

Mathematical Methods for Computer Science

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Michaelmas Term 2005/6
(Last revised on 28 Nov 2005)



Outline

- ▶ Probability methods
 - ▶ Limits and inequalities (3 lectures)
 - ▶ Markov chains (3 lectures)
- ▶ Fourier and related methods
 - ▶ Inner product spaces, Fourier series and transforms (3 lectures)
 - ▶ Discrete Fourier Transform and Fast Fourier Transform (2 lectures)
 - ▶ Wavelets (1 lecture)



Reference books

-  (*) Ross, Sheldon M.
Probability Models for Computer Science.
Harcourt/Academic Press, 2002
-  Mitzenmacher, Michael & Upfal, Eli.
Probability and Computing: Randomized Algorithms and Probabilistic Analysis.
Cambridge University Press, 2005
-  (*) Pinkus, A. & Zafrany, S.
Fourier series and integral transforms.
Cambridge University Press, 1997
-  Oppenheim, A.V. & Willsky, A.S.
Signals and systems.
Prentice-Hall, 1997

Limits and inequalities

We are familiar with limits of real numbers. If $x_n = 1/n$ for $n = 1, 2, \dots$ then $\lim_{n \rightarrow \infty} x_n = 0$ 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.



Notation

	RV	random variable
	IID	independent, identically distributed
$X \sim U(0, 1)$		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 $n = 1, 2, \dots$
	$F_X(x)$	distribution function, $F_X(x) = \mathbb{P}(X \leq x)$
	$f_X(x)$	density of RV X given, when it exists, by $F'_X(x)$



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 μ and finite variance σ^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 for which this expectation exists.

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

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

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



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 $0, 1, 2, \dots$ 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 $t < \lambda$

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

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

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



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,

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



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 $M(t)$ and $a > 0$ then for all $t \geq 0$

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

Proof.

Using Markov's inequality, we have that

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

□

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



Notions of convergence: $X_n \rightarrow X$ as $n \rightarrow \infty$

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

Definition (Convergence in distribution)

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

Definition (Convergence in probability)

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

Definition (Convergence almost surely)

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

Definition (Convergence in r^{th} mean)

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



Convergence theorems

Theorem

If $X_n \xrightarrow{\text{a.s.}} X$ 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

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

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 $\mathbb{P}(|X_n - X| > \epsilon) \rightarrow 0$. So, as $n \rightarrow \infty$, $F_{X_n}(x)$ is squeezed between $F_X(x - \epsilon)$ and $F_X(x + \epsilon)$.

Hence, if F_X is continuous at x , $F_{X_n}(x) \rightarrow F_X(x)$ and so $X_n \xrightarrow{D} X$. \square



Theorem

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

Proof.

Set $Y_n = |X_n - X|$ then by Lyapunov's inequality

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

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



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

$$S_n = X_1 + X_2 + \cdots + X_n \quad \text{and} \quad \bar{X}_n = S_n/n.$$

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

Theorem (Weak Law of Large Numbers/WLLN)

Suppose $(X_n)_{n \geq 1}$ are IID RVs with finite mean μ (and finite variance σ^2) then $\bar{X}_n \xrightarrow{P} \mu$.

Theorem (Strong Law of Large Numbers/SLLN)

Suppose $(X_n)_{n \geq 1}$ are IID RVs with finite mean μ (and finite fourth moment) then $\bar{X}_n \xrightarrow{\text{a.s.}} \mu$.



WLLN

Theorem (Weak Law of Large Numbers/WLLN)

Suppose $(X_n)_{n \geq 1}$ are IID RVs with finite mean μ and finite variance σ^2 then $\bar{X}_n \xrightarrow{P} \mu$.

Proof.

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

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

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

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

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



SLLN

Theorem (Strong Law of Large Numbers/SLLN)

Suppose $(X_n)_{n \geq 1}$ are IID RVs with finite mean μ (and finite fourth moment) then $\bar{X}_n \xrightarrow{\text{a.s.}} \mu$.

Proof.

Omitted. □



Applications: estimating probabilities

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

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

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

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

by the SLLN.

Thus we have shown the important result that the empirical estimate of the probability of some event 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

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

where Shannon's *entropy* is defined by

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

and

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

is the joint probability distribution of the n IID RVs X_1, X_2, \dots, X_n .



Proof.

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

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



AEP implications

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

$$\lim_{n \rightarrow \infty} \mathbb{P}\left(\left| -\frac{1}{n} \log_2 p(X_1, X_2, \dots, X_n) - H(X) \right| \leq \epsilon\right) = 1$$

$$\lim_{n \rightarrow \infty} \mathbb{P}(H(X) - \epsilon \leq -\frac{1}{n} \log_2 p(X_1, X_2, \dots, X_n) \leq H(X) + \epsilon) = 1$$

$$\lim_{n \rightarrow \infty} \mathbb{P}(-n(H(X) + \epsilon) \geq \log_2 p(X_1, X_2, \dots, X_n) \geq -n(H(X) - \epsilon)) = 1$$

$$\lim_{n \rightarrow \infty} \mathbb{P}(2^{-n(H(X)+\epsilon)} \leq p(X_1, X_2, \dots, X_n) \leq 2^{-n(H(X)-\epsilon)}) = 1$$

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

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

have a high probability and are referred 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 $(X_n)_{n \geq 1}$ be a sequence of IID RVs with mean μ , variance σ^2 and whose moment generating function converges in some interval $-a < t < a$ with $a > 0$. Then

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



Proof of CLT

Set $Y_i = (X_i - \mu)/\sigma$ then $\mathbb{E}(Y_i) = 0$ and $\mathbb{E}(Y_i^2) = \text{Var}(Y_i) = 1$ 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 $t \rightarrow 0$. Also,

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

Hence,

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

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, \dots, X_n are the IID RVs showing the n sample outcomes of a 6-sided die with common distribution

