected total number of successes stays approximately constant. Then we will show that  $W_n$  converges in distribution to Poisson( $\lambda$ ).

It is enough to show (check!) that for each fixed k = 0, 1, ...,

$$\mathbb{P}(W_n = k) \to \frac{\lambda^k}{k!} e^{-\lambda}$$

(since the RHS is the probability that a  $Poisson(\lambda)$  random variable takes the value k). We have

$$\mathbb{P}(W_n = k) = \binom{n}{k} p_n^k (1 - p_n)^{n-k}$$

$$= \binom{n}{k} \left(\frac{\lambda_n}{n}\right)^k \left(1 - \frac{\lambda_n}{n}\right)^{n-k}$$

$$= \frac{n(n-1)\cdots(n-k+1)}{n^k} \frac{\lambda_n^k}{k!} \left(1 - \frac{\lambda_n}{n}\right)^n \left(1 - \frac{\lambda_n}{n}\right)^{-k}$$

$$\to 1 \cdot \frac{\lambda^k}{k!} e^{-\lambda} \cdot 1$$

as  $n \to \infty$ , as desired.

#### Generating functions

#### 3.1 Review of probability generating functions

Let X be a random variable taking non-negative integer values, and let  $p_X$  be its probability mass function. The **probability generating function** of X is defined by  $G: \mathcal{S} \to \mathbb{R}$ , where

$$\mathcal{S} = \left\{ s \in \mathbb{R} \colon \sum_{k=0}^{\infty} |s|^k p_X(k) < \infty \right\}$$

and

$$G(s) := \mathbb{E}\left(s^X\right) = \sum_{k=0}^{\infty} p_X(k) s^k, \quad s \in \mathcal{S}.$$

G is a power series whose radius of convergence is at least 1. We can recover the coefficients of the power series, i.e. the values of the function  $p_X$ , from the behaviour of G and its derivatives at the point 0, and we can compute the moments of X from the behaviour of G and its derivatives at 1:

#### Theorem 3.1.

- (a)  $G^{(k)}(0) = k! p_X(k)$  for k = 0, 1, 2, ...
- (b) G(1) = 1 and  $G^{(k)}(1) = \mathbb{E}[X(X-1)\cdots(X-k+1)]$  for  $k = 1, 2, \dots$

Here if the radius of convergence of G is exactly 1, then  $G^{(k)}(1)$  should be taken to mean  $\lim_{s\uparrow 1} G^{(k)}(s)$ . In this case, the limit may be finite or infinite.

From Theorem 3.1(a), we see immediately that a distribution is determined by its generating function:

**Theorem 3.2** (Uniqueness theorem for probability generating functions). If X and Y have the same generating function, then they have the same distribution.

From Theorem 3.1(b), we have, for example,  $\mathbb{E}(X) = G'(1)$ ,  $\operatorname{var}(X) = G''(1) + G'(1) - [G'(1)]^2$ .

Generating functions are extremely useful tools for dealing with sums of independent random variables. Let X and Y be independent random variables with generating functions

 $G_X$  and  $G_Y$ . Then the generating function of their sum is given by

$$G_{X+Y}(s) = \mathbb{E} \left( s^{X+Y} \right)$$

$$= \mathbb{E} \left( s^X s^Y \right)$$

$$= \mathbb{E} \left( s^X \right) \mathbb{E} \left( s^Y \right) \quad \text{(by independence)}$$

$$= G_X(s)G_Y(s).$$

(Again, "independence means multiply").

We can also treat the sum of a random number of random variables. Let  $X_1, X_2, \ldots$  be i.i.d. random variables (taking non-negative integer values), and let N be another random variable, also taking non-negative integer values, independent of the sequence  $X_i$ . Define  $S = X_1 + \cdots + X_N$ . Then we can write the generating function of S in terms of the common generating function of the  $X_i$  and the generating function of N by the law of total probability for expectations

$$G_{S}(z) = \mathbb{E} \left( z^{S} \right)$$

$$= \mathbb{E} \left( z^{X_{1} + \dots + X_{N}} \right)$$

$$= \sum_{n=0}^{\infty} \mathbb{E} \left( z^{X_{1} + \dots + X_{n}} \middle| N = n \right) \mathbb{P}(N = n)$$

$$= \sum_{n=0}^{\infty} \mathbb{E} \left( z^{X_{1} + \dots + X_{n}} \middle| \mathbb{P}(N = n) \right) \text{ (by independence)}$$

$$= \sum_{n=0}^{\infty} \left( \mathbb{E} \left( z^{X_{1}} \right) \right)^{n} \mathbb{P}(N = n) \text{ (by independence)}$$

$$= \mathbb{E} \left( \left( G_{X}(z) \right)^{N} \right)$$

$$= G_{N} \left( G_{X}(z) \right).$$

#### 3.2 Moment generating functions

The probability generating function is well adapted for handling random variables which take non-negative integer values. To treat random variables with general distribution, we now introduce two related objects, the moment generating function and the characteristic function.

The moment generating function of a random variable X is defined by

$$M_X(t) := \mathbb{E}\left(e^{tX}\right). \tag{3.1}$$

This expectation may be finite or infinite, so  $M_X$  is a function  $M_X : \mathbb{R} \to [0, \infty]$ , or we might alternatively consider the function  $M_X$  to be defined on the domain  $\{t \in \mathbb{R} : \mathbb{E}\left(e^{tX}\right) < \infty\}$ , where it takes values in  $[0, \infty)$ .

(Note that we could obtain the moment generating function by substituting  $s = e^t$  in the definition of the probability generating function above. An advantage of this form is that we can conveniently consider an expansion around t = 0, whereas the expansion around s = 0,

convenient when the random variables took only non-negative integer values, no longer gives a power series in the general case.)

We will state (but not prove) Uniqueness and Convergence theorems that are similar to the ones stated for probability generating functions, subject, however, to assuming that the moment generating functions are finite on an interval around 0, which does not hold for all random variables! We will provide a fuller discussion of these points later.

#### 3.2.1 Examples and basic results about moment generating functions

For the same reason as for probability generating functions, the mgf of a sum of independent random variables is the product of the mgfs:

#### Theorem 3.3.

- (a) If Y = aX + b, then  $M_Y(t) = e^{bt}M_X(at)$ .
- (b) Let  $X_1, \ldots, X_n$  be independent random variables, with mgfs  $M_{X_1}, \ldots, M_{X_n}$ . Then the mgf of their sum is given by

$$M_{X_1 + \dots + X_n}(t) = M_{X_1}(t) \dots M_{X_n}(t).$$

*Proof.* (a): easy exercise. Part (b) is also straightforward:

$$M_{X_1 + \dots + X_n}(t) = \mathbb{E} \left( e^{tX_1 + \dots + tX_n} \right)$$

$$= \mathbb{E} \left( e^{tX_1} \dots e^{tX_n} \right)$$

$$= \mathbb{E} \left( e^{tX_1} \right) \dots \mathbb{E} \left( e^{tX_n} \right) \quad \text{(by independence)}$$

$$= M_{X_1}(t) \dots M_{X_n}(t).$$

An immediate disadvantage of the moment generating function is that it may not be well defined. If the positive tail of the distribution is too heavy, the expectation in the definition in (3.1) may be infinite for all t > 0: while if the negative tail is too heavy, the expectation may be infinite for all t < 0.

For the moment generating function to be useful, we will require  $\mathbb{E} e^{t_0|X|} < \infty$  for some  $t_0 > 0$ . That is, X has "finite exponential moments" of some order (equivalently, the tails of the distribution function decay at least exponentially fast). Then (exercise!) the moment generating function is finite for all  $t \in (-t_0, t_0)$ , and also all the moments  $\mathbb{E} X^k$  are finite.

Most of the classical distributions that we have looked at are either bounded or have tails that decay at least exponentially (for example uniform, geometric/exponential, normal, Poisson...). However, distributions with heavier tails are also of great importance, especially in many modelling contexts. For those distributions, the moment generating function is of no use; however, we can consider a variant of it, the characteristic function (see later).

The next result explains the terminology "moment generating function"; the mgf of X can be expanded as a power series around 0, in which the coefficients are the moments of X.

**Theorem 3.4.** Suppose  $M_X(t)$  is finite for  $|t| \le t_0$ , for some  $t_0 > 0$ . Then

(a) 
$$M_X(t) = \sum_{k=0}^{\infty} \frac{t^k \mathbb{E}(X^k)}{k!}$$
 for  $|t| \le t_0$ .

(b) 
$$M_X^{(k)}(0) = \mathbb{E}(X^k)$$
.

Informal proof.

$$M_X(t) = \mathbb{E}(e^{tX})$$

$$= \mathbb{E}\left(1 + tX + \frac{(tX)^2}{2!} + \frac{(tX)^3}{3!} + \dots\right)$$

$$= 1 + t\mathbb{E}(X) + \frac{t^2\mathbb{E}(X^2)}{2!} + \frac{t^3\mathbb{E}(X^3)}{3!} + \dots,$$

using linearity of expectation. This gives (a) and taking derivatives at 0 gives (b). Exchanging expectation with an infinite sum, as we did here, really needs extra justification, which is not in our technical toolkit at this stage. In this case there is no problem (for example, it can be formally justified in the case where the sum of the absolute values also has finite expectation – in this case this gives  $\mathbb{E} e^{|tX|} < \infty$  which is easily seen to be true); but we do not pursue it further here.

The following **uniqueness** and **continuity** results will be key to our applications of the moment generating function.

**Theorem 3.5.** If X and Y are random variables with the same moment generating function, which is finite on  $[-t_0, t_0]$  for some  $t_0 > 0$ , then X and Y have the same distribution.

**Theorem 3.6.** Suppose Y and  $X_1, X_2, \ldots$  are random variables whose moment generating functions  $M_Y$  and  $M_{X_1}, M_{X_2}, \ldots$  are all finite on  $[-t_0, t_0]$  for some  $t_0 > 0$ . If

$$M_{X_n}(t) \to M_Y(t)$$
 as  $n \to \infty$ , for all  $t \in [-t_0, t_0]$ ,

then

$$X_n \stackrel{d}{\to} Y \text{ as } n \to \infty.$$

The proofs of the uniqueness and continuity results for mgfs are beyond the scope of the course. They correspond to an inversion theorem from Fourier analysis, by which the distribution function of X can be written in a suitable way as a linear mixture over t of terms  $\mathbb{E} e^{itX}$ .

**Example 3.7.** Find the moment generating function of the exponential distribution with parameter  $\lambda$ .

Solution:

$$M(t) = \mathbb{E}(e^{tX})$$

$$= \int_0^\infty e^{tx} f(x) dx$$

$$= \int_0^\infty \lambda e^{tx} e^{-\lambda x} dx$$

$$= \frac{\lambda}{\lambda - t} \int_0^\infty (\lambda - t) \exp^{-(\lambda - t)x} dx$$
$$= \frac{\lambda}{\lambda - t} \text{ for } t \in (-\infty, \lambda).$$

In the last step we used the fact that the integrand is the density function of a random variable, namely one with  $\operatorname{Exp}(\lambda-t)$  distribution, so that the integral is 1. Note that this last step is meaningless when  $t \geq \lambda$  although  $\lambda/(\lambda-t)$  is well-defined for  $t > \lambda$ . Therefore, it is important to **specify the domain of** M on which this argument is valid.

**Example 3.8.** Find the moment generating function of a random variable with  $N(\mu, \sigma^2)$  distribution. If  $Y_1 \sim N(\mu_1, \sigma_1^2)$  and  $Y_2 \sim N(\mu_2, \sigma_2^2)$  are independent, show that  $Y_1 + Y_2 \sim N(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2)$ .

**Solution:** Let  $X \sim N(\mu, \sigma^2)$ . Then  $X = \sigma Z + \mu$ , where Z is standard normal. We have

$$M_Z(t) = \mathbb{E}\left(e^{tZ}\right)$$

$$= \int_{-\infty}^{\infty} \exp(tz) \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-z^2}{2}\right) dz$$

$$= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-(z^2 - 2tz)}{2}\right) dz$$

$$= \int_{-\infty}^{\infty} \exp\left(\frac{t^2}{2}\right) \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-(z - t)^2}{2}\right) dz$$

(this is "completing the square")

$$= \exp\left(\frac{t^2}{2}\right) \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-(z-t)^2}{2}\right) dz$$
$$= e^{t^2/2}$$

(the same trick as before: the integrand is the density function of N(t,1) so the integral is 1). Then from the first part of Theorem 3.3,  $M_X(t) = e^{\mu t} M_Z(\sigma t) = e^{\mu t + \sigma^2 t^2/2}$ . For the second part,

$$\begin{split} M_{Y_1+Y_2}(t) &= M_{Y_1}(t) M_{Y_2}(t) \\ &= e^{\mu_1 t + \sigma_1^2 t^2/2} e^{\mu_2 t + \sigma_2^2 t^2/2} \\ &= e^{(\mu_1 + \mu_2)t + (\sigma_1^2 + \sigma_2^2)t^2/2} \end{split}$$

Since this is the mgf of  $N(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2)$ , and it is finite on an interval  $[-t_0, t_0]$  (in fact, for all  $t \in \mathbb{R}$ ), the uniqueness theorem for mgfs tells us that indeed that must be the distribution of  $Y_1 + Y_2$ .

#### 3.2.2 Proof of WLLN and CLT using moment generating functions

Let  $X_1, X_2,...$  be a sequence of i.i.d. random variables with finite exponential moments of some order (i.e. their moment generating function is finite on some interval containing the origin in its interior).

Let  $S_n = X_1 + X_2 + \cdots + X_n$ . We can use moment generating functions to give a very compact proof of the Central Limit Theorem for the sequence  $S_n$  (and, even more simply, the Weak Law of Large Numbers).

Let the  $X_i$  have mean  $\mu$  and variance  $\sigma^2$ , and let M be their moment generating function.

#### Weak law of large numbers

From Taylor's Theorem and the expansion of M as a power series around 0 (Theorem 3.4) we can write, as  $h \to 0$ ,

$$M(h) = M(0) + hM'(0) + o(h)$$
  
= 1 + h\mu + o(h).

Here, we use notation "f(h) = o(g(h)) as  $h \to 0$ " to mean  $f(h)/g(h) \to 0$  as  $h \to 0$ . We will similarly use notation " $a_n = o(b_n)$  as  $n \to \infty$ " to mean  $a_n/b_n \to 0$  as  $n \to \infty$ . Here, specifically, we therefore have  $(M(h) - M(0) - hM'(0))/h \to 0$  as  $h \to 0$ .

Let  $\overline{M}_n$  be the mgf of  $S_n/n$ . Using the independence of the  $X_i$ , we have

$$\overline{M}_n(t) = \mathbb{E}\left(e^{tS_n/n}\right)$$

$$= \mathbb{E}\left(e^{tX_1/n} \dots e^{tX_n/n}\right)$$

$$= (M(t/n))^n$$

$$= \left(1 + \frac{t}{n}\mu + o(t/n)\right)^n \text{ as } n \to \infty$$

$$\to e^{t\mu} \text{ as } n \to \infty.$$

But  $e^{t\mu}$  is the mgf of a random variable which takes the constant value  $\mu$  with probability 1. From the continuity theorem for mgfs,  $S_n/n \stackrel{d}{\to} \mu$  as  $n \to \infty$ , and we have proved the weak law of large numbers.

