Mathematical Foundations of Information Theory / Discrete Stochastics and Information Theory

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Preface

The course is based on the lecture notes of Wolfgang Woess.

1 Introduction to Probability Theory

Probability is a mathematical phenomenon that we see in every day life that we perhaps intuitively understand. As a motivating example, consider what is called the *law of large numbers* if we toss a fair coin 1000 times every day, then each day we will get heads *about* 500 times. Of course, we won't get exactly 500 heads, but the *deviations* we observe, over the repeated trials, should be *small*. Similarly, if we roll a fair die many times, the relative frequency of the outcome "6" will be approximately 1/6. From a certain philosophical viewpoint, this is what we mean when we say "The probability of rolling a 6 is 1/6".

More generally, the law of large numbers says that if we have some random experiment, whose outcome is a real number, and we repeat the experiment many times, then the average of the outcomes should *converge* to some specific, deterministic number, which is the *expected* outcome of the experiment.

In some ways this is intuitive, in other ways almost tautological, but what we want then from a theory of probability is a set of axioms which behaves like how we experience probability in the real world, and so in particular statements like the law of large numbers should follow as a mathetmatical theorem from these axioms.

1.1 Probability Spaces

Definition 1.1. A probability space is a triple $(\Omega, \mathcal{A}, \mathbb{P})$, where

- 1. Ω is a non-empty set, the sample space,
- 2. \mathcal{A} is a σ -algebra, that is, a collection of subsets of Ω such that
 - (i) $\Omega \in \mathcal{A}$,
 - (ii) $A \in \mathcal{A} \Rightarrow A^c = \Omega \setminus A \in \mathcal{A}$,
 - (iii) if $A_n \in \mathcal{A}$ for n = 1, 2, ..., then $\bigcup_{n=1}^{\infty} A_n \in \mathcal{A}$.
- 3. \mathbb{P} is a probability measure on \mathcal{A} , that is, a function $\mathbb{P}: \mathcal{A} \to [0,1]$ such that
 - (i) $\mathbb{P}(\emptyset) = 0$ and $\mathbb{P}(\Omega) = 1$,
 - (ii) if $A_n \in \mathcal{A}$ are pairwise disjoint for n = 1, 2, ..., that is, $A_n \cap A_m = \emptyset$ for all $m \neq n$, then

$$\mathbb{P}\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{n=1}^{\infty} \mathbb{P}(A_n).$$

We should think of the sample space Ω as consisting of all possible outcomes of some random experiment.

Example 1.2. (a) Our experiment is a coin toss. Our two outcomes are "Heads" and "Tails" and so our sample space is $\Omega = \{\text{Heads, Tails}\}$. We could equally 'encode' the outcomes as Heads = 1 and Tails = 0, in which case our sample space is $\Omega = \{0, 1\}$.

(b) Our experiment is again a coin toss, but we don't just measure the side that the coin lies on, but also its position on the ground, which is some point (x, y) in the plane with the coin-tosser standing at the origin, as well as the number m of times that the coin rotates whilst in the air. Then, a possible sample space would be

$$\Omega = \{(\ell, x, y, m) : \ell \in \{0, 1\}, (x, y) \in \mathbb{R}^2, m \in \mathbb{N}_0\}.$$

(c) Our experiment is sequence of n coin tosses, and we measure the sequence of outcomes. We can take our sample space to be

$$\Omega = \{0, 1\}^n$$

sequences of 0s and 1s of length n, which we call *bitstrings*, where the kth element of the sequence is the outcome of the kth coin toss.

(d) Our (theoretical) experiment is an infinite sequence of coin tosses. Our sample space is then

$$\Omega = \{0, 1\}^{\mathbb{N}}$$

all infinite sequences of 0s and 1s (an uncountable set!).

The function \mathbb{P} then tells us, for an *event*, a particular subset of the possible outcomes, how likely it is that this event occurs, that is, how likely it is that the outcome lies in this subset.

It turns out, for complicated mathematical reasons, even if the sample space Ω is something familiar like the real numbers \mathcal{R} or the unit interval [0,1], there is no way to define a consistent notion of measure that will assign a probability to *every* subset of Ω - very weird sets exist! For this reason we have to restrict ourselves to some 'well-behaved' collection of sets, this σ -algebra \mathcal{A} . However, this is no great restriction, as we can choose \mathcal{A} such that any event that you can actually physically describe will lie inside \mathcal{A} .

When Ω is *countable*, one can usually take $\mathcal{A} = \mathcal{P}(\Omega)$, the *power set* of Ω , consisting of all subsets of Ω . However, when Ω is uncountable, such as $\Omega = \mathbb{R}$, then there is no way to define any function \mathbb{P} satisfying the definition of a probability space with $\mathcal{A} = \mathcal{P}(\mathbb{R})$.

For the most part we will work with discrete probability spaces, those where Ω is countable, and so avoid these difficulties. In this case, if Ω is countable and $\mathcal{A} = \mathcal{P}(\Omega)$, then the probability measure is determined by the measure of the elementary events $\omega \in \Omega$ since

$$\mathbb{P}(A) = \sum_{\omega \in A} \mathcal{P}(\{\omega\})$$
 for all $A \in \mathcal{P}(\Omega)$.

Definition 1.3. Given a logical expression Φ concerning the elements of Ω , we will write $[\Phi]$ for the event

$$A = \{ \omega \in \Omega \colon \Phi \text{ is true for } \omega \},$$

and if $A \in \mathcal{A}$ (which will usually be the case) we define

$$\mathbb{P}[\Phi] := \mathbb{P}(A).$$

Example 1.4. (a) Our experiment is to roll two fair dice. Our sample space is

$$\Omega = \{(i,j) \colon 1 \leq i,j \leq 6\}$$

and we can take our σ -algebra to be $\mathcal{A} = \mathcal{P}(\Omega)$.

An event we could consider is the event that the total value of the two dice is 11, that is, we consider the event A = [the total value of the dice is 11], or in other words

$$A = \{(i, j) \in \Omega : i + j = 11\}.$$

(b) Our experiment is as in Example 1.2 (b). We consider the event

$$A = [$$
the coin lands at distance at most r from the coin tosser $] = \{(\ell, x, y, m) \colon x^2 + y^2 \le r^2\}.$

Similarly the event

$$A = [$$
the coin spins at least 3 times and lands on Heads $]$ $= \{(\ell, x, y, m) \colon \ell = 1, m \geq 3\}.$

One can easily deduce the following properties from Definition 1.1.

Proposition 1.5. (i) $\emptyset \in \mathcal{A}$,

- (ii) If $A_n \in \mathcal{A}$ for $n = 1, 2, ..., then <math>\bigcap_{n=1}^{\infty} A_n \in \mathcal{A}$,
- (iii) If $A, B \in \mathcal{A}$ then $A \cup B, A \cap B \in \mathcal{A}$ and

$$\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B) - \mathbb{P}(A \cap B),$$

- (iv) If $A \in \mathcal{A}$, then $\mathbb{P}(A^c) = 1 \mathbb{P}(A)$,
- (v) If $A, B \in \mathcal{A}$ and $A \subseteq B$, then $\mathbb{P}(A) < \mathbb{P}(B)$.

The next lemma is fundamental.

Lemma 1.6 (Continuity of the probability measure). If $(A_n : n \in \mathbb{N})$ is an increasing sequence, that is $A_n \subseteq A_{n+1}$ for all $n \in \mathbb{N}$, with $A_n \in \mathcal{A}$ for all n, then

$$\mathbb{P}\left(\bigcup_{n=1}^{\infty} A_n\right) = \lim_{N \to \infty} \mathbb{P}(A_N).$$

Similarly, if $(A_n: n \in \mathbb{N})$ is an decreasing sequence, that is $A_n \supseteq A_{n+1}$ for all $n \in \mathbb{N}$, with $A_n \in \mathcal{A}$ for all n, then

$$\mathbb{P}\left(\bigcap_{n=1}^{\infty} A_i\right) = \lim_{N \to \infty} \mathbb{P}(A_N).$$

Proof.

Definition 1.7 (Conditional probability, Independence). Given two events $A, B \in \mathcal{A}$ we define

$$\mathbb{P}(A \mid B) = \begin{cases} \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}, & \text{if } \mathbb{P}(B) > 0, \\ 0, & \text{if } \mathbb{P}(B) = 0. \end{cases}$$

Given two logical expression Φ_1 and Φ_2 , where $A = \{\omega \in \omega : \Phi_1 \text{ is true for } \omega\}$ and $B = \{\omega \in \omega : \Phi_2 \text{ is true for } \omega\}$, we will write

$$\mathbb{P}[\Phi_1 \mid \Phi_2] = \mathbb{P}(A \mid B).$$

We say A and B are independent if $\mathbb{P}(A \cap B) = \mathbb{P}(A) \cdot \mathbb{P}(B)$. A sequence (finite or infinite) of events $(A_n : n \in I)$ is called (mutually) independent if for all choices of indices $J \subseteq I$

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

We note that this condition is stronger than asking for *pairwise* independence of the events A_i, A_j for $i, j \in I$.

Example 1.8. Suppose we flip two fair coins, so that $\Omega = \{0,1\}^2$, $\mathcal{A} = \mathcal{P}(\Omega)$. We can check that each outcome is equally likely, and so for all events $A \subseteq \Omega$

$$\mathbb{P}(A) = \frac{|A|}{|\Omega|} = \frac{|A|}{4}.$$

Let us consider the events

 $A_1 = [\text{the first coin lands Heads}],$

 $A_2 = [$ the second coin lands Heads],

 $A_3 = [both coins land on the same side],$

so that $A_1 = \{(1,0), (1,1)\}, A_2 = \{(0,1), (1,1)\}$ and $A_3 = \{(0,0), (1,1)\}$ and $A_i \cap A_j = \{(1,1)\}$ for all i, j.

In particular $\mathbb{P}(A_i) = \frac{2}{4} = \frac{1}{2}$ for all $i \leq 3$ and $\mathbb{P}(A_i \cap A_j) = \frac{1}{4} = \mathbb{P}(A_i) \cdot \mathbb{P}(A_j)$ for all $i, j \leq 3$, and hence all pairs of events are independent.

However, $A_1 \cap A_2 \cap A_3 = \{(1,1)\}$ and so $\mathbb{P}(A_1 \cap A_2 \cap A_3) = \frac{1}{4}$, but

$$\prod_{i=1}^{3} \mathbb{P}(A_i) = \left(\frac{1}{2}\right)^3 = \frac{1}{8} \neq \frac{1}{4}.$$

Hence, whilst these three events are pairwise independent, we shouldn't intuitively think of the sequence as being independent. Indeed, if we know that both A_1 and A_2 happens, then it is already determined that A_3 must happen!

1.2 Random Variables

Definition 1.9 (Discrete Random Variable, Distribution). Given a probability space $(\Omega, \mathcal{A}, \mathbb{P})$, a discrete random variable is a function $X : \Omega \to \mathcal{X}$, where $|\mathcal{X}|$ is countable, such that for every $B \subseteq \mathcal{X}$ the set

$$X^{-1}(B) = \{ \omega \in \Omega \colon X(\omega) \in B \} = [X \in B],$$

is a member of the σ -algebra \mathcal{A} .

That is, a discrete random variable is some function of our sample space which takes values in some discrete set \mathcal{X} , such that for any possible subset of \mathcal{X} , the probability that X lies in this subset is well-defined.

The distribution of X is the function $P_X : \mathcal{P}(\mathcal{X}) \to [0,1]$ given by

$$P_X(B) = \mathbb{P}[X \in B].$$

When One can check that $(\mathcal{X}, \mathcal{P}(\mathcal{X}), P_X)$ is a probability space. If $\mathcal{X} \subseteq \mathbb{R}$ we say that X is a discrete *real* random variable.