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

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

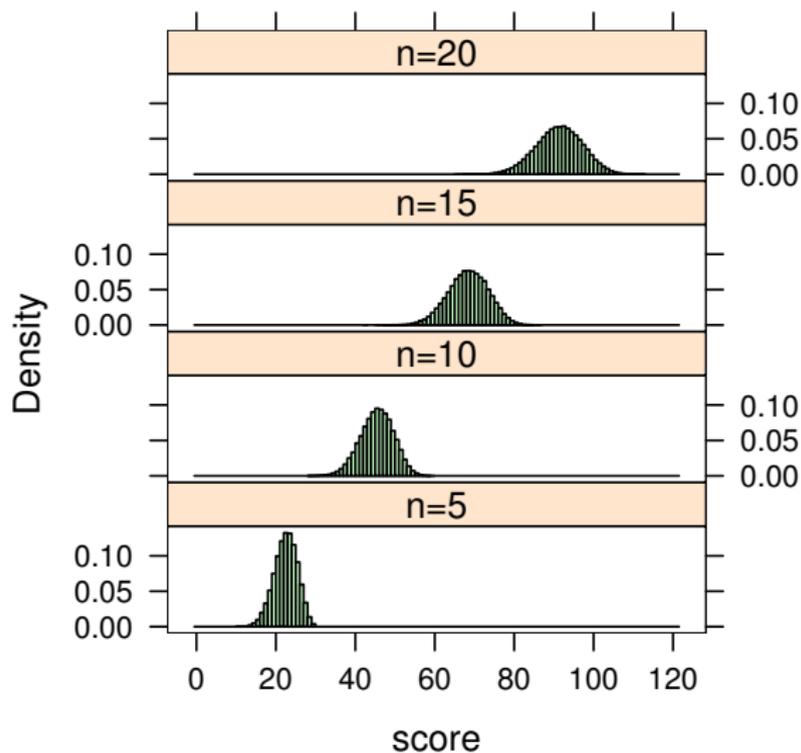
- ▶ **symmetric**: $(p_j) = (1/6, 1/6, 1/6, 1/6, 1/6, 1/6)$
- ▶ **asymmetric**: $(p_j) = (0.2, 0.1, 0.0, 0.0, 0.3, 0.4)$

for varying sample sizes $n = 5, 10, 15$ and 20 .

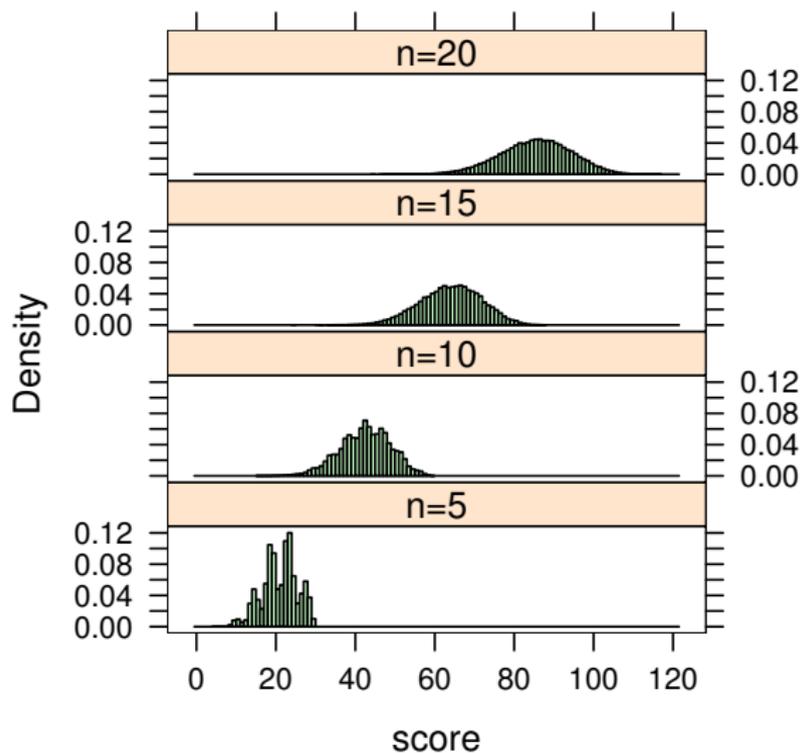
The CLT tells us that for large n , S_n is approximately distributed as $N(n\mu, n\sigma^2)$ where μ and σ^2 are the mean and variance, respectively, of X_i .



CLT example: symmetric



CLT example: asymmetric



Confidence intervals I

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

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

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

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

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

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

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



Confidence intervals II

Define z_α 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,

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

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

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



Confidence intervals: example

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

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

with mean $\mathbb{E}(X_i) = \lambda$.

Then a 95% confidence interval for the mean value λ is given by

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

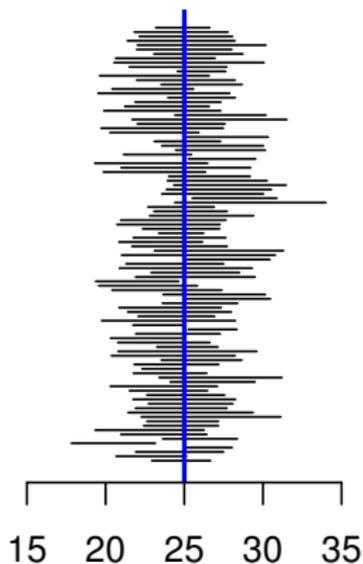
where $z_{0.025} = 1.96$.

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



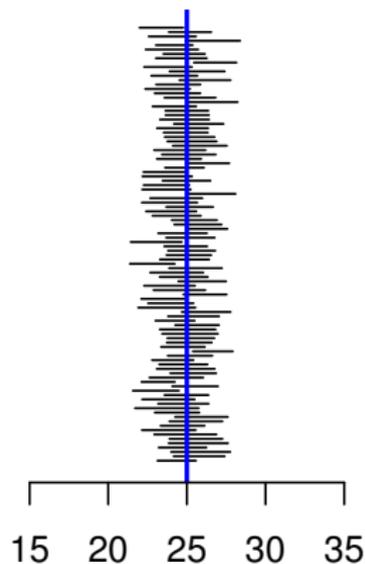
Confidence intervals: illustration

100 runs, $n = 10$



confidence interval

100 runs, $n = 40$



confidence interval



Monte Carlo simulation

Suppose we wish to estimate the value of π . 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

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

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

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

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-Kolmogorov 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 following holds.