#### Central limit theorem

Let  $Y_i = X_i - \mu$ , and let  $M_Y$  be the mgf of the common distribution of the  $Y_i$ . Taking one more term in the Taylor expansion, we have that as  $h \to 0$ ,

$$M_Y(h) = M_Y(0) + hM'_Y(0) + \frac{h^2}{2}M''_Y(0) + o(h^2)$$
$$= 1 + h\mathbb{E}(Y) + \frac{h^2}{2}\text{var}(Y) + o(h^2)$$
$$= 1 + h^2\sigma^2/2 + o(h^2).$$

Let  $\widetilde{M}_n$  be the mgf of  $\frac{S_n - \mu n}{\sigma \sqrt{n}}$ . Then we have

$$\widetilde{M}_n(t) = \mathbb{E}\left(\exp\left(\frac{t(S_n - \mu n)}{\sigma\sqrt{n}}\right)\right)$$
$$= \mathbb{E}\left(\exp\left(\frac{t(X_1 - \mu)}{\sigma\sqrt{n}}\right) \dots \exp\left(\frac{t(X_n - \mu)}{\sigma\sqrt{n}}\right)\right)$$

$$= M_Y \left(\frac{t}{\sigma\sqrt{n}}\right)^n$$

$$= \left(1 + \frac{t^2}{2n} + o\left(\frac{t^2}{n}\right)\right)^n \text{ as } n \to \infty$$

$$\to \exp\left(\frac{t^2}{2}\right) \text{ as } n \to \infty.$$

But the last line is the mgf of N(0,1). Using the continuity theorem again,

$$\frac{S_n - \mu n}{\sigma \sqrt{n}} \stackrel{d}{\to} N(0, 1),$$

and we have proved the CLT.

#### 3.3 Using moment generating functions for tail bounds

Using a version of Markov's inequality applied to a random variable like  $e^{tX}$ , we can get bounds on the tail of a distribution in terms of the moment generating function which are much better than we would get from, for example, Chebyshev's inequality, which is the application of Markov's inequality to the random variable  $(X - \mu)^2$ . (Of course, this can only work if the moment generating function exists!)

For example, we can apply this to simple random walk. Let  $X_i$  be i.i.d. taking values -1 and 1 with probability 1/2 each. Let  $S_n = X_1 + \cdots + X_n$ , so that  $S_n$  is the position of simple random walk on  $\mathbb{Z}$  after n steps.

We know from the central limit theorem that, for large n,  $S_n$  is typically on the order of  $\sqrt{n}$ . So an event like  $\{|S_n| > na\}$ , for some a > 0, ought to have probability which gets small as  $n \to \infty$ .

First we bound the probability using Chebyshev. We have  $\mathbb{E} S_n = 0$  and  $\text{var} S_n = n$ . So

$$\mathbb{P}(|S_n| > na) \le \frac{\text{var}S_n}{(na)^2}$$
$$= \frac{1}{na^2}.$$

This goes to 0 as desired but not very quickly!

Let us try instead using the moment generating function. We have

$$\mathbb{E} e^{tX_i} = \frac{e^t + e^{-t}}{2}$$

$$= \cosh t$$

$$\leq \exp\left(\frac{t^2}{2}\right) \text{ for all } t.$$

(The inequality  $\cosh t \leq \exp(t^2/2)$  can be checked directly by expanding the exponential functions and comparing coefficients in the power series).

For t > 0, we can now write

$$\mathbb{P}(S_n > na) = \mathbb{P}\left(\exp(tS_n) > \exp(tna)\right)$$

$$\leq \frac{\mathbb{E} \exp(tS_n)}{\exp(tna)} \text{ (this is from Markov's inequality)}$$

$$= \left(\frac{\mathbb{E} \exp(tX_i)}{\exp(ta)}\right)^n$$

$$\leq \left(\exp\left(t^2/2 - ta\right)\right)^n.$$

Note that this is true for any positive t, so we are free to choose whichever one we like. Naturally, we want to minimise the RHS. It is easy to check (just differentiate) that this is done by choosing t = a, which gives

$$\mathbb{P}(S_n > na) \le \exp\left(-na^2/2\right).$$

By symmetry the bound on  $\mathbb{P}(S_n < -na)$  is exactly the same. Combining the two we get

$$\mathbb{P}(|S_n| > na) \le 2 \exp\left(-na^2/2\right).$$

This decays much quicker than the bound from Chebyshev above!

This is a version of the *Chernoff bound*. The same method above can be used to prove "large deviations" bounds for sums of i.i.d. random variables with any distribution whose moment generating function exists in a neighbourhood of the origin.

Remark 3.9. For a moment generating function of a random variable to exist on an interval  $[-t_0, t_0]$  for some  $t_0 > 0$ , we need "light tails"  $a \mapsto \mathbb{P}(|X| \ge a)$ . Indeed, applying Markov's inequality as above, we find

$$\mathbb{P}(|X| \ge a) = \mathbb{P}(e^{t_0|X|} \ge e^{t_0 a}) \le e^{-t_0 a} \mathbb{E} e^{t_0|X|},$$

which decreases exponentially as  $a \to \infty$ .

Distributions of random variables can be classified according to the asymptotic behaviour of their tails  $\mathbb{P}(|X| \geq a)$  as  $a \to \infty$ .

- Distributions on bounded intervals such as Bernoulli, binomial and uniform distributions on intervals or on finite sets have a tail that vanishes eventually. The moment generating function is finite for all  $t \in \mathbb{R}$ .
- We have seen that  $N(\mu, \sigma^2)$  has a moment generating function that is finite everywhere the tails have "superexponential" decay like  $e^{-cx^2}$ . The same can be shown for the Poisson distribution.
- We have seen that Exp(λ) has a moment generating function defined on an interval.
   The tail is "exponential". The same can be shown for the geometric distribution and the Gamma distribution.
- Some distributions have "polynomial tails", e.g. the Pareto distribution given by

$$\mathbb{P}(X > x) = x^{-\alpha - 1}, \qquad x \ge 1,$$

for some  $\alpha > 0$ . Distributions with polynomial tails only have moments up to a certain order, here for  $k < \alpha$ . The Cauchy distribution with probability density function

$$f_X(x) = \frac{1}{\pi} \frac{1}{1 + x^2}, \quad x \in \mathbb{R},$$

is also in this category. In this category, the moment generating function is infinite for all  $t \neq 0$ . In particular, the Uniqueness and Convergence theorems do not apply.

#### 3.4 Characteristic functions

The **characteristic function** is defined by replacing t by it in the definition of the moment generating function. The characteristic function of X is given by

$$\phi_X(t) := \mathbb{E}\left(e^{itX}\right),$$

for  $t \in \mathbb{R}$ , i.e.

$$\phi_X(t) = \mathbb{E}\left(\cos(tX)\right) + i\mathbb{E}\left(\sin(tX)\right).$$

As a result we can see that the characteristic function is finite for every t, whatever the distribution of X. In fact,  $|\phi_X(t)| \leq 1$  for all t.

This means that many of the results for the moment generating function which depended on exponential tails of the distribution have analogues for the characteristic function which hold for any distribution. Just as before we have  $\phi_{X+Y}(t) = \phi_X(t)\phi_Y(t)$ . The uniqueness and continuity theorems given for mgfs hold in a similar way for characteristic functions. The Taylor expansion of the characteristic function around the origin involves the moments of the distribution in a similar way (except now with an added factor of  $i^k$  for the kth term):

$$\phi_X(t) = 1 + it \mathbb{E} X + i^2 t^2 \frac{\mathbb{E} X^2}{2} + \dots + i^k t^k \frac{\mathbb{E} X^k}{k!} + o(t^k)$$
(3.2)

as  $t \to 0$ , whenever  $\mathbb{E} X^k$  is finite. Hence by following exactly the same strategy, we could give a proof of the central limit theorem using characteristic functions instead of mgfs. This would now prove the CLT without any additional assumption on the distribution (only finiteness of the variance is needed). Apart from working with complex power series instead of real power series, there are no additional complications when translating the proof from mgfs to cfs.

When the mgf is finite in an interval containing the origin in its interior, the theory of analytic continuation of complex functions allows us to obtain the characteristic function easily, by replacing t with it in the mgf.

**Example 3.10.** (a) The mgf of N(0,1) is  $\exp(t^2/2)$ , and the cf is  $\exp((it)^2/2) = \exp(-t^2/2)$ .

- (b) The mgf of Exp(1) is 1/(1-t), and the cf is 1/(1-it).
- (c) Suppose X has Cauchy distribution with density  $f(x) = \frac{1}{\pi(1+x^2)}$ . The moment generating function is infinite for all  $t \neq 0$  (in fact, even the mean does not exist as  $\mathbb{E}|X| = \infty$  exercise). The characteristic function is given by

$$\phi_X(t) = \mathbb{E} e^{itX} = \int_{-\infty}^{\infty} \frac{e^{itx}}{\pi (1 + x^2)} dx$$

and this can be evaluated by contour integration to give  $e^{-|t|}$ .

Note that  $\phi_X$  is not differentiable at 0; from (3.2), this corresponds to the fact that the mean does not exist.

In fact, consider  $X_1, X_2, \dots X_n$  i.i.d. Cauchy, and  $S_n = X_1 + \dots + X_n$ . Then

$$\phi_{S_n/n}(t) = \phi \left(\frac{t}{n}\right)^n = \left(e^{-|t|/n}\right)^n = e^{-|t|} = \phi_X(t).$$

So  $S_n/n$  and  $X_i$  have the same distribution! The law of large numbers and the CLT do not apply (since the mean does not exist).

# Joint distribution of continuous random variables

#### 4.1 Review of jointly continuous random variables

The **joint cumulative distribution function** of two random variables X and Y is defined by

$$F_{X,Y}(x,y) = \mathbb{P}(X \le x, Y \le y).$$

X and Y are said to be **jointly continuous** if their joint cdf can be written as an integral:

$$F_{X,Y}(x,y) = \int_{u=-\infty}^{x} \int_{v=-\infty}^{y} f(u,v) du dv.$$

Then f is said to be the joint pdf of X and Y, often written as  $f_{X,Y}$ . As in the case of a single random variable, we might more properly say "a joint pdf" rather than "the joint pdf" because we can, for example, change the value of f at finitely many points without changing the value of any integrals of f. But it is natural to put

$$f_{X,Y}(x,y) = \frac{\partial^2}{\partial x \partial y} F_{X,Y}(x,y)$$

whenever  $F_{X,Y}$  is differentiable at (x,y).

For general (suitably nice<sup>1</sup>) sets  $A \subset \mathbb{R}^2$  we have

$$\mathbb{P}\left((X,Y)\in A\right) = \iint_A f_{X,Y}(x,y)dx\,dy. \tag{4.1}$$

If  $f_{X,Y}$  satisfies (4.1) for all (nice)  $A \subset \mathbb{R}^2$ , then, clearly,  $f_{X,Y}$  is a joint pdf of (X,Y). It suffices to check (4.1) for rectangles A or just for sets of the form  $A = (-\infty, u] \times (-\infty, v]$ , which yield the joint cdf.

We can recover the distribution of one of the random variables X or of Y by integrating over the other one. (In this context the distribution of one of the variables is called the **marginal distribution**).

$$f_X(x) = \int_{y=-\infty}^{\infty} f_{X,Y}(x,y)dy$$

<sup>&</sup>lt;sup>1</sup>The suitable definition of "nice" is "Borel measurable". See Part A Integration.

$$f_Y(y) = \int_{x = -\infty}^{\infty} f_{X,Y}(x, y) dx$$

A function of X and Y is itself a random variable. Its expectation is given by

$$\mathbb{E} h(X,Y) = \int_{x=-\infty}^{\infty} \int_{y=-\infty}^{\infty} h(x,y) f_{X,Y}(x,y) dx dy.$$

Recall that X and Y are independent if  $F_{X,Y}(x,y) = F_X(x)F_Y(y)$  for all x,y. Equivalently, the joint density can be written as a product:

$$f_{X,Y}(x,y) = f_X(x)f_Y(y).$$

All the above can be naturally generalised to describe the joint distribution of more than two random variables.

## 4.2 Transformation formula for bivariate probability density functions

Often there is more than one natural coordinate system in which to view a model. We have the following **change of variables** result:

**Theorem 4.1.** Suppose  $T:(x,y)\mapsto (u,v)$  is a one-to-one mapping from some domain  $D\subseteq \mathbb{R}^2$  onto some range  $R\subseteq \mathbb{R}^2$ .

Define the **Jacobian** J as a function of (u, v) by

$$J = \det \begin{pmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} \end{pmatrix} = \frac{\partial x}{\partial u} \frac{\partial y}{\partial v} - \frac{\partial x}{\partial v} \frac{\partial y}{\partial u}.$$

Assume that the partial derivatives involved exist and are continuous.

If X, Y have joint probability density function  $f_{X,Y}$ , then the random variables U, V defined by (U, V) = T(X, Y) are jointly continuous with joint probability density function  $f_{U,V}$  given by

$$f_{U,V}(u,v) = \begin{cases} f_{X,Y}(x(u,v),y(u,v))|J(u,v)| & \text{if } (u,v) \in R, \\ 0 & \text{otherwise.} \end{cases}$$

*Proof.* The proof is simple using the familiar formula for change of variables in an integral. Suppose that  $A \subseteq D$  and T(A) = B. Then, since T is one-to-one,

$$\mathbb{P}\left((U,V) \in B\right) = \mathbb{P}\left((X,Y) \in A\right)$$

$$= \iint_{A} f_{X,Y}(x,y) dx dy$$

$$= \iint_{B} f_{X,Y}\left(x(u,v), y(u,v)\right) |J(u,v)| du dv.$$

Hence the final integrand is the joint pdf of (U, V).

The formula for change of variables in the integral appeared in various contexts last year. Recall the general idea: after a suitable translation, the transformation T looks locally like a linear transformation whose matrix is the matrix of partial derivatives above. We know that the factor by which the area of a set changes under a linear transformation is given by the determinant of the matrix of the transformation. So, locally, the Jacobian J(u, v) gives the ratio between the area of a rectangle  $(x, x + dx) \times (y, y + dy)$  and its image under T (which is a parallelogram). Since we want the probability to stay the same, and probability is area times density, we should rescale the density by the same amount J(u, v).

#### 4.2.1 Examples of transformed bivariate pdfs

**Example 4.2.** Let X, Y be i.i.d. exponentials with rate  $\lambda$ . Let U = X/(X+Y), V = X+Y. What is the joint distribution of (U, V)?

