# *Mathematical Methods for CS*
# *Probability*

UNIVERSITY OF
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*Michaelmas 2009*

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This handout includes copies of the slides that will be used in lectures together with some suggested exercises for supervisions. These notes do not constitute a complete transcript of all the lectures and they are not a substitute for text books. They are intended to give a reasonable synopsis of the subjects discussed, but they give neither complete descriptions nor all the background material.

## Some notation

| | |
|---|---|
| RV | random variable |
| IID | independent, identically distributed |
| PGF | probability generating function $G_X(z)$ |
| mgf | moment generating function $M_X(t)$ |
| $X \sim U(0,1)$ | RV X has the distribution $U(0,1)$, etc |
| $\mathbb{I}(A)$ | indicator function of the event $A$ |
| $\mathbb{P}(A)$ | probability that event $A$ occurs, e.g. $A = \{X = n\}$ |
| $\mathbb{E}(X)$ | expected value of RV $X$ |
| $\mathbb{E}(X^n)$ | $n^{th}$ moment of RV $X$, for $n = 1, 2, \ldots$ |
| $F_X(x)$ | distribution function, $F_X(x) = \mathbb{P}(X \leq x)$ |
| $f_X(x)$ | density of RV $X$ given, when it exists, by $F'_X(x)$ |



## Limits and inequalities



## Limits and inequalities

We are familiar with limits of real numbers. If $x_n = 1/n$ for $n = 1, 2, \ldots$ then $\lim_{n\to\infty} x_n = 0$ whereas if $x_n = (-1)^n$ no such limit exists. Behaviour in the long-run or on average is an important characteristic of everyday life.
In this section we will be concerned with these notions of limiting behaviour when the real numbers $x_n$ are replaced by random variables $X_n$. As we shall see there are several distinct notions of convergence that can be considered.
To study these forms of convergence and the limiting theorems that emerge we shall on the way also gather a potent collection of concepts and tools for the probabilistic analysis of models and systems.



## Probabilistic inequalities

To help assess how close RVs are to each other it is useful to have methods that provide upper bounds on probabilities of the form

$$\mathbb{P}(X > a)$$

for fixed constants $a$, and where, for example, $X = |X_1 - X_2|$.
We shall consider several such bounds and related inequalities.

- Markov's inequality
- Chebychev's inequality
- Lyapunov's inequality



### Theorem (Markov's inequality)

*If $\mathbb{E}(X) < \infty$ then for any $a > 0$,*

$$\mathbb{P}(|X| \geq a) \leq \frac{\mathbb{E}(|X|)}{a}\,.$$

### Proof.

We have that

$$\mathbb{I}(|X| \geq a) = \begin{cases} 1 & |X| \geq a \\ 0 & \text{otherwise}\,. \end{cases}$$

Clearly,

$$|X| \geq a\mathbb{I}(|X| \geq a)$$

hence

$$\mathbb{E}(|X|) \geq \mathbb{E}(a\mathbb{I}(|X| \geq a)) = a\mathbb{P}(|X| \geq a)$$

which yields the result. □



### Theorem (Chebychev's inequality)

*Let $X$ be a RV with mean $\mu$ and finite variance $\sigma^2$ then for all $a > 0$*

$$\mathbb{P}(|X - \mu| \geq a) \leq \frac{\sigma^2}{a^2}\,.$$

### Proof.

Consider, for example, the case of a continuous RV $X$ and put $Y = |X - \mu|$ then

$$\sigma^2 = \mathbb{E}(Y^2) = \int y^2 f_Y(y)dy = \int_{0\leq y<a} y^2 f_Y(y)dy + \int_{y\geq a} y^2 f_Y(y)dy$$

so that

$$\sigma^2 \geq 0 + a^2\mathbb{P}(Y \geq a)\,.$$

□

### Theorem (Lyapunov's inequality)

*If $r \geq s > 0$ then $\mathbb{E}(|X|^r)^{1/r} \geq \mathbb{E}(|X|^s)^{1/s}$.*

### Proof.

Omitted. □



## Moment generating function

### Definition

The moment generating function (mgf) of a RV $X$ is given by

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

and is defined for those values of $t \in \mathbb{R}$ for which this expectation exists.

Using the power series $e^x = 1 + x + x^2/2! + x^3/3! + \cdots$ we see that

$$M_X(t) = \mathbb{E}(e^{tX}) = 1 + \mathbb{E}(X)t + \mathbb{E}(X^2)t^2/2! + \mathbb{E}(X^3)t^3/3! + \cdots$$

and so the $n^{th}$ moment of $X$, $\mathbb{E}(X^n)$, is given by the coefficient of $t^n/n!$ in the power series expansion of the mgf $M_X(t)$.



## Elementary properties of the mgf

1. If $X$ has mgf $M_X(t)$ then $Y = aX + b$ has mgf $M_Y(t) = e^{bt}M_X(at)$.
2. If $X$ and $Y$ are independent then $X + Y$ has mgf $M_{X+Y}(t) = M_X(t)M_Y(t)$.
3. $\mathbb{E}(X^n) = M_X^{(n)}(0)$ where $M_X^{(n)}$ is the $n^{th}$ derivative of $M_X$.
4. If $X$ is a discrete RV taking values $0, 1, 2, \ldots$ with probability generating function $G_X(z) = \mathbb{E}(z^X)$ then $M_X(t) = G_X(e^t)$.



## Fundamental properties of the mgf

1. Uniqueness: to each mgf there corresponds a unique distribution function having that mgf.
   In fact, if $X$ and $Y$ are RVs with the same mgf in some region $-a < t < a$ where $a > 0$ then $X$ and $Y$ have the same distribution.
2. Continuity: if distribution functions $F_n(x)$ converge pointwise to a distribution function $F(x)$, the corresponding mgf's (where they exist) converge to the mgf of $F(x)$. Conversely, if a sequence of mgf's $M_n(t)$ converge to $M(t)$ which is continuous at $t = 0$, then $M(t)$ is a mgf, and the corresponding distribution functions $F_n(x)$ converge to the distribution function determined by $M(t)$.



## Example: exponential distribution

If $X$ has an exponential distribution with parameter $\lambda > 0$ then $f_X(x) = \lambda e^{-\lambda x}$ for $0 < x < \infty$. Hence, for $t < \lambda$,

$$\begin{aligned} M_X(t) &= \int_0^\infty e^{tx}\lambda e^{-\lambda x}dx = \int_0^\infty \lambda e^{-(\lambda-t)x}dx \\ &= \left[-\frac{\lambda}{(\lambda-t)}e^{-(\lambda-t)x}\right]_0^\infty = \frac{\lambda}{\lambda-t}\,. \end{aligned}$$

For $t < \lambda$

$$\frac{\lambda}{(\lambda-t)} = \left(1 - \frac{t}{\lambda}\right)^{-1} = 1 + \frac{t}{\lambda} + \frac{t^2}{\lambda^2} + \cdots$$

and hence $\mathbb{E}(X) = 1/\lambda$ and $\mathbb{E}(X^2) = 2/\lambda^2$ so that

$$\mathrm{Var}(X) = \mathbb{E}(X^2) - (\mathbb{E}(X))^2 = 1/\lambda^2\,.$$



## Example: normal distribution

Consider a normal RV $X \sim N(\mu, \sigma^2)$ then $f_X(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-(x-\mu)^2/2\sigma^2}$ so that

$$\begin{aligned} M_X(t) &= \int_{-\infty}^\infty e^{tx}\frac{1}{\sigma\sqrt{2\pi}}e^{-(x-\mu)^2/2\sigma^2}dx \\ &= \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^\infty e^{-(2tx\sigma^2+(x-\mu)^2)/2\sigma^2}dx\,. \end{aligned}$$

So, by completing the square,

$$\begin{aligned} M_X(t) &= e^{\mu t+\sigma^2t^2/2}\left\{\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^\infty e^{-(x-(\mu+t\sigma^2))^2/2\sigma^2}\right\}dx \\ &= e^{\mu t+\sigma^2t^2/2}\,. \end{aligned}$$