Lemma

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

and so,

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

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

Proof.

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



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 $i \leftrightarrow j$.

Observe that the relation **communicates** \leftrightarrow 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 $n \geq 1$

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

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 $f_{ij} < 1$ then state i is **transient**
- ▶ If $f_{ij} = 1$ 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 $f_{ii}^N \rightarrow 0$ as $N \rightarrow \infty$ 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 $m = 1, 2, \dots$ 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 $F_{ii}(z) \rightarrow F_{ii}(1) = f_{ii}$ and $P_{ii}(z) \rightarrow \sum_n p_{ii}^{(n)}$.

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, $\mathbb{P}(T_j = \infty | X_0 = i) > 0$ if and only if i is transient in which case $\mathbb{E}(T_j | X_0 = i) = \infty$.

Definition (Mean recurrence time)

The **mean recurrent time**, μ_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 μ_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 $\mu_i = \infty$.



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.



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.



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 π then X_n has distribution π for all n . Moreover, π is the **limiting distribution** of X_n as $n \rightarrow \infty$.



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 {vowel, 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 $n \rightarrow \infty$,

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

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



Limiting behaviour as $n \rightarrow \infty$

Theorem (Erdős-Feller-Pollard)

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

1. if the chain is transient, $p_{ij}^{(n)} \rightarrow 0$
2. if the chain is recurrent, $p_{ij}^{(n)} \rightarrow \pi_j$, 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 π 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. □



Remarks

- ▶ The limiting distribution, π , is seen to be a stationary one. Suppose the current distribution is given by π and consider the evolution of the MC for a further period of T steps. Since π is stationary, the probability of being in any state i remains π_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 $\lambda^{(n)} \rightarrow 0$, that is, $\mathbb{P}(X_n = j) \rightarrow 0$ for all states j
 2. for a positive recurrent state, $p^{(n)} \rightarrow \pi > 0$, that is, $\mathbb{P}(X_n = j) \rightarrow \pi_j > 0$ for all j , where π 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, positive recurrent MC with transition matrix P and unique stationary distribution π . Suppose also that X_n has the distribution π for all $-\infty < n < \infty$. Now define the **reversed chain** by

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

Then (Y_n) is also a MC and where Y_n has the distribution π .

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

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

Proof.

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

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

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 π such that

1. $0 \leq \pi_i \leq 1$ and $\sum_i \pi_i = 1$
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 π .

Proof.

Suppose that π 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

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

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

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

which yields $\pi_i = \binom{m}{i} \left(\frac{1}{2}\right)^m$, 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

$$\begin{aligned}\pi_i p_{ij} &= \pi_j p_{ji} \\ \pi_i \frac{1}{v_i} &= \pi_j \frac{1}{v_j} \\ \frac{\pi_i}{\pi_j} &= \frac{v_j}{v_i}.\end{aligned}$$

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

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

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

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

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

But

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

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

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

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



Hence,

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

However, by the SLLN,

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

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

So,

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

which implies

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



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

$$p_{ij} = (1 - \alpha)\hat{p}_{ij} + \alpha \mathbf{e}\mathbf{e}^T / |V|$$

where \mathbf{e}^T is a row vector of ones with length $|V|$.

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 α we jump to a random page selected uniformly from the entire set of pages while 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).



PageRank

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

$$\pi = \pi P$$

They report typical values for α of between 0.1 and 0.2.

The ergodic theorem now tells us that the random surfer in this model spends a proportion π_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>



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

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

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.



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.



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” Lawrence R. Rabiner. Proceedings of the IEEE, Vol 77, No 2, February 1988.



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, \dots, 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

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

that is, the probability of the observed sequence given the model?

Such problems are solved in practice by the **forward algorithm**.



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, \dots, 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, \dots, i_n of the MC?

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



The third important problem is the **learning problem**.

Definition (Learning problem)

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

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

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.



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



Fourier and related methods



Introduction

In this section we shall consider what it means to represent a function $f(x)$ in terms of other, perhaps simpler, functions. One example is Fourier series of the form

$$\frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(nx) + b_n \sin(nx)] .$$

How are the coefficients a_n and b_n related to the choice of $f(x)$ and what other representations can we use?

We shall take a quite general approach to these questions and derive the necessary framework that underpins a wide range of applications.



Linear space

Definition (Linear space)

A non-empty set V of **vectors** is a **linear space** over a field F of **scalars** if the following are satisfied.

1. Binary operation $+$ such that if $u, v \in V$ then $u + v \in V$
2. $+$ is associative: for all $u, v, w \in V$
then $(u + v) + w = u + (v + w)$
3. There exists a zero vector, written $\vec{0}$, such that $\vec{0} + v = v$ for all $v \in V$.
4. For all $v \in V$, there exists an inverse vector, written $-v$, such that $v + (-v) = \vec{0}$
5. $+$ is commutative: for all $u, v \in V$ then $u + v = v + u$
6. For all $v \in V$ and $a \in F$ then $av \in V$ is defined
7. For all $a \in F$ and $u, v \in V$ then $a(u + v) = au + av$
8. For all $a, b \in F$ and $v \in V$ then $(a + b)v = av + bv$
and $a(bv) = (ab)v$
9. For all $v \in V$ then $1v = v$, where $1 \in F$ is the unit scalar.



Linear subspaces

Two common choices of scalar fields are the real numbers, \mathbb{R} , and the complex numbers \mathbb{C} , giving rise to **real** and **complex** linear spaces, respectively.

Definition (Linear subspace)

A subset $W \subset V$ is a **linear subspace** of V if the W is again a linear space over the same field of scalars.

Thus W is a linear subspace if $W \neq \emptyset$ and for all $u, v \in W$ and $a, b \in F$ we have that $au + bv \in W$.