We can think of random variables as "functions of chance". When our probability space models the outcome of some random experiment, a random variable extracts some aspect of the experiment which can be measured.

A lot of very natural random variables are not discrete, for example when the observable is not a discrete, but a continuous quantity, and there is a corresponding theory of *continuous* random variables. However, this won't be relevant until the very last part of the course, and dealing with them formally is a bit more involved. In particular, unless otherwise stated, every random variable we consider in the course will be discrete, and we will only state the relevant results for discrete random variables. However, in almost all cases, analogous statements can be shown to hold for continuous random variables.

So, a random variable X assigns to each outcome ω in the sample space an element $X(\omega) = x \in \mathcal{X}$. It is important then to keep track of the difference between the random variable X and one of the possible values x that X can take.

Example 1.10. Suppose we toss a sequence of n fair coins, so that we have a sample space $\Omega = \{0,1\}^n$ (and since Ω is finite we can take $\mathcal{A} = \mathcal{P}(\Omega)$). Since the coin is fair, each possible outcome, each sequence $\omega \in \Omega$, is equally likely to occur, and so $\mathbb{P}(\{\omega\}) = 2^{-n}$ for all ω , and $\mathbb{P}(A) = |A|2^{-n}$ for all $A \in \mathcal{A}$.

Now we can look at some random variables, functions from Ω to \mathbb{R} , which are observable quantities from this experiment. For example I could define $X_k(\omega)$ to be the kth element in the sequence ω , the outcome of the kth coin toss.

Then X_k is a discrete random variable, it takes values in $\mathcal{X}_k = \{0, 1\}$, and we can calculate the distribution

$$P_{X_k}(\{0\}) = \mathbb{P}[X_k = 0] = \mathbb{P}[\text{The kth coin toss is tails}] = \frac{1}{2},$$

and similarly $P_{X_k}(\{1\}) = \frac{1}{2}, P_{X_k}(\emptyset) = 0, P_{X_k}(\{0,1\}) = 1.$

Or we could define $S_n(\omega)$ to be the sum of the elements of ω , or in other words the number of heads thrown. Again, S_n is a discrete random variable, taking values in $S_n = \{0, \ldots, n\}$. In

this case for each $k \in \{0, ..., n\}$ we can calculate $P_{S_n}(\{k\}) = \mathbb{P}[S_n = k]$. Indeed, this is just a combinatorial exercise

$$\mathbb{P}[S_n = k] = |[S_n = k]|2^{-n}$$

$$= |\{\omega \colon \omega \text{ has precisely } k \text{ zeroes}\}|2^{-n}$$

$$= \binom{n}{k}2^{-n}.$$

It is then easy to see that for every $A \subseteq \{0, \ldots, n\}$

$$P_{S_n}(A) = \sum_{k \in A} P_{S_n}(\{k\})$$

Definition 1.11 (Discrete density function). Given a discrete random variable X taking values in \mathcal{X} the discrete density function $p_X \colon \mathcal{X} \to [0, 1]$ is defined by

$$p_X(x) = \mathbb{P}[X = x] = P_X(\{x\}).$$

This, $p_X(x) \neq 0$ if and only if $x = x_i$ for some $i \in I$. In particular,

$$1 = \mathbb{P}[X \in \mathcal{X}] = \sum_{x \in \mathcal{X}} p_X(x),$$

and for any $B \subseteq \mathcal{X}$

$$P_X(B) = \sum_{x \in B} p_X(x),$$

and so the discrete density function and the distribution of X determine one another. For this reason, we will often refer to the discrete density function as the distribution of the random variable.

We will often think of the discrete density function as a vector $\mathbf{p} \in \mathbb{R}^{\mathcal{X}}$ with $||\mathbf{p}||_1 = 1$. Conversely, for any such vector \mathbf{p} there is a random variable X whose density function satisfies $p_X = \mathbf{p}$.

During the course we will normally just introduce random variables by specifying their distributions or discrete density function, rather than making reference to any specific probability space.

Example 1.12. (a) Given $q \in [0, 1]$ a Bernoulli random variable Ber(q) takes values in $\{0, 1\}$ and has distribution given by

$$p_{\text{Ber}(q)}(1) = p$$
 and $p_{\text{Ber}(q)}(0) = 1 - p$,

so that $p_{Ber(q)} = (1 - q, q)$. We can think of this random variable as the outcome of a biased coin flip.

(b) Given an event A, the indicator random variable of the event A

$$\mathbb{1}_{A}(\omega) = \begin{cases} 0 & \text{if } \omega \notin A, \\ 1 & \text{if } \omega \in A. \end{cases}$$

In particular, if $\mathbb{P}(A) = q$, then $p_{\mathbb{I}_A} = (1 - q, q)$, and so \mathbb{I}_A has the same distribution as Ber(q).

(c) Given $n \in \mathbb{N}$ and $q \in [0, 1]$ a binomial random variable Bin(n, q) takes values in $\{0, \ldots, n\}$ and has distribution given by

$$p_{\operatorname{Bin}(n,q)}(k) = \binom{n}{k} q^k (1-q)^{n-k}.$$

We can think of this random variable as counting the number of heads in a sequence of n consecutive flips of a random coin.

However, in this way, if I have two random variables X and Y, given just in terms of their distributions, this doesn't necessarily tell us 'the whole story'. Indeed, if X and Y are both observables from the same random experiment, then their values may be related in some way if X is the height of a random person on the street and Y is the weight, then for most outcomes, most people, the values of X and Y will be positively correlated, if X is large then Y is more likely to be large and vice versa.

Definition 1.13 (Joint distribution). If we have two discrete random variables X and Y defined on the same probability space, the *joint discrete density function* (which again we will usually refer to as the joint distribution) is defined as

$$p_{X,Y}(x,y) = \mathbb{P}[X = x, Y = y],$$

and from the joint density function we can reconstruct the marginal density functions of X and Y, which are given by

$$p_X(x) = \sum_{y \in \mathcal{Y}} p_{X,Y}(x,y)$$
 and $p_Y(y) = \sum_{x \in \mathcal{X}} p_{X,Y}(x,y)$.

Note that there can be many different joint density functions $p_{X,Y}$ with the same marginal density functions p_X and p_Y .

More generally, if X_1, \ldots, X_n are all discrete random variables, defined on the same probability space, taking values in sets $\mathcal{X}_1, \ldots, \mathcal{X}_n$, then the 'vector' of random variables (X_1, \ldots, X_n) is also a discrete random variable, which takes values in some subset of the product set $\mathcal{X}_1 \times \ldots, \times \mathcal{X}_n$. In this case, the *joint discrete density function* is defined as

$$p_{X_1,\ldots,X_n}(x_1,\ldots,x_n) = \mathbb{P}[X_1 = x_1, X_2 = x_2,\ldots,X_n = x_n],$$

and the marginal distributions are defined in the obvious way.

Definition 1.14 (Conditional distribution). Given jointly distributed discrete random variables X and Y, and some value $x \in \mathcal{X}$ with $p_X(x) > 0$, the conditional density function (conditional distribution) of Y, given that X = x, is

$$p_{Y|X}(y|x) = \mathbb{P}[Y = y | X = x] = \frac{p_{X,Y}(x,y)}{p_X(x)} = \frac{p_{X,Y}(x,y)}{\sum_{y' \in \mathcal{Y}} p_{X,Y}(x,y')}.$$

Note that, p_X and $p_{Y|X}$ together determine the joint distribution $p_{X,Y}$ and hence also the marginal density function p_Y .

When the random variables that we are dealing with are clear from the context, we will often drop the subscripts in the notation above and simply write expressions likes p(x), p(x,y) or p(y|x).

Example 1.15. Suppose we toss three coins and we let X be the number of heads in the first two coin tosses and Y be the number of heads in the last two coin tosses.

Then we can calculate the joint distribution of X and Y:

$$\begin{array}{c|cccc} (x,y) & 0 & 1 & 2 \\ \hline 0 & 1/8 & 1/8 & 0 \\ 1 & 1/8 & 1/4 & 1/8 \\ 2 & 0 & 1/8 & 1/8 \\ \end{array}$$

The marginal distribution p_X is given by the sum of the rows, which is $p_X = (1/4, 1/2, 1/4)$ and the marginal distribution p_Y is given by the sum of the columns, which is $p_Y = (1/4, 1/2, 1/4)$. Note that, as expected, both are distributed as Bin(3, 1/2).

The conditional distribution $p_{X|Y}$ is then :

$$\begin{array}{c|cccc} (x|y) & 0 & 1 & 2 \\ \hline 0 & 1/2 & 1/4 & 0 \\ 1 & 1/2 & 1/2 & 1/2 \\ 2 & 0 & 1/4 & 1/2 \\ \end{array}$$

Definition 1.16 (Independence). A sequence of discrete random variables X_1, \ldots, X_n are *independent*, if for any sequence of subsets $B_1 \subseteq \mathcal{X}_1, \ldots, B_n \subseteq \mathcal{X}_n$ the events

$$[X_1 \in B_1], \dots, [X_n \in B_n]$$

are independent. In particular

$$\mathbb{P}[X_1 \in B_1, \dots, X_n \in B_n] = \prod_{i=1}^n \mathbb{P}[X_i \in B_i].$$

One can check that it is equivalent to show that the joint density of the sequence is equal to the product of the marginal distributions, that is

$$p_{X_1,\dots,X_n}(x_1,\dots,x_n) = \prod_{i=1}^n p_{X_i}(x_i) \qquad \text{whenever } x_i \in \mathcal{X}_i \text{ for all } i.$$
 (1.1)

An infinite sequence $(X_n)_{n\in\mathbb{N}}$ of discerete random variables is *independent* if the sequence X_1, \ldots, X_n is independent for all n, or equivalently if (1.1) holds for all $n \in \mathbb{N}$.

1.3 Markov's and Chebyshev's inequality

Definition 1.17 (Expectation). The expectation or expected value or mean of a discrete real random variable X is

$$\mathbb{E}(X) := \sum_{x \in \mathcal{X}} x \cdot \mathbb{P}[X = x] = \sum_{x \in \mathcal{X}} x \cdot p_X(x),$$

if the sum converges. Otherwise we informally say that the expectation is infinite.

If $(\Omega, \mathcal{P}(\Omega), \mathbb{P})$ is the underlying probability space, it can sometimes be simpler to use the formula

$$\mathbb{E}(X) = \sum_{\omega \in \Omega} X(\omega) \mathbb{P}(\{\omega\}).$$

When $\mathcal{X} \subseteq \mathbb{R}$, so that X is not a real random variable, it does not make sense to talk about the expectation of X. However, for any function $g \colon \mathcal{X} \to \mathbb{R}$, we have that g(X) is a real random variable (defined as $g(X)(\omega) = g(X(\omega))$ for all ω) whose expectation we can compute as

$$\mathbb{E}(g(X)) = \sum_{g \in \mathcal{X}} g(x) \cdot p_X(x).$$

Lemma 1.18 (Linearity of expectation). Let X and Y be jointly distributed discrete real random variables with finite expectations and let $c \in \mathbb{R}$. Then

- (i) $\mathbb{E}(c) = c$,
- (ii) $\mathbb{E}(X+Y) = \mathbb{E}(X) + \mathbb{E}(Y)$,
- (iii) $\mathbb{E}(c \cdot X) = c \cdot \mathbb{E}(X)$,
- (iv) $x \ge 0$ for all $x \in \mathcal{X} \Rightarrow \mathbb{E}(X) \ge 0$.

Proof.

However, it is not true in general that $\mathbb{E}(X \cdot Y) = \mathbb{E}(X) \cdot \mathbb{E}(Y)$! This does however hold in the special case where X and Y are independent.