## Example: uniform distribution

Consider a uniform RV $X \sim U(a, b)$. Then

$$f_X(x) = \begin{cases} \frac{1}{b-a} & a < x < b \\ 0 & \text{otherwise}. \end{cases}$$

Hence,

$$\begin{aligned} M_X(t) &= \int_a^b \frac{e^{tx}}{b-a} dx \\ &= \left[\frac{e^{tx}}{(b-a)t}\right]_a^b \\ &= \frac{e^{bt} - e^{at}}{(b-a)t}. \end{aligned}$$



### Theorem (Chernoff's bound)

*Suppose that $X$ has mgf $M_X(t)$ and $a \in \mathbb{R}$ then for all $t \geq 0$*

$$\mathbb{P}(X \geq a) \leq e^{-ta} M_X(t).$$

### Proof.

Using Markov's inequality, we have that

$$\begin{aligned} \mathbb{P}(X \geq a) &= \mathbb{P}(e^{tX} \geq e^{ta}) \\ &\leq \frac{\mathbb{E}(e^{tX})}{e^{ta}} \\ &= e^{-ta} M_X(t) \end{aligned}$$

□

Note that the above bound holds for all $t > 0$ so we can select the best such bound by choosing $t$ to minimize $e^{-ta} M_X(t)$.



## Notions of convergence: $X_n \to X$ as $n \to \infty$

For a sequence of RVs $(X_n)_{n \geq 1}$, we shall define several distinct notions of convergence to some RV $X$ as $n \to \infty$.

### Definition (Convergence in distribution)

$X_n \xrightarrow{D} X$ if $F_{X_n}(x) \to F_X(x)$ for all points $x$ at which $F_X$ is continuous.

### Definition (Convergence in probability)

$X_n \xrightarrow{P} X$ if $\mathbb{P}(|X_n - X| > \epsilon) \to 0$ for all $\epsilon > 0$.

### Definition (Convergence almost surely)

$X_n \xrightarrow{a.s.} X$ if $\mathbb{P}(X_n \to X) = 1$.

### Definition (Convergence in $r^{th}$ mean)

$X_n \xrightarrow{r} X$ if $\mathbb{E}(|X_n - X|^r) \to 0$.



## Convergence theorems

### Theorem

*If $X_n \xrightarrow{a.s.} X$ then $X_n \xrightarrow{P} X$.*

### Theorem

*If $X_n \xrightarrow{P} X$ then $X_n \xrightarrow{D} X$.*

### Theorem

*If $r > s \geq 1$ and $X_n \xrightarrow{r} X$ then $X_n \xrightarrow{s} X$.*

### Theorem

*If $r \geq 1$ and $X_n \xrightarrow{r} X$ then $X_n \xrightarrow{P} X$.*



### Theorem

*If $X_n \xrightarrow{a.s.} X$ then $X_n \xrightarrow{P} X$.*

### Proof.

Omitted. □



### Theorem

*If $X_n \xrightarrow{P} X$ then $X_n \xrightarrow{D} X$.*

### Proof

We prove this theorem as follows. Fix, $\epsilon > 0$ then

$$F_{X_n}(x) = \mathbb{P}(X_n \leq x \cap X > x + \epsilon) + \mathbb{P}(X_n \leq x \cap X \leq x + \epsilon)$$

since $X > x + \epsilon$ and $X \leq x + \epsilon$ form a partition. But if $X_n \leq x$ and $X > x + \epsilon$ then $|X_n - X| > \epsilon$ and $\{X_n \leq x \cap X \leq x + \epsilon\} \subset \{X \leq x + \epsilon\}$. Therefore,

$$F_{X_n}(x) \leq \mathbb{P}(|X_n - X| > \epsilon) + F_X(x + \epsilon).$$

Similarly,

$$\begin{aligned} F_X(x - \epsilon) &= \mathbb{P}(X \leq x - \epsilon \cap X_n > x) + \mathbb{P}(X \leq x - \epsilon \cap X_n \leq x) \\ &\leq \mathbb{P}(|X_n - X| > \epsilon) + F_{X_n}(x). \end{aligned}$$

The proof is completed by noting that together these inequalities show that

$$F_X(x-\epsilon) - \mathbb{P}(|X_n - X| > \epsilon) \leq F_{X_n}(x) \leq \mathbb{P}(|X_n - X| > \epsilon) + F_X(x+\epsilon)\,.$$

But $X_n \xrightarrow{P} X$ implies that $\mathbb{P}(|X_n - X| > \epsilon) \to 0$. So, as $n \to \infty$, $F_{X_n}(x)$ is squeezed between $F_X(x-\epsilon)$ and $F_X(x+\epsilon)$.
Hence, if $F_X$ is continuous at $x$, $F_{X_n}(x) \to F_X(x)$ and so $X_n \xrightarrow{D} X$. □



### Theorem
*If $r > s \geq 1$ and $X_n \xrightarrow{r} X$ then $X_n \xrightarrow{s} X$.*

### Proof.
Set $Y_n = |X_n - X| \geq 0$ then by Lyapunov's inequality

$$\mathbb{E}(Y_n^r)^{1/r} \geq \mathbb{E}(Y_n^s)^{1/s}\,.$$

Hence, if $\mathbb{E}(Y_n^r) \to 0$ then $\mathbb{E}(Y_n^s) \to 0$. □



### Theorem
*If $r \geq 1$ and $X_n \xrightarrow{r} X$ then $X_n \xrightarrow{P} X$.*

### Proof.
By Markov's inequality, for all $\epsilon > 0$

$$\mathbb{P}(|X_n - X| > \epsilon) \leq \frac{\mathbb{E}(|X_n - X|)}{\epsilon}\,.$$

But $X_n \xrightarrow{r} X$ implies $X_n \xrightarrow{1} X$ and so the right hand side tends to zero and as required $X_n \xrightarrow{P} X$. □



## Limit theorems

Given a sequence of RVs $(X_n)_{n\geq 1}$, let

$$S_n = X_1 + X_2 + \cdots + X_n \qquad \text{and} \qquad \overline{X}_n = S_n/n\,.$$

What happens to $\overline{X}_n$ for large $n$?

### Theorem (Weak Law of Large Numbers/WLLN)
*Suppose $(X_n)_{n\geq 1}$ are IID RVs with finite mean $\mu$ (and finite variance $\sigma^2$) then $\overline{X}_n \xrightarrow{P} \mu$.*

### Theorem (Strong Law of Large Numbers/SLLN)
*Suppose $(X_n)_{n\geq 1}$ are IID RVs with finite mean $\mu$ (and finite fourth moment) then $\overline{X}_n \xrightarrow{a.s.} \mu$.*

Note that convergence to $\mu$ in the WLLN and SLLN actually means convergence to a degenerate RV, $X$, with $\mathbb{P}(X = \mu) = 1$.



## WLLN

### Theorem (Weak Law of Large Numbers/WLLN)
*Suppose $(X_n)_{n\geq 1}$ are IID RVs with finite mean $\mu$ and finite variance $\sigma^2$ then $\overline{X}_n \xrightarrow{P} \mu$.*

### Proof.
Recall that $\mathbb{E}(\overline{X}_n) = \mu$ and $\mathrm{Var}(\overline{X}_n) = \sigma^2/n$. Hence, by Chebychev's inequality, for all $\epsilon > 0$

$$\mathbb{P}(|\overline{X}_n - \mu| > \epsilon) \leq \frac{\sigma^2/n}{\epsilon^2} = \frac{\sigma^2}{n\epsilon^2}$$

and so, letting $n \to \infty$,

$$\mathbb{P}(|\overline{X}_n - \mu| > \epsilon) \to 0$$

hence $\overline{X}_n \xrightarrow{P} \mu$ as required. □



## SLLN

### Theorem (Strong Law of Large Numbers/SLLN)
*Suppose $(X_n)_{n\geq 1}$ are IID RVs with finite mean $\mu$ (and finite fourth moment) then $\overline{X}_n \xrightarrow{a.s.} \mu$.*

### Proof.
Omitted. □

## Applications: estimating probabilities

Suppose we wish to estimate the probability, $p$, that we succeed when we play some game. For $i = 1, \ldots, n$, let

$$X_i = \mathbb{I}(\{i^{th}\text{game is success}\}) .$$

So $\overline{X}_n = m/n$ if we succeed $m$ times in $n$ attempts.
We have that $\mu = \mathbb{E}(X_i) = \mathbb{P}(X_i = 1) = p$ so then

$$m/n \xrightarrow{a.s.} p$$

by the SLLN.
Thus we have shown the important result that the empirical estimate of the probability of some event by its observed sample frequency converges to the correct value as the number of samples grows. This result forms the basis of all simulation methods.