Linear combinations and spans

Definition (Linear combinations)

If V is a linear space and $v_1, v_2, \dots, v_n \in V$ are vectors in V then $u \in V$ is a **linear combination** of v_1, v_2, \dots, v_n if there exist scalars a_1, a_2, \dots, a_n such that

$$u = a_1 v_1 + a_2 v_2 + \dots + a_n v_n .$$

We also define

$$\text{span}\{v_1, v_2, \dots, v_n\} = \{u \in V : u \text{ is a linear combination of } v_1, v_2, \dots, v_n\} .$$

Thus, $W = \text{span}\{v_1, v_2, \dots, v_n\}$ is a linear subspace of V .



Linear independence

Definition (Linear independence)

Let V be a linear space. The vectors $v_1, v_2, \dots, v_n \in V$ are **linearly independent** if whenever

$$a_1 v_1 + a_2 v_2 + \dots + a_n v_n = \vec{0} \quad a_1, a_2, \dots, a_n \in F$$

then $a_1 = a_2 = \dots = a_n = 0$

The vectors v_1, v_2, \dots, v_n are **linearly dependent** otherwise.



Bases

Definition (Basis)

A finite set of vectors $v_1, v_2, \dots, v_n \in V$ is a **basis** for the linear space V if v_1, v_2, \dots, v_n are linearly independent and $V = \text{span}\{v_1, v_2, \dots, v_n\}$. The number n is called the **dimension** of V , written $n = \dim(V)$.

A result from linear algebra is that while there are infinitely many choices of basis vectors any two bases will always consist of the same number of element vectors. Thus, the dimension of a linear space is well-defined.



Inner product

Suppose that V is either a real or complex linear space (that is, $F = \mathbb{R}$ or \mathbb{C}).

Definition (Inner product)

The inner product of two vectors $u, v \in V$, written $\langle u, v \rangle \in F$, is a scalar value satisfying

1. For each $v \in V$, $\langle v, v \rangle$ is a non-negative real number, so $\langle v, v \rangle \geq 0$
2. For each $v \in V$, $\langle v, v \rangle = 0$ if and only if $v = \vec{0}$
3. For all $u, v, w \in V$ and $a, b \in F$, $\langle au + bv, w \rangle = a\langle u, w \rangle + b\langle v, w \rangle$
4. For all $u, v \in V$ then $\langle u, v \rangle = \overline{\langle v, u \rangle}$.

A linear space together with an inner product is called an **inner product space**. Here, $\overline{\langle v, u \rangle}$ denotes the complex conjugate of the complex number $\langle v, u \rangle$. When the field of scalars, F , is the real numbers, \mathbb{R} , then $\langle v, u \rangle = \langle v, u \rangle$.



Useful properties of the inner product

Before looking at some examples of inner products there are several consequences of the definition of an inner product that are useful in calculations.

1. For all $v \in V$ and $a \in \mathbb{C}$ then $\langle av, av \rangle = |a|^2 \langle v, v \rangle$
2. For all $v \in V$, $\langle \vec{0}, v \rangle = 0$
3. For all $v \in V$ and finite sequences of vectors $u_1, u_2, \dots, u_n \in V$ and scalars a_1, a_2, \dots, a_n then

$$\left\langle \sum_{i=1}^n a_i u_i, v \right\rangle = \sum_{i=1}^n a_i \langle u_i, v \rangle$$

$$\left\langle v, \sum_{i=1}^n a_i u_i \right\rangle = \sum_{i=1}^n \bar{a}_i \langle v, u_i \rangle$$



Inner product: examples

Example (Euclidean space, \mathbb{R}^n)

$V = \mathbb{R}^n$ with the usual operations of vector addition and multiplication by a scalar is a linear space over \mathbb{R} . Given two vectors $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ in \mathbb{R}^n we can define an inner product

$$\langle x, y \rangle = \sum_{i=1}^n x_i y_i.$$

Often, this inner product is known as the **dot product** and is written $x \cdot y$.

Example

Similarly, for $V = \mathbb{C}^n$, we can define an inner product by

$$\langle x, y \rangle = x \cdot y = \sum_{i=1}^n x_i \bar{y}_i.$$



Example (Space of continuous functions)

$V = C[a, b]$, the space of continuous functions $f : [a, b] \rightarrow \mathbb{C}$ with the standard operations of the sum of two functions and multiplication by a scalar, is a linear space over \mathbb{C} and we can define an inner product for $f, g \in C[a, b]$ by

$$\langle f, g \rangle = \int_a^b f(x) \overline{g(x)} dx .$$



Norms

The concept of a norm is closely related to an inner product and we shall see that there is a natural way to define a norm given an inner product.

Definition (Norm)

Let V be a real or complex linear space. A **norm** on V is a function from V to \mathbb{R}_+ , written $\|v\|$, that satisfies

1. For all $v \in V$, $\|v\| \geq 0$
2. $\|v\| = 0$ if and only if $v = \vec{0}$
3. For each $v \in V$ and $a \in \mathbb{C}$, $\|av\| = |a| \|v\|$
4. For all $u, v \in V$, $\|u + v\| \leq \|u\| + \|v\|$ (the **triangle inequality**).

A norm can be thought of as a generalisation of the notion of **distance**, where for any two vectors $u, v \in V$ the number $\|u - v\|$ is the distance between u and v .



Norms: examples

Example (Euclidean norm)

If $V = \mathbb{R}^n$ or \mathbb{C}^n then for $x = (x_1, x_2, \dots, x_n) \in V$ define

$$\|x\| = \sqrt{\sum_{i=1}^n |x_i|^2}.$$

Example (Uniform norm)

If $V = \mathbb{R}^n$ or \mathbb{C}^n then for $x = (x_1, x_2, \dots, x_n) \in V$ define

$$\|x\|_{\infty} = \max \{|x_i| : i = 1, 2, \dots, n\}.$$

Example (Uniform norm)

If $V = C[a, b]$ then for each function $f \in V$, define

$$\|f\|_{\infty} = \max \{|f(x)| : x \in [a, b]\}.$$



Cauchy-Schwarz inequality

Theorem (Cauchy-Schwarz inequality)

Let V be a real or complex inner product space then for all $u, v \in V$

$$|\langle u, v \rangle|^2 \leq \langle u, u \rangle \langle v, v \rangle.$$

Proof.