Lemma 1.19. Let X and Y be independent discrete real random variables with finite expectations. Then $\mathbb{E}(X \cdot Y) = \mathbb{E}(X) \cdot \mathbb{E}(Y)$.

Proof.

Another important quantity comes from considering how far a random variable deviates from it's expectation.

Definition 1.20 (Variance). Let X be a discrete real random variable with $\mu = \mathbb{E}(X) < \infty$. The *variance* of X is defined as

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

It can easily be shown, using the linearity of expectation, that

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

In general, the variance is also not linear, but again for independent random variables, we do have a nice formula.

Lemma 1.21. Let X and Y be independent discrete real random variables with finite expectations and variances and let $c \in \mathbb{R}$. Then $\mathbb{V}(cX) = c^2 \mathbb{V}(X)$ and $\mathbb{V}(X \pm Y) = \mathbb{V}(X) + \mathbb{V}(Y)$.

$$Proof.$$
 (Exercise)

It turns out that we can get some control over the distribution of a random variable X just by controlling its expectation or variance. In practise, since many of the random variables that arise are 'simple' combinations of 'simple' random variables, it it often possible to calculate, estimate or bound the expectation or variance of these random variables, and in this way obtain information about their distributions.

In particular, given an event A, it is easy to calculate the expectation and variance of the indicator random variable $\mathbb{1}_A$. Indeed

$$\mathbb{E}\left(\mathbb{1}_{A}\right) = 1 \cdot \mathbb{P}\left[\mathbb{1}_{A} = 1\right] + 0 \cdot \mathbb{P}\left[\mathbb{1}_{A} = 0\right] = \mathbb{P}(A),$$

and since $\mathbb{1}_A^2 = \mathbb{1}_A$, we see that

$$\mathbb{V}(\mathbb{1}_A) = \mathbb{E}(\mathbb{1}_A^2) - (\mathbb{E}(\mathbb{1}_A))^2 = \mathbb{E}(\mathbb{1}_A) - (\mathbb{E}(\mathbb{1}_A))^2 = \mathbb{P}(A) - \mathbb{P}(A)^2.$$

Lemma 1.22 (Markov's inequality). Let X be a non-negative discrete real random variable such that $0 < \mathbb{E}(X) < \infty$ and let a > 0. Then

$$\mathbb{P}[X \ge a] \le \frac{\mathbb{E}(X)}{a}.$$

A simple, but powerful consequence of Markov's inequality is Chebyshev's inequality.

Corollary 1.23 (Chebyshev's inequality). Let X be a real random variable such that $\mathbb{E}(X)$, $\mathbb{V}(X) < \infty$ and let a > 0. Then

$$\mathbb{P}[|X - \mathbb{E}(X)| \ge a] \le \frac{\mathbb{V}(X)}{a^2}.$$

Proof.

1.4 Convergence of Random Variables and the Law of Large Numbers

Definition 1.24 (Convergence of random variables). Let $(X_n)_{n\in\mathbb{N}}$ be a sequence of real random variables and X a random variable, all defined on the same probability space.

(i) $X_n \longrightarrow X$ in probability if for every a > 0

$$\lim_{n \to \infty} \mathbb{P}\big[|X_n - X| > a\big] = 0.$$

(ii) $X_n \longrightarrow X$ almost surely if

$$\mathbb{P}[X_n \to X] = 1,$$

that is, if

$$\mathbb{P}(\{\omega \in \Omega : \lim_{n \to \infty} X_n(\omega) = X(\omega)\}) = 1.$$

We will see that convergence almost surely implies convergence in probability, and so the second is a stronger notion of convergence. We note that converse is not true! There exist sequences of random variables which converge in probability but no almost surely.

Example 1.25. Let us consider a sequence of independent random variables $(X_n)_{n\in\mathbb{N}}$ each taking values in $\{0,1\}$ such that

$$\mathbb{P}(X_n = i) = \begin{cases} \frac{1}{n} & \text{if } i = 1\\ 1 - \frac{1}{n} & \text{if } i = 0. \end{cases}$$

For all a > 0, it is clear that

$$\mathbb{P}(|X_n - 0| \ge a) \le \mathbb{P}(X_n = 1) = \frac{1}{n}$$

and hence, X_n tend to 0 in probability.

On the other hand, $X_n \to 0$ if and only there is some N such that $X_n = 0$ for all $n \ge N$. However for any fixed N, since the X_n are independent,

$$\mathbb{P}[\forall n \ge N : X_n = 0] = \lim_{M \to \infty} \mathbb{P}[\forall N \le n \le M : X_n = 0]$$

$$\le \lim_{M \to \infty} \prod_{n=N}^{M} \left(1 - \frac{1}{n}\right)$$

$$\le \lim_{M \to \infty} \exp\left(-\sum_{n=N}^{M} \frac{1}{n}\right)$$

$$= 0,$$

where we used that $1-x \leq e^{-x}$, which holds for all x, and also that $\sum_{n=N}^{M} \frac{1}{n} \approx \ln M - \ln N$.

Hence,

$$\mathbb{P}[X_n \to 0] \le \sum_{N=1}^{\infty} \mathbb{P}[\forall n \ge N : X_n = 0] = 0.$$

Whilst convergence in probability is not enough to guarantee convergence almost surely, it does guarantee the existence of an almost surely convergent subsequence.

Theorem 1.26. Let $(X_n)_{n\in\mathbb{N}}$ and X be as above. If $X_n \to X$ in probability, then there is a subsequence $(n_k)_{k\in\mathbb{N}}$ such that $X_n \to X$ almost surely.

Theorem 1.27 (Weak law of large numbers). Let $(X_n)_{n\in\mathbb{N}}$ be a sequence of independent random variables with finite mean $\mathbb{E}(X_n) = \mu < \infty$ and finite variance $\mathbb{V}(X_n) = \sigma^2 < \infty$ (the same for all n). Then

$$\overline{X}_n = \frac{1}{n} (X_1 + X_2 + \ldots + X_n) \to \mu \text{ in probability.}$$

Proof.

As we saw, convergence in probability is weaker than convergence almost surely, and at times we will need the stronger statement that the *sample mean* converges to the mean almost surely.

Theorem 1.28 (Strong law of large numbers). Let $(X_n)_{n\in\mathbb{N}}$ be a sequence of independent, identically distributed (i.i.d) random variables (that is, each X_n has the same distribution) with finite mean $\mathbb{E}(X_n) = \mu < \infty$. Then

$$\overline{X}_n = \frac{1}{n}(X_1 + X_2 + \ldots + X_n) \to \mu \text{ almost surely.}$$

The proof of this theorem is a bit beyond the focus of the course, however we will at time want to relate the two notions of convergence, and will prove a few short lemmas on this topic.

One useful thing for a notion of convergence is that limits should be unique, although here we only have uniqueness up to a set of measure 0.

Lemma 1.29. Let $X, (X_n)_{n \in \mathbb{N}}$ be jointly distributed real random variables. If $X_n \to X$ and $X_n \to X'$ in probability, then $\mathbb{P}[X = X'] = 1$.

Finally, let us prove that convergence almost surely implies convergence in probability.

Theorem 1.30. Let $X, (X_n)_{n \in \mathbb{N}}$ be jointly distributed real random variables. If $X_n \to X$ almost surely, then $X_n \to X$ in probability.

Moreover, if we write $U_k = \sup\{|X_n - X| : n \ge k\}$, then $X_n \to X$ almost surely if and only if $U_k \to 0$ in probability.

2 Discrete Entropy

2.1 Hartley's formula and Shannon's formula

Information theory deals with the mathematical problems that arise in the *storage*, *transformation* and *transmission* of information.

We would like to have some sort of theory that measures the *informational content* of some data, which in some way should not depend on the particular form the data takes

Example 2.1. Suppose I have written down secretly a number from 0 to 31 and you wish to identify the number asking only yes/no questions.

It is, intuitively, clear that the 'best' question to start with is "Is your number at most 15?", since either answer will reduce the number of possibilities by $\frac{1}{2}$. In a similar fashion each question can reduce the number of possibilities by $\frac{1}{2}$, and so after 5 questions you can also identify the number.

Considering a question as a unit of information, we might say that this hidden number then contains 5 of these units, which we will call *bits*, of information.

If we think of encoding the numbers from 0 to 31 in binary, each number corresponds to a sequence in $\{0,1\}^5$, and the questions that we ask correspond to asking about the value of the kth digit in the sequence.

Hartley made this idea formal in 1928 when he defined the notion of the *uncertainty* of a uniform random sample.

Definition 2.2 (Hartley's formula). Suppose some element is chosen from a collection U_N of N different elements, with each being equally likely. The *uncertainty* of this random element (which one can think of the *informational cost* to identify the element) is given by

$$H(U_N) = \log_2 N.$$

This can be justified in terms of the follow (heuristic) axiomatic requirements

- (A) $H(U_2) = 1$,
- (B) $H(U_{N+1}) \ge H(U_N)$,
- (C) $H(U_{N \cdot M}) = H(U_N) + H(U_M)$.

The first two are relatively intuitive - the amount of information needed to identify one of two elements is a single question or bit (alternatively, this is just some arbitrary choice to normalise this measure with respect to the units we've chosen). Furthermore, clearly there is more information needed to identify an element from a larger set.

For the third we can think of grouping our elements into N disjoint groups consisting of M elements

$$U_{N \cdot M} = U_M^{(1)} \cup \ldots \cup U_M^{(N)}.$$

In order to identify one element from $U_{N\cdot M}$ we could identify first the group $U_M^{(i)}$ that the element lies in, and so identify a uniformly chosen unknown group from a collection of N many groups, and then identify the unknown element of $U_M^{(i)}$, which is equally likely to be any of these elements. Hence, the cost to identify this element is at most $H(U_N) + H(U_M)$.

However, conversely, suppose we choose our random element by first choosing a random group, and then choosing a random element of our group. If we can identify the random element, we can identify both of these random choices, and so the cost to identify this element must be at least $H(U_N) + H(U_M)$.

In fact, Rényi showed that these three properties uniquely determine Hartley's formula.

Lemma 2.3. The function $H(U_N) = \log_2 N$ is the unique function satisfying properties (A)–(C).

Suppose now that our elements are not equally likely to be chosen, but that the kth element is instead chosen with some probability p_k . Can we justify, using the previous heuristic, what the informational cost of identifying the chosen element is?

Well, in some sense the 'cost' to identify the hidden element does not change, we still might need to identify any one of N elements. However, if one of the p_k s were much larger than all the others, so in almost every case the kth element is chosen, it would be much more sensible to start by asking "is the hidden element the kth element"? In the worst case we would have to ask more questions, but on average we'd identify the element with many fewer questions!

So, it makes sense instead to consider the *expected uncertainty*, or the expected informational cost to identify the unknown element. The following is a *heuristic* argument for how we should define this quantity.

Let us assume that the probabilities p_k are all rational, otherwise we can take some rational approximations and argue "in the limit". Instead of an element from U_N where the kth element is chosen with probability p_k , I could choose an element from a larger set

$$U_M = U_{M_1} \cup \ldots \cup U_{M_N}$$
.

where U_{M_i} contains p_iM elements, for some large M such that all these numbers are integers. There is then a clear equivalence between identifying the group U_{M_i} in which this element lies, and of identifying the element in the original problem.

By a similar argument as before, the expected informational cost of identify the random element of U_M , which should be $\log_2 M$ by Hartley's formula, should be given by the expected cost to identify the correct group U_{M_i} , which is the quantity we are interested in, which we denote by H_1 , plus the expected cost to identify the correct element of this group, which we denote by H_2 . Now the element lies in M_i with probability p_i , and if the element lies in U_{M_i} then the informational cost to identify it is $\log_2 M_i$ by Hartley's formula. Hence, the expected cost is

$$H_2 = \sum_i p_i \log_2 M_i = \sum_i p_i \log_2 p_i M = \sum_i p_i \log_2 p_i + \sum_i p_i \log_2 M = \log_2 M + \sum_i p_i \log_2 p_i.$$

Since $H_1 + H_2 = \log_2 M$, it follows that

$$H_1 = -\sum_i p_i \log_2 p_i$$

which is known as *Shannon's formula*. In the following section we will make this informal discussion mathematically rigorous.