Solution:

$$f_{X,Y}(x,y) = \lambda e^{-\lambda x} \lambda e^{-\lambda y}$$
  
=  $\lambda^2 e^{-\lambda(x+y)}$ 

for  $(x,y) \in (0,\infty)^2$ . The transformation (u,v) = (x/(x+y),x+y) takes  $(0,\infty)^2$  to  $(0,1) \times (0,\infty)$ . It is inverted by x = uv, y = v(1-u). The Jacobian is given by

$$J(u,v) = \det \begin{pmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} \end{pmatrix} = \det \begin{pmatrix} v & u \\ -v & 1-u \end{pmatrix}$$
$$= v(1-u) + uv$$

So we have

$$f_{U,V}(u,v) = f_{X,Y}(x(u,v),y(u,v))|J(u,v)|$$
$$= \lambda^2 e^{-\lambda(x(u,v)+y(u,v))}|J(u,v)|$$
$$= v\lambda^2 e^{-\lambda v}$$

for  $(u, v) \in (0, 1) \times (0, \infty)$ .

This factorises into a product of a function of u and a function of v (the function of u is trivial). So U and V are independent, with

$$f_U(u) = 1, \ u \in (0,1)$$
  
 $f_V(v) = \lambda^2 v e^{-\lambda v}, \ v \in (0,\infty).$ 

So  $U \sim U[0,1]$  and  $V \sim \text{Gamma}(2,\lambda)$ , independently.

**Example 4.3.** Let X and Y be independent  $\text{Exp}(\lambda)$  as in the previous example, and now let V = X + Y, W = X - Y. This transformation takes  $(0, \infty)^2$  to the set  $\{(v, w) : |w| < v\}$ . The inverse transformation is

$$x = \frac{v+w}{2}, \ y = \frac{v-w}{2}$$

with Jacobian

$$J(v, w) = \det \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} = -\frac{1}{2}.$$

(Notice that any linear transformation always has constant Jacobian). So we have

$$f_{V,W}(v,w) = \begin{cases} f_{X,Y}\left(\frac{v+w}{2}, \frac{v-w}{2}\right) |J(v,w)| & \text{for } |w| < v \\ 0 & \text{otherwise} \end{cases}$$
$$= \begin{cases} \frac{1}{2}\lambda^2 e^{-\lambda v} & \text{for } |w| < v \\ 0 & \text{otherwise} \end{cases}$$

It looks like the pdf factorises into a product as in the previous example. But here this is not really the case! – because of the restriction to |w| < v. In fact, V and W could not be independent here, otherwise we could not have  $\mathbb{P}(|W| < V) = 1$ .

From the previous example we already know that  $V \sim \text{Gamma}(2, \lambda)$ . What is the marginal distribution of W?

$$f_W(w) = \int_{v=|w|}^{\infty} \frac{1}{2} \lambda^2 e^{-\lambda v} dv$$
$$= \left[ -\frac{1}{2} \lambda e^{-\lambda v} \right]_{|w|}^{\infty}$$
$$= \frac{1}{2} \lambda e^{-\lambda |w|}.$$

We see that the distribution of W is symmetric around 0, and by adding the density at w and -w, the distribution of |W| has pdf  $\lambda e^{-\lambda|w|}$  and so again has  $\text{Exp}(\lambda)$  distribution.

**Example 4.4** (General formula for the sum of continuous random variables). If X and Y are jointly continuous with density function  $f_{X,Y}$ , what is the distribution of X + Y? We can change variables to U = X + Y, V = X. This transformation has Jacobian 1 (check!), and we obtain  $f_{U,V}(u,v) = f_{X,Y}(v,u-v)$ .

To obtain the marginal distribution of X + Y, which is U, we integrate over v:

$$f_{X+Y}(u) = \int_{-\infty}^{\infty} f_{X,Y}(v, u - v) dv.$$

An important case is when X and Y are independent. Then we obtain the **convolution** formula:

$$f_{X+Y}(u) = \int_{-\infty}^{\infty} f_X(v) f_Y(u-v) dv.$$

#### 4.3 Multivariate normal distribution

The transformation formula and its proof can be generalised to the case of the joint distribution of n > 2 random variables. The Jacobian is now the determinant of an  $n \times n$  matrix.

Let  $Z_1, Z_2, \ldots, Z_n$  be i.i.d. standard normal random variables. Their joint density function can be written as

$$f_{\mathbf{Z}}(\mathbf{z}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z_i^2}{2}\right)$$
$$= \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}\mathbf{z}^T\mathbf{z}\right).$$

Define  $W_1, \ldots, W_n$  by

$$\begin{pmatrix} W_1 \\ W_2 \\ \vdots \\ W_n \end{pmatrix} = A \begin{pmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_n \end{pmatrix} + \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{pmatrix}$$

where A is some  $n \times n$  matrix.

Assume A is invertible. Then by change of variables (the Jacobian is constant) we get

$$f_{\mathbf{W}}(\mathbf{w}) = \frac{1}{(2\pi)^{n/2}|\det A|} \exp\left(-\frac{1}{2}(\mathbf{w} - \boldsymbol{\mu})^T (AA^T)^{-1} (\mathbf{w} - \boldsymbol{\mu})\right).$$

The matrix  $\Sigma := AA^T$  is the *covariance matrix* in the sense that  $cov(W_i, W_j) = (AA^T)_{ij}$  (check, e.g. for n = 2 if you want an easy case).  $W_1, \ldots, W_n$  are said to have the **multivariate** normal distribution with mean vector  $\boldsymbol{\mu}$  and covariance matrix  $\Sigma$ .

For the case n=2, one can manipulate to obtain (with  $X=W_1,\,Y=W_2$ )

 $f_{X,Y}(x,y)$ 

$$= \frac{1}{2\pi\sigma_{X}\sigma_{Y}\sqrt{1-\rho^{2}}} \exp\left(-\frac{1}{2(1-\rho^{2})} \left[ \frac{(x-\mu_{X})^{2}}{\sigma_{X}^{2}} - \frac{2\rho(x-\mu_{X})(y-\mu_{Y})}{\sigma_{X}\sigma_{Y}} + \frac{(y-\mu_{Y})^{2}}{\sigma_{Y}^{2}} \right] \right)$$

where  $\sigma_X^2$  and  $\sigma_Y^2$  are the variances of X and Y,  $\mu_X$  and  $\mu_Y$  are the means, and  $\rho$  is the correlation coefficient between X and Y which is defined by

$$\rho = \frac{\text{cov}(X, Y)}{\sigma_X \sigma_Y}$$

and lies in (-1,1).

Note that

- (1) The density depends only on  $\mu_X$ ,  $\mu_Y$ ,  $\sigma_X$ ,  $\sigma_Y$  and  $\rho$ .
- (2) X and Y are independent  $\Leftrightarrow \rho = 0$ . ( $\Rightarrow$  is true for any joint distribution;  $\Leftarrow$  is a special property of joint normal.)

A special case is the **standard bivariate normal** where  $\sigma_X = \sigma_Y = 1$  and  $\mu_X = \mu_Y = 0$ . Then

$$f_{X,Y}(x,y) = \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left(-\frac{x^2 - 2\rho xy + y^2}{2(1-\rho^2)}\right).$$

In this case  $\Sigma = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$ .

#### 4.4 Conditional densities

#### 4.4.1 Conditioning on events of positive probability

The basic definition of conditional probability: for two events A and B with  $\mathbb{P}(A) > 0$ , the conditional probability of B given A is

$$\mathbb{P}(B|A) := \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(A)}.$$
(4.2)

Applying this to the distribution of a random variable, we have for example

$$\mathbb{P}(X \le x|A) = \frac{\mathbb{P}(\{X \le x\} \cap A)}{\mathbb{P}(A)}.$$

The left-hand side is a cumulative distribution function. It gives the **conditional distribution** of X, given A. We might denote it by  $F_{X|A}(x)$ .

In the case where X is discrete, we can write the conditional probability mass function:

$$p_{X|A}(x) = \mathbb{P}(X = x|A).$$

If X is continuous, we can differentiate the conditional distribution function to get a conditional density function  $f_{X|A}(x)$ , and then for a set C,

$$\mathbb{P}(X \in C|A) = \int_{x \in C} f_{X|A}(x) dx.$$

The conditional expectation of X given A is the expectation of the conditional distribution, which is given by

$$\mathbb{E}\left(X|A\right) = \sum_{x} x p_{X|A}(x)$$

in the discrete case, and by

$$\mathbb{E}\left(X|A\right) = \int x f_{X|A}(x) dx$$

in the continuous case.

**Example 4.5.** Suppose X and Y are independent random variables which both have uniform distribution on [0,1]. Find the conditional distribution and conditional expectation of Y given X+Y>1.

Solution:

$$\mathbb{P}(Y < y|X+Y>1) = \frac{\mathbb{P}(Y < y, X+Y>1)}{\mathbb{P}(X+Y>1)}.$$

Since X, Y are uniform on the square  $[0,1]^2$ , the probability of a set is equal to its area.

The set  $\{x + y > 1\}$  has area 1/2, while for fixed y, the set  $\{(x, v) : v < y, x + v > 1\}$  has area  $y^2/2$ .

So the distribution function of Y given X + Y > 1 is  $F(y) = (y^2/2)/(1/2) = y^2$ , and the conditional density is 2y on [0, 1], and 0 elsewhere.

The conditional expectation  $\mathbb{E}(Y|X+Y>1)$  is  $\int_0^1 y \times 2y \, dy = 2/3$ .

A common way in which conditional distributions arise is when we have two random variables X and Y with some joint distribution; we observe the value of X and want to know what this tells us about the value of Y. That is, what is the conditional distribution of Y given X = x?

When X is a discrete random variable, everything works fine; since  $\mathbb{P}(X = x)$  will be positive, we can use the approach above.

However, if X is continuous, then  $\mathbb{P}(X = x)$  will be 0 for every x. Now we have a problem, since if the event A in (4.2) has probability 0, then the definition makes no sense.

### 4.4.2 Definition of conditional probability density functions, and an example

To resolve this problem, rather than conditioning directly on  $\{X = x\}$ , we look at the distribution of Y conditioned on  $\{x \le X \le x + \epsilon\}$ . If the joint distribution is well-behaved (as it will be in all the cases that we wish to consider), we can obtain a limit as  $\epsilon \downarrow 0$ , which we define as the distribution of Y given X = x.

As  $\epsilon \to 0$ , we have (if  $f_{X,Y}$  is sufficiently smooth)

$$\mathbb{P}(Y \le y | x \le X \le x + \epsilon) = \frac{\int_{v=-\infty}^{y} \int_{u=x}^{x+\epsilon} f_{X,Y}(u,v) du \, dv}{\int_{u=x}^{x+\epsilon} f_{X}(u) du}$$

$$\sim \frac{\epsilon \int_{v=-\infty}^{y} f_{X,Y}(x,v) dv}{\epsilon f_{X}(x)}$$

$$= \int_{v=-\infty}^{y} \frac{f_{X,Y}(x,v)}{f_{X}(x)} dv. \tag{4.3}$$

So we define  $F_{Y|X=x}(y)$ , the **conditional distribution function of** Y **given** X=x, as the right-hand side of (4.3), whenever this is well-defined.

Differentiating with respect to y, we obtain the **conditional density function of** Y **given** X = x, written as  $f_{Y|X=x}(y)$ :

$$f_{Y|X=x}(y) = \frac{f_{X,Y}(x,y)}{f_X(x)}.$$

These definitions make sense whenever  $f_X(x) > 0$ . In that case, note that  $f_{Y|X=x}$  is indeed a density function, because we have defined  $f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x,y)dy$ . (Notice that the denominator  $f_X(x)$  does not involve y at all; it is just a normalising constant).

The idea is that the following two procedures are equivalent:

- (1) generate (X,Y) according to the joint density function  $f_{X,Y}$ ;
- (2) first generate X according to the density function  $f_X$ , and then having observed X = x, generate Y according to the density function  $f_{Y|X=x}$ .

**Example 4.6** (Simple example). Let (X, Y) be uniform on the triangle  $\{0 < y < x < 1\}$ . Then

$$f_{X,Y}(x,y) = \begin{cases} 2 & 0 < y < x < 1, \\ 0 & \text{otherwise.} \end{cases}$$

For the conditional density of Y given X = x,

$$\begin{split} f_{Y|X=x}(y) &= \frac{f_{X,Y}(x,y)}{f_X(x)} \\ &= \begin{cases} 2/f_X(x) & 0 < y < x, \\ 0 & \text{otherwise,} \end{cases} \end{split}$$

provided  $x \in (0,1)$ . We do not need to calculate  $f_X(x)$ , since it is just a normalising constant. Since the conditional density function of Y is constant in y, we see that Y is uniform on [0,x], with distribution function given by

$$F_{Y|X=x}(y) = \begin{cases} 0 & y < 0, \\ \frac{y}{x} & 0 \le y \le x, \\ 1 & y > x. \end{cases}$$

The conditional mean of Y given X = x is x/2.

## 4.4.3 Example: bivariate normal distribution

**Example 4.7** (Bivariate normal). Let X and Y be jointly normal with means  $\mu_1$  and  $\mu_2$  respectively, variances  $\sigma_1^2$  and  $\sigma_2^2$  respectively, and correlation coefficient  $\rho$ . What is the conditional distribution of Y given X = x?

Rather than working directly from the joint density function, we can proceed by writing Y as the sum of two terms, one which is a function of X and one which is independent of X.

First let us write X and Y as functions of independent standard normals  $Z_1$  and  $Z_2$ . If we put

$$X = \sigma_1 Z_1 + \mu_1$$
  
 $Y = \rho \sigma_2 Z_1 + \sqrt{1 - \rho^2} \sigma_2 Z_2 + \mu_2$ 

then indeed X and Y have the desired means, variances and covariance (check!).

Then we can write

$$Y = \rho \frac{\sigma_2}{\sigma_1} (X - \mu_1) + \sqrt{1 - \rho^2} \sigma_2 Z_2 + \mu_2.$$

The first term is a function of X and the second term, involving only  $Z_2$ , is independent of X.

So conditional on X = x, the distribution of Y is the distribution of

$$\rho \frac{\sigma_2}{\sigma_1}(x-\mu_1) + \sqrt{1-\rho^2}\sigma_2 Z_2 + \mu_2,$$

which is normal with mean  $\rho \frac{\sigma_2}{\sigma_1}(x-\mu_1) + \mu_2$  and variance  $(1-\rho^2)\sigma_2^2$ .

Note the way the variance of this conditional distribution depends on  $\rho$ . We say that  $\rho^2$  is the "amount of the variance of Y explained by X". Consider the extreme cases. If  $\rho = \pm 1$ , then the conditional variance is 0. That is, Y is a function of X and once we observe X, there is no longer any uncertainty about the value of Y. If  $\rho = 0$ , the conditional variance and the unconditional variance are the same; observing X tells us nothing about Y.