If $v = \vec{0}$ then the result holds trivially. Now assume $v \neq \vec{0}$ so that $\langle v, v \rangle \neq 0$ and let $\lambda \in \mathbb{C}$ then

$$0 \leq \langle u - \lambda v, u - \lambda v \rangle = \langle u, u \rangle - \bar{\lambda} \langle u, v \rangle - \lambda \langle v, u \rangle + |\lambda|^2 \langle v, v \rangle$$

Now set $\lambda = \frac{\langle u, v \rangle}{\langle v, v \rangle}$ so that

$$0 \leq \langle u, u \rangle - \frac{|\langle u, v \rangle|^2}{\langle v, v \rangle}$$

and hence

$$|\langle u, v \rangle|^2 \leq \langle u, u \rangle \langle v, v \rangle.$$



Inner products and norms

Given an inner product space, V , with inner product $\langle \cdot, \cdot \rangle$ there is a natural choice of norm, namely, for all $v \in V$

$$\|v\| = \sqrt{\langle v, v \rangle}$$

that is, the non-negative square root.

Most of the properties that make this a norm follow simply from the properties of the inner product but we shall use the Cauchy-Schwarz inequality to establish the triangle inequality. We have,

$$\begin{aligned}\|u + v\|^2 &= \langle u + v, u + v \rangle \\ &= \|u\|^2 + \langle u, v \rangle + \langle v, u \rangle + \|v\|^2 \\ &\leq \|u\|^2 + 2|\langle u, v \rangle| + \|v\|^2 \\ &\leq \|u\|^2 + 2\|u\| \|v\| + \|v\|^2 \\ &= (\|u\| + \|v\|)^2.\end{aligned}$$

Hence, the triangle inequality, $\|u + v\| \leq \|u\| + \|v\|$ holds.



Orthogonal and orthonormal systems

Let V be an inner product space.

Definition (Orthogonality)

We say that $u, v \in V$ are **orthogonal** if $\langle u, v \rangle = 0$, written $u \perp v$.

Definition (Orthogonal system)

A finite or infinite sequence of vectors (u_i) in V is an **orthogonal system** if

1. $u_i \neq \vec{0}$ for all such vectors u_i
2. $u_i \perp u_j$ for all $i \neq j$.

Definition (Orthonormal system)

An orthogonal system is called an **orthonormal system** if, in addition, $\|u_i\| = 1$ for all such vectors u_i .

A vector $v \in V$ such that $\|v\| = 1$ is called a **unit vector**.



Theorem

Suppose that $\{e_1, e_2, \dots, e_n\}$ is an orthonormal system in the inner product space V . If $u = \sum_{i=1}^n a_i e_i$ then $a_i = \langle u, e_i \rangle$.

Proof.

$$\begin{aligned}\langle u, e_i \rangle &= \langle a_1 e_1 + a_2 e_2 + \dots + a_n e_n, e_i \rangle \\ &= a_1 \langle e_1, e_i \rangle + a_2 \langle e_2, e_i \rangle + \dots + a_n \langle e_n, e_i \rangle \\ &= a_i.\end{aligned}$$



Hence, if $\{e_1, e_2, \dots, e_n\}$ is an orthonormal system then for all $u \in \text{span}\{e_1, e_2, \dots, e_n\}$ we have

$$u = \sum_{i=1}^n a_i e_i = \sum_{i=1}^n \langle u, e_i \rangle e_i.$$



Fourier coefficients

Let V be an inner product space and e_1, e_2, \dots, e_n an orthonormal system (n being finite or infinite).

Definition (Generalized Fourier coefficients)

Given a vector $u \in V$, the scalars $\langle u, e_i \rangle$ ($i = 1, 2, \dots, n$) are called the **Generalized Fourier coefficients** of u with respect to the given orthonormal system.

These coefficients are generalized in the sense that they refer to a general orthonormal system.



Let V be an inner product space and e_1, e_2, \dots, e_n an orthonormal system. If a_1, a_2, \dots, a_n and b_1, b_2, \dots, b_n are any sequences of scalars then

$$\left\langle \sum_{i=1}^n a_i e_i, \sum_{i=1}^n b_i e_i \right\rangle = \sum_{i=1}^n a_i \overline{b_i}.$$

Equivalently, for $u, v \in \text{span}\{e_1, e_2, \dots, e_n\}$

$$\langle u, v \rangle = \sum_{i=1}^n \langle u, e_i \rangle \overline{\langle v, e_i \rangle}.$$

A consequence of these relations is the following theorem.

Theorem (Generalized Pythagorean Theorem)

Suppose that $\{u_1, u_2, \dots, u_n\}$ is an orthogonal system in V and a_1, a_2, \dots, a_n are scalars then

$$\left\| \sum_{i=1}^n a_i u_i \right\|^2 = \sum_{i=1}^n |a_i|^2 \|u_i\|^2.$$



Orthogonal projections

Suppose that V is an inner product space and e_1, e_2, \dots, e_n an orthonormal system. Define $W = \text{span}\{e_1, e_2, \dots, e_n\}$ and let $u \in V$ be any vector. We have seen that for $u \in W$

$$u = \sum_{i=1}^n \langle u, e_i \rangle e_i$$

but if $u \notin W$ then certainly

$$u \neq \sum_{i=1}^n \langle u, e_i \rangle e_i$$

since u is not a linear combination of the vectors e_1, e_2, \dots, e_n . Nevertheless, there is a close connection between u and the expression $\sum_{i=1}^n \langle u, e_i \rangle e_i$.