2.2 Entropy

The idea of entropy originated in statistical mechanics. Roughly, given a thermodynamic system, such as a gas or a liquid, if we know some global properties of the system, e.g temperature, volume, energy, there are many different *microstates*, that is configurations of the individual particles within the system, which are consistent with these measurements.

As an example imagine flipping 1000 coins. We have a global measurement, the number of heads, but for each particular value for this, there are many different configurations of the specific states each of the 1000 coins landed in which achieve this number of heads.

Under a broad assumption that each of these microstates are equally likely, Boltzmann defined entropy of the system to be $k_B \log(\# \text{ of microstates})$ where k_B is some constant. Gibbs generalized this to microstates with unequal probabilities and gave the formula

$$S = -k_B \sum p_i \log(p_i),$$

where S is the *entropy*, p_i is the probability of the ith microstates, and the sum ranges over all the microstates. This reduces to Boltzmann's formula when the p_i are equal.

The second law of thermodynamics states that the entropy of an isolated system never decreases, and so such systems naturally 'tend' towards the state with maximum entropy, known as thermodynamic equilibrium. This was an attempt to formalise the idea that there is a natural 'direction' to natural processes, for example to explain why heat is transferred from hotter objects to cooler objects, rather than the other way round (which would not by itself contradict the conservation of energy in a process).

In the early 20th Century Hartley and Shannon found that similar equations arise naturally in the study of information theory, and at the suggestion of Von Neumann, Shannon also named it *entropy*.

"You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, nobody knows what entropy really is, so in a debate you will always have the advantage." - John von Neumann

Definition 2.4 (Entropy). Let X be a discrete random variable taking values in a *finite* set \mathcal{X} , and let

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

be the distribution of X. The *entropy* of X, which we will also call the entropy of the distribution p, is defined as

$$H(X) = H(p) = -\sum_{x \in \mathcal{X}} p(x) \log_2 p(x).$$
 (2.1)

If we enumerate $\mathcal{X} = \{x_1, \dots, x_n\}$ and set $p_k = p(x_k)$ then we might also use the following notation, that $p = (p_1, \dots, p_n)$ and

$$H(p) = H(p_1, \dots, p_n) = -\sum_{i=1}^{n} p_i \log_2 p_i.$$

Remark 2.5. For ease of notation, it will often be convenient to define

$$0 \log 0 := 0$$
,

whenever it appears in such a sum.

Example 2.6. Suppose the X is uniformly distributed on a set $\mathcal{X} = \{x_1, \dots, x_n\}$ of size n, so that $p_k = p(x_k) = \frac{1}{n}$ for each k.

In this case

$$H(X) = H(p) = H\left(\frac{1}{n}, \dots, \frac{1}{n}\right) = -\sum_{i=1}^{n} p_i \log_2 p_i = -\sum_{i=1}^{n} \frac{1}{n} \log_2 \frac{1}{n} = -\log_2 \frac{1}{n} = \log_2 n.$$

Another way to think of entropy is as a measure of the expected amount of information we gain from learning the value of X. Indeed, suppose we have some function g(x) which measure the information we gain from learning that X takes the value x. We clearly gain more information by knowing that a low probability event happens, so this function g(x) should a decreasing function of p(x). In fact, as we will see later, there are other natural assumptions to make about g(x) which, similar to Hartley's formula, imply that the only 'reasonable' choice for this function g is to take $g(x) = -\log_2 p(x)$.

In this way, we can view (2.1) as an expectation - we have the weighted sum over some probability distribution of a quantity, where this quantity is the function $g: \mathcal{X} \to \mathbb{R}$ given by $g(x) = -\log_2 p(x)$ (note that this is a deterministic function, even though it encodes the probability distribution of the random variable X), then (2.1) can be rewritten as

$$H(X) = \sum_{x \in \mathcal{X}} p(x)g(x) = \mathbb{E}(g(X)) = \mathbb{E}(-\log_2 p(X)),$$

and it represents the expected amount of information we gain from learning the value of X.

Let us collect a few basic facts about the entropy function, some of which are obvious and some of which we will prove formally later.

Remark 2.7. (1) $H(X) \ge 0$, with equality if and only if X is constant.

(2) H(X) doesn't depend on the values of the random variable X, just the distribution of probabilities between these values. In other words, if we relabel the outcomes, that is, if we take some bijection $f: \mathcal{X} \to \mathcal{X}'$ and let X' = f(X), then H(X') = H(X).

In other words if (p_1, \ldots, p_n) and (p'_1, \ldots, p'_n) are the same up to some permutation, then

$$H(p_1,\ldots,p_n)=H(p_1',\ldots,p_n').$$

- (3) The function $p_1 \mapsto H(p_1, 1 p_1)$ is continuous for $p_1 \in [0, 1]$. Furthermore this function is symmetric, takes values 0 at $p_1 = 0, 1$ and is maximised at $p_1 = \frac{1}{2}$ where it takes the value 1.
- (4) More generally, for fixed n,

$$\max\{H(p): p = (p_1, \dots, p_n)\} = H\left(\frac{1}{n}, \dots, \frac{1}{n}\right) = \log_2 n,$$

which the last equality is equivalent to Hartley's formula.

In other words, the uniform distribution has the maximum expected uncertainty, or the maximum expected information.

A discrete random variable X determines another jointly distributed random variable Y if there is an function $f: \mathcal{X} \to \mathcal{Y}$ such that Y = f(X)

Lemma 2.8. Let X and Y be jointly distributed discrete random variables taking finitely many values such that X determines Y. Then $H(Y) \leq H(X)$.

Proof.

In particular, if X determines Y and Y determines X, then H(X) = H(Y).

Given jointly distributed discrete random variable X and Y, taking values in finite sets \mathcal{X} and \mathcal{Y} , as mentioned the random vector Z = (X, Y) is again a discrete random variable and we can define the *joint entropy* of X and Y as the entropy of Z. That is, since for any $z = (x, y) \in \mathcal{X} \times \mathcal{Y}$

$$\mathbb{P}[Z = z] = \mathbb{P}[X = x, Y = y] = p_{X,Y}(x, y),$$

we can calculate

$$H(X,Y) := H(Z) = -\sum_{(x,y)\in\mathcal{X}\times\mathcal{Y}} p(x,y)\log_2 p(x,y)$$

Similarly, given $x \in \mathcal{X}$ we can consider the conditional distribution of Y, given that X = x, which we recall is

$$p_{Y|X}(y|x) = \frac{p_{X,Y}(x,y)}{p_X(x)}$$

assuming that $p_X(x) > 0$. We can thus write the entropy of this conditional distribution as

$$H(Y \mid X = x) := -\sum_{y \in \mathcal{Y}} p(y|x) \log_2 p(y|x) = -\sum_{y \in \mathcal{Y}} \frac{p(x,y)}{p(x)} \log_2 \frac{p(x,y)}{p(x)}.$$

Example 2.9. Suppose X and Y are both distributed on $\{1, 2, 3\}$ and have joint distribution given by

so that $p_X = (1/4, 1/2, 1/4)$ and $p_Y = (3/8, 1/2, 1/8)$. In this case we can calculate

$$H(X) = \frac{1}{4}\log_2 4 + \frac{1}{2}\log_2 2 + \frac{1}{4}\log_2 4 = \frac{3}{2}.$$

$$H(Y) = \frac{3}{8}\log_2 \frac{8}{3} + \frac{1}{2}\log 2 + \frac{1}{8}\log_2 8 = 2 - \frac{3}{8}\log_2 3.$$

$$H(X,Y) = 4 \cdot \frac{1}{8}\log_2 8 + 2 \cdot \frac{1}{4}\log_2 4 = \frac{5}{2}.$$

$$H(Y|X=1) = \frac{1}{2}\log_2 2 + \frac{1}{2}\log_2 2 + 0\log_2 0 = 1.$$

Definition 2.10 (Conditional entropy). The conditional entropy of a discrete random variable Y given a discrete random variable X, both taking finitely many values, is the average value of H(Y|X=x) with respect to the possible values of X

$$\begin{split} H(Y \mid X) &= \sum_{x \in \mathcal{X}} p_X(x) H(Y \mid X = x) \\ &= -\sum_{x \in \mathcal{X}} p(x) \sum_{y \in \mathcal{Y}} p(y \mid x) \log_2 p(y \mid x) \\ &= -\sum_{x \in \mathcal{X}, y \in \mathcal{Y}} p(x, y) \log_2 \frac{p(x, y)}{p(x)} \end{split}$$

So in the previous example we can calculate

$$H(Y \mid X) = \frac{1}{8}\log_2 2 + \frac{1}{8}\log_2 2 + \frac{1}{4}\log_2 2 + \frac{1}{8}\log_2 4 + \frac{1}{8}\log_2 4 + \frac{1}{4}\log_2 1 = 1.$$

We can think of H(Y|X) as the expected amount of information contained in the random variable Y if we already know the value of X. In particular, if H(X,Y) represents the expected total information in both X and Y, then since discovering the value of X and Y is the same as first discovering the value of X, and then discovering the value of Y, heuristically it should be the case that $H(X,Y) = H(X) + H(Y \mid X)$, and indeed in the example above

$$\frac{5}{2} = H(X,Y) = H(X) + H(Y \mid X) = \frac{3}{2} + 1.$$

It should heuristically be true that conditioning can only decreases the entropy, and indeed this is the case. Later we will show a far more general statement.

Lemma 2.11. For any two jointly distributed discrete random variables X and Y taking finitely many values $H(Y) \ge H(Y \mid X)$.

Theorem 2.12 (Chain rule). For any two jointly distributed discrete random variables X and Y taking finitely many values

$$H(X,Y) = H(X) + H(Y \mid X) = H(Y) + H(X \mid Y).$$

More generally, using Theorem 2.12 it can be shown by induction that the following holds.

Theorem 2.13 (Chain rule). For any sequence of discrete random variables X_1, X_2, \ldots, X_n taking finitely many values

$$H(X_1, \dots, X_n) = \sum_{k=1}^n H(X_k \mid X_{k_1}, \dots, X_1).$$

In fact, the chain rule holds in a slightly more general form, for conditional entropies, which can be proved in much the same way.

Lemma 2.14 (Conditional Chain Rule). For any three jointly distributed random variables X, Y and Z taking finitely many values

$$H(X,Y \mid X) = H(X \mid Z) + H(Y \mid X,Z)$$

Example 2.15. Suppose Z takes values in $\{1, \ldots, n\}$ and has probability distribution (p_1, \ldots, p_n) . Let us define two new random variables : $X = Z + \mathbb{1}_{[Z=1]}$ and $Y = \mathbb{1}_{[Z=1]}$. In particular, $p_X = (p_1 + p_2, p_3, \ldots, p_n)$ and $p_Y = (1 - p_1, p_1)$.

Now, since Z = X - Y, the pair (X, Y) determine Z, and clearly X and Y are determined by Z, and so

$$H(X,Y) = H(Z) = H(p_1, \dots, p_n), \qquad H(X) = H(p_1 + p_2, p_3, \dots, p_n), \qquad H(Y) = H(1 - p_1, p_1).$$

Now, if $X = x \ge 3$, then Y = 0 and so $H(Y \mid X = x) = 0$. If X = 2, which happens with probability $p_X(2) = p_1 + p_2$, then Z is either 1 or 2, with probabilities p_1 and p_2 , and so Y is either 1 or 0 with the same probabilities, that is,

$$p_{Y|X}(1 \mid 2) = \frac{p_1}{p_1 + p_2}$$
 and $p_{Y|X}(0 \mid 2) = \frac{p_2}{p_1 + p_2}$.