## Applications: Shannon's entropy

### Theorem (Asymptotic Equipartition Property/AEP)

*If $X_n$ is a sequence of IID discrete RV with probability distribution given by $\mathbb{P}(X_i = x) = p(x)$ for each $x \in I$ then*

$$-\frac{1}{n}\log_2 p(X_1, X_2, \ldots, X_n) \xrightarrow{P} H(X)$$

*where Shannon's entropy is defined by*

$$H(X) = H(X_1) = \cdots = H(X_n) = -\sum_{x \in I} p(x)\log_2 p(x)$$

*and*

$$p(x_1, x_2, \ldots, x_n) = \prod_{i=1}^{n} p(x_i)$$

*is the joint probability distribution of the n IID RVs $X_1, X_2, \ldots, X_n$.*



### Proof.

Observe that $p(X_i)$ is a RV taking the value $p(x)$ with probabilty $p(x)$ and similarly $p(X_1, X_2, \ldots, X_n)$ is a RV taking a value $p(x_1, x_2, \ldots, x_n)$ with probability $p(x_1, x_2, \ldots, x_n)$. Therefore,

$$\begin{aligned}
-\frac{1}{n}\log_2 p(X_1, X_2, \ldots, X_n) &= -\frac{1}{n}\log_2 \prod_{i=1}^{n} p(X_i) \\
&= -\frac{1}{n}\sum_{i=1}^{n} \log_2 p(X_i) \\
&= \frac{1}{n}\sum_{i=1}^{n} (-\log_2 p(X_i)) \\
&\xrightarrow{P} \mathbb{E}(-\log_2 p(X_i)) \qquad \text{by WLLN} \\
&= -\sum_{x \in I} p(x)\log_2 p(x) \\
&= H(X)
\end{aligned}$$

□



## AEP implications

By the AEP, for all $\epsilon > 0$,

$$\begin{aligned}
\lim_{n\to\infty} \mathbb{P}(|-\frac{1}{n}\log_2 p(X_1, X_2, \ldots, X_n) - H(X)| \le \epsilon) &= 1 \\
\lim_{n\to\infty} \mathbb{P}(H(X) - \epsilon \le -\frac{1}{n}\log_2 p(X_1, X_2, \ldots, X_n) \le H(X) + \epsilon) &= 1 \\
\lim_{n\to\infty} \mathbb{P}(-n(H(X) - \epsilon) \ge \log_2 p(X_1, X_2, \ldots, X_n) \ge -n(H(X) + \epsilon)) &= 1 \\
\lim_{n\to\infty} \mathbb{P}(2^{-n(H(X)+\epsilon)} \le p(X_1, X_2, \ldots, X_n) \le 2^{-n(H(X)-\epsilon)}) &= 1
\end{aligned}$$

Thus, the sequences of outcomes $(x_1, x_2, \ldots, x_n)$ for which

$$2^{-n(H(X)+\epsilon)} \le p(x_1, x_2, \ldots, x_n) \le 2^{-n(H(X)-\epsilon)}$$

have a high probability and are refered to as typical sequences. An efficient (optimal) coding is to assign short codewords to such sequences leaving longer codewords for any non-typical sequence. Such long codewords must arise only rarely in the limit.



## Central limit theorem

### Theorem (Central limit theorem/CLT)

*Let $(X_n)_{n\ge1}$ be a sequence of IID RVs with mean $\mu$, variance $\sigma^2$ and whose moment generating function converges in some interval $-a < t < a$ with $a > 0$. Then*

$$Z_n = \frac{\overline{X}_n - \mu}{\sigma/\sqrt{n}} \xrightarrow{D} Z \sim N(0, 1) .$$



## Proof of CLT

Set $Y_i = (X_i - \mu)/\sigma$ then $\mathbb{E}(Y_i) = 0$ and $\mathbb{E}(Y_i^2) = \mathrm{Var}(Y_i) = 1$ so

$$M_{Y_i}(t) = 1 + \frac{t^2}{2} + o(t^2)$$

where $o(t^2)$ refers to terms of higher order than $t^2$ which will therefore tend to 0 as $t \to 0$. Also,

$$Z_n = \frac{\overline{X}_n - \mu}{\sigma/\sqrt{n}} = \frac{1}{\sqrt{n}}\sum_{i=1}^{n} Y_i .$$

Hence,

$$\begin{aligned}
M_{Z_n}(t) &= \left(M_{Y_i}\left(\frac{t}{\sqrt{n}}\right)\right)^n \\
&= \left(1 + \frac{t^2}{2n} + o\left(\frac{t^2}{n}\right)\right)^n \\
&\to e^{t^2/2} \qquad \text{as} \qquad n \to \infty .
\end{aligned}$$

But $e^{t^2/2}$ is the mgf of the $N(0, 1)$ distribution so, together with the continuity property, the CLT now follows as required.

## CLT example

Suppose $X_1, X_2, \ldots, X_n$ are the IID RVs showing the $n$ sample outcomes of a 6-sided die with common distribution

$$\mathbb{P}(X_i = j) = p_j\,, \qquad j = 1, 2, \ldots, 6$$

Set $S_n = X_1 + X_2 + \cdots + X_n$, the total score obtained, and consider the two cases

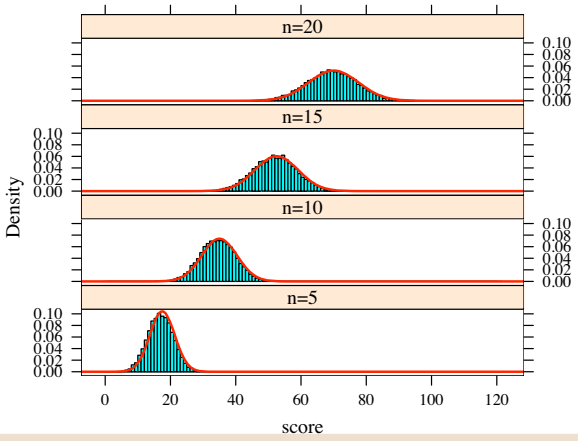
- symmetric: $(p_j) = (1/6, 1/6, 1/6, 1/6, 1/6, 1/6)$ so that $\mu = \mathbb{E}(X_i) = 3.5$ and $\sigma^2 = \mathrm{Var}(X_i) \approx 2.9$
- asymmetric: $(p_j) = (0.2, 0.1, 0.0, 0.0, 0.3, 0.4)$ so that $\mu = \mathbb{E}(X_i) = 4.3$ and $\sigma^2 = \mathrm{Var}(X_i) \approx 4.0$

for varying sample sizes $n = 5, 10, 15$ and 20.
The CLT tells us that for large $n$, $S_n$ is approximately distributed as $N(n\mu, n\sigma^2)$ where $\mu$ and $\sigma^2$ are the mean and variance, respectively, of $X_i$.