Definition (Orthogonal projection)

For all $u \in V$ we define the **orthogonal projection of u in W** , \tilde{u} , by

$$\tilde{u} = \sum_{i=1}^n \langle u, e_i \rangle e_i.$$



Theorem

For each $u \in V$ and for all $w \in W$

1. $\langle u - \tilde{u}, w \rangle = 0$
2. $\|u - w\|^2 = \|u - \tilde{u}\|^2 + \|\tilde{u} - w\|^2.$

Proof

First $\langle u - \tilde{u}, e_j \rangle = 0$ for all $j = 1, 2, \dots, n$ since

$$\begin{aligned}\langle u - \tilde{u}, e_j \rangle &= \langle u, e_j \rangle - \left\langle \sum_{i=1}^n \langle u, e_i \rangle e_i, e_j \right\rangle = \langle u, e_j \rangle - \sum_{i=1}^n \langle u, e_i \rangle \langle e_i, e_j \rangle \\ &= \langle u, e_j \rangle - \langle u, e_j \rangle \langle e_j, e_j \rangle = \langle u, e_j \rangle - \langle u, e_j \rangle = 0.\end{aligned}$$



So take any $w \in W$ with $w = \sum_{j=1}^n b_j e_j$ for some scalars b_1, b_2, \dots, b_n and

$$\langle u - \tilde{u}, w \rangle = \left\langle u - \tilde{u}, \sum_{j=1}^n b_j e_j \right\rangle = \sum_{j=1}^n \overline{b_j} \langle u - \tilde{u}, e_j \rangle = \sum_{j=1}^n \overline{b_j} \cdot 0 = 0.$$

Now $(u - \tilde{u}) \perp w$ for all $w \in W$ and so since $\tilde{u} - w \in W$
 $(u - \tilde{u}) \perp (\tilde{u} - w)$. Hence,

$$\|u - w\|^2 = \|u - \tilde{u} + \tilde{u} - w\|^2 = \|u - \tilde{u}\|^2 + \|\tilde{u} - w\|^2.$$



Best approximation

Theorem

Let V be an inner product space and $\{e_1, e_2, \dots, e_n\}$ an orthonormal system. Let $W = \text{span}\{e_1, e_2, \dots, e_n\}$ and $u \in V$ be any vector then $\tilde{u} = \sum_{i=1}^n \langle u, e_i \rangle e_i$ is the closest vector to u in W . Moreover, \tilde{u} is the unique such vector in W .

Proof.

For all $w \in W$,

$$\|u - w\|^2 = \|u - \tilde{u}\|^2 + \|\tilde{u} - w\|^2$$

and so $\|u - \tilde{u}\| \leq \|u - w\|$ for all $w \in W$.

To show uniqueness, suppose that $\|u - \tilde{u}\| = \|u - w\|$ for some $w \in W$ then $\|\tilde{u} - w\| = 0$ and so $w = \tilde{u}$. □



Infinite orthonormal systems

We now consider the situation of an inner product space, V , with $\dim(V) = \infty$ and consider orthonormal systems $\{e_1, e_2, \dots\}$ consisting of infinitely many vectors.

Definition (Convergence in norm)

Let $\{u_1, u_2, \dots\}$ be an infinite sequence of vectors in the normed linear space V and let $\{a_1, a_2, \dots\}$ be a sequence of scalars. We say that the series

$$\sum_{n=1}^{\infty} a_n u_n$$

converges in norm to $w \in V$ if

$$\lim_{m \rightarrow \infty} \left\| w - \sum_{n=1}^m a_n u_n \right\| = 0.$$



Closure and completeness

Two further properties are defined for an infinite orthonormal system $\{e_1, e_2, \dots\}$ in an inner product space V .

Definition (Closed)

The system is called **closed** in V if for all $u \in V$

$$\lim_{m \rightarrow \infty} \left\| u - \sum_{n=1}^m \langle u, e_n \rangle e_n \right\| = 0.$$

Definition (Complete)

The system is called **complete** in V if the zero vector $u = \vec{0}$ is the only solution to the set of equations

$$\langle u, e_n \rangle = 0 \quad n = 1, 2, \dots$$



Remarks on closure and completeness

- ▶ It can be shown that a closed infinite orthonormal system $\{e_1, e_2, \dots\}$ is necessarily complete (but not the converse).
- ▶ If a system is **not** closed then there must exist some $u \in V$ such that the linear combination

$$\sum_{n=1}^m \langle u, e_n \rangle e_n$$

cannot be made arbitrarily close to u , for all choices of m .

- ▶ If the system is closed it may still be that the required number of terms in the above linear combination for a “good” approximation is too great for practical purposes.
- ▶ Seeking alternative closed systems of orthonormal vectors may produce “better” approximations in the sense of requiring fewer terms for a given accuracy.



Representing functions

In seeking to represent functions as linear combinations of simpler functions we shall need to consider spaces of functions with closed orthonormal systems.

Definition (piecewise continuous)

A function is **piecewise continuous** if it is continuous, except at a finite number of points and at each such point of discontinuity, the right and left limits exist and are finite.

The space, E , of piecewise continuous functions $f : [-\pi, \pi] \rightarrow \mathbb{C}$ is seen to be a linear space, under the convention that we regard two functions in E as identical if they are equal at all but a finite number of points.

For $f, g \in E$, then

$$\langle f, g \rangle = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \overline{g(x)} dx$$

defines an inner product on E .



A closed infinite orthonormal system for E

An important result is that

$$\left\{ \frac{1}{\sqrt{2}}, \sin x, \cos x, \sin 2x, \cos 2x, \sin 3x, \cos 3x, \dots \right\}$$

is a closed infinite orthonormal system in the space E .

Here we shall just demonstrate orthonormality and omit establishing that this system is closed.