## 4.5 Cautionary tale

The definition above of conditional distribution given the value of a continuous random variable makes sense in context, but keep in mind that conditioning directly on events on probability zero is not valid, and as a result the objects involved are not robust to seemingly innocent manipulation! Consider the following example:

**Example 4.8** (Borel's paradox). Consider the uniform distribution on the half-disc  $C = \{(x,y) : y \ge 0, x^2 + y^2 \le 1\}$ . The joint density of X and Y is given by

$$f(x,y) = \begin{cases} \frac{2}{\pi} & (x,y) \in C, \\ 0 & \text{otherwise.} \end{cases}$$

What is the conditional distribution of Y given X = 0? Its density is given by

$$f_{Y|X=0}(y) = \frac{2/\pi}{f_X(0)}$$

for  $y \in [0, 1]$ , and 0 elsewhere. So the distribution is uniform on [0, 1] (we do not need to calculate  $f_X(0)$  to see this, since it is only a normalising constant).

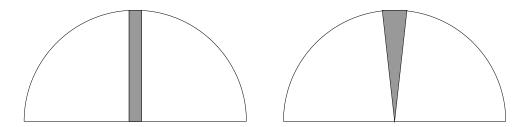
We could change variables and represent the same distribution in polar coordinates. Then R and  $\Theta$  are independent; R has density 2r on [0,1] and  $\Theta$  is uniform on  $[0,\pi)$ . (See first question on problem sheet 2 for the transformation to polar coordinates. But in this case where the density of X, Y is uniform on a set, one can also easily derive the joint distribution of R and  $\Theta$  directly by considering areas of subsets of the set C).

Note that the events  $\{X=0\}$  and  $\{\Theta=\pi/2\}$  are the same.

What is the conditional distribution of R given  $\Theta = \pi/2$ ? Since R and  $\Theta$  are independent, it still has density 2r on [0,1]. This is *not* uniform on [0,1].

But when X = 0, i.e. when  $\Theta = \pi/2$ , R and Y are the same thing. So the distribution of R given  $\Theta = \pi/2$  ought to be the same as the distribution of Y given X = 0, should it not?

What is happening is that, although the events  $\{X=0\}$  and  $\{\Theta=\pi/2\}$  are the same, it is *not* the case that the events  $\{|X|<\epsilon\}$  and  $\{|\Theta-\pi/2|<\epsilon\}$  are the same. When we condition X to be within  $\epsilon$  of 0, we restrict to a set which is approximately a rectangle (the left-hand picture below). However, when we condition  $\Theta$  to be near  $\pi/2$ , we restrict to a thin sector of the circle, which is approximately a triangle (the right-hand picture below). In the second case, we bias the point chosen to lie higher up. As  $\epsilon \to 0$ , this bias persists; the two limits are not the same!



What this "paradox" illustrates is that conditioning for continuous random variables involves a limit, and that it can be important exactly how the limit is taken. The procedure whereby we generate X from  $f_X$  and then Y from  $f_{Y|X}$  makes sense in terms of a particular set of variables; but the conditional densities involved are not robust to a change of variables.

## Markov chains: Introduction

Let  $X_n, n = 0, 1, 2, ...$  be a "random process", taking values in some set I called the *state* space. That is,  $X_0, X_1, X_2, ...$  are random variables with  $X_n \in I$  for all n.

Often  $X_n$  represents some quantity evolving in time. So far we have been working with random variables taking values which are real numbers of some kind, but there is no problem in considering a more general state space. For example, we might consider processes of the following kind:

- $I = \mathbb{Z}^2$ ,  $X_n$ =position at nth step of a "random walk" on the two-dimensional lattice.
- $I = \{A, B, C, \dots, a, b, c, \dots, ?, !, \dots\}, X_n = n$ th character in a text or in an email.
- $I = \{C, G, A, T\}$  (representing cytosine, guanine, adenine, thymine, the four bases of DNA),  $X_n$ =base appearing in nth position in a DNA sequence.

We will assume that the state space I is finite or countably infinite (i.e. discrete). A **(probability) distribution** on I is a collection  $\lambda = (\lambda_i, i \in I)$  with  $\lambda_i \geq 0$  for all i, and  $\sum \lambda_i = 1$ . This is really just the same idea as the probability mass function of a discrete random variable. We will often think of  $\lambda$  as a **row vector**. We will say that a random variable Y taking values in I has distribution  $\lambda$  if  $\mathbb{P}(Y = i) = \lambda_i$  for all i.

## 5.1 Markov chains

Let  $X = (X_0, X_1, X_2, ...)$  be a sequence of random variables taking values in I. The process X is called a **Markov chain** if for any  $n \ge 0$  and any  $i_0, i_1, ..., i_{n+1} \in I$ ,

$$\mathbb{P}\left(X_{n+1} = i_{n+1} | X_n = i_n, \dots, X_0 = i_0\right) = \mathbb{P}\left(X_{n+1} = i_{n+1} | X_n = i_n\right). \tag{5.1}$$

(To be precise, we should restrict (5.1) to cases where these conditional probabilities are well-defined, i.e. where the event  $\{X_n = i_n, \dots, X_0 = i_0\}$  has positive probability.)

The Markov chain is called **(time-)homogeneous** if in addition  $\mathbb{P}(X_{n+1} = j | X_n = i)$  depends only on i and j, not on n. In that case we write

$$p_{ij} = \mathbb{P}\left(X_{n+1} = j \middle| X_n = i\right)$$

(or we will often write  $p_{i,j}$  rather than  $p_{ij}$ , according to convenience). The quantities  $p_{ij}$  are known as the **transition probabilities** of the chain.

We will work almost always with homogeneous chains. To describe such a chain, it's enough to specify two things:

- the initial distribution  $\lambda$  of  $X_0$ . For each  $i \in I$ ,  $\lambda_i = \mathbb{P}(X_0 = i)$ .
- the transition matrix  $P = (p_{ij})_{i,j \in I}$ .

P is a square (maybe infinite) matrix, whose rows and columns are indexed by I. P is a "stochastic matrix" which means that all its entries are non-negative and every row sums to 1. Equivalently, every row of P is a probability distribution. The ith row of P is the distribution of  $X_{n+1}$  given  $X_n = i$ .

**Theorem 5.1.** For  $i_0, i_1, ..., i_n \in I$ ,

$$\mathbb{P}(X_0 = i_0, X_1 = i_1, \dots, X_n = i_n) = \lambda_{i_0} p_{i_0 i_1} p_{i_1 i_2} \dots p_{i_{n-1} i_n}.$$

Proof.

$$\begin{split} \mathbb{P}\left(X_{0} = i_{0}, X_{1} = i_{1}, \dots, X_{n} = i_{n}\right) \\ &= \mathbb{P}\left(X_{0} = i_{0}\right) \mathbb{P}\left(X_{1} = i_{1} \middle| X_{0} = i_{0}\right) \mathbb{P}\left(X_{2} = i_{2} \middle| X_{1} = i_{1}, X_{0} = i_{0}\right) \times \dots \\ & \cdots \times \mathbb{P}\left(X_{n} = i_{n} \middle| X_{n-1} = i_{n-1}, \dots, X_{0} = i_{0}\right) \\ &= \mathbb{P}\left(X_{0} = i_{0}\right) \mathbb{P}\left(X_{1} = i_{1} \middle| X_{0} = i_{0}\right) \mathbb{P}\left(X_{2} = i_{2} \middle| X_{1} = i_{1}\right) \dots \mathbb{P}\left(X_{n} = i_{n} \middle| X_{n-1} = i_{n-1}\right) \\ &= \lambda_{i_{0}} p_{i_{0}i_{1}} p_{i_{1}i_{2}} \dots p_{i_{n-1}i_{n}}, \end{split}$$

where we used the definition of a Markov chain to get the penultimate line.  $\Box$ 

If X is a Markov chain with initial distribution  $\lambda$  and transition matrix P, we will sometimes write " $X \sim \text{Markov}(\lambda, P)$ ".

Markov chains are "memoryless". If we know the current state, any information about previous states is irrelevant to the future evolution of the chain. We can say that "the future is independent of the past, given the present". This is known as the **Markov property**.

Notation: it will be convenient to write  $\mathbb{P}_i$  for the distribution conditioned on  $X_0 = i$ . For example  $\mathbb{P}_i(X_1 = j) = p_{ij}$ . Similarly  $\mathbb{E}_i$  for expectation conditioned on  $X_0 = i$ .

## 5.2 *n*-step transition probabilities

Write  $p_{ij}^{(n)} = \mathbb{P}(X_{r+n} = j | X_r = i)$ . This is an *n*-step transition probability of the Markov chain.

**Theorem 5.2.** (Chapman-Kolmogorov equations)

(i) 
$$p_{ij}^{(n+m)} = \sum_{k \in I} p_{ik}^{(n)} p_{kj}^{(m)}$$
.

(ii) 
$$p_{ij}^{(n)} = (P^n)_{i,j}$$
.

Here  $P^n$  is the *n*th power of the transition matrix. As ever, matrix multiplication is given by  $(AB)_{i,j} = \sum_k (A)_{i,k}(B)_{k,j}$ , whether the matrices are finite or infinite.

*Proof.* (i) We partition according to the value of the intermediate state  $X_n$ , and apply the law of total probability.

$$\mathbb{P}\left(X_{n+m} = j \middle| X_0 = i\right) = \sum_{k} \mathbb{P}\left(X_n = k \middle| X_0 = i\right) \mathbb{P}\left(X_{n+m} = j \middle| X_n = k, X_0 = i\right)$$
$$= \sum_{k} \mathbb{P}\left(X_n = k \middle| X_0 = i\right) \mathbb{P}\left(X_{n+m} = j \middle| X_n = k\right)$$

(using the Markov property)

$$= \sum_{k} p_{ik}^{(n)} p_{kj}^{(m)}.$$

(ii) Inductively,

$$p_{ij}^{(2)} = \sum_{k} p_{ik} p_{kj} = (P^2)_{i,j}$$

$$p_{ij}^{(3)} = \sum_{k} p_{ik}^{(2)} p_{kj}^{(1)} = \sum_{k} (P^2)_{i,k} (P)_{k,j} = (P^2 P)_{i,j} = (P^3)_{i,j},$$

and so on.

**Theorem 5.3.** Let  $\lambda$  be the initial distribution (i.e. the distribution of  $X_0$ ). Then the distribution of  $X_1$  is  $\lambda P$ , and more generally the distribution of  $X_n$  is  $\lambda P^n$ .

Here we are thinking of  $\lambda$  as a row vector, so that  $\lambda P^n$  is also a row vector;  $(\lambda A)_i = \sum_k \lambda_k A_{ki}$  as usual, whether the dimensions are finite or infinite.

Proof.

$$\mathbb{P}(X_1 = j) = \sum_{i} \mathbb{P}(X_0 = i) \mathbb{P}(X_1 = j | X_0 = i)$$
$$= \sum_{i} \lambda_i p_{ij}$$
$$= (\lambda P)_j,$$

and similarly for  $X_n$  with  $p_{ij}$  and P replaced by  $p_{ij}^{(n)}$  and  $P^n$ .

Using this result and the Markov property it's easy to get the following property: if  $(X_0, X_1, X_2, \ldots)$  is a Markov chain with initial distribution  $\lambda$  and transition matrix P, then  $(X_0, X_k, X_{2k}, \ldots)$  is a Markov chain with initial distribution  $\lambda$  and transition matrix  $P^k$ .

**Example 5.4** (General two-state Markov chain). Let  $I = \{1, 2\}$  and

$$P = \begin{pmatrix} 1 - \alpha & \alpha \\ \beta & 1 - \beta \end{pmatrix}$$

What is  $p_{11}^n$ ? Two approaches:

(1) P has eigenvalues 1 and  $1 - \alpha - \beta$  (check! Every Markov transition matrix has 1 as an eigenvalue – why?). So we can diagonalise:

$$P = U^{-1} \begin{pmatrix} 1 & 0 \\ 0 & 1 - \alpha - \beta \end{pmatrix} U,$$
  
$$P^{n} = U^{-1} \begin{pmatrix} 1 & 0 \\ 0 & (1 - \alpha - \beta)^{n} \end{pmatrix} U.$$

We get  $(P^n)_{11} = A + B(1 - \alpha - \beta)^n$  for some constants A and B.

Since we know  $p_{11}^{(0)} = 1$  and we have  $p_{11}^{(1)} = 1 - \alpha$ , we can solve for A and B to get

$$p_{11}^{(n)} = \frac{\beta}{\alpha + \beta} + \frac{\alpha}{\alpha + \beta} (1 - \alpha - \beta)^n. \tag{5.2}$$

(2) Alternatively, we can condition on the state at step n-1:

$$\begin{split} p_{11}^{(n)} &= p_{11}^{(n-1)}(1-\alpha) + p_{12}^{(n-1)}\beta \\ &= p_{11}^{(n-1)}(1-\alpha) + \left(1-p_{11}^{(n-1)}\right)\beta \\ &= (1-\alpha-\beta)p_{11}^{(n-1)} + \beta. \end{split}$$

This gives a linear recurrence relation for  $p_{11}^{(n)}$ , which we can solve using standard methods to give (5.2) again.

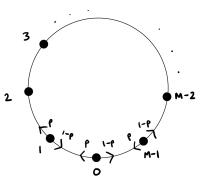
## 5.3 A few examples

**Example 5.5** (Random walk on a cycle).  $I = \{0, 1, 2, ..., M - 1\}$ . At each step the walk increases by 1 (mod M) with probability p and decreases by 1 (mod M) with probability 1 - p. That is,

$$p_{ij} = \begin{cases} p & \text{if } j \equiv i+1 \mod M \\ 1-p & \text{if } j \equiv i-1 \mod M \\ 0 & \text{otherwise} \end{cases}$$

or

$$P = \begin{pmatrix} 0 & p & 0 & 0 & \cdots & 0 & 1-p \\ 1-p & 0 & p & 0 & \cdots & 0 & 0 \\ 0 & 1-p & 0 & p & \cdots & 0 & 0 \\ \vdots & & & \ddots & & & \\ p & 0 & 0 & 0 & \cdots & 1-p & 0 \end{pmatrix}.$$



**Example 5.6** (Simple symmetric random walk on  $\mathbb{Z}^d$ ).  $I = \mathbb{Z}^d$ . At each step the walk moves from its current site to one of its 2d neighbours chosen uniformly at random.

$$p_{ij} = \begin{cases} \frac{1}{2d} & \text{if } |i-j| = 1\\ 0 & \text{otherwise} \end{cases}.$$

**Example 5.7** (A card-shuffling chain). Let I be the set of orderings of 52 cards. We can regard I as the permutation group  $S_{52}$ . There are many interesting Markov chains on permutation groups. We can think of shuffling a pack of cards. A simple and not very practical example of a shuffle: at each step, choose a and b independently and uniformly in  $\{1, 2, \ldots, 52\}$  and exchange the cards in positions a and b. This gives

$$p_{\alpha\beta} = \begin{cases} \frac{2}{52^2} & \text{if } \alpha = \beta\tau \text{ for some transposition } \tau \\ \frac{1}{52} & \text{if } \alpha = \beta \\ 0 & \text{otherwise} \end{cases}$$

## 5.4 Exploring the Markov property

Let's look at a few examples of simple processes where the Markov property holds or fails. We can do this in the context of a simple random walk on  $\mathbb{Z}$ .