## CLT example: symmetric

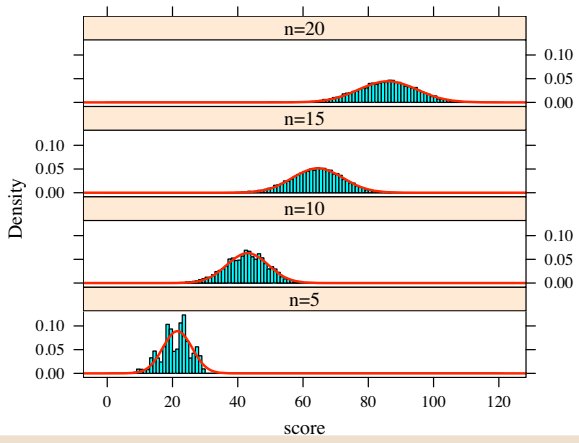
10,000 replications






## CLT example: asymmetric

10,000 replications






## Confidence intervals I

One of the major statistical applications of the CLT is to the construction of confidence intervals. The CLT shows that

$$Z_n = \frac{\overline{X}_n - \mu}{\sigma/\sqrt{n}}$$

is asymptotically distributed as $N(0, 1)$. If, the true value of $\sigma^2$ is unknown we may estimate it by the sample variance given by

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \overline{X}_n)^2\,.$$

For instance, it can be shown that $\mathbb{E}(S^2) = \sigma^2$ and then

$$\frac{\overline{X}_n - \mu}{S/\sqrt{n}}$$

is approximately distributed as $N(0, 1)$ for large $n$.



## Confidence intervals II

Define $z_\alpha$ so that $\mathbb{P}(Z > z_\alpha) = \alpha$ where $Z \sim N(0, 1)$ and so

$$\mathbb{P}(-z_{\alpha/2} < Z < z_{\alpha/2}) = 1 - \alpha\,.$$

Hence,

$$\mathbb{P}\left(-z_{\alpha/2} < \frac{\overline{X}_n - \mu}{S/\sqrt{n}} < z_{\alpha/2}\right) \approx 1 - \alpha$$

$$\mathbb{P}\left(\overline{X}_n - z_{\alpha/2}\frac{S}{\sqrt{n}} < \mu < \overline{X}_n + z_{\alpha/2}\frac{S}{\sqrt{n}}\right) \approx 1 - \alpha\,.$$

The interval $\overline{X}_n \pm z_{\alpha/2}S/\sqrt{n}$ is thus an (approximate) $100(1-\alpha)$ percent confidence interval for the unknown parameter $\mu$.



## Confidence intervals: example

Consider a collection of $n$ IID RVs, $X_i$, with common distribution $X_i \sim \mathrm{Pois}(\lambda)$. Hence,

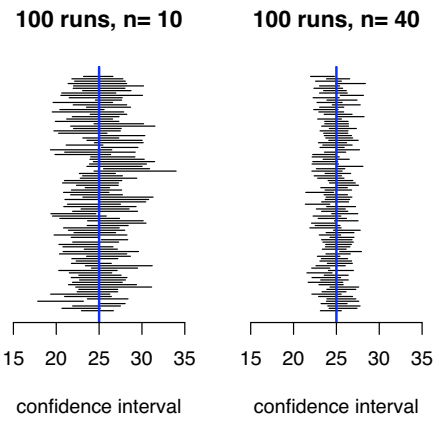
$$\mathbb{P}(X_i = j) = \frac{\lambda^j e^{-\lambda}}{j!} \qquad j = 0, 1, \ldots$$

with mean $\mathbb{E}(X_i) = \lambda$.
Then a 95% confidence interval for the (unknown) mean value $\lambda$ is given by

$$\overline{X}_n \pm 1.96S/\sqrt{n}$$

where $z_{0.025} = 1.96$.
Alternatively, to obtain 99% confidence intervals replace 1.96 by $z_{0.005} = 2.58$.

## Confidence intervals: illustration with $\lambda = 25$






## Monte Carlo simulation

Suppose we wish to estimate the value of $\pi$. One way to proceed is to perform the following experiment. Select a point $(X, Y) \in [-1, 1] \times [-1, 1]$, the square of side 2 and area 4 units, with $X$ and $Y$ chosen independently and uniformly in $[-1, 1]$. Now consider those points within unit distance of the origin then

$$\mathbb{P}((X, Y) \text{ lies in unit circle}) = \mathbb{P}(X^2 + Y^2 \leq 1) = \frac{\text{area of circle}}{\text{area of square}} = \frac{\pi}{4}.$$

Suppose we have access to a stream of random variables $U_i \sim U(0, 1)$ then $2U_i - 1 \sim U(-1, 1)$. Now set $X_i = 2U_{2i-1} - 1$, $Y_i = 2U_{2i} - 1$ and $H_i = \mathbb{I}(\{X_i^2 + Y_i^2 \leq 1\})$ so that

$$\mathbb{E}(H_i) = \mathbb{P}(X_i^2 + Y_i^2 \leq 1) = \frac{\pi}{4}.$$

Then by the SLLN the proportion of points $(X_i, Y_i)$ falling within the unit circle converges almost surely to $\pi/4$.



## Markov Chains



## Markov chains

### Definition (Markov chain)

Suppose that $(X_n)$ $n \geq 0$ is a sequence of discrete random variables taking values in some countable state space $S$. The sequence $(X_n)$ is a Markov chain if

$$\mathbb{P}(X_n = x_n | X_0 = x_0, X_1 = x_1, \ldots, X_{n-1} = x_{n-1}) = \mathbb{P}(X_n = x_n | X_{n-1} = x_{n-1})$$

for all $n \geq 1$ and for all $x_0, x_1, \ldots, x_n \in S$.

Since, $S$ is countable we can always choose to label the possible values of $X_n$ by integers and say that when $X_n = i$ the Markov chain is in the "$i^{th}$ state at the $n^{th}$ step" or "visits $i$ at time $n$".



## Transition probabilities

The dynamics of the Markov chain are governed by the transition probabilites $\mathbb{P}(X_n = j | X_{n-1} = i)$.

### Definition (time-homogeneous MC)

A Markov chain $(X_n)$ is time-homogeneous if

$$\mathbb{P}(X_n = j | X_{n-1} = i) = \mathbb{P}(X_1 = j | X_0 = i)$$

for all $n \geq 1$ and states $i, j \in S$.

- We shall assume that our MCs are time-homogeneous unless explicitly stated otherwise.



## Transition matrix

### Definition (Transition matrix)

The transition matrix, $P$, of a MC $(X_n)$ is given by $P = (p_{ij})$ where for all $i, j \in S$

$$p_{ij} = \mathbb{P}(X_n = j | X_{n-1} = i).$$

- Note that $P$ is a stochastic matrix, that is, it has non-negative entries ($p_{ij} \geq 0$) and the row sums all equal one ($\sum_j p_{ij} = 1$).
- The transition matrix completely characterizes the dynamics of the MC.

## Example

Suppose the states of the MC are $S = \{1, 2, 3\}$ and that the transition matrix is given by

$$P = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/2 & 0 & 1/2 \\ 2/3 & 0 & 1/3 \end{pmatrix}.$$

- Thus, in state 1 we are equally likely to be in any of the three states at the next step.
- In state 2, we can move with equal probabilities to 1 or 3 at the next step.
- Finally in state 3, we either move to state 1 with probability $2/3$ or remain in state 3 at the next step.



## $n$-step transition matrix

### Definition ($n$-step transition matrix)

The $n$-step transition matrix is $P^{(n)} = (p_{ij}^{(n)})$ where

$$p_{ij}^{(n)} = \mathbb{P}(X_n = j | X_0 = i).$$

Thus $P^{(1)} = P$ and we also set $P^{(0)} = I$, the identity matrix.