Writing $\|f\| = \sqrt{\langle f, f \rangle}$ as the norm associated with our inner product, it can be established that

$$\left\| \frac{1}{\sqrt{2}} \right\|^2 = 1$$

and similarly that for each $n = 1, 2, \dots$

$$\|\sin nx\|^2 = \|\cos nx\|^2 = 1$$

and that for $m, n \in \mathbb{N}$

- ▶ $\left\langle \frac{1}{\sqrt{2}}, \sin nx \right\rangle = 0$
- ▶ $\left\langle \frac{1}{\sqrt{2}}, \cos nx \right\rangle = 0$
- ▶ $\langle \sin mx, \cos nx \rangle = 0$
- ▶ $\langle \sin mx, \sin nx \rangle = 0, m \neq n$
- ▶ $\langle \cos mx, \cos nx \rangle = 0, m \neq n.$



Fourier series

From our knowledge of closed orthonormal systems $\{e_1, e_2, \dots\}$ we know that we can represent any function $f \in E$ by a linear combination

$$\sum_{n=1}^{\infty} \langle f, e_n \rangle e_n.$$

We now turn to consider the individual terms $\langle f, e_n \rangle e_n$ in the case of the closed orthonormal system

$$\left\{ \frac{1}{\sqrt{2}}, \sin x, \cos x, \sin 2x, \cos 2x, \sin 3x, \cos 3x, \dots \right\}.$$

There are three cases, either $e_n = \frac{1}{\sqrt{2}}$ or $\sin nx$ or $\cos nx$. Recall that the vectors e_n are actually functions in $E = \{f : [-\pi, \pi] \rightarrow \mathbb{C} : f \text{ is piecewise continuous}\}$



If $e_n = 1/\sqrt{2}$ then

$$\langle f, e_n \rangle e_n = \frac{1}{\pi} \left(\int_{-\pi}^{\pi} f(t) \frac{1}{\sqrt{2}} dt \right) \frac{1}{\sqrt{2}} = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) dt.$$

If $e_n = \sin nx$ then

$$\langle f, e_n \rangle e_n = \frac{1}{\pi} \left(\int_{-\pi}^{\pi} f(t) \sin nt dt \right) \sin nx.$$

If $e_n = \cos nx$ then

$$\langle f, e_n \rangle e_n = \frac{1}{\pi} \left(\int_{-\pi}^{\pi} f(t) \cos nt dt \right) \cos nx.$$



Fourier coefficients

Thus the linear combination $\sum_{n=1}^{\infty} \langle f, e_n \rangle e_n$ becomes the familiar Fourier series for a function f , namely

$$\frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos nx + b_n \sin nx]$$

where

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx \, dx, \quad n = 0, 1, 2, \dots$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx \, dx, \quad n = 1, 2, 3, \dots$$

Note how the constant term is written $a_0/2$ where $a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx$.



Periodic functions

Our Fourier series

$$\frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos nx + b_n \sin nx]$$

defines a function, $g(x)$, say, that is 2π -periodic in the sense that

$$g(x + 2\pi) = g(x), \quad \text{for all } x \in \mathbb{R}.$$

Hence, it is convenient to extend $f \in E$ to a 2π -periodic function defined on \mathbb{R} instead of being restricted to $[-\pi, \pi]$.



Even and odd functions

A particularly useful simplification occurs when the function $f \in E$ is either an **even** function, that is, for all x ,

$$f(-x) = f(x)$$

or an **odd** function, that is, for all x ,

$$f(-x) = -f(x).$$

The following properties can be easily verified.

1. If f, g are even then fg is even
2. If f, g are odd then fg is even
3. If f is even and g is odd then fg is odd
4. If g is odd then for any $h > 0$ then $\int_{-h}^h g(x) dx = 0$
5. If g is even then for any $h > 0$ then $\int_{-h}^h g(x) dx = 2 \int_0^h g(x) dx$.



Even functions and cosine series

Recall that the Fourier coefficients are given by

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx \, dx, \quad n = 0, 1, 2, \dots$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx \, dx, \quad n = 1, 2, 3, \dots$$

so if f is **even** then they become

$$a_n = \frac{2}{\pi} \int_0^{\pi} f(x) \cos nx \, dx, \quad n = 0, 1, 2, \dots$$

$$b_n = 0, \quad n = 1, 2, 3, \dots$$



Odd functions and sine series

Similarly, the Fourier coefficients

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx \, dx, \quad n = 0, 1, 2, \dots$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx \, dx, \quad n = 1, 2, 3, \dots,$$

for the case where f is an **odd** function become

$$a_n = 0, \quad n = 0, 1, 2, \dots$$

$$b_n = \frac{2}{\pi} \int_0^{\pi} f(x) \sin nx \, dx, \quad n = 1, 2, \dots$$



Fourier series: examples I

Consider $f(x) = x$ for $x \in [-\pi, \pi]$ then f is clearly odd and so we need to calculate a sine series with coefficients, b_n , $n = 1, 2, \dots$ given by

$$\begin{aligned} b_n &= \frac{2}{\pi} \int_0^\pi x \sin nx \, dx = \frac{2}{\pi} \left\{ \left[-x \frac{\cos nx}{n} \right]_0^\pi + \int_0^\pi \frac{\cos nx}{n} dx \right\} \\ &= \frac{2}{\pi} \left\{ -\pi \frac{(-1)^n}{n} + \left[\frac{\sin nx}{n^2} \right]_0^\pi \right\} \\ &= \frac{2}{\pi} \left\{ -\pi \frac{(-1)^n}{n} + 0 \right\} = \frac{2(-1)^{n+1}}{n}. \end{aligned}$$

Hence the Fourier series of $f(x) = x$ is

$$\sum_{n=1}^{\infty} \frac{2(-1)^{n+1}}{n} \sin nx.$$

Observe that the series does **not** agree with $f(x)$ at $x = \pm\pi$ — a matter that we shall return to later.