Let 
$$X_i$$
 be i.i.d. with  $\mathbb{P}(X_i=1)=p$  and  $\mathbb{P}(X_i=-1)=1-p$ .  
Let  $S_0=0$  and  $S_n=\sum_{i=1}^n X_i$ .  
Then:

- (1)  $X_n$  is a Markov chain. In fact,  $X_n$  are i.i.d., which is a stronger property. Given any history, the next state is equal to 1 with probability p and -1 with probability 1-p. The matrix of the chain  $X_n$  (with rows and columns indexed by  $\{-1,1\}$ ) is  $P = \begin{pmatrix} 1-p & p \\ 1-p & p \end{pmatrix}$ .
- (2) The random walk  $S_n$  is also a Markov chain. Its transition probabilities are  $p_{i,i+1} = p$  and  $p_{i,i-1} = p$  for all  $i \in \mathbb{Z}$ .
- (3) Consider the process  $M_n = \max_{0 \le k \le n} S_k$ . Try drawing some possible paths of the process  $S_n$ , and the corresponding paths of the "maximum process"  $M_n$ . Is this maximum process a Markov chain?

We can consider two different ways of arriving at the same state. Suppose  $(M_0, \ldots, M_4) = (0, 0, 0, 1, 2)$ . This implies  $S_4 = 2$  (the maximum process has just increased, so now the walk must be at its current maximum.) In that case, if the random walk moves up at the next step, then the maximum will also increase. So

$$\mathbb{P}(M_5 = 3 | (M_0, \dots, M_4) = (0, 0, 0, 1, 2)) = p.$$

Suppose instead that  $(M_0, ..., M_4) = (0, 1, 2, 2, 2)$ . In that case, both  $S_4 = 2$  and  $S_4 = 0$  are possible (check! – find the corresponding paths). As a consequence, sometimes the maximum will stay the same at the next step, even when the random walk moves up. So we have

$$\mathbb{P}(M_5 = 3 | (M_0, \dots, M_4) = (0, 1, 2, 2, 2)) < p.$$

We see that the path to  $M_4 = 2$  affects the conditional probability of the next step of the process. So  $M_n$  is not a Markov chain.

The next result gives a criterion for the Markov property to hold.

**Proposition 5.8.** Suppose that  $(Y_n, n \ge 0)$  is a random process, and for some function f we can write, for each n,

$$Y_{n+1} = f(Y_n, X_{n+1}),$$

where  $X_{n+1}$  is independent of  $Y_0, Y_1, \ldots, Y_n$ . Then  $(Y_n)$  is a Markov chain.

*Proof.* The idea is that to update the chain, we use only the current state and some "new" randomness. We have

$$\begin{split} \mathbb{P}\big(Y_{n+1} = i_{n+1} \big| Y_n = i_n, \dots, Y_0 = i_0 \big) \\ &= \mathbb{P}\left(f(i_n, X_{n+1}) = i_{n+1} \big| Y_n = i_n, \dots, Y_0 = i_0 \right) \\ &= \mathbb{P}\left(f(i_n, X_{n+1}) = i_{n+1} \right) \quad \text{(by independence of } X_{n+1} \text{ from } Y_0, \dots, Y_n \text{)} \\ &= \mathbb{P}\left(f(i_n, X_{n+1}) = i_{n+1} \big| Y_n = i_n \right) \quad \text{(by independence of } X_{n+1} \text{ from } Y_n \text{)} \\ &= \mathbb{P}\left(Y_{n+1} = i_{n+1} \big| Y_n = i_n \right). \end{split}$$

For example, for the simple random walk above, we can put  $S_{n+1} = f(S_n, X_{n+1})$ , where f(s,x) = s + x. For the card-shuffling example in the previous section, if  $Y_n \in S_{52}$  is the permutation after step n, we can put  $Y_{n+1} = f(Y_n, X_{n+1})$  where for a permutation  $\beta$  and a transposition  $\tau$ ,  $f(\beta,\tau) = \beta\tau$ , and where  $(X_n)$  is an i.i.d. sequence in which each member is uniform in the set of transpositions.

## 5.5 Class structure

Let  $i, j \in I$ . We say that "i leads to j" and write " $i \to j$ " if  $\mathbb{P}_i(X_n = j) > 0$  for some  $n \ge 0$ , i.e.  $p_{ij}^{(n)} > 0$  for some  $n \ge 0$ .

If  $i \to j$  and  $j \to i$  then we say "i communicates with j" and write  $i \leftrightarrow j$ .

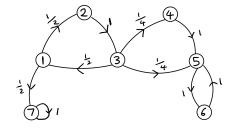
Then  $\leftrightarrow$  is an equivalence relation (check!). It partitions the state space I into **communicating classes**.

A class C is called **closed** if  $p_{ij} = 0$  whenever  $i \in C, j \notin C$ , or equivalently  $i \not\to j$  for any  $i \in C, j \notin C$ . Once the chain enters a closed class, it can never escape from it. If  $\{i\}$  is a closed class then  $p_{ii} = 1$ , and i is called an **absorbing state**. If C is not closed it is called **open**.

A chain (or more precisely a transition matrix) for which I consists of a single communicating class is called **irreducible**. Equivalently,  $i \to j$  for all  $i, j \in I$ .

**Example 5.9.** Let  $I = \{1, 2, 3, 4, 5, 6, 7\}$ . The communicating classes for the transition matrix

$$P = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

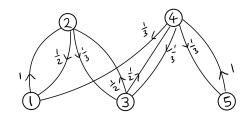


are  $\{1,2,3\}$ ,  $\{4\}$ ,  $\{5,6\}$  and  $\{7\}$ . The closed classes are  $\{5,6\}$  and  $\{7\}$  (so 7 is an absorbing state).

#### 5.6Periodicity

Consider the transition matrix

$$\begin{pmatrix}
0 & 1 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\
0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\
\frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\
0 & 0 & 0 & 1 & 0
\end{pmatrix}$$



Note that whenever  $p_{ij} > 0$ , the states i and j have different parity mod 2 (in the diagram, all the arcs go between the set  $\{2,4\}$  shown above and the set  $\{1,3,5\}$  shown below). It follows that  $p_{ii}^{(n)} = 0$  whenever n is odd.

For a general chain and a state  $i \in I$ , the **period** of the state i is defined to be the greatest common divisor of the set  $\left\{n: p_{ii}^{(n)} > 0\right\}$ . (If  $p_{ii}^{(n)} = 0$  for all n > 0, then the period is not defined). All the states in the chain above have period 2.

i is called **aperiodic** if this g.c.d. is 1 (and otherwise **periodic**). Equivalently (check!), i is aperiodic if  $p_{ii}^{(n)} > 0$  for all sufficiently large n.

Fact. All states in a communicating class have the same period.

*Proof.* Suppose  $i \leftrightarrow j$  and d|n whenever  $p_{ii}^{(n)} > 0$ .

Since i and j communicate, we can find a and b with  $p_{ij}^{(a)} > 0$  and  $p_{ji}^{(b)} > 0$ . Then also  $p_{ii}^{(a+b)} > 0.$ 

Suppose  $p_{jj}^{(m)} > 0$ . Then also  $p_{ii}^{(a+m+b)} > 0$ .

Then d|a+b and d|a+m+b, so also d|m.

This demonstrates that the sets  $\left\{n:p_{ii}^{(n)}>0\right\}$  and  $\left\{m:p_{jj}^{(m)}>0\right\}$  have the same divisors, and hence the same greatest common divisor.

In particular, if a chain is irreducible, then all states have the same period, and we call this the period of the chain. If this period is 1, we say that the chain is aperiodic (otherwise we say the chain is periodic).

Remark. Notice that both irreducibility and periodicity are "structural properties" in the following sense: they depend only on which transition probabilities  $p_{ij}$  are positive and which are zero, not on the particular values taken by those which are positive.

**Example.** Look back at the three examples in Section 5.3 and consider which are irreducible and which are periodic.

The random walk on the cycle is irreducible (since every site is accessible from every other). It has period 2 if M is even, and is aperiodic if M is odd.

The random walk on  $\mathbb{Z}^d$  is irreducible and has period 2 for any d.

The card-shuffling chain is irreducible (because the set of transpositions is a set of generators for the group  $S_{52}$ ). It is aperiodic, since there is a positive transition probability from any state to itself.

Remark. Later we will show results about convergence to equilibrium for Markov chains. The idea will be that after a long time, a Markov chain should more or less "forget where it started". There are essentially two reasons why this might not happen: (a) periodicity; for example if a chain has period 2, then it alternates between, say, "odd" and "even" states; even an arbitrarily long time, the chain will still remember whether it started at an "odd" or "even" state. (b) lack of irreducibility. A chain with more than one closed class can never move from one to the other, and so again will remember its starting state for ever. When we prove results about convergence to equilibrium, it will be under the condition that the chain is irreducible and aperiodic.

## 5.7 Hitting probabilities

Let A be a subset of the state space I. Define  $h_i^A = \mathbb{P}_i$  ( $X_n \in A$  for some  $n \geq 0$ ), the **hitting** probability of A starting from state i.

If A is a closed class, we might call  $h_i^A$  the absorption probability.

**Example.** Let  $I = \{1, 2, 3, 4\}$  and

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Starting from 2, what is the probability of absorption at 4?

Write  $h_i = \mathbb{P}_i(X_n = 4 \text{ for some } n \geq 0)$ . Then  $h_4 = 1$ , and  $h_1 = 0 \text{ since } 1$  is itself absorbing. Also by conditioning on the first jump we have

$$h_2 = \frac{1}{2}h_1 + \frac{1}{2}h_3,$$
  
$$h_3 = \frac{1}{2}h_2 + \frac{1}{2}h_4.$$

Solving, we get  $h_2 = 1/3$  and  $h_3 = 2/3$ .

**Theorem 5.10.** The vector of hitting probabilities  $(h_i^A, i \in I)$  is the minimal non-negative solution to the equations

$$h_i^A = \begin{cases} 1 & \text{if } i \in A \\ \sum_j p_{ij} h_j^A & \text{if } i \notin A \end{cases}$$
 (5.3)

Here by "minimal" we mean that if  $(x_i, i \in I)$  is another non-negative solution to the system (5.3), then  $h_i \leq x_i$  for all i.

*Proof.* To see that  $h_i^A$  satisfies (5.3), we condition on the first jump of the process. If  $i \notin A$ , then

$$\begin{aligned} h_i^A &= \mathbb{P}_i \left( X_n \in A \text{ for some } n \geq 0 \right) \\ &= \mathbb{P}_i \left( X_n \in A \text{ for some } n \geq 1 \right) \\ &= \sum_j \mathbb{P}_i (X_1 = j) \mathbb{P} \left( X_n \in A \text{ for some } n \geq 1 \middle| X_0 = i, X_1 = j \right) \\ &= \sum_j p_{ij} \mathbb{P} \left( X_n \in A \text{ for some } n \geq 1 \middle| X_1 = j \right) \\ &= \sum_j p_{ij} h_j^A. \end{aligned}$$

To obtain the penultimate line we applied the Markov property. Meanwhile for  $i \in A$ ,  $h_i^A = 1$  by definition. So indeed (5.3) holds.

To prove minimality, suppose  $(x_i, i \in I)$  is any non-negative solution to (5.3). We want to show that  $h_i^A \leq x_i$  for all i.

We make the following claim: for any  $M \in \mathbb{N}$ , and for all i,

$$x_i \ge \mathbb{P}_i(X_n \in A \text{ for some } n \le M).$$
 (5.4)

We will prove (5.4) by induction on M.

The case M=0 is easy; the LHS is 1 for  $i \in A$ , while the RHS is 0 for  $i \notin A$ .

For the induction step, suppose that for all  $i, x_i \geq \mathbb{P}_i(X_n \in A \text{ for some } n \leq M-1)$ . If  $i \in A$ , then again  $x_i = 1$  and (5.4) is clear. If  $i \notin A$ , then

$$\mathbb{P}_i(X_n \in A \text{ for some } n \leq M) = \sum_j p_{ij} \mathbb{P}_i(X_n \in A \text{ for some } n \in \{1, 2, \dots, M\} | X_1 = j)$$

$$= \sum_j p_{ij} \mathbb{P}_j \left( X_n \in A \text{ for some } n \in \{0, 1, \dots, M - 1\} \right)$$

$$\leq \sum_j p_{ij} x_i$$

$$= x_i,$$

and the induction step is complete. Hence (5.4) holds for all i and M as desired. Then, using the fact that the sequence of events in (5.4) is increasing in M, we have

$$x_i \ge \lim_{M \to \infty} \mathbb{P}_i(X_n \in A \text{ for some } n \le M)$$
  
=  $\mathbb{P}_i(\bigcup_M \{X_n \in A \text{ for some } n \le M\})$   
=  $\mathbb{P}_i(X_n \in A \text{ for some } n)$   
=  $h_i^A$ .

## Important example: "Gambler's ruin"

Let  $I = \{0, 1, 2...\}$ . Let  $p \in (0, 1)$  and q = 1 - p, and consider the transition probabilities given by

$$p_{00} = 1$$
 $p_{i,i-1} = q \text{ for } i \ge 1$ 
 $p_{i,i+1} = p \text{ for } i \ge 1.$ 
(5.5)

The name "gambler's ruin" comes from the interpretation where the state is the current capital of a gambler, who repeatedly bets 1 (against an infinitely rich bank). Will the gambler inevitably go broke? But chains like this come up in a wide range of settings. Chains on  $\mathbb{Z}_+$  in which all transitions are steps up and down by 1 are called "birth-and-death chains" (modelling the size of a population). This is one of the simplest examples.

Let  $h_i = \mathbb{P}_i(\text{hit } 0)$ . To find  $h_i$ , we need the minimal non-negative solution to

$$h_0 = 1 \tag{5.6}$$

$$h_i = ph_{i+1} + qh_{i-1} \text{ for } i \ge 1.$$
 (5.7)

If  $p \neq q$ , (5.7) has general solution

$$h_i = A + B\left(\frac{q}{p}\right)^i.$$

We look at three cases:

- Jumps downwards are more likely than jumps upward. From (5.6), A + B = 1. Then for minimality, we take A = 1 and B = 0, since  $\left(\frac{q}{p}\right)^i \ge 1$  for all i.

  We obtain  $h_i = 1$  for all i. So with probability 1, the chain will hit 0.
- p > q Again A + B = 1. Also  $\left(\frac{q}{p}\right)^i \to 0$  as  $i \to \infty$ , so we need  $A \ge 0$  for a non-negative solution. Then for a minimal solution, we will want A = 0, B = 1, since  $1 \ge \left(\frac{q}{p}\right)^i$  for all i.
  - Hence  $h_i = \left(\frac{q}{p}\right)^i$ . The chain has a positive probability of "escaping to infinity".
- p=q Now the general solution of (5.7) is  $h_i=A+Bi$ . From i=0 we get A=1. For non-negativity we need  $B\geq 0$ , and then for minimality B=0. We get  $h_i=1$  again. Now there is no drift, but still with probability 1 the chain will hit 0 eventually.