## Chapman-Kolmogorov equations

### Theorem (Chapman-Kolmogorov)

*For all states $i, j$ and for all steps $m, n$*

$$p_{ij}^{(m+n)} = \sum_k p_{ik}^{(m)} p_{kj}^{(n)}.$$

*Hence, $P^{(m+n)} = P^{(m)} P^{(n)}$ and $P^{(n)} = P^n$, the $n^{th}$ power of $P$.*

### Proof.

$$\begin{aligned} p_{ij}^{(m+n)} &= \mathbb{P}(X_{m+n} = j | X_0 = i) = \sum_k \mathbb{P}(X_{m+n} = j, X_m = k | X_0 = i) \\ &= \sum_k \mathbb{P}(X_{m+n} = j | X_m = k, X_0 = i) \mathbb{P}(X_m = k | X_0 = i) \\ &= \sum_k \mathbb{P}(X_{m+n} = j | X_m = k) \mathbb{P}(X_m = k | X_0 = i) \\ &= \sum_k p_{kj}^{(n)} p_{ik}^{(m)} \end{aligned}$$



The Chapman-Kolmorgorov equations tell us how the long-term evolution of the MC depends on the short-term evolution specified by the transition matrix.
If we let $\lambda_i^{(n)} = \mathbb{P}(X_n = i)$ be the elements of a row vector $\lambda^{(n)}$ specifying the distribution of the MC at the $n^{th}$ time step then the follow holds.

### Lemma

$$\lambda^{(m+n)} = \lambda^{(m)} P^{(n)}$$

*and so,*

$$\lambda^{(n)} = \lambda^{(0)} P^{(n)}$$

*where $\lambda^{(0)}$ is the initial distribution $\lambda_i^{(0)} = \mathbb{P}(X_0 = i)$.*

### Proof.

$$\begin{aligned} \lambda_j^{(m+n)} &= \mathbb{P}(X_{m+n} = j) = \sum_i \mathbb{P}(X_{m+n} = j | X_m = i) \mathbb{P}(X_m = i) \\ &= \sum_i \lambda_i^{(m)} p_{ij}^{(n)} = \left(\lambda^{(m)} P^{(n)}\right)_j \end{aligned}$$



## Classification of states

### Definition (Accessibility)

If, for some $n \geq 0$, $p_{ij}^{(n)} > 0$ then we say that state $j$ is accessible from state $i$, written $i \rightsquigarrow j$.
If $i \rightsquigarrow j$ and $j \rightsquigarrow i$ then we say that $i$ and $j$ communicate, written $i \leftrightsquigarrow j$.

Observe that the relation communicates $\leftrightsquigarrow$ is

- reflexive
- symmetric
- transitive

and hence is an equivalence relation. The corresponding equivalence classes partition the state space into subsets of states, called communicating classes, that communicate with each other.



## Irreducibility

- A communicating class, $C$, that once entered can not be left is called closed, that is $p_{ij} = 0$ for all $i \in C, j \notin C$.
- A closed communicating class consisting of a single state is called absorbing.
- When the state space forms a single communicating class, the MC is called irreducible and is called reducible otherwise.

## Recurrence and transience

Write for $n \geq 1$

$$f_{ij}^{(n)} = \mathbb{P}(X_1 \neq j, \ldots, X_{n-1} \neq j, X_n = j | X_0 = i)$$

so that $f_{ij}^{(n)}$ is the probability starting in state $i$ that we visit state $j$ for the first time at time $n$. Also, let

$$f_{ij} = \sum_{n \geq 1} f_{ij}^{(n)}$$

the probability that we ever visit state $j$, starting in state $i$.

### Definition

- If $f_{ii} < 1$ then state $i$ is transient
- If $f_{ii} = 1$ then state $i$ is recurrent.



## Recurrence and transience, ctd

- Observe that if we return to a state $i$ at some time $n$ then the evolution of the MC is independent of the path before time $n$. Hence, the probability that we will return at least $N$ times is $f_{ii}^N$.
- Now, if $i$ is recurrent $f_{ii}^N = 1$ for all $N$ and we are sure to return to state $i$ infinitely often.
- Conversely, if state $i$ is transient then $f_{ii}^N \to 0$ as $N \to \infty$ and so there is zero probability of returning infinitely often.



### Theorem

- *$i$ is transient* $\Leftrightarrow \sum_{n \geq 1} p_{ii}^{(n)}$ *converges*
- *$i$ is recurrent* $\Leftrightarrow \sum_{n \geq 1} p_{ii}^{(n)}$ *diverges*

*If $i$ and $j$ belong to the same communicating class then they are either both recurrent or both transient — the solidarity property.*

### Proof

First, define generating functions

$$P_{ii}(z) = \sum_{n=0}^{\infty} p_{ii}^{(n)} z^n \quad \text{and} \quad F_{ii}(z) = \sum_{n=0}^{\infty} f_{ii}^{(n)} z^n$$

where we take $p_{ii}^{(0)} = 1$ and $f_{ii}^{(0)} = 0$.



By examining the first time, $r$, that we return to $i$, we have for $m = 1, 2, \ldots$ that

$$p_{ii}^{(m)} = \sum_{r=1}^{m} f_{ii}^{(r)} p_{ii}^{(m-r)} .$$

Now multiply by $z^m$ and summing over $m$ we get

$$\begin{aligned} P_{ii}(z) &= 1 + \sum_{m=1}^{\infty} z^m p_{ii}^{(m)} \\ &= 1 + \sum_{m=1}^{\infty} z^m \sum_{r=1}^{m} f_{ii}^{(r)} p_{ii}^{(m-r)} \\ &= 1 + \sum_{r=1}^{\infty} f_{ii}^{(r)} z^r \sum_{m=r}^{\infty} p_{ii}^{(m-r)} z^{m-r} \\ &= 1 + F_{ii}(z) P_{ii}(z) \end{aligned}$$



Thus, $P_{ii}(z) = 1/(1 - F_{ii}(z))$. Now let $z \nearrow 1$ then $F_{ii}(z) \to F_{ii}(1) = f_{ii}$ and $P_{ii}(z) \to \sum_n p_{ii}^{(n)}$.
If $i$ is transient then $f_{ii} < 1$ so $\sum_n p_{ii}^{(n)}$ converges. Conversely, if $i$ is recurrent then $f_{ii} = 1$ and $\sum_n p_{ii}^{(n)}$ diverges.
Furthermore, if $i$ and $j$ are in the same class then there exist $m$ and $n$ so that $p_{ij}^{(m)} > 0$ and $p_{ji}^{(n)} > 0$. Now, for all $r \geq 0$

$$p_{ii}^{(m+r+n)} \geq p_{ij}^{(m)} p_{jj}^{(r)} p_{ji}^{(n)}$$

so that $\sum_r p_{jj}^{(r)}$ and $\sum_k p_{ii}^{(k)}$ diverge or converge together. □



## Mean recurrence time

First, let

$$T_j = \min\{n \geq 1 : X_n = j\}$$

be the time of the first visit to state $j$ and set $T_j = \infty$ if no such visit ever occurs.
Thus, $\mathbb{P}(T_i = \infty | X_0 = i) > 0$ if and only if $i$ is transient in which case $\mathbb{E}(T_i | X_0 = i) = \infty$.

### Definition (Mean recurrence time)

The mean recurrent time, $\mu_i$, of a state $i$ is defined as

$$\mu_i = \mathbb{E}(T_i | X_0 = i) = \begin{cases} \sum_n n f_{ii}^{(n)} & \text{if } i \text{ is recurrent} \\ \infty & \text{if } i \text{ is transient} . \end{cases}$$

- Note that $\mu_i$ may still be infinite when $i$ is recurrent.

## Positive and null recurrence

### Definition

A recurrent state $i$ is

- positive recurrent if $\mu_i < \infty$ and
- null recurrent if $\mu_i = \infty$.

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## Example: simple random walk

Recall the simple random walk where $X_n = \sum_{i=1}^{n} Y_i$ where $(Y_n)$ are IID RVs with $\mathbb{P}(Y_i = 1) = p = 1 - \mathbb{P}(Y_i = -1)$. Thus $X_n$ is the position after $n$ steps where we take unit steps up or down with probabilities $p$ and $1 - p$, respectively.
It is clear that return to the origin is only possible after an even number of steps. Thus the sequence $(p_{00}^{(n)})$ alternates between zero and a positive value.