Hence we can calculate.

$$H(Y|X) = \sum_{i=2}^{n} p_X(i)H(X|Y=i) = (p_1 + p_2)H\left(\frac{p_1}{p_1 + p_2}, \frac{p_2}{p_1 + p_2}\right),$$

and the chain rule H(X,Y) = H(X) + H(Y|X) in this case implies

$$H(p_1, \dots, p_n) = H(p_1 + p_2, p_3, \dots, p_n) + (p_1 + p_2)H\left(\frac{p_1}{p_1 + p_2}, \frac{p_2}{p_1 + p_2}\right),$$
 (2.2)

which holds for any probability distribution (p_1, \ldots, p_n) (if we interpret the second term as 0 when $p_1 + p_2 = 0$).

For Hartley's formula, there was a heuristic collections of axioms that determine what we should expect from a measure of uncertainty that in fact determined Hartley's formula as the unique way to capture these axioms mathematically. It turns out that there is a similar axiomatic basis for Shannon's formula, in terms of some natural axioms that any measure of expected uncertainty should satisfy.

Theorem 2.16. Let $\mathcal{B} = \{(p_1, \dots, p_n) : n \in \mathbb{N}, p_k \geq 0 \text{ for all } k \leq n, p_1 + \dots + p_n = 1\}$ be the set of all finite probability distributions. Suppose that we have some function $H : \mathcal{B} \to \mathbb{R}$ which satisfies the following axioms:

(I) H is transposition invariant: if $1 \le i < j \le n$ then

$$H(p_1,\ldots,p_i,\ldots,p_j,\ldots,p_n)=H(p_1,\ldots,p_j,\ldots,p_i,\ldots,p_n).$$

(II) Normalisation : H(1/2, 1/2) = 1.

- (III) Continuity: The function $p_1 \to H(p_1, 1 p_1)$ is continuous
- (IV) Equation (2.2) holds for all $p \in \mathcal{B}$ with $n \geq 2$.

Then

$$H(p_1, \dots, p_n) = -\sum_{k=1}^{n} p_k \log_2 p_k.$$

Proof. For mathematical students only.

In order to do this we will need the following variant of Lemma 2.3

Proposition 2.17. The function $H(U_N) = \log_2 N$ is the unique function satisfying properties (A),(C) of Lemma 2.3 and the following variant of property (B):

$$(B^*)$$
 $\lim_{N\to\infty} H(U_{N+1}) - H(U_N) = 0.$

2.3 Kullback-Leibler Divergence and Mutual Information

Definition 2.18. Let p and q be probability distributions on the same finite set \mathcal{X} . The relative entropy or Kullback-Leibler Divergence of p with respect to q is

$$D(p \parallel q) = \sum_{x \in \mathcal{X}} p(x) \log_2 \frac{p(x)}{q(x)} = \mathbb{E}\left(\log_2 \frac{p(X)}{q(X)}\right),$$

where X is some random variable with distribution p.

Remark 2.19. Again here we need some convenition to deal with the cases where the quantity $p(x) \log_2 \frac{p(x)}{g(x)}$ is not defined. If p(x) = 0 then we define

$$0\log_2\frac{0}{q(x)} = 0 \text{ for any } q(x) \ge 0,$$

and if $p(x) \neq 0, q(x) = 0$ we define

$$p(x)\log_2\frac{p(x)}{q(x)} = \infty \text{ for any } p(x) > 0.$$

In particular, if there is any $x \in \mathcal{X}$ such that p(x) > 0 and q(x) = 0, then $D(p \parallel q) = \infty$.

This quantity is also sometimes called the *Kullbakc-Liebler distance*, however one should be careful that this function does not behave as we would expect a distance function to behave in particular, it is not always *symmetric* and it does not satisfy the *triangle inequality*. In fact, it is not even obvious that this quantity is *non-negative*, although we will later show that this is the case.

Example 2.20. Let $\mathcal{X} = \{0, 1\}$, $p = (p_1, p_2)$ and $q = (q_1, q_2)$, with $p_1 + p_2 = q_1 + q_2 = 1$. Then

$$D(p \parallel q) = p_1 \log_2 \frac{p_1}{q_1} + p_2 \log_2 \frac{p_2}{q_2}.$$

For example, for p = (1/2, 1/2) and q = (1/4, 3/4) we can compute

$$D(p \parallel q) = \frac{1}{2}\log_2 2 + \frac{1}{2}\log_2 \frac{2}{3} = 1 - \frac{1}{2}, \log_2 3$$

and

$$D(q \parallel p) = \frac{1}{4} \log_2 \frac{1}{2} + \frac{3}{4} \log_2 \frac{3}{2} = \frac{3}{4} \log_2 3 - 1.$$

Definition 2.21. Let X and Y be two jointly distributed discrete random variables taking values in finite sets X and Y. The *mutual information* of X and Y is defined as

$$I(X ; Y) = D(p_{X,Y} \parallel p_X \otimes p_Y)$$

where $p_X \otimes p_Y(x, y) = p_X(x)p_Y(y) = \mathbb{P}[X = x]\mathbb{P}[Y = y]$.

In other words, if we think of the Kullback-Liebler divergence as a distance between distributions, the mutual information of X and Y measures how far their joint distribution is from the joint distribution of independent copies of X and Y, and so we can think of the mutual information as a measure of dependence between random variables.

Plugging Definition 2.18 into Definition 2.21 we get the following explicit formula for the mutual information

$$I(X ; Y) = \sum_{x \in \mathcal{X}, y \in \mathcal{Y}} p_{X,Y}(x, y) \log_2 \frac{p_{X,Y}(x, y)}{p_X(x)p_y(y)}.$$

In particular, if X and Y are independent, then the term inside the log is always one, and so I(X;Y)=0. The larger the mutual information, the further in some sense X and Y are from being independent.

Lemma 2.22. Let X and Y be two jointly distributed discrete random variables taking finitely many values. Then

$$I(X ; Y) = H(X) + H(Y) - H(X, Y) = H(Y) - H(Y | X) = H(X) - H(X|Y) = I(Y ; X).$$

In particular, I(X ; X) = H(X).

Example 2.23 (Secure encryption). Suppose we have a set of *messages* \mathcal{M} that we wish to encrypt and a set of *keys* \mathcal{K} that we can use to encrypt these messages. That is, every pair $m \in \mathcal{M}$ and $k \in \mathcal{K}$ of a message and a key can be used to generate some encrypted text $c \in \mathcal{C}$, or *ciphertext*.

Normally we have some (pseudo)-random method of generating keys $k \in \mathcal{K}$, which determines some random variable K on \mathcal{K} , and there is some underlying distribution M on the messages \mathcal{M} . An encryption scheme for M is a pair of random variables K and C, representing the key

and the encrypted text such that K and C together determine M. This last condition is just saying that we can decrypt the message given the key and the ciphertext.

A classical encryption scheme would consist of some deterministic function $e: \mathcal{M} \times \mathcal{K} \to \mathcal{C}$ such that for each $k \in \mathcal{K}$ the function $e(\cdot, k) \to \mathcal{C}$ is injective, and then taking C = e(M, K).

What does it mean for an encryption scheme to be secure? We want that someone who doesn't know the key cannot infer any information about the message from the ciphertext. To put this in terms of entropy, we want that there is no mutual information between C and M.

Definition 2.24 (Perfectly secure encryption scheme). An encryption scheme K, C for M is perfectly secure if I(M; C) = 0.

There is an obvious example of a perfectly secure encryption scheme which is known as a one-time pad. We assume (essentially wlog) that $\mathcal{M} = \{0,1\}^n$ and that we have a uniformly distributed set of keys on the same set $\mathcal{K} = \{0,1\}^n$. We take then a classical encryption scheme where e(m,k) = m+k where addition is taken in \mathbb{Z}_2^n .

Theorem 2.25. The one time pad is perfectly secure.

Proof. (Exercise)
$$\Box$$

However this clearly isn't a very efficient method of encryption, since it requires the two parties to share a key which is as large as the message itself. However Shannon showed that this is essentially necessary for a secure encryption scheme, in the sense that, in an perfectly secure encryption scheme the set of keys must contain as least as much information as the messages.

Theorem 2.26. If K, C is a perfectly secure encryption scheme for M then $H(K) \geq H(M)$.

As a more concrete example, if both M and K are uniformly distributed then Theorem 2.26 says that

$$\log_2 |\mathcal{K}| = H(K) \ge H(M) = \log_2 |\mathcal{M}|.$$

That is, $|\mathcal{K}| \geq |\mathcal{M}|$ and so we need at least as many different keys as we have messages.

As with entropy, we can extend the concept of mutual information to conditional spaces.

Definition 2.27 (Conditional mutual information). Let X, Y, Z be three jointly distributed discrete random variables taking finitely many values. The *conditional mutual information* of X and Y given Z is defined as

$$I(X \; ; \; Y \mid Z) = \sum_{z \in \mathcal{Z}} p_Z(z) I(X \; ; \; Y \mid Z = z)$$

Let us briefly clarify the meaning of the above definition. Suppose $p_{X,Y,Z}(x,y,z)$ is the joint distribution of the three random variables. We can define the joint distribution of X and Y conditioned on Z as

$$p_{X,Y|Z}(x,y|z) = \frac{p_{X,Y,Z}(x,y,z)}{p_Z(z)}.$$

Then

$$I(X \; ; \; Y \; | \; Z = z) = \sum_{x \in \mathcal{X}, y \in \mathcal{Y}} p_{X,Y|Z}(x,y|z) \log_2 \frac{p_{X,Y|Z}(x,y,z)}{p_{X|Z}(x|z)p_{Y|Z}(y|z)},$$

so that

$$I(X \; ; \; Y \mid Z) = \sum_{x \in \mathcal{X}, y \in \mathcal{Y}, z \in \mathcal{Z}} p_{X,Y,Z}(x,y,z) \log_2 \frac{p_{X,Y\mid Z}(x,y,z)}{p_{X\mid Z}(x\mid z) p_{Y\mid Z}(y\mid z)}.$$

Lemma 2.28. Let X, Y, Z be three jointly distributed discrete random variables taking finitely many values. Then

$$I(X ; Y | Z) = H(X | Z) + H(Y | Z) - H(X, Y | Z)$$

= $H(X | Z) - H(X | Y, Z) = H(Y | Z) - H(Y | X, Z).$

Proof.

As a consequence it is easy to deduce the following variant of the chain rule for mutual information.

Theorem 2.29 (Chain rule for mutual information). Let $X_1, \ldots X_n$ and Y be jointly distributed discrete random variables taking finitely many values. Then

$$I(X_1, \dots, X_n ; Y) = \sum_{k=1}^n I(X_k ; Y \mid X_{k-1}, \dots, X_1).$$

Proof. Exercise - Use Theorem 2.13 and induct on n.

So far we have only proved various equalities about entropy, just by rearranging the formulas. At various points it will be useful to be able to *estimate*, that is, bound from above or below, entropies and related quantities, and a particularly useful tool for this come from *Jensen's inequality*. To state this inequality we will require a little background from analysis.

Definition 2.30 (Convex and concave). Let $I \subseteq \mathbb{R}$ be an open interval. A function $f: I \to \mathbb{R}$ is *convex* if for every $x, y \in I$ and $\lambda \in (0, 1)$

$$f(\lambda x + (1 - \lambda)y) \le \lambda f(x) + (1 - \lambda)f(y) \tag{2.3}$$

We can think of this as taking a weighted average $z = \lambda x + (1 - \lambda)y$ of the points x and y, which lies somewhere between x and y. f is convex if the value of the function at this point is smaller than the same weighted average of f(x) and g(y).