*Remark.* Notice that we could have seen  $h_i = \alpha^i$  for some  $\alpha$ , by a direct argument. Since the chain can only descend by one step at a time,

$$\mathbb{P}_i(\text{hit }0) = \mathbb{P}_i(\text{hit }i-1)\mathbb{P}_{i-1}(\text{hit }i-2)\dots\mathbb{P}_1(\text{hit }0), \tag{5.8}$$

and all terms in the product are the same, since the transition probabilities are the same at every level.

## 5.8 Recurrence and transience

If the chain starts in state i, what is the chance that it returns to i at some point in the future? We can distinguish two possibilities:

(1) 
$$\mathbb{P}_i(X_n = i \text{ for some } n > 1) = p < 1.$$

Then the total number of visits to i has geometric distribution with parameter 1 - p (since each time we return to i, we have chance 1 - p of never returning again). We have

$$\mathbb{P}_i(\text{hit } i \text{ infinitely often}) = 0.$$

The state i is called **transient**.

(2) 
$$\mathbb{P}_i(X_n = i \text{ for some } n \ge 1) = 1.$$

Then

$$\mathbb{P}_i(\text{hit } i \text{ infinitely often}) = 1.$$

The state i is called **recurrent**.

The definition is very simple, but the concept of recurrence and transience is extremely rich (mainly for infinite chains).

There is an important criterion for recurrence and transience in terms of the transition probabilities:

**Theorem 5.11.** State i is recurrent if and only if  $\sum_{n=0}^{\infty} p_{ii}^{(n)} = \infty$ .

*Proof.* The total number of visits to i is  $\sum_{n=0}^{\infty} I(X_n = i)$  which has expectation  $\sum_{n=0}^{\infty} \mathbb{E} I(X_n = i) = \sum_{n=0}^{\infty} \mathbb{P}(X_n = i) = \sum_{n=0}^{\infty} p_{ii}^{(n)}$ .

If i is transient, the number of visits to i is geometric with parameter 1-p, and hence with mean  $\frac{1}{1-p} < \infty$ .

On the other hand if i is recurrent, the number of visits to i is infinite with probability 1, and so has mean  $\infty$ .

This gives the statement of the theorem.

**Theorem 5.12.** (a) Let C be a communicating class. Either all states in C are recurrent, or all are transient (so we may refer to the whole class as transient or recurrent).

- (b) Every recurrent class is closed.
- (c) Every finite closed class is recurrent.

*Proof.* Exercises – see example sheet 3. For part (a), use Theorem 5.11 to show that if i is recurrent and  $i \leftrightarrow j$ , then j is also recurrent.

The theorem tells us that recurrence and transience are quite boring for finite chains: state i is recurrent if and only if its communicating class is closed. But infinite chains are more interesting! An infinite closed class may be either transient or recurrent.

## 5.9 Random walk in $\mathbb{Z}^d$

Consider a simple symmetric random walk on the d-dimensional integer lattice. This is a Markov chain with state space  $\mathbb{Z}^d$  and transition probabilities  $p_{xy} = 1/2d$  if |x - y| = 1, and  $p_{xy} = 0$  otherwise. The chain is irreducible, with period 2.

In this section we will show that the random walk is recurrent when d = 1 or d = 2 but transient in higher dimensions.

#### **5.9.1** d = 1

The analysis after (5.7) (for p = q = 1/2) shows us that for the simple symmetric random walk on  $\mathbb{Z}$ , the hitting probability of 0 from any i > 0 is 1. By symmetry, the same is true from any negative state. This shows that starting from 0, the probability of returning to 0 is 1. Hence state 0 is recurrent (and so by irreducibility the whole chain is recurrent).

An alternative approach uses Theorem 5.11. This gives a good warm-up for the approach we will use in higher dimensions.

We need to show that  $\sum_{n=0}^{\infty} p_{00}^{(n)} = \infty$ . We will use Stirling's formula, which tells us that

$$n! \sim \sqrt{2\pi} \, n^{n+1/2} e^{-n} \text{ as } n \to \infty.$$
 (5.9)

(The constant  $\sqrt{2\pi}$  won't be important.)

Suppose  $X_0 = 0$ . If n is odd, then  $\mathbb{P}_0(X_n = 0) = 0$ , since the chain has period 2. For  $X_{2m} = 0$  we need m "ups" and m "downs" in the first 2m steps. Applying Stirling's formula to the binomial probability we obtain

$$p_{00}^{(2m)} = {2m \choose m} \left(\frac{1}{2}\right)^{2m}$$

$$= \frac{(2m)!}{m!m!} \left(\frac{1}{2}\right)^{2m}$$

$$\sim \frac{1}{\sqrt{\pi}} \frac{1}{m^{1/2}}.$$
(5.10)

Since  $\sum m^{-1/2} = \infty$ , we have  $\sum p_{00}^{(n)} = \infty$  and the chain is recurrent.

**Exercise.** Use Stirling's formula to show that if  $p \neq q$ , then the chain is transient. (We could also deduce this from the hitting probability analysis after (5.7).)

#### **5.9.2** d=2

Why should the walk be recurrent in 1 and 2 dimensions but transient in 3 dimensions? An intuitive answer is as follows. A d-dimensional random walk behaves in some sense like d independent 1-dimensional walks. For the d-dimensional walk to be back at the origin, we require all d of the 1-dimensional walks to be at 0. From (5.10), the probability that a 1-dimensional walk is at 0 decays like  $m^{-1/2}$ . Hence the probability that a 2-dimensional walk is at the origin decays like  $m^{-1}$ , which sums to infinity, leading to recurrence, while the corresponding probability for a 3-dimensional walk decays like  $m^{-3/2}$  which has finite sum, leading to transience.

In two dimensions we can make this precise in a very direct way. Let  $X_n$  be the walk in  $\mathbb{Z}^2$  and consider its projections onto the diagonal lines x = y and x = -y in the plane.

Each step of the walk increases or decreases the projection onto x = y by  $1/\sqrt{2}$ , and also increases or decreases the projection onto x = -y by  $1/\sqrt{2}$ . All four possibilities are equally likely.

Hence if we write  $W_n^+$  and  $W_n^-$  for the two projections of  $X_n$ , we have that the processes  $W_n^+$  and  $W_n^-$  are independent of each other, and both of them are simple symmetric random walks on  $2^{-1/2}\mathbb{Z}$ .

Then we have

$$\mathbb{P}(X_{2m} = 0) = \mathbb{P}(W_{2m}^{+} = 0)\mathbb{P}(W_{2m}^{-} = 0)$$
$$\sim \left(\frac{1}{\sqrt{\pi}} \frac{1}{m^{1/2}}\right)^{2}$$
$$= \frac{1}{\pi m}.$$

Hence  $\sum p_{00}^{(2m)} = \infty$  and the walk is recurrent.

#### **5.9.3** d = 3

The trick from the previous section doesn't work in d=3, so we need to do a little more combinatorics. As the walk has period 2 we have a positive chance of return to the origin only when n is even. Each step is  $\pm e_1, \pm e_2$  or  $\pm e_3$  where  $e_i, i=1,2,3$  are the three unit coordinate vectors. To return to the origin after 2m steps, we should have made, say, i steps in each of the directions  $\pm e_1$ , j steps in each of the directions  $\pm e_2$ , and k steps in each of the directions  $\pm e_3$  for some i, j, k with i + j + k = m. Considering all the possible orderings of these steps among the first 2m steps of the walk, we get

$$p_{00}^{(2m)} = \sum_{\substack{i,j,k \ge 0 \\ i+j+k=m}} \frac{(2m)!}{i!^2 j!^2 k!^2} \left(\frac{1}{6}\right)^{2m}$$

$$= \left(\frac{2m}{m}\right) \left(\frac{1}{2}\right)^{2m} \sum_{\substack{i,j,k \ge 0 \\ i+j+k=m}} {m \choose i,j,k}^2 \left(\frac{1}{3}\right)^{2m}$$

$$\leq \left(\frac{2m}{m}\right) \left(\frac{1}{2}\right)^{2m} \left(\sum_{\substack{i,j,k \ge 0 \\ i+j+k=m}} {m \choose i,j,k} \left(\frac{1}{3}\right)^{m} \right) \max_{\substack{i,j,k \ge 0 \\ i+j+k=m}} {m \choose i,j,k} \left(\frac{1}{3}\right)^{m}. \quad (5.11)$$

Here, if i + j + k = m, we write  $\binom{m}{i,j,k} = \frac{m!}{i!j!k!}$ . Note that

$$\sum_{\substack{i,j,k \ge 0\\ i+j+k=m}} \binom{m}{i,j,k} \left(\frac{1}{3}\right)^m = 1,$$

since it is the sum of the mass function of a "trinomial(1/3, 1/3, 1/3)" distribution (consider the number of ways of putting 3 balls into m boxes).

If m is divisible by 3, say m = 3r, then it's easy to check that the max in (5.11) is attained when i = j = k = r, giving

$$\begin{aligned} p_{00}^{(2m)} &\leq \binom{2m}{m} \left(\frac{1}{2}\right)^{2m} \binom{m}{m/3, m/3, m/3} \left(\frac{1}{3}\right)^m \\ &\sim \frac{1}{\sqrt{2\pi}} \frac{1}{m^{1/2}} \times \frac{1}{2\pi} \frac{1}{m} \\ &\sim \frac{1}{(2\pi)^{3/2}} m^{-3/2}, \end{aligned}$$

where we used Stirling's formula again for the last line. Hence we have  $\sum_{r=0}^{\infty} p_{00}^{(6r)} < \infty$ . Note also that  $p_{00}^{(6r)} \geq \left(\frac{1}{6}\right)^2 p_{00}^{(6r-2)}$  and  $p_{00}^{(6r)} \geq \left(\frac{1}{6}\right)^4 p_{00}^{(6r-4)}$ , so overall,  $\sum_{n=0}^{\infty} p_{00}^{(n)} < \infty$ , and the walk is transient.

#### **5.9.4** $d \ge 4$

If we have a walk on  $\mathbb{Z}^d$  for  $d \geq 4$ , we can obtain from it a walk on  $\mathbb{Z}^3$  by looking only at the first 3 coordinates, and ignoring any transitions that don't change them. Since we know that a walk on  $\mathbb{Z}^3$  only visits the origin finitely often, the same must be true for the walk in higher dimensions also. Hence we have transience for all  $d \geq 3$ .

## 5.9.5 Mean hitting time

Let  $H^A = \min\{n : X_n \in A\}$ , the first hitting-time of the set A. Notice that  $H^A$  is allowed to take the value  $\infty$ . In fact if  $h_i^A$  is the hitting probability defined above, then  $h_i^A = \mathbb{P}_i(H^A < \infty)$ .

Let  $k_i^A = \mathbb{E}_i(H^A)$ , the mean hitting time of A from i. If  $h_i^A < 1$ , then  $\mathbb{P}_i(H^A = \infty) > 0$  and certainly  $k_i^A = \infty$ . Also maybe  $k_i^A = \infty$  even when  $h_i^A = 1$ .

**Theorem 5.13.** The vector of mean hitting times  $k^A = (k_i^A, i \in S)$  is the minimal non-negative solution to

$$k_i^A = \begin{cases} 0 & \text{if } i \in A \\ 1 + \sum_j p_{ij} k_j^A & \text{if } i \notin A \end{cases}.$$

*Proof.* "Condition on the first jump" again. For  $i \notin A$ ,

$$k_i^A = \mathbb{E}_i(H^A) = \sum_j \mathbb{E}_i(H^A|X_1 = j)\mathbb{P}_i(X_1 = j)$$
  
=  $\sum_j p_{ij}(1 + k_j^A)$   
=  $1 + \sum_i p_{ij}k_j^A$ .

For the minimality, one can use a similar idea to that at (5.4) in the proof of Theorem 5.10 above. Specifically, one can show by induction that if  $(y_i)$  is any non-negative solution to the recursions, then  $y_i \geq \mathbb{E}_i \min(H^A, m)$  for all  $m \geq 0$ ; we omit the details.

#### 5.9.6 Gambler's ruin, continued

What is the expected hitting time of 0 from state i in the gambler's ruin chain at (5.5)?

Let  $k_i$  be the mean time to hit 0 starting from i. We give brief details (of course, one can be more formal!).

If  $k_i < \infty$ , one can see that  $k_i = \beta i$  for some  $\beta$ , since (compare the remark at (5.8) above),

$$\mathbb{E}_i(\text{time to }0) = \mathbb{E}_i(\text{time to }i-1) + \mathbb{E}_{i-1}(\text{time to }i-2) + \cdots + \mathbb{E}_1(\text{time to }0).$$

To satisfy the recursion in Theorem (5.13), we need

$$k_i = 1 + qk_{i-1} + pk_{i+1}$$

which leads to  $(q - p)\beta = 1$ . We obtain:

p < q  $k_i = \frac{1}{q-p}i$ ; the chain takes a finite time on average to hit 0.

p > q We already know  $h_i < 1$ , so certainly  $k_i = \infty$ .

p=q There is no suitable  $\beta$ , so  $k_i=\infty$  here also, even though  $h_i=1$ . The chain hits 0 with probability 1, but the mean time to arrive there is infinite.

## 5.10 Null recurrence and positive recurrence

Define  $m_i$ , the **mean return time** to a state i by

$$m_i := \mathbb{E}_i \left( \min\{n \ge 1 : X_n = i\} \right)$$
  
=  $1 + \sum_{i \ge j} p_{ij} k_j^{\{i\}}$  (5.12)

(where  $k_j^{\{i\}}$  is the mean hitting time of i starting from j).

This quantity will be particularly important when we consider equilibrium behaviour of a Markov chain – loosely speaking, the long-run proportion of time spent in state i ought to be the reciprocal of the mean return time.

If i is transient, then certainly  $m_i = \infty$  (since the return time itself is infinite with positive probability).

If i is recurrent, then the return time is also finite, but nonetheless the mean could be infinite.

If i is recurrent but  $m_i = \infty$ , the state i is said to be **null recurrent**.

If  $m_i < \infty$  then the state i is said to be **positive recurrent**.

For similar reasons to those in Theorem 5.12, null recurrence and positive recurrence are *class properties*; if one state in a communicating class is null (resp. positive) recurrent, then every state in the class is null (resp. positive) recurrent.

If the chain is irreducible, we can therefore call the whole chain either transient, or null recurrent, or positive recurrent.

# Markov chains: stationary distributions, convergence to equilibrium, and time-reversal

Let  $\pi = (\pi_i, i \in I)$  be a distribution on the state space I.

We say that  $\pi$  is a stationary distribution, or invariant distribution, or equilibrium distribution, for the transition matrix P if

$$\pi P = \pi$$

That is, for all j,  $\pi_j = \sum_i \pi_i p_{ij}$ . The row vector  $\pi$  is a left eigenvector for the matrix P, with eigenvalue 1.