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## Periodicity

Let $d_i$ be the greatest common divisor of $\{n : p_{ii}^{(n)} > 0\}$.

### Definition

- If $d_i = 1$ then $i$ is aperiodic.
- If $d_i > 1$ then $i$ is periodic with period $d_i$.

- It may be shown that the period is a class property, that is, if $i, j \in C$ then $d_i = d_j$.

We will now concentrate on irreducible and aperiodic Markov chains.

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## Stationary distributions

### Definition

The vector $\pi = (\pi_j; j \in S)$ is a stationary distribution for the MC with transition matrix $P$ if

1. $\pi_j \geq 0$ for all $j \in S$ and $\sum_{j \in S} \pi_j = 1$
2. $\pi = \pi P$, or equivalently, $\pi_j = \sum_{i \in S} \pi_i p_{ij}$.

Such a distribution is stationary in the sense that $\pi P^2 = (\pi P)P = \pi P = \pi$ and for all $n \geq 0$

$$\pi P^n = \pi .$$

Thus if $X_0$ has distribution $\pi$ then $X_n$ has distribution $\pi$ for all $n$. Moreover, $\pi$ is the limiting distribution of $X_n$ as $n \to \infty$.

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## Markov's example

Markov was lead to the notion of a Markov chain by study the patterns of vowels and consonants in text. In his original example, he found a transition matrix for the states $\{\text{vowel}, \text{consonant}\}$ as

$$P = \begin{pmatrix} 0.128 & 0.872 \\ 0.663 & 0.337 \end{pmatrix} .$$

Taking successive powers of $P$ we find

$$P^2 = \begin{pmatrix} 0.595 & 0.405 \\ 0.308 & 0.692 \end{pmatrix} \quad P^3 = \begin{pmatrix} 0.345 & 0.655 \\ 0.498 & 0.502 \end{pmatrix} \quad P^4 = \begin{pmatrix} 0.478 & 0.522 \\ 0.397 & 0.603 \end{pmatrix} .$$

As $n \to \infty$,

$$P^n \to \begin{pmatrix} 0.432 & 0.568 \\ 0.432 & 0.568 \end{pmatrix} .$$

Check that $\pi = (0.432, 0.568)$ is a stationary distribution, that is $\pi P = \pi$.

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## Limiting behaviour as $n \to \infty$

### Theorem (Erdös-Feller-Pollard)

*For all states $i$ and $j$ in an irreducible, aperiodic MC,*

1. *if the chain is transient, $p_{ij}^{(n)} \to 0$*
2. *if the chain is recurrent, $p_{ij}^{(n)} \to \pi_j$, where*
   - 2.1 *(null recurrent) either, every $\pi_j = 0$*
   - 2.2 *(positive recurrent) or, every $\pi_j > 0$, $\sum_j \pi_j = 1$ and $\pi$ is the unique probability distribution solving $\pi P = \pi$.*
3. *In case (2), let $T_i$ be the time to return to $i$ then $\mu_i = \mathbb{E}(T_i) = 1/\pi_i$ with $\mu_i = \infty$ if $\pi_i = 0$.*

### Proof.

Omitted. □

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## Remarks

- The limiting distribution, $\pi$, is seen to be a stationary one. Suppose the current distribution is given by $\pi$ and consider the evolution of the MC for a further period of $T$ steps. Since $\pi$ is stationary, the probability of being in any state $i$ remains $\pi_i$, so we will make around $T\pi_i$ visits to $i$. Consequently, the mean time between visits to $i$ would be $T/(T\pi_i) = 1/\pi_i$.
- Using $\lambda_j^{(n)} = \mathbb{P}(X_n = j)$ and since $\lambda^{(n)} = \lambda^{(0)}P^n$
  1. for transient or null recurrent states $\lambda^{(n)} \to 0$, that is, $\mathbb{P}(X_n = j) \to 0$ for all states $j$
  2. for a positive recurrent state, $p^{(n)} \to \pi > 0$, that is, $\mathbb{P}(X_n = j) \to \pi_j > 0$ for all $j$, where $\pi$ is the unique probability vector solving $\pi P = \pi$.
- Note the distinction between a transient and a null recurrent chain is that in a transient chain we might never make a return visit to some state $i$ and there is zero probability that we will return infinitely often. However, in a null recurrent chain we are sure to make infinitely many return visits but the mean time between consecutive visits is infinite.



## Time-reversibility

Suppose now that $(X_n : -\infty < n < \infty)$ is an irreducible, postive recurrent MC with transition matrix $P$ and unique stationary distribution $\pi$. Suppose also that $X_n$ has the distribution $\pi$ for all $-\infty < n < \infty$. Now define the reversed chain by

$$Y_n = X_{-n} \qquad \text{for } -\infty < n < \infty$$

Then $(Y_n)$ is also a MC and where $Y_n$ has the distribution $\pi$.

### Definition (Reversibility)

A MC $(X_n)$ is reversible if the transition matrices of $(X_n)$ and $(Y_n)$ are equal.



### Theorem

*A MC $(X_n)$ is reversible if and only if*

$$\pi_i p_{ij} = \pi_j p_{ji} \qquad \text{for all } i, j \in S\,.$$

### Proof.

Consider the transition probabilities $q_{ij}$ ofthe MC $(Y_n)$ then

$$\begin{aligned} q_{ij} &= \mathbb{P}(Y_{n+1} = j | Y_n = i) \\ &= \mathbb{P}(X_{-n-1} = j | X_{-n} = i) \\ &= \mathbb{P}(X_m = i | X_{m-1} = j)\mathbb{P}(X_{m-1} = j)/\mathbb{P}(X_m = i) \qquad \text{where } m = -n \\ &= p_{ji}\pi_j/\pi_i\,. \end{aligned}$$

Hence, $p_{ij} = q_{ij}$ if and only if $\pi_i p_{ij} = \pi_j p_{ji}$. □



### Theorem

*For an irreducible chain, if there exists a vector $\pi$ such that*

1. $0 \le \pi_i \le 1$ *and* $\sum_i \pi = 1$
2. $\pi_i p_{ij} = \pi_j p_{ji}$ *for all* $i, j \in S$

*then the chain is reversible and positive recurrent, with stationary distribution $\pi$.*

### Proof.

Suppose that $\pi$ satisfies the conditions of the theorem then

$$\sum_i \pi_i p_{ij} = \sum_i \pi_j p_{ji} = \pi_j \sum_i p_{ji} = \pi_j$$

and so $\pi = \pi P$ and the distribution is stationary. □

The conditions $\pi_i p_{ij} = \pi_j p_{ji}$ for all $i, j \in S$ are known as the local balance conditions.



## Ehrenfest model

Suppose we have two containers $A$ and $B$ containing a total of $m$ balls. At each time step a ball is chosen uniformly at random and switched between containers. Let $X_n$ be the number of balls in container $A$ after $n$ units of time. Thus, $(X_n)$ is a MC with transition matrix given by

$$p_{i,i+1} = 1 - \frac{i}{m}\,, \qquad p_{i,i-1} = \frac{i}{m}\,.$$

Instead of solving the equations $\pi = \pi P$ we look for solutions to

$$\pi_i p_{ij} = \pi_j p_{ji}$$

which yields $\pi_i = \binom{m}{i}(\frac{1}{2})^m$, a binomial distribution with parameters $m$ and $\frac{1}{2}$.