Geometrically, this asserts that the line between f(x) and f(y) lies above the graph of the function f between x and y.

We say f is strictly convex if (2.3) is strict for any $x \neq y$. Similarly we say f is concave or strictly concave if the inequality in (2.3) is reversed.

Theorem 2.31 (Jensen's inequality). Let $f: I \to \mathbb{R}$ be a convex function on an open interval I and let X be a real random variable taking values in I. If $\mathbb{E}(X)$ and $\mathbb{E}(f(X))$ exist, then

$$\mathbb{E}(f(X)) \ge f(\mathbb{E}(X)).$$

Furthermore, if f is strictly convex then the inequality is strict unless X is almost surely constant.

Proof.

Probably the most important application of Jensen's inequality in information theory is the following:

Theorem 2.32 (Information Inequality). Let p and q be distributions on a finite set \mathcal{X} . Then $D(p \parallel q) \geq 0$ with equality if and only if p = q.

Proof.

Let us note then some immediate, and incredibly useful, corrolaries of this Theorem.

Corollary 2.33. Let X, Y, Z and X_1, \ldots, X_n be jointly distributed discrete random variables taking values in a finite set.

- 1. $I(X; Y) \ge 0$, with equality if and only if X and Y are independent,
- 2. $H(X \mid Y) \leq H(X)$, with equality if and only if X and Y are independent,
- 3. $I(X ; Y | Z) \ge 0$, with equality if and only if X and Y are independent conditional upon Z.
- 4. $H(X_1, ..., X_n) \leq H(X_1) + ... + H(X_n)$ with equality if and only if the X_k are mutually independent.

Proof.

Another important consequence of Theorem 2.32 is the following.

Lemma 2.34 (Log sum inequality). Let $a_1, b_1, \ldots, a_n, b_n \ge 0$ and let $a = \sum_{k=1}^n a_k$ and $b = \sum_{k=1}^n b_k$. Then

$$\sum_{k=1}^{n} a_k \log_2 \frac{a_k}{b_k} \ge a \log_2 \frac{a}{b}.$$

Proof.

As a corollary we get a weird looking statement asserting a sort of multivariable concavity of the Kullback-Liebler divergence.

Corollary 2.35. Let $p^{(1)}, p^{(2)}, q^{(1)}$ and $q^{(2)}$ be probability distributions on the same finite set \mathcal{X} and let $\lambda \in (0,1)$.

$$D(\lambda \cdot p^{(1)} + (1 - \lambda) \cdot p^{(2)} \parallel \lambda \cdot q^{(1)} + (1 - \lambda) \cdot q^{(2)}) \le \lambda D(p^{(1)} \parallel q^{(1)}) + (1 - \lambda) D(p^{(2)} \parallel q^{(2)})$$

As a simple corollary we find that the entropy function is also concave.

Corollary 2.36. Let p,q be probability distributions on a finite set \mathcal{X} and let $\lambda \in (0,1)$. Then

$$H(\lambda p + (1 - \lambda)q) \ge \lambda H(p) + (1 - \lambda)H(q).$$

Remark 2.37. From the inequality

$$D(p \parallel u) = \log_2 |\mathcal{X}| - H(p) \ge 0,$$

we can conclude from Theorem 2.32 that $H(p) \leq \log_2 |\mathcal{X}|$ with equality if and only if p is the uniform distribution.

Suppose we are given the conditional distribution of a random variable Y with respect to a random variable X, but no the distribution of X or Y. That is, we have the function

$$p_{Y|X}(y,x) = p(y|x),$$

where for each x we can think of the function $p(\cdot|x)$ as a distribution on \mathcal{Y} .

Then, any probability distribution p_X on \mathcal{X} gives rise to a joint distribution $p_{X,Y}$ via

$$p_{X,Y}(x,y) = p_X(x)p_{Y|X}(y,x),$$

from which we can also derive the distribution $p(y) = \mathbb{E}_{p_X} p(y|X) = \sum_{x \in \mathcal{X}} p(x) p(y|x)$.

In other words, if we fix ahead of time the conditional distribution, then the joint distribution (X, Y), and so in particular the distribution of Y, is determined by the distribution of X. We can think of this as the evolution of a random process in time, where X and Y represent the outcome at two specific times. In order to calculate the probability that we saw the outcome (x, y) we need to know the probability that at the first time we had the outcome x, and then the outcome that the process developed from x to become y at the second time.

We can think of this in terms of a transition matrix P, whose columns are indexed by \mathcal{X} and rows by \mathcal{Y} and whose entry $P_{xy} = p(y|x)$ is the probability that we observe y after observing x, the probability that our process evolves from x to become y. The rows of this matrix $p(\cdot|x)$ correspond to the conditional distribution of Y given that X = x, and so given a distribution p_X on \mathcal{X} we can compute the marginal distribution on \mathcal{Y} as $p_Y = p_X P$ and the joint distribution (as an $\mathcal{X} \times \mathcal{Y}$ matrix) can be seen to be the product $\operatorname{diag}(p_X) \cdot P$ of a diagonal matrix with entries $p_X(x)$ together with P, so that that xth row is $p_X(x)p(\cdot|x) = p_{X,Y}(x,\cdot)$.

Theorem 2.38. Suppose $p_{Y|X}$ is the conditional distribution of some discrete random variable Y taking values in a finite set \mathcal{Y} with respect to some unknown discrete random variable X taking values in a finite set \mathcal{X} . Then the function $f(p_X) = I(X; Y) = D(p_{X,Y} \parallel p_X \otimes p_Y)$ is concave, that is, for any two distributions p and q on \mathcal{X} and $\lambda \in (0,1)$

$$f(\lambda \cdot p + (1 - \lambda) \cdot q) \ge \lambda f(p) + (1 - p)f(q).$$

Conversely, if p_X is known, then the function $F(p_{Y|X}) = I(X; Y)$ is convex.

Definition 2.39. Let X, Y and Z be jointly distributed discrete random variables taking values in a finite set. The triple (X, Y, Z) is called a Markov(ian) triple, which we write as $X \to Y \to Z$, if for all x, y with $\mathbb{P}[X = x \mid Y = y] > 0$

$$\mathbb{P}[Z=z\mid X=x,Y=y]=\mathbb{P}[Z=z\mid Y=y]$$

If we think of $X \to Y \to Z$ as the evolution of some random process over time, then this says that if we know the "present", the value of Y, then the future evolution does not depend on the past.

For a Markov triple we can write the joint distribution as the product

$$p_{X,Y,Z}(x,y,z) = p_X(x) \cdot p_{Y|X}(y \mid x) \cdot p_{Z|X,Y}(z \mid x,y) = p_X(x) \cdot p_{Y|X}(y \mid x) \cdot p_{Z|Y}(z \mid y). \quad (2.4)$$

There is another nice equivalent description in terms of the conditional distributions.

Lemma 2.40. (X,Y,Z) is a Markovian triple if and only if X and Z are conditionally independent, given Y. That is, if whenever $p_Y(y) > 0$,

$$p_{X,Z|Y}(x,z \mid y) = p_{X|Y}(x \mid y)p_{Z|Y}(z \mid y).$$

Note that the condition in Lemma 2.40 is symmetric in X and Z. In other words, we see that $X \to Y \to Z$ is a Markovian triple if and only if $Z \to Y \to X$ is as well.

If we think about our random process as some method of processing some data, our input data X is encoded or transmitted say, and we have as output data Y. Then, if forget about our original data X, there should be no way to increase the amount of information about X that the output Y contains by further processing (via some deterministic, or random, process).

As an example, we can think about the transmission of some message X from Alice to Bob, who receives the transmitted message Y (perhaps some random noise has been added in the channel). Without access to the message X, there should be no way that Bob can deduce more information about X than what is contained in Y.

Theorem 2.41 (Data processing inequality). If $X \to Y \to Z$, then $I(X; Z) \le I(X; Y)$.

Note that, since $Z \to Y \to X$ is also a Markovian triple, we can also deduce from Theorem 2.41 that $I(Z; Y) \ge I(Z; X) = I(X; Z)$, and so

$$I(X ; Z) \le \max\{I(X ; Y), I(Y ; Z)\}.$$

Suppose, in the previous example, Alice transmit a message X to Bob, who receives Y, and Bob wishes to reconstruct the message X from Y, via some process. Perhaps Alice is sending pictures of some letters, and Bob receives slightly perturbed pictures, and so has to guess which letter fits the picture best. This might be some deterministic process, or maybe when Bob is unsure he makes some random choice, weighted by how likely he thinks each letter is. In this way Bob makes a (potentially random) guess $Z = \hat{X}$ based on Y, and we have a Markov triple $X \to Y \to Z$.

How accurate can Bob be? There are many ways we could measure this, but one way would be to look at the probability that Bob's guess is correct, the probability that $\hat{X} = X$.

Now, from the Data processing inequality, we know that if lots of information is lost in transmission, and so I(X; Y) is small, it shouldn't be the case that \hat{X} is well-correlated with \hat{X} , since $I(X; \hat{X})$, which is a measure of dependence, is also small. So, we should expect to be able to bound the probability of success, as some function of the mutual information I(X; Y), and the following inequality makes this precise (in fact, we bound instead the probability of failure, as a function of the conditional entropy H(X|Y)).

Theorem 2.42 (Fano's inequality). Let $X \to Y \to \hat{X}$ be a Markov triple, where we think of \hat{X} as an estimation of X on the basis of Y. Define $p_{err} = \mathbb{P}[\hat{X} \neq X]$. Then

$$H(p_{err}, 1 - p_{err}) + p_{err} \log_2 |\mathcal{X}| \ge H(X \mid \hat{X}) \ge H(X \mid Y).$$

In particular

$$p_{err} \geq \frac{H(X\mid \hat{X}) - 1}{\log_2|\mathcal{X}|} \geq \frac{H(X\mid Y) - 1}{\log_2|\mathcal{X}|}.$$

Proof.

It is reasonable to ask why we mention also the weaker bounds in terms of $H(X \mid Y)$ rather than $H(X \mid \hat{X})$. This is useful if we're interested in an *a priori estimate*, one that only depends on the message X and the transmitted message Y, and not the method of reconstruction \hat{X} . This bound then holds for *every* possible \hat{X} - no matter how Bob attempts to guess the message X, he must always have a failure probability of at least this quantity.

Remark 2.43. All the material in this section extends straightforwardly to arbitrary discrete random variables, respectively probability distributions, taking values in countable sets.

That is, given a random variable X taking values in $\mathcal{X} = \{x_k : x \in \mathbb{N}\}$ with distribution $p = (p_1, p_2, \ldots)$ we can define the entropy

$$H(X) = H(p) = -\sum_{k=1}^{\infty} p_k \log_2 p_k,$$

which may also take the value $+\infty$.

3 Entropy Rate and Asymptotic Equipartition

3.1 Entropy Rate

Definition 3.1 (Stochastic process, state space). A stochastic process in discrete time is a sequence $(X_n)_{n\in\mathbb{N}}$ of jointly distributed random variables. The state space of the process is the set \mathcal{X} of possible values which the X_n can take.

Example 3.2. Pick a random page of a book and let X_n be the nth letter on the page.

Let $X_1 = 100$ be constant, and let X_n be the bankroll after n spins of a roulette wheel of a gambler who bets his entire stake on red each time.

Let $X_1 = (0,0) \in \mathbb{Z}^2$ and let X_n be the position after n steps of a 'random walk', where in each time step we choose uniformly at random one of the four neighbours in the grid of our current position and move there.

Given a stochastic process $(X_n)_{n\in\mathbb{N}}$ we can think of $H(X_1,\ldots,X_n)$ as the total amount of information in the system at time n. This is clearly an increasing function of n. What we're interested in is the rate at which this function is increasing.