If  $X_0$  has distribution  $\pi$ , then we know that  $X_n$  has distribution  $\pi P^n$ . Hence if  $\pi$  is stationary, then  $X_n$  has distribution  $\pi$  for all n. It follows that the sequence

$$(X_n, X_{n+1}, X_{n+2}, \dots)$$

has the same distribution as

$$(X_0, X_1, X_2, \dots)$$

for any n.

## 6.1 Stationary distributions and convergence to equilibrium: main theorems

**Theorem 6.1** (Existence and uniqueness of stationary distributions). Let P be an irreducible transition matrix.

- (a) P has a stationary distribution if and only if P is positive recurrent.
- (b) In that case, the stationary distribution  $\pi$  is unique, and is given by  $\pi_i = 1/m_i$  for all i (where  $m_i$  is the mean return time to state i defined at (5.12)).

**Theorem 6.2** (Convergence to equilibrium). Suppose P is irreducible and aperiodic, with stationary distribution  $\pi$ . If  $X_n$  is a Markov chain with transition matrix P and any initial distribution, then for all  $j \in I$ ,

$$\mathbb{P}(X_n = j) \to \pi_j \text{ as } n \to \infty.$$

In particular,

$$p_{ij}^{(n)} \to \pi_j \text{ as } n \to \infty, \text{ for all } i \text{ and } j.$$

**Theorem 6.3** (Ergodic theorem). Let P be irreducible. Let  $V_i(n)$  be the number of visits to state i before time n, that is

$$V_i(n) = \sum_{r=0}^{n-1} I(X_r = i).$$

Then for any initial distribution, and for all  $i \in I$ ,

$$\frac{V_i(n)}{n} \to \frac{1}{m_i}$$
 almost surely, as  $n \to \infty$ .

That is,

$$\mathbb{P}\left(\frac{V_i(n)}{n} \to \frac{1}{m_i} \text{ as } n \to \infty\right) = 1.$$

The ergodic theorem concerns the "long-run proportion of time" spent in a state.

In the positive recurrent case,  $1/m_i = \pi_i$  where  $\pi$  is the stationary distribution, so the ergodic theorem says that (with probability 1) the long-run proportion of time spent in a state is the stationary probability of that state.

In the null-recurrent or transient case,  $1/m_i = 0$ , so the ergodic theorem says that with probability 1 the long-run proportion of time spent in a state is 0.

We can see the ergodic theorem as a generalisation of the strong law of large numbers. If  $X_n$  is an i.i.d. sequence, then the strong law tells us that, with probability 1, the long run proportion of entries in the sequence which are equal to i is equal to the probability that any given entry is equal to i. The ergodic theorem can be seen as extending this to the case where  $X_n$  is not i.i.d. but is a Markov chain.

## 6.2 Examples of stationary distributions

**Example 6.4.** Let  $P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \end{pmatrix}$ . (You may like to draw the diagram of the chain.)

For  $\pi$  to be stationary, we need

$$\pi_1 = \frac{1}{2}\pi_3$$

$$\pi_2 = \pi_1 + \frac{1}{2}\pi_2$$

$$\pi_3 = \frac{1}{2}\pi_2 + \frac{1}{2}\pi_3.$$

One of these equations is redundant, and we need the added relation  $\pi_1 + \pi_2 + \pi_3 = 1$  to normalise the solution (so that  $\pi$  is a distribution).

Solving, we obtain  $(\pi_1, \pi_2, \pi_3) = (1/5, 2/5, 2/5)$ .

Correspondingly, the vector of mean return times is given by  $(m_1, m_2, m_3) = (5, 5/2, 5/2)$ .

From any initial state, the distribution at time n converges to  $\pi$  as  $n \to \infty$ . For example,  $p_{11}^{(n)} \to 1/5$  as  $n \to \infty$ .

By the way, be careful to solve the equation  $\pi P = \pi$  and not to solve  $P\pi = \pi$  by mistake! For any transition matrix P, the equation  $P\pi = \pi$  is solved by any vector  $\pi$  all of whose entries are the same (why is this?) which could trap you into thinking that the uniform distribution is stationary, which, of course, is not the case in general. We want the left eigenvector, rather than the right eigenvector.

**Example 6.5.** Recall the example of a simple symmetric random walk on a cycle of size M in Section 5.3. Each step goes clockwise with probability p and anticlockwise with probability 1 - p. The distribution  $\pi$  with  $\pi_i = 1/M$  for all i is stationary, since it solves

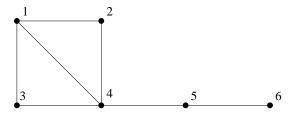
$$\pi_i = (1 - p)\pi_{i+1} + p\pi_{i-1}$$

for each i (where addition on states is mod M). Because of the symmetry of the chain, it is not surprising that the stationary distribution is uniform.

Is it the true that  $p_{00}^{(n)} \to 1/M$  as  $n \to \infty$ ? If M is odd, then the chain is aperiodic (check this!), so the answer is yes.

However, if M is even then the chain has period 2. Then  $p_{00}^{(n)} = 0$  whenever n is odd. In fact  $p_{00}^{(2m)} \to 2\pi_0 = 2/M$  as  $m \to \infty$  (exercise; consider the 2-step chain  $X_0, X_2, X_4, \ldots$  on the subset of the state space which consists just of even sites. Is it irreducible? What is its stationary distribution?)

**Example 6.6** (Random walk on a graph). A "graph" in the combinatorial sense is a collection of *vertices* joined by *edges*. For example, the following graph has 6 vertices and 7 edges.



Let I be the set of vertices. Two vertices are *neighbours* in the graph if they are joined by an edge. The *degree* of a vertex is its number of neighbours. Let  $d_i$  be the degree of vertex i. In the graph above, the vector of vertex degrees is  $(d_i, i \in I) = (3, 2, 2, 4, 2, 1)$ .

Assume  $d_i > 0$  for all i. A random walk on the graph is a Markov chain with state space I, evolving as follows; if i is the current vertex, then at the next step move to each of the neighbours of i with probability  $1/d_i$ .

Assume irreducibility of the chain (equivalently, that there is a path between any two vertices in the graph). Then the stationary distribution of the chain  $\pi$  is unique.

In fact, the stationary probability of a vertex is proportional to its degree. To show this, we will check that dP = d where d is the vector of vertex degrees and P is the transition matrix of the chain:

$$d_j = \sum_i I(i \text{ is a neighbour of } j)$$
 
$$= \sum_i d_i \frac{1}{d_i} I(i \text{ is a neighbour of } j)$$

$$= \sum_{i} d_i p_{ij},$$

as required.

To obtain the stationary distribution we simply need to normalise d. So we obtain  $\pi_i = d_i / \sum_j d_j$ .

For the graph above,  $\sum_{j} d_{j} = 14$ , and we obtain

$$\pi = \left(\frac{3}{14}, \frac{1}{7}, \frac{1}{7}, \frac{2}{7}, \frac{1}{7}, \frac{1}{14}\right).$$

From this we can deduce the mean return times. For example,  $m_1 = 1/\pi_1 = 14/3$ .

Notice that the chain is aperiodic. As a result, we also have convergence to the stationary distribution. For example, starting from any initial distribution, the probability that the walk is at vertex 1 at step n converges to 3/14 as  $n \to \infty$ .

**Example 6.7** (One-dimensional random walk). Consider again the familiar example of a one-dimensional random walk. Let  $I = \{0, 1, 2, ...\}$  and let

$$p_{i,i+1} = p \text{ for } i \ge 0,$$
  
 $p_{i,i-1} = q = 1 - p \text{ for } i \ge 1,$   
 $p_{0,0} = q.$ 

If p > q, we found previously that the walk is transient, so no stationary distribution will exist.

If p = q, the walk is recurrent, but the mean return time is infinite, so again there is no stationary distribution.

If p < q, the walk is positive recurrent. For stationarity, we need  $\pi_i = \pi_{i-1}p + \pi_{i+1}q$  for  $i \geq 1$ . This is (not coincidentally) reminiscent of the hitting probability equation we previously found for the model (except the values of p and q are reversed). It has general solution  $\pi_i = A + B(p/q)^i$ .

We need  $\sum \pi_i = 1$ , which forces A = 0 and B = (1 - p/q), giving

$$\pi_i = \left(1 - \frac{p}{q}\right) \left(\frac{p}{q}\right)^i.$$

That is, the stationary distribution of the walk is geometric with parameter  $1 - \frac{p}{q}$ .

Example 6.8 (A two-state chain and a non-irreducible chain).

Consider the two-state chain on  $\{1,2\}$  with transition matrix  $P = \begin{pmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{pmatrix}$ .

Solving  $\pi P = \pi$  and normalising we obtain that  $\pi = \left(\frac{\beta}{\alpha + \beta}, \frac{\alpha}{\alpha + \beta}\right)$ .

Notice that this agrees with what we found in Example 5.4; the expression for  $p_{11}^{(n)}$  given in (5.2) satisfies  $p_{11}^{(n)} \to \pi_1 = \frac{\beta}{\alpha + \beta}$  as  $n \to \infty$ , as it should do because of the convergence to equilibrium in Theorem 6.2.

Now consider the chain on  $\{1, 2, 3, 4\}$  whose transition matrix is

$$P = \begin{pmatrix} 1 - \alpha & \alpha & 0 & 0 \\ \beta & 1 - \beta & 0 & 0 \\ 0 & 0 & 1 - \gamma & \gamma \\ 0 & 0 & \delta & 1 - \delta \end{pmatrix}.$$

This chain is not irreducible. We can view it as two separate two-state chains, on  $\{1,2\}$  and  $\{3,4\}$ , with no communication between them. Both  $\left(\frac{\beta}{\alpha+\beta},\frac{\alpha}{\alpha+\beta},0,0\right)$  and  $\left(0,0,\frac{\delta}{\gamma+\delta},\frac{\gamma}{\gamma+\delta}\right)$  are stationary distributions. But also any mixture of these is stationary (since if  $\pi^{(1)}$  and  $\pi^{(2)}$ ) are eigenvectors of P with eigenvalue 1, then so is any linear combination of  $\pi^{(1)}$  and  $\pi^{(2)}$ ).

So any distribution

$$\left(x\frac{\beta}{\alpha+\beta}, x\frac{\alpha}{\alpha+\beta}, (1-x)\frac{\delta}{\gamma+\delta}, (1-x)\frac{\gamma}{\gamma+\delta}\right),$$

where  $x \in [0, 1]$ , is stationary. (In fact, these are all the stationary distributions – exercise). The uniqueness result in Theorem 6.1 does not apply because the transition matrix is not irreducible.

**Example 6.9** (A random-to-front chain on permutations). A student keeps m books in a row on their bookshelf, which we will label as 1, 2, ..., m. Each day they take out a book to read before going to sleep, choosing book i with probability  $q_i$  where  $\sum_i q_i = 1$  (independently of all previous choices). The book is then replaced at the front of the row.

We can think of the process as a Markov chain whose state space is  $S_m$ , the set of all permutations of m objects, of size m!. What is the stationary distribution of the chain?

Rather than trying to calculate directly from the stationarity relations, we can alternatively think about the long-run behaviour of the process. Imagine running the chain until some large time N. Let  $\sigma$  be the state we find the chain in at that time (whose distribution will be close to the stationary distribution). Suppose  $Y_r$  is the book chosen at step r, so that  $(Y_n)_{1 \le n \le N}$  are i.i.d. with distribution  $q = (q_i)_{1 \le i \le m}$ .

The book in first position is simply the most recently chosen book. So  $\mathbb{P}(\sigma_1 = i) = \mathbb{P}(Y_N = i) = q_i$ .

The book in second position is then the most recently chosen book other than  $\sigma_1$ . We get

$$\mathbb{P}(\sigma_2 = j | \sigma_1 = i) = \frac{q_j}{1 - q_i}.$$

More generally,

$$\mathbb{P}(\sigma_r = i_r | (\sigma_1, \dots, \sigma_{r-1}) = (i_1, \dots, i_{r-1})) = \frac{q_{i_r}}{1 - q_{i_1} - \dots - q_{i_{r-1}}} = \frac{q_{i_r}}{\sum_{j \notin \{i_1, \dots, i_{r-1}\}} q_j}.$$

So the stationary probability of observing the books in order  $i_1, i_2, \dots i_m$  is

$$\prod_{r=1}^{m} \frac{q_{i_r}}{\sum_{j \ge r} q_{i_j}}.$$

(The final term in the product, with r = m, is simply equal to 1.)

For example, for the case m=3, the stationary probability of seeing the books in order 1,2,3 is

$$q_1 \frac{q_2}{q_2 + q_3}.$$

The expressions for the other 5 possible orders of the three books are analogous. As an exercise, try checking this stationary distribution for the case m=3 directly from the stationarity relations.

## 6.3 Proof of Theorems 6.1, 6.2 and 6.3. (non-examinable)

The proofs below are given partly rather informally. They are not examinable; however, they are very helpful in developing your intuition about the results. The "coupling" idea used in the proof of Theorem 6.2 is particularly pretty and I certainly recommend thinking about it, but it won't be examined. (The results themselves are very much examinable!)

*Proof of Theorem 6.3.* This proof is essentially an application of the strong law of large numbers

If the chain is transient, then with probability 1 there are only finitely many visits to any state, so  $V_i(n)$  is bounded with probability 1. So

$$\mathbb{P}\left(\frac{V_i(n)}{n} \to 0 \text{ as } n \to \infty\right) = 1,$$

which is the result we want since  $m_i = \infty$ .

Suppose instead that the chain is recurrent. In this case we will visit state i infinitely often. Let  $X_k$  be the time between the kth and the (k+1)st visits to i. Then  $X_1, X_2, X_3, \ldots$  are i.i.d. with mean  $m_i$  (which is finite in the positive recurrent case and infinite in the null recurrent case).

So by the strong law of large numbers,

$$\mathbb{P}\left(\frac{X_1 + X_2 + \dots + X_K}{K} \to m_i \text{ as } K \to \infty\right) = 1.$$
(6.1)

Let  $T_K$  be the time of the Kth visit to i. Then  $T_K = T_1 + X_1 + X_2 + \cdots + X_{K-1}$ . It's easy to obtain that, for any c,  $T_K/K \to c$  if and only if  $(X_1 + \cdots + X_K)/K \to c$  (this is a determinantic fact – no probability involved). Hence from (6.1) we have

$$\mathbb{P}\left(\frac{T_K}{K} \to m_i \text{ as } k \to \infty\right) = 1. \tag{6.2}$$

Notice that  $T_K/K$  is the time per visit (averaged over the first K visits) whereas  $V_i(n)/n$  is the number of visits per unit time (averaged over the first n times). It's straightforward to obtain (check!) that, for any c,  $T_K/K \to c$  as  $K \to \infty$  if and only if  $V_i(n)/n \to 1/c$  as  $n \to \infty$ .

Hence from (6.2) we have

$$\mathbb{P}\left(\frac{V_i(n)}{n} \to \frac{1}{m_i} \text{ as } n \to \infty\right) = 1$$

as required.  $\Box$ 

**Lemma 6.10.** If P is positive recurrent, then it has stationary distribution  $\pi$  with  $\pi_i = 1/m_i$ .

*Proof.* We give an informal version of the proof, which could quite easily be made rigorous.