## Random walk on a graph

Consider a graph $G$ consisting of a countable collection of vertices $i \in N$ and a finite collection of edges $(i, j) \in E$ joining (unordered) pairs of vertices. Assume also that $G$ is connected. A natural way to construct a MC on $G$ uses a random walk through the vertices. Let $v_i$ be the number of edges incident at vertex $i$. The random walk then moves from vertex $i$ by selecting one of the $v_i$ edges with equal probability $1/v_i$. So the transition matrix, $P$, is

$$p_{ij} = \begin{cases} \frac{1}{v_i} & \text{if } (i,j) \text{ is an edge} \\ 0 & \text{otherwise}\,. \end{cases}$$

Since $G$ is connected, $P$ is irreducible. The local balance conditions for $(i,j) \in E$ are

$$\pi_i p_{ij} = \pi_j p_{ji}$$
$$\pi_i \frac{1}{v_i} = \pi_j \frac{1}{v_j}$$
$$\frac{\pi_i}{\pi_j} = \frac{v_i}{v_j}.$$

Hence,

$$\pi_i \propto v_i$$

and the normalization condition $\sum_{i \in N} \pi_i = 1$ gives

$$\pi_i = \frac{v_i}{\sum_{j \in N} v_j}$$

and $P$ is reversible.



## Ergodic results

Ergodic results tell us about the limiting behaviour of averages taken over time. In the case of Markov Chains we shall consider the long-run proportion of time spent in a given state.
Let $V_i(n)$ be the number of visits to $i$ before time $n$ then

$$V_i(n) = \sum_{k=0}^{n-1} \mathbb{I}(\{X_k = i\}).$$

Thus, $V_i(n)/n$ is the proportion of time spent in state $i$ before time $n$.

### Theorem (Ergodic theorem)

*Let $(X_n)$ be a MC with irreducible transition matrix $P$ then*

$$\mathbb{P}\left(\frac{V_i(n)}{n} \to \frac{1}{\mu_i} \quad as \quad n \to \infty\right) = 1$$

*where $\mu_i = \mathbb{E}(T_i | X_0 = i)$ is the expected return time to state $i$.*



### Proof

If $P$ is transient then the total number of visits, $V_i$, to $i$ is finite with probability one, so

$$\frac{V_i(n)}{n} \leq \frac{V_i}{n} \to 0 = \frac{1}{\mu_i} \quad n \to \infty.$$

Alternatively, if $P$ is recurrent let $Y_i^{(r)}$ be the $r^{th}$ duration between visits to any given state $i$. Then $Y_i^{(1)}, Y_i^{(2)}, \ldots$ are non-negative IID RVs with $\mathbb{E}(Y_i^{(r)}) = \mu_i$.
But

$$Y_i^{(1)} + \cdots + Y_i^{(V_i(n)-1)} \leq n - 1$$

since the time of the last visit to $i$ before time $n$ occurs no later than time $n-1$ and

$$Y_i^{(1)} + \cdots + Y_i^{(V_i(n))} \geq n$$

since the time of the first visit to $i$ after time $n-1$ occurs no earlier than time $n$.



Hence,

$$\frac{Y_i^{(1)} + \cdots + Y_i^{(V_i(n)-1)}}{V_i(n)} \leq \frac{n}{V_i(n)} \leq \frac{Y_i^{(1)} + \cdots + Y_i^{(V_i(n))}}{V_i(n)}.$$

However, by the SLLN,

$$\mathbb{P}\left(\frac{Y_i^{(1)} + \cdots + Y_i^{(n)}}{n} \to \mu_i \quad \text{as} \quad n \to \infty\right) = 1$$

and for $P$ recurrent we know that $\mathbb{P}(V_i(n) \to \infty \quad \text{as} \quad n \to \infty) = 1$.
So,

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

which implies

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

□



## Example: random surfing on web graphs

Consider a web graph, $G = (V, E)$, with vertices given by a finite collection of web pages $i \in V$ and (directed) edges given by $(i,j)$ whenever there is a hyperlink from page $i$ to page $j$.
Random walks through the web graph have received much attention in the last few years.
Consider the following model, let $X_n \in V$ be the location (that is, web page visited) by the surfer at time $n$ and suppose we choose $X_{n+1}$ uniformly from the, $L(i)$, outgoing links from $i$, in the case where $L(i) > 0$ and uniformly among all pages in $V$ if $L(i) = 0$ (the dangling page case).



Hence, the transition matrix, $\hat{P}_{ij}$, say, is given by

$$\hat{p}_{ij} = \begin{cases} \frac{1}{L(i)} & \text{if } (i,j) \in E \\ \frac{1}{|V|} & \text{if } L(i) = 0 \\ 0 & \text{otherwise} \end{cases}$$

where $|V|$ is the number of pages (that is, vertices) in the web graph.
A potential problem remains in that $\hat{P}$ may not be irreducible or may be periodic.

We make a further adjustment to ensure irreducibility and aperiodicity as follows.
For $0 \leq \alpha \leq 1$ set

$$p_{ij} = (1-\alpha)\hat{p}_{ij} + \frac{\alpha}{|V|}.$$

We can interpret this as an "easily bored web surfer" model and see that the transitions take the form of a mixture of two distributions.
With probability $1-\alpha$ we follow the randomly chosen outgoing link (unless the page is dangling in which case we move to a randomly chosen page) while with probability $\alpha$ we jump to a random page selected uniformly from the entire set of pages $V$.

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## PageRank

Brin *et al* (1999) used this approach to define PageRank through the limiting distribution of this Markov Chain, that is $\pi_i$ where the vector $\pi$ satisfies

$$\pi = \pi P$$

They report typical values for $\alpha$ of between 0.1 and 0.2.
The ergodic theorem now tells us that the random surfer in this model spends a proportion $\pi_i$ of the time visiting page $i$ — a notion in some sense of the importance of page $i$.
Thus, two pages $i$ and $j$ can be ranked according to the total order defined by

$$i \geq j \quad \text{if and only if} \quad \pi_i \geq \pi_j.$$

See, "The PageRank Citation Ranking: Bring Order to the Web" Sergey Brin, Lawrence Page, Rajeev Motwani and Terry Winograd (1999) Technical Report, Computer Science Department, Stanford University.
`http://dbpubs.stanford.edu:8090/pub/1999-66`

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## Computing PageRank: the power method

We seek a solution to the system of equations

$$\pi = \pi P$$

that is, we are looking for an eigenvector of $P$ (with corresponding eigenvalue of one). Google's computation of PageRank is one of the world's largest matrix computations.
The power method starts from an initial distribution $\pi^{(0)}$, updating $\pi^{(k-1)}$ by the iteration

$$\pi^{(k)} = \pi^{(k-1)}P = \cdots = \pi^{(0)}P^k$$

Advanced methods from linear algebra can be used to speed up convergence of the power method and there has been much study of related MCs, to include web browser back buttons and many other properties and alternative notions of the "importance" of a web page.

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## Hidden Markov Models

An extension of Markov Chains is provided by Hidden Markov Models (HMM) where a statistical model of observed data is constructed from an underlying but usually hidden Markov Chain.
Such models have proved very popular in a wide variety of fields including

- speech and optical character recognition
- natural language processing
- bioinformatics and genomics.

We shall not consider these applications in any detail but simply introduce the basic ideas and questions that Hidden Markov Models address.

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## A Markov model with hidden states

Suppose we have a MC with transition matrix $P$ but that the states $i$ of the chain are not directly observable. Instead, we suppose that on visiting any state $i$ at time $n$ there is a randomly chosen output value or token, $Y_n$, that is observable.
The probability of observing the output token $t$ when in state $i$ is given by some distribution $b_i$, depending on the state $i$ that is visited.
Thus,

$$\mathbb{P}(Y_n = t | X_n = i) = (b_i)_t$$

where $(b_i)_t$ is the $t^{th}$ component of the distribution $b_i$.
For an excellent introduction to HMM, see "A Tutorial on Hidden Markov Models and Selected Applications in Speech Recognition" Lawence R. Rabiner. Proceedings of the IEEE, Vol 77, No 2, February 1988.

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## Three central questions

There are many variants of this basic setup but three central problems are usually addressed.