Definition 3.3 (Entropy rate). If $(X_n)_{n\in\mathbb{N}}$ is a stochastic process whose state space is finite, then the *entropy rate* or *asymptotic entropy* of the stochastic process is defined as

$$h := \lim_{n \to \infty} \frac{1}{n} H(X_1, \dots, X_n),$$

if the limit exists. The unit of h is bits per time unit.

We will see that the entropy rate represents a theoretical limit on how efficiently we can encode the data stream $(X_n)_{n\in\mathbb{N}}$. Conversely, we will find for a broad class of processes, we can achieve this theoretical limit asymptotically, using the idea of asymptotic equipartition.

We can think of h as the average amount of new information introduced in each step of the stochastic process. Indeed, by the chain rule (Theorem 2.13)

$$\frac{1}{n}H(X_1,\dots,X_n) = \frac{1}{n}\sum_{k=1}^n H(X_k \mid X_1,\dots,X_{k-1}),$$
(3.1)

where $H(X_k \mid X_1, \dots, X_{k-1})$ is the amount of information introduced at the kth step.

What we will find is that the entropy rate represents a theoretical limit on how efficiently we can encode the data stream $(X_n)_{n\in\mathbb{N}}$. Conversely, the idea of asymptotic equipartition is that for a broad class of processes, we can achieve this theoretical limit asymptotically.

Lemma 3.4. If $(X_n)_{n\in\mathbb{N}}$ is a stochastic process whose state space is finite and the limit $h' = \lim_{k\to\infty} H(X_k \mid X_1,\ldots,X_{k-1})$ exists, then h exists and h = h'.

Proof.

For i.i.d sequences, it is trivial to compute h using Lemma 3.4

Lemma 3.5. If $(X_n)_{n\in\mathbb{N}}$ is a sequence of i.i.d discrete random variables taking values in a finite set, then the entropy rate h exists and is equal to $H(X_1)$.

Definition 3.6. A stochastic process $(X_n)_{n\in\mathbb{N}}$ is *stationary* if for every $\ell, k \in \mathbb{N}$ the two random vectors

$$(X_1, ..., X_{\ell})$$
 and $(X_{k+1}, ..., X_{k+\ell})$

have the same distribution. In other words, for every choice of elements $x_1, \ldots, x_\ell \in \mathcal{X}$ in the state space,

$$\mathbb{P}[X_1 = x_1, \dots, X_\ell = x_\ell] = \mathbb{P}[X_{k+1} = x_1, \dots, X_{k+\ell} = x_\ell].$$

Example 3.7. The simplest example of stationary processes are sequences of independent and identically distributed random variables. For example, if we repeatedly roll a dice and let X_n be the value of the nth roll.

As another example, suppose we have two biased coins with different probabilities p and q of heads, and I choose randomly, say with probability $\frac{1}{2}$ one of the coins to flip, and then let X_n be the (bit) value of the nth coin toss. Then the X_n are not independent, if p is very close to one and q is very close to 0, then if $X_1 = 1$, it's very likely that I picked the first coin and so very likely that $X_2 = 1$ as well. However, it is easy to show that this process is stationary.

The random walk on \mathbb{Z}^2 from the previous example is not stationary - X_0 is deterministic, whereas X_1 is uniformly distributed on $\{(\pm 1, 0), (0, \pm 1)\}$.

Lemma 3.8. If $(X_n)_{n\in\mathbb{N}}$ is a stationary process with a finite state space, then the entropy rate h exists.

Whilst Lemma 3.8 asserts the existence of the entropy rate for stationary processes, it is non-constructive - it does not provide us a formula to calculate h. It is reasonable to ask if there is a broader class of stochastic processes (than i.i.d) for which we can compute h explicitly.

3.2 Time-homogeneous Markov Chains

Definition 3.9. A stochastic process $(X_n)_{n\geq 0}$ with finite state space \mathcal{X} is a *Markov chain* (MC) if for all $n \in \mathbb{N}$ and for all $x_0, \ldots, x_n \in \mathcal{X}$,

$$\mathbb{P}[X_n = x_n \mid X_0 = x_0, \dots, X_{n-1} = x_{n-1}] = \mathbb{P}[X_n = x_n \mid X_{n-1} = x_{n-1}] := p_n(x_n \mid x_{n-1}),$$
whenever $\mathbb{P}[X_1 = x_0, \dots, X_{n-1} = x_{n-1}] > 0.$

A Markov chain is time-homogeneous if $p_n(y|x) := p(y|x)$ does not depend on n. In this case the matrix $P = \Big(p(y|x)\Big)_{x,y \in \mathcal{X}}$ is the $transition\ matrix$ of the time-homogeneous Markov chain and the distribution of X_0

$$\nu(x) = \mathbb{P}[X_0 = x]$$

is the *initial distribution* or *starting distribution*.

We note that the transition matrix P is always a *stochastic* matrix - the entries are all non-negative and each row sums to one, that is for all $x \in \mathcal{X}$

$$\sum_{y \in \mathcal{X}} p(y|x) = 1.$$

We can think of a Markov chain as a *memoryless* stochastic process - given the state of the process at some time n, the future distribution does not depend on the past. In particular, it is easy to check that each consecutive triple is Markovian and so

$$X_0 \to X_1 \to \ldots \to X_n$$
.

Example 3.10. Suppose we're playing some board game with a number of possible states \mathcal{X} . Each turn we roll a dice and play according to some fixed strategy, so that the probability that we move from a state x to a state y in any particular turn is fixed. The state X_n of some player is then a time-homogeneous Markov chain.

A random walk is also an example of a time-homogeneous Markov chain - if we are currently at a vertex x the probability that we move to a vertex y only depends on the current state, and not the history of the walk.

Lemma 3.11. If $(X_n)_{n\geq 0}$ is a Markov chain, then for any $k\in \mathbb{N}$ $((X_n,X_{n+1},\ldots,X_{n+k}))_{n\geq 0}$ is a Markov chain.

Proof. Exercise.
$$\Box$$

Definition 3.12 (The (di)graph of a Markov chain). Given a time-homogeneous Markov chain $(X_n)_{n\geq 0}$ with state space \mathcal{X} , we can draw an associated (weighted) (di)graph whose vertex set is \mathcal{X} and for any two states x and y we draw an arc from x to y with weight p(y|x) if p(y|x) > 0.

We can think of the Markov chain as a simple random walk on this graph, where the probability of moving from state x to y is given by the weight of the arc from x to y and the distribution of the starting vertex is given by X_0 .

Example 3.13. We can think of the following simplified model of the evolution of the weather. Our stochastic process has three state $\mathcal{X} = \{\text{sun, rain, snow}\} = \{N, R, S\}$

Our transition matrix is given as follows

$$P = \begin{array}{c|cccc} & N & R & S \\ \hline N & 0 & 1/2 & 1/2 \\ R & 1/4 & 1/2 & 1/4 \\ S & 1/4 & 1/4 & 1/2 \end{array}.$$

So, we never have two sunny days in a row - if a day is sunny then the next day is equally likely to be rainy or snowy. On rainy or snow days the next day has probability 1/2 to have the same weather, and probability 1/2 to change to one of the other options uniformly.

In this case the digraph of this Markov chain has vertex set $V = \{N, R, S\}$ and arcs

$$e_1 = (N, R), e_2 = (N, S), e_3 = (R, N), e_4 = (R, R),$$

 $e_5 = (R, S), e_6 = (S, N), e_7 = (S, R), e_8 = (S, S).$

with weights

$$w(e_1) = 1/2$$
, $w(e_2) = 1/2$, $w(e_3) = 1/4$, $w(e_4) = 1/2$, $w(e_5) = 1/4$, $w(e_6) = 1/4$, $w(e_7) = 1/4$, $w(e_8) = 1/2$.

.

By the Markovian property it is relatively easy to write down the joint distribution of (X_0, \ldots, X_n) as

$$\mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] = \nu(x_0)p(x_1|x_0)p(x_2|x_1)\dots p(x_n|x_{n-1}), \tag{3.2}$$

and from this it is also clear what the conditional distribution of X_n , given X_0 is.

Lemma 3.14. Let $(X_n)_{n\geq 0}$ be a Markov chain with initial distribution ν and transition matrix P. Then

$$p^{(n)}(y|x) := \mathbb{P}[X_n = y \mid X_0 = x] = (P^n)_{xy},$$

that is, the matrix given by $\left(p^{(n)}(y|x)\right)_{x,y\in\mathcal{X}}$ is the nth power of P.

If we consider ν as a row vector, then $p_{X_n} = \nu P^n$, that is

$$p_{X_n}(y) = \sum_{x \in \mathcal{X}} \nu(x) p^{(n)}(y|x).$$

Proof.

We will show that for a natural class of time-homoegenous Markov chains the entropy rate exists, and can be easily calculated, and furthermore is independent of the choice of the initial distribution ν .

The existence of the entropy rate would be clear if the Markov chain were stationary, by Lemma 3.8. However, whilst is easy to verify that every stationary Markov chain is time-homogeneous (exercise). The converse is not true in general, but will hold for sensible choices of initial distribution.

Lemma 3.15. Let $(X_n)_{n\geq 0}$ be a time-homogeneous Markov chain with initial distribution ν and transition matrix P. Then the Markov chain is stationary if and only if $\nu P = \nu$, that is, only if ν is an eigenvector of P with eigenvalue one.

In this case we call ν a stationary distribution for P, or for the Markov chain.

Lemma 3.16. Let $(X_n)_{n\geq 0}$ be a time-homogeneous Markov chain with a stationary initial distribution ν . Then the entropy rate exists and is given by

$$h = \sum_{x \in \mathcal{X}} \nu(x) H(p(\cdot|x)),$$

where

$$H(p(\cdot|x)) = -\sum_{y \in \mathcal{X}} p(y|x) \log_2 p(y|x)$$

is the entropy of the probability vector which is the row of the transition matrix P indexed by x.

We note that there is a trivial right eigenvector of P with eigenvalue one given by the all ones vector $\mathbf{1} = (1, ..., 1)$. Indeed, since P is stochastic, for all $x \in \mathcal{X}$

$$(P\mathbf{1})_x = \sum_{y \in \mathcal{X}} p(y|x) = 1.$$

More generally, a function $f: \mathcal{X} \to \mathbb{R}$ is called *harmonic* (with respect to P) if, when viewed as a column vector, it satisfies Pf = f. Since

$$(Pf)_x = \sum_{y \in \mathcal{X}} p(y|x)f(y) = \sum_{y: p(y|x) > 0} p(y|x)f(y),$$

we can think of this as saying that the weighted average of the function f over the neighbourhood of x in the digraph of the Markov chain is equal to f(x).

Hence, since the left and right eigenvalues of a matrix agree, there must be *some* vector ν which is a left eigenvector of P with eigenvalue one. It remains to show that ν is a probability vector. Arranging that ν sums to one is trivial, any linear scaling of an eigenvector lies in the same eigenspace, however it is not obvious that ν is non-negative.

Lemma 3.17. Let $(X_n)_{n\geq 0}$ be a time-homogeneous Markov chain with a finite state space \mathcal{X} and transition matrix P. Then there is at least one stationary probability distribution ν for P.

Note that the same argument would apply to any accumulation point μ of the sequence μ_n . Can we say when this stationary distribution is unique?

Definition 3.18. Let $(X_n)_{n\geq 0}$ be a time-homogeneous Markov chain with a finite state space \mathcal{X} and transition matrix P. The Markov chain, and transition matrix, are called *irreducible* if for every pair $x, y \in \mathcal{X}$ there is some $n \in \mathbb{N}$ such that $p^{(n)}(y|x) > 0$. That is, for any pair of states, there is some n such that we can transition from one state to the other in n steps with positive probability.