From the ergodic theorem, we know that (with probability 1) the long-run proportion of visits to state i is  $1/m_i$ .

Each time the chain visits state i, it has probability  $p_{ij}$  of jumping from there to state j. We can obtain that the long-run proportion of jumps from i to j is  $\frac{1}{m_i}p_{ij}$ .

First consider the case where the state space I is finite. By summing over  $i \in I$ , we get that the long-run proportion of jumps into state j is  $\sum_{i} \frac{1}{m_i} p_{ij}$ .

But the long-run proportion of jumps into j is the same as the long-run proportion of visits to j, which (by the ergodic theorem) is  $1/m_j$ .

We obtain

$$\frac{1}{m_j} = \sum_i \frac{1}{m_i} p_{ij},$$

i.e.  $\pi_j = \sum_i \pi_i p_{ij}$ , so that  $\pi$  satisfies  $\pi P = \pi$  and is stationary as desired.

If i is infinite, it is not immediate that the long-run proportion of jumps into j is the sum over i of the long-run proportions of jumps from i to j. However (by considering as large a finite set of i as desired) the second quantity does give an upper bound for the first, so we get

$$\frac{1}{m_j} \le \sum_{i} \frac{1}{m_i} p_{ij}$$

for all  $j \in I$ . But summing both sides over j gives the same (finite) amount, since  $\sum_{j} p_{ij} = 1$  for all i. So in fact we must have equality for all j as required.

**Lemma 6.11.** If  $\pi$  is any stationary distribution then  $\pi_i = 1/m_i$ .

*Proof.* Suppose  $\pi$  is stationary for P, and let X be a Markov chain with initial distribution  $\pi$  and transition matrix P. Then by stationarity,  $\mathbb{P}(X_n = i) = \pi_i$  for all n, and

$$\frac{\mathbb{E} V_n(i)}{n} = \frac{1}{n} \sum_{r=0}^{n-1} \mathbb{E} \left( I(X_n = i) \right)$$

$$= \frac{1}{n} \sum_{r=0}^{n-1} \mathbb{P}(X_n = i)$$

$$= \pi_i.$$
(6.3)

From the ergodic theorem, for any  $\epsilon$ 

$$\mathbb{P}\left(\left|\frac{V_n(i)}{n} - \frac{1}{m_i}\right| > \epsilon\right) < \epsilon \tag{6.4}$$

for large enough n (since almost sure convergence implies convergence in probability).

But since  $V_n(i)/n$  is bounded between 0 and 1, it follows from (6.4) (check!) that

$$\frac{\mathbb{E} V_n(i)}{n} \to \frac{1}{m_i} \text{ as } n \to \infty.$$

Comparing to (6.3), we obtain  $\pi_i = 1/m_i$ .

This gives uniqueness of the stationary distribution for positive recurrent chains, and shows that no stationary distribution can exist for null recurrent and transient chains. So we have proved Theorem 6.1.

Finally, we prove the result on convergence to equilibrium.

Proof of Theorem 6.2. Let P be irreducible and aperiodic, with stationary distribution  $\pi$ .

Let  $\lambda$  be any initial distribution, and let  $(X_n, n \geq 0)$  be  $\operatorname{Markov}(\lambda, P)$ . We wish to show that  $\mathbb{P}(X_n = j) \to \pi_j$  as  $n \to \infty$ , for any j.

Consider another chain  $(Y_n, n \ge 0)$  which is Markov $(\pi, P)$ , and which is independent of Z. Since  $\pi$  is stationary,  $Y_n$  has distribution  $\pi$  for all n.

Let  $T = \inf\{n \geq 0 : X_n = Y_n\}$ . We will claim that  $\mathbb{P}(T < \infty) = 1$ ; that is, the chains X and Y will meet at some point.

Suppose this claim is true. Then define another chain Z by

$$Z_n = \begin{cases} X_n & \text{if } n < T \\ Y_n & \text{if } n \ge T \end{cases}.$$

The idea is that Z starts in distribution  $\lambda$ , and evolves independently of the chain Y, until they first meet. As soon as that happens, Z copies the moves of Y exactly.

Then Z is also Markov( $\lambda$ , P), since  $Z_n$  starts in distribution  $\lambda$  and each jump is done according to P, first by copying X up to time T, and then by copying Y after time T.

The idea is that the chain Y is "in equilibrium" (since it starts in the equilibrium distribution  $\pi$ ) so that if there is high probability that  $Y_n = Z_n$ , then the distribution of  $Z_n$  must be close to  $\pi$ . More precisely:

$$|\mathbb{P}(Z_n = j) - \pi_j| = |\mathbb{P}(Z_n = j) - \mathbb{P}(Y_n = j)|$$

$$\leq \mathbb{P}(Z_n \neq Y_n)$$

$$= \mathbb{P}(T > n)$$

$$\to 0 \text{ as } n \to \infty.$$

Then we have  $\mathbb{P}(Z_n = j) \to \pi_j$ .

But the chains X and Z have the same distribution (they are both  $Markov(\lambda, P)$ ). So we have also shown that  $\mathbb{P}(X_n = j) \to \pi_j$ , as required.

It remains to prove the claim that T is finite with probability 1. Fix any state  $b \in I$  and define  $T_b = \inf\{n \geq 0 : X_n = Y_n = b\}$ . Then  $T \leq T_b$ . We will show that  $T_b$  is finite with probability 1.

Consider the process  $W_n = (X_n, Y_n)$ . Since  $X_n$  and  $Y_n$  evolve independently,  $W_n$  is a Markov chain on the state space  $I \times I$  with transition probabilities

$$\tilde{p}_{(i,k)(i,l)} = p_{ij}p_{kl},$$

and initial distribution

$$\mu_{(i,k)} = \lambda_i \pi_k.$$

P is aperiodic and irreducible, so for all i, j, k, l, we have that

$$\tilde{p}_{(i,k)(j,l)}^{(n)} = p_{ij}^{(n)} p_{kl}^{(n)} > 0$$

for all large enough n. So  $\tilde{P}$  is irreducible.

 $\tilde{P}$  has an invariant distribution given by

$$\tilde{\pi}_{(i,k)} = \pi_i \pi_k$$
.

Hence  $\tilde{P}$  is recurrent (by Theorem 6.1). But  $T_b = \inf\{n \geq 0 : W_n = (b,b)\}$ . Then indeed  $\mathbb{P}(T_b < \infty) = 1$  (since an irreducible recurrent chain visits every state with probability 1).  $\square$ 

Notice where the argument above fails when P is periodic. The chain  $W_n = (X_n, Y_n)$  still has the stationary distribution of the form above, but it is not irreducible, so it may never reach the state (b, b). (For example, if P has period 2, and the chains X and Y start out with "opposite parity", then they will never meet).

#### 6.4 Time-reversal

Consider an irreducible positive-recurrent Markov chain, started in its stationary distribution  $\pi$ .

The Markov property tells us that conditional on the state of the process at some given time, the past and the future of the chain are independent. This property is symmetrical in time, suggesting that the *time-reversal* of the process should also be a Markov chain.

**Theorem 6.12.** Let P be an irreducible transition matrix, with stationary distribution  $\pi$ . Let  $(X_0, X_1, \ldots, X_N)$  be  $Markov(\pi, P)$ .

For  $0 \le n \le N$ , define  $Y_n = X_{N-n}$ . Then  $(Y_0, Y_1, \dots, Y_N)$  is Markov $(\pi, Q)$  with transition matrix  $Q = (q_{ij})$  given by

$$q_{ij} = \frac{\pi_j}{\pi_i} p_{ji}. (6.5)$$

The matrix Q also has stationary distribution  $\pi$ .

*Proof.* First we check that Q is a stochastic matrix: Its entries  $q_{ij}$  defined by (6.5) are non-negative (since all of  $\pi_i$ ,  $\pi_j$  and  $p_{ji}$  are non-negative), and we also have, for any i,

$$\sum_{j} q_{ij} = \frac{1}{\pi_i} \sum_{j} \pi_j p_{ji} = \frac{1}{\pi_i} \pi_i = 1$$

using the fact that  $\pi$  is stationary for P.

To see that  $\pi$  is also stationary for Q: for any j, (6.5) gives

$$\sum_{i} \pi_i q_{ij} = \pi_j \sum_{i} p_{ji} = \pi_j$$

using the fact that P is a stochastic matrix.

Finally, consider any sequence of states  $i_0, i_1, \ldots, i_N$ . We have

$$\mathbb{P}(Y_0 = i_0, Y_1 = i_1, \dots, Y_N = i_N)$$

$$= \mathbb{P}(X_0 = i_N, X_1 = i_{N-1}, \dots, X_N = i_0)$$

$$= \pi_{i_N} p_{i_N i_{N-1}} p_{i_{N-1} i_{N-2}} \dots p_{i_2 i_1} p_{i_1 i_0}$$

$$= \pi_{i_N} \left( q_{i_{N-1}i_N} \frac{\pi_{i_{N-1}}}{\pi_{i_N}} \right) \left( q_{i_{N-2}i_{N-1}} \frac{\pi_{i_{N-2}}}{\pi_{i_{N-1}}} \right) \dots \left( q_{i_1i_2} \frac{\pi_{i_1}}{\pi_{i_2}} \right) \left( q_{i_0i_1} \frac{\pi_{i_0}}{\pi_{i_1}} \right)$$

$$= \pi_{i_0} q_{i_0i_1} q_{i_1i_2} \dots q_{i_{N-2}i_{N-1}} q_{i_{N-1}i_N},$$

so that  $Y \sim \text{Markov}(\pi, Q)$  as claimed.

The chain Y is called the *time-reversal* of the chain X (or more specifially its *time-reversal* in equilibrium). We can interpret (6.5) as follows. As we argued in the previous section, for a stationary chain with matrix P and stationary distribution  $\pi$ , the long-run rate of jumps from j to i is  $\pi_j p_{ji}$ . This ought to be the same as the long-run rate of jumps from i to j in the time-reversal of the chain – if the time-reversal has matrix Q and stationary distribution  $\pi$ , then this is  $\pi_i q_{ij}$ . The equality of those two quantities is precisely the relation (6.5).

If P and Q are the same – that is, if the distribution of the original process and its time-reversal are the same – we say that the chain (or the matrix) is reversible (or time-reversible, or even more fully time-reversible in equilibrium).

The relations (6.5) immediately give us the following characterisation of time-reversibility:

**Theorem 6.13.** Let P be an irreducible transition matrix with stationary distribution  $\pi$ . P is reversible iff

$$\pi_i p_{ij} = \pi_j p_{ji} \text{ for all } i, j. \tag{6.6}$$

The relations (6.6) are known as the *detailed balance equations*. If a matrix P and a distribution  $\pi$  satisfy (6.6), they are sometimes said to be "in detailed balance".

**Theorem 6.14.** If the matrix P and the distribution  $\pi$  are in detailed balance, i.e. satisfy (6.6), then  $\pi$  is stationary for P.

*Proof.* For any 
$$j$$
,  $\pi_j = \pi_j \sum_i p_{ji} = \sum_i \pi_j p_{ji} = \sum_i \pi_i p_{ij}$  as required.

This result is very useful in practice when looking for stationary distributions. When they do have a solution, the detailed balance equations are often much easier to deal with than the more general stationarity relations.

Remark 6.15. Suppose we have, for example, a finite irreducible chain, and we want to determine whether or not it's time-reversible in equilibrium. We could solve the stationarity equations to find the stationary distribution, and then look at whether the stationary distribution solves the detailed balance equations. It's usually much simpler to attempt to solve the detailed balance equations themselves. If a solution exists, then that is the stationary distribution and the chain is reversible in equilibrium. If on the other hand we find that no solution exists, then the chain is not reversible in equilibrium.

#### 6.4.1 Examples

**Example 6.16** (Random walk on a cycle). Recall the random walk on a cycle with M states from Example 5.5 and Example 6.5. At each step, the walk moves clockwise around the cycle

with probability p, and anticlockwise with probability 1 - p. That is,

$$p_{ij} = \begin{cases} p & \text{if } j \equiv i+1 \mod M \\ 1-p & \text{if } j \equiv i-1 \mod M \\ 0 & \text{otherwise} \end{cases}$$

The stationary distribution is uniform on  $\{0, 1, 2, \dots, M-1\}$ .

If p > 1/2, in the long run the walk moves clockwise more often than it moves anticlockwise. Hence we could tell the difference between the chain and its time-reversal (which would move more often anticlockwise). The chain is not reversible. It's easy to obtain from (6.5) that the time-reversal in equilibrium is a similar chain but with the opposite drift; the transition probabilities  $q_{ij}$  of the time-reversal are

$$q_{ij} = \begin{cases} 1 - p & \text{if } j \equiv i + 1 \mod M \\ p & \text{if } j \equiv i - 1 \mod M \\ 0 & \text{otherwise} \end{cases}.$$

If p=1/2, the chain is reversible. For every i,j, either  $\pi_i p_{ij}=\pi_j p_{ji}=0$ , or (when i and j are neighbours on the cycle)  $\pi_i p_{ij}=\pi_j p_{ji}=\frac{1}{M}\frac{1}{2}$ , so that the detailed balance equations hold.

**Example 6.17** (One-dimensional random walk). Consider again the one-dimensional random walk on the non-negative integers, from Example 6.7. Let  $I = \{0, 1, 2, ...\}$  and let

$$p_{i,i+1} = p \text{ for } i \ge 0,$$
  
 $p_{i,i-1} = 1 - p \text{ for } i \ge 1,$   
 $p_{0,0} = 1 - p.$ 

Suppose p < 1/2 so that the walk has a downward drift. We saw that there exists a stationary distribution given by

$$\pi_i = \left(1 - \frac{p}{1 - p}\right) \left(\frac{p}{1 - p}\right)^i$$

i.e. a geometric distribution with parameter  $1 - \frac{p}{1-p}$ .

Although the walk has a "drift", nonetheless the process is reversible. Unlike the previous example, there are no cycles in the graph of transitions. For every edge (i, i + 1), upward transitions across it must alternate with downward transitions across it. Hence they have equal long-run frequency, which gives the detailed balance equations.

The same argument applies to any chain on the integers that can change by at most 1 at each step. In fact, it applies more generally to any irreducible chain whose graph of transitions is a "tree" (i.e. contains no cycles).

**Example 6.18** (Random walk on a graph). The random walk on a connected graph from Example 6.6 is always reversible. Consider any neighbours i and j in the graph, with degrees  $d_i$  and  $d_j$ . Then  $p_{ij} = 1/d_i$  and  $p_{ji} = 1/d_j$ . We also saw that the stationary distribution of a state is proportional to its degree. In particular  $\pi_i/d_i = \pi_j/d_j$ . We deduce  $\pi_i p_{ij} = \pi_j p_{ji}$  as required for the detailed balance equations.

Further examples to come in lectures!