### Definition (Evaluation problem)

Given a sequence $y_1, y_2, \ldots, y_n$ of observed output tokens and the parameters of the HMM (namely, $P$, $b_i$ and the distribution for the initial state $X_0$) how do we compute

$$\mathbb{P}(Y_1 = y_1, Y_2 = y_2, \ldots, Y_n = y_n | \text{HMM parameters})$$

that is, the probability of the observed sequence given the model?
Such problems are solved in practice by the forward algorithm.

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A second problem that may occur in an application is the decoding problem.

### Definition (Decoding problem)

Given an observed sequence of output tokens $y_1, y_2, \ldots, y_n$ and the full description of the HMM parameters, how do we find the best fitting corresponding sequence of (hidden) states $i_1, i_2, \ldots, i_n$ of the MC?

Such problems are solved in practice by a dynamic programming approach called the Viterbi algorithm.

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The third important problem is the learning problem.

### Definition (Learning problem)

Given an observed sequence of output tokens $y_1, y_2, \ldots, y_n$, how do we adjust the parameters of the HMM to maximize

$$\mathbb{P}(Y_1 = y_1, Y_2 = y_2, \ldots, Y_n = y_n | \text{HMM parameters})$$

The observed sequence used to adjust the model parameters is called a training sequence. Learning problems are crucial in most applications since they allow us to create the "best" models in real observed processes.
Iterative procedures, known as the Baum-Welch method, are used to solve this problem in practice.

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## Applications of Markov Chains

These and other applications of Markov Chains are important topics in a variety of Part II courses, including

- Artificial Intelligence II
- Bioinformatics
- Computer Systems Modelling

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## §2: Limits and inequalities

1. Suppose that $X$ is a random variable with the $U(-1,1)$ distribution. Find the exact value of $\mathbb{P}(|X| \geq a)$ for each $a > 0$ and compare it to the upper bounds obtained from the Markov and Chebychev inequalities.

2. Let $X$ be the random variable giving the number of heads obtained in a sequence of $n$ fair coin flips. Compare the upper bounds on $\mathbb{P}(X \geq 3n/4)$ obtained from the Markov and Chebychev inequalities.

3. Let $A_i$ $(i = 1, 2, \ldots, n)$ be a collection of random events and set $N = \sum_{i=1}^{n} \mathbb{I}(A_i)$. By considering Markov's inequality applied to $\mathbb{P}(N \geq 1)$ show Boole's inequality, namely,

$$\mathbb{P}\left(\cup_{i=1}^{n} A_i\right) \leq \sum_{i=1}^{n} \mathbb{P}(A_i)\,.$$

4. Let $h : \mathbb{R} \to [0, \infty)$ be a non-negative function. Show that

$$\mathbb{P}(h(X) \geq a) \leq \frac{\mathbb{E}(h(X))}{a} \qquad \text{for all} \qquad a > 0\,.$$

   By making suitable choices of $h(x)$, show that we may obtain the Markov and Chebychev inequalities as special cases.

5. Show the following properties of the moment generating function.

   (a) If $X$ has mgf $M_X(t)$ then $Y = aX + b$ has mgf $M_Y(t) = e^{bt} M_X(at)$.

   (b) If $X$ and $Y$ are independent then $X + Y$ has mgf $M_{X+Y}(t) = M_X(t) M_Y(t)$.

   (c) $\mathbb{E}(X^n) = M_X^{(n)}(0)$ where $M_X^{(n)}$ is the $n^{th}$ derivative of $M_X$.

   (d) If $X$ is a discrete random variable taking values $0, 1, 2, \ldots$ with probability generating function $G_X(z) = \mathbb{E}(z^X)$ then $M_X(t) = G_X(e^t)$.

6. Let $X$ be a random variable with moment generating function $M_X(t)$ which you may assume exists for any value of $t$. Show that for any $a > 0$

$$\mathbb{P}(X \leq a) \leq e^{-ta} M_X(t) \qquad \text{for all} \qquad t < 0\,.$$

7. Show that, if $X_n \xrightarrow{D} X$, where $X$ is a degenerate random variable (that is, $\mathbb{P}(X = \mu) = 1$ for some constant $\mu$) then $X_n \xrightarrow{P} X$.

8. Suppose that you estimate your monthly phone bill by rounding all amounts to the nearest pound. If all rounding errors are independent and distributed as $U(-0.5, 0.5)$, estimate the probability that the total error exceeds one pound when your bill has 12 items. How does this procedure suggest an approximate method for constructing Normal random variables?

9. 2006 Paper 3 Question 10

## §3: Markov chains

1. Suppose that $(X_n)$ is a Markov chain with $n$-step transition matrix, $P^{(n)}$, and let $\lambda_i^{(n)} = \mathbb{P}(X_n = i)$ be the elements of a row vector $\lambda^{(n)}$ $(n = 0, 1, 2, \ldots)$. Show that

   (a) $P^{(m+n)} = P^{(m)}P^{(n)}$ for $m, n = 0, 1, 2, \ldots$

   (b) $\lambda^{(n)} = \lambda^{(0)}P^{(n)}$ for $n = 0, 1, 2, \ldots$.

2. Suppose that $(X_n)$ is a Markov chain with transition matrix $P$. Define the relations *"state $j$ is accessible from state $i$"* and *"states $i$ and $j$ communicate"*. Show that the second relation is an equivalence relation and define the communicating classes as the equivalence classes under this relation. What is meant by the terms *closed class*, *absorbing class* and *irreducible*?

3. Show that
$$P_{ij}(z) = \delta_{ij} + F_{ij}(z)P_{jj}(z)$$
where
$$P_{ij}(z) = \sum_{n=0}^{\infty} p_{ij}^{(n)} z^n, \qquad F_{ij}(z) = \sum_{n=0}^{\infty} f_{ij}^{(n)} z^n$$
and $\delta_{ij} = 1$ if $i = j$ and 0 otherwise. [You should assume that $p_{ij}^{(n)}$ and $f_{ij}^{(n)}$ are as defined in lectures with $p_{ij}^{(0)} = \delta_{ij}$ and $f_{ij}^{(0)} = 0$ for all states $i, j$.]

4. Suppose that $(X_n)$ is a finite state Markov chain and that for some state $i$ and for all states $j$
$$\lim_{n\to\infty} p_{ij}^{(n)} = \pi_j$$
for some collection of numbers $(\pi_j)$. Show that $\pi = (\pi_j)$ is a stationary distribution.

5. Consider the Markov chain with transition matrix
$$P = \begin{pmatrix} 0.128 & 0.872 \\ 0.663 & 0.337 \end{pmatrix}$$
for Markov's example of a chain on the two states $\{\text{vowel}, \text{consonant}\}$ for consecutive letters in a passage of text. Find the stationary distribution for this Markov chain. What are the mean recurrence times for the two states?

6. Define what is meant by saying that $(X_n)$ is a reversible Markov chain and write down the local balance conditions. Show that if a vector $\pi$ is a distribution over the states of the Markov chain that satisfies the local balance conditions then it is a stationary distribution.

7. Consider the Erhenfest model for $m$ balls moving between two containers with transition matrix
$$p_{i,i+1} = 1 - \frac{i}{m}, \qquad p_{i,i-1} = \frac{i}{m}$$
where $i$ $(0 \le i \le m)$ is the number of balls in a given container. Show that the Markov chain is irreducible and periodic with period 2. Derive the stationary distribution.

8. Consider a random walk, $(X_n)$, on the states $i = 0, 1, 2, \ldots$ with transition matrix

$$\begin{aligned} p_{i,i-1} &= p \qquad i = 1, 2, \ldots \\ p_{i,i+1} &= 1 - p \qquad i = 0, 1, \ldots \\ p_{0,0} &= p \end{aligned}$$

where $0 < p < 1$. Show that the Markov chain is irreducible and aperiodic. Find a condition on $p$ to make the Markov chain positive recurrent and find the stationary distribution in this case.

9. Describe PageRank as a Markov chain model for the motion between nodes in a graph. Explain the main mathematical results that underpin PageRank's connection to a notion of web page *"importance"*.

10. 2007 Paper 4 Question 5