If we think about the associated digraph of the Markov chain, then irreducibility is equivalent to the property that this digraph is strongly connected - for any pair of vertices x and y there is a directed path from x to y.

Proposition 3.19. Let $(X_n)_{n\geq 0}$ be a irreducible time-homogeneous Markov chain with a finite state space \mathcal{X} and transition matrix P. Then there is a unique stationary distribution ν and furthermore $\nu(x) > 0$ for all $x \in \mathcal{X}$.

Proof.

Corollary 3.20. Let $(X_n)_{n\geq 0}$ be a irreducible time-homogeneous Markov chain with a finite state space \mathcal{X} and transition matrix P. Then

$$\lim_{n\to\infty} \frac{1}{n} \left(\mu + \mu P + \mu P^2 + \ldots + \mu P^{n-1} \right)$$

exists and is equal to the unique stationary distribution ν .

Proof.

Corollary 3.21. Let $(X_n)_{n\geq 0}$ be a irreducible time-homogeneous Markov chain with a finite state space \mathcal{X} and transition matrix P. Then for any initial distribution μ , the entropy rate of the Markov chain exists and is equal to the entropy rate of the Markov chain under its unique stationary distribution (see Lemma 3.16).

Proof.

Definition 3.22 (Return time). If $(X_n)_{n\geq 0}$ is a Markov chain with a finite state space \mathcal{X} , then for any $x\in\mathcal{X}$ we define

$$\tau^x = \inf\{n > 1 : X_n = x\},\$$

which is the first time the chain is in state x after the start (where we define $\inf \emptyset = \infty$). Note that τ_x is a random variable! If $X_0 = x$ then we call τ^x the return time to x. A state x is called recurrent if the Makrov chain returns to x almost surely, that is, if

$$\mathbb{P}[\tau^x < \infty \mid X_0 = x] = 1,$$

and it is positive recurrent if in addition the return time has finite expectation, that is,

$$\mathbb{E}\left(\tau^{x}\mid X_{0}=x\right)<\infty.$$

Theorem 3.23 (Ergodic Theorem for Markov chains). Let $(X_n)_{n\geq 0}$ be a irreducible, time-homogeneous Markov chain with a finite state space \mathcal{X} . Then every state $x\in\mathcal{X}$ is positive recurrent, and the (unique) stationary distribution ν is given by

$$\nu(x) = \frac{1}{\mathbb{E}\left(\tau^x \mid X_0 = x\right)}.$$

Furthermore, for any initial distribution μ and any function $f: \mathcal{X} \to \mathbb{R}$

$$\lim_{n \to \infty} \frac{1}{n} \sum_{k=0}^{n-1} f(X_k) = \sum_{x \in \mathcal{X}} f(x) \nu(x) \qquad almost \ surely.$$

The expression on the right hand side is a determinstic quantity, the *space average* of the value f(x) - the average of f over the state space \mathcal{X} under the stationary distribution ν . On

the left hand side we have a random quantity, the time average of f over the trajectory of the random process X_n and the theorem asserts that the two are almost surely equal.

In applications, we are often interested in the value of the right hand side, however if the state space is large then it can be hard, or inefficient to compute the space average directly. On the other hand, the time average can be approximated by simulating the Markov chain for a large number of steps and calculating the time average. In this way we get a tool for approximating the sum on the right hand side, which is know as the *Markov chain Monte Carlo* method.

3.3 The Asymptotic Equipartition Property

Let $(X_n)_{n\geq 1}$ be a stochastic process with a finite state space \mathcal{X} . For each $n\in\mathbb{N}$ we can consider the joint distribution $p_n=p_{X_1,\ldots,X_n}$ on \mathcal{X}^n , that is

$$p_n(x_1,\ldots,x_n) = \mathbb{P}[X_1 = x_1, X_2 = x_2,\ldots,X_n = x_n].$$

Note that the sequence of distributions $(p_n)_{n\geq 1}$ (which are deterministic functions on \mathcal{X}^n), determines all the probabilistic characteristics of the stochastic process.

Suppose that the entropy rate of the stochastic process

$$h = \lim_{n \to \infty} \frac{1}{n} H(X_1, \dots, X_n) = \lim_{n \to \infty} \frac{1}{n} H(p_n)$$

exists. Since for any random variable X we can write

$$H(X) = \mathbb{E}(-\log_2 p_X(X)),$$

as the expected value of the deterministic function $-\log_2 \circ p_X$ applied to the random variable X, we can apply this to the random vector (X_1, \ldots, X_n) to conclude that

$$\frac{1}{n}H(X_1,\ldots,X_n) = \mathbb{E}\left(-\frac{1}{n}\log_2 p_n(X_1,\ldots,X_n)\right).$$

Then the entropy rate h is the limit of the expected value of the random variables $Y_n = -\frac{1}{n}\log_2 p_n(X_1,\ldots,X_n)$. A much stronger property than the limit of the expectation existing would be that the random variables themselves converge (in probability or almost surely) to some limiting random variable with finite expectation h.

Definition 3.24 (Asymptotic equipartition property). Let $(X_n)_{n\geq 1}$ be a stochastic process with a finite state space \mathcal{X} whose entropy rate h exists. We say X has the asymptotic equipartition property (AEP), if

$$-\frac{1}{n}\log_2 p_n(X_1,\ldots,X_n) \longrightarrow h$$
 almost surely, as $n \to \infty$.

The asymptotic equipartition property makes a very strong *prediction* about the observed outcome $(x_n)_{n\geq 1}$ of the stochastic process - with very high probability the quantity $-\frac{1}{n}\log_2 p_n(x_1,\ldots,x_n)$ will be close to the entropy rate h, where the error in probability and in approximation to h is tending to 0 with n.

Example 3.25. Let $\mathcal{X} = \{0,1\}$ and let $(X_n)_{n\geq 1}$ be i.i.d with distribution $\mathrm{Ber}(\theta)$, that is,

$$\mathbb{P}[X_n = 1] = \theta \quad \text{and} \quad \mathbb{P}[X_n = 0] = 1 - \theta,$$

where $0 < \theta < 1$. For any bitstring $(x_1, \ldots, x_n) \in \{0, 1\}^n$, let

$$s_n = x_1 + \ldots + x_n,$$

be the total number of ones, so that $n - s_n$ is the total number of zeroes. Let us write S_n for the random variable $X_1 + \ldots + X_n$.

Since the sequence is i.i.d we can compute

$$p_n(x_1, \dots, x_n) = \theta^{s_n} (1 - \theta)^{n - s_n}$$
 and so $p_n(X_1, \dots, X_n) = \theta^{S_n} (1 - \theta)^{n - S_n}$.

Hence,

$$-\frac{1}{n}\log_2 p_n(X_1, \dots, X_n) = -\frac{1}{n}\log_2 \left(\theta^{S_n}(1-\theta)^{n-S_n}\right) = -\frac{S_n}{n}\log_2 \theta - \left(1 - \frac{S_n}{n}\right)\log_2(1-\theta).$$

On the other hand, since the X_n are i.i.d, by Lemma 3.5 the entropy rate h exists and is equal to

$$h = H(X_1) = H(\theta, 1 - \theta) = -\theta \log_2 \theta - (1 - \theta) \log_2 (1 - \theta).$$

So, in this case, the statement that $(X_n)_{n\geq 1}$ satisfies the AEP would be that almost surely

$$-\frac{S_n}{n}\log_2\theta - \left(1 - \frac{S_n}{n}\right)\log_2(1 - \theta) \longrightarrow -\theta\log_2\theta - (1 - \theta)\log_2(1 - \theta).$$

Or, in other words, the AEP is equivalent to the statement that $\frac{S_n}{n} \to \theta$ almost surely, which is the strong law of large numbers.

In fact the argument above works for general for i.i.d sequences.

Lemma 3.26. Let $(X_n)_{n\geq 1}$ be an i.i.d stochastic process with a finite state space \mathcal{X} . Then $(X_n)_{n\geq 1}$ satisfies the AEP, where the entropy rate $h=H(X_1)$.

There are perhaps two natural questions to ask at this point:

- (I) Which classes of stochastic process have the AEP (does this include a nice large natural class)?
- (II) What is the practical application of knowing that we have the AEP?

Theorem 3.27. Let $(X_n)_{n\geq 0}$ be a irreducible, time-homogeneous Markov chain with a finite state space \mathcal{X} . Then for any initial distribution, $(X_n)_{n\geq 0}$ satisfies the AEP, where the entropy rate h is given by the formula in Corollary 3.21 / Lemma 3.16.

Proof.

What can we conclude from the fact that the AEP holds? Since convergence almost surely implies convergence in probability, if the AEP holds then for any $\epsilon > 0$

$$\mathbb{P}\left[\left|-\frac{1}{n}\log_2 p_n(X_1,\dots,X_n) - h\right| < \epsilon\right] \to 1. \tag{3.3}$$

In other words, there is some deterministic set inside the set of trajectories \mathcal{X}^n , which we can specify ahead of time in terms of the deterministic function p_n and the quantity h, such that with very high probability the trajectory of the process lies inside this set.

Definition 3.28 (Typical set). Given a stochastic process $(X_n)_{n\geq 1}$ which satisfies the AEP with entropy rate h. For every n and (small) $\epsilon > 0$ the typical set is given by

$$A_{\epsilon}^{(n)} = \left\{ \boldsymbol{x} = (x_1, \dots, x_n) \in \mathcal{X}^n : \left| -\frac{1}{n} \log_2 p_n(x_1, \dots, x_n) - h \right| < \epsilon \right\}.$$

The following properties of typical sets follow immediately from the definitions.

Proposition 3.29. Given a stochastic process $(X_n)_{n\geq 1}$ which satisfies the AEP with entropy rate h. Then for all (small) $\epsilon > 0$ the typical set has the following properties:

(a) There exists $N(\epsilon)$ such that for all $n \geq N(\epsilon)$

$$\mathbb{P}[(X_1, \dots, X_n) \in A_{\epsilon}^{(n)}] > 1 - \epsilon.$$

(b) For all $\mathbf{x} = (x_1, ..., x_n) \in A_{\epsilon}^{(n)}$,

$$2^{-n(h+\epsilon)} < p_n(\boldsymbol{x}) < 2^{-n(h-\epsilon)}.$$

(c) The size of the typical set satisfies

$$(1-\epsilon)2^{n(h-\epsilon)} < \left| A_{\epsilon}^{(n)} \right| < 2^{n(h+\epsilon)},$$

where the second inequality holds for all n, and the first for all $n \geq N(\epsilon)$.

Proof.

So, from (a) we see that p_n is almost concentrated on the set $A_{\epsilon}^{(n)}$, and from (b) and (c) we see furthermore that it is almost *equidistributed* on this set (and this is where the name asymptotic equipartition property comes from)!

In general, the fact that p_n is concentrated on this 'smaller' set $A_{\epsilon}^{(n)}$ will be most useful when $\left|A_{\epsilon}^{(n)}\right| \ll |\mathcal{X}^n|$, which in light of (c) will be the case when

$$2^{n(h+\epsilon)} \ll |\mathcal{X}^n| \Longleftrightarrow h + \epsilon < \log_2 |\mathcal{X}|,$$

in which case $A_{\epsilon}^{(n)}$ will be exponentially smaller than \mathcal{X}^n . When the X_n are i.i.d and uniformly distributed, then $h = \log_2 |\mathcal{X}|$, and the typical set consists of almost all of the possible trajectories.

Whilst there are possibly many more possible trajectories in \mathcal{X}^n than typical sequences in $A_{\epsilon}^{(n)}$, it is vanishingly unlikely that the observed trajectory lies outside of $A_{\epsilon}^{(n)}$, and so these non-typical trajectories play no significant role in the analysis of the process.