Fourier series: examples II

Now suppose $f(x) = |x|$ for $x \in [-\pi, \pi]$ which is clearly an even function so we need to construct a cosine series with coefficients

$$a_0 = \frac{2}{\pi} \int_0^{\pi} x dx = \frac{2}{\pi} \frac{\pi^2}{2} = \pi$$

and for $n = 1, 2, \dots$

$$\begin{aligned} a_n &= \frac{2}{\pi} \int_0^{\pi} x \cos nx \, dx = \frac{2}{\pi} \left\{ \left[\frac{x \sin nx}{n} \right]_0^{\pi} - \int_0^{\pi} \frac{\sin nx}{n} dx \right\} \\ &= \frac{2}{\pi} \left\{ \left[\frac{\cos nx}{n^2} \right]_0^{\pi} \right\} = \frac{2}{\pi} \left\{ \frac{(-1)^n - 1}{n^2} \right\} = \begin{cases} -\frac{4}{\pi n^2} & n \text{ is odd} \\ 0 & n \text{ is even} \end{cases} . \end{aligned}$$

Hence, the Fourier series of $f(x) = |x|$ is

$$\frac{\pi}{2} - \sum_{k=1}^{\infty} \frac{4}{\pi(2k-1)^2} \cos(2k-1)x .$$



Complex Fourier series I

We have used real-valued functions $\sin nx$ and $\cos nx$ as our orthonormal system for the linear space E but we can also use complex-valued functions. In this case, we should amend our inner product to

$$\langle f, g \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) \overline{g(x)} dx .$$

A suitable orthonormal system in this case is the collection of functions

$$\{1, e^{ix}, e^{-ix}, e^{i2x}, e^{-i2x}, \dots\} .$$

Then if $f \in E$ we have a representation, known as the **complex Fourier series** of $f \in E$, given by

$$\sum_{n=-\infty}^{\infty} c_n e^{inx}$$

where

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-inx} dx, \quad , n = 0, \pm 1, \pm 2, \dots .$$



Complex Fourier series II

Euler's formula ($e^{ix} = \cos x + i \sin x$) gives for $n = 1, 2, \dots$ that

$$\begin{aligned}e^{inx} &= \cos nx + i \sin nx \\e^{-inx} &= \cos nx - i \sin nx\end{aligned}$$

and $e^{i0x} = 1$. Using these relations it can be shown that for $n = 1, 2, \dots$

$$c_n = \frac{a_n - ib_n}{2}, \quad c_{-n} = \frac{a_n + ib_n}{2}.$$

Hence,

$$a_n = c_n + c_{-n}, \quad b_n = i(c_n - c_{-n})$$

and

$$c_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-i0x} dx = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) dx = \frac{a_0}{2}.$$



Pointwise convergence and Dirichlet's conditions

The closure property of the trigonometric orthonormal system guarantees that the Fourier series for any function $f \in E$ converges in norm to f . That is,

$$\lim_{m \rightarrow \infty} \left\| f(x) - \left(\frac{a_0}{2} + \sum_{n=1}^m [a_n \cos nx + b_n \sin nx] \right) \right\| = 0$$

or, equivalently,

$$\lim_{m \rightarrow \infty} \int_{-\pi}^{\pi} \left| f(x) - \left(\frac{a_0}{2} + \sum_{n=1}^m [a_n \cos nx + b_n \sin nx] \right) \right|^2 dx = 0.$$

As we have already seen in the example of $f(x) = x$, this does not imply convergence to $f(x)$ at every point x .



The Dirichlet conditions

We now consider conditions on the space of functions that allow us to determine how the Fourier series behaves at individual points x .

Definition (Dirichlet conditions)

We define a subspace, E' , of E by the **Dirichlet conditions**:

1. $f \in E$
2. For all $x \in [-\pi, \pi)$ both the left and right derivatives exist (and are finite).

Recall, that in the space E each function has a left and right limit at every point. Let these values be $f(x-)$ and $f(x+)$, respectively.



Theorem (Dirichlet's theorem)

For all $x \in [-\pi, \pi]$ the Fourier series of a function $f \in E'$ converges to the value of the expression

$$\frac{f(x-) + f(x+)}{2}.$$

- ▶ Here we should consider f not just defined on $[-\pi, \pi]$ but also make it 2π -periodic to handle the end points $\pm\pi$ correctly.
- ▶ Recall that functions $f \in E$ can have at most a finite number of points of discontinuity (that is, points where $f(x-)$ and $f(x+)$ differ).
- ▶ Hence, we can conclude that if a function f satisfies the Dirichlet conditions its Fourier series converges to f at all points where f is continuous and at points of discontinuity it converges to the average of the left and right hand limits. This was indeed the case in our earlier example where $f(x) = x$.



General intervals

We have so far considered functions defined on the interval $[-\pi, \pi]$ but we may readily extend our approach to a general interval of the form $[a, b]$. If we define $E[a, b]$ to be the space of piecewise continuous functions $f : [a, b] \rightarrow \mathbb{C}$ then we may define the Fourier series of $f \in E[a, b]$ as

$$\frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \frac{2n\pi x}{(b-a)} + b_n \sin \frac{2n\pi x}{(b-a)} \right]$$

where

$$a_n = \frac{2}{(b-a)} \int_a^b f(x) \cos \frac{2n\pi x}{(b-a)} dx, \quad n = 0, 1, 2, \dots$$
$$b_n = \frac{2}{(b-a)} \int_a^b f(x) \sin \frac{2n\pi x}{(b-a)} dx, \quad n = 1, 2, 3, \dots$$



This may be justified by showing, for example, that

$$\left\{ \frac{1}{\sqrt{2}}, \cos \frac{2n\pi x}{(b-a)}, \sin \frac{2n\pi x}{(b-a)} \quad \text{for } n = 1, 2, \dots \right\}$$

is an infinite orthonormal system for functions in $E[a, b]$ with respect to the inner product

$$\langle f, g \rangle = \frac{2}{(b-a)} \int_a^b f(x) \overline{g(x)} dx.$$



Fourier transforms



Introduction

- ▶ We have seen how functions $f : [-\pi, \pi] \rightarrow \mathbb{C}$, $f \in E$ can be represented in alternative ways using closed orthonormal systems, such as

$$\sum_{n=-\infty}^{\infty} c_n e^{inx}$$

where

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-inx} dx \quad n = 0, \pm 1, \pm 2, \dots$$

The domain $[-\pi, \pi]$ can be swapped for a general interval $[a, b]$ and the function can be regarded as L -periodic and defined for all \mathbb{R} , where $L = (b - a) < \infty$ is the length of the interval.

- ▶ We shall now consider the situation where $f : \mathbb{R} \rightarrow \mathbb{C}$ may be a non-periodic function.



Fourier transform

Definition (Fourier transform)

For $f : \mathbb{R} \rightarrow \mathbb{C}$ define the **Fourier transform** of f to be the function $F : \mathbb{R} \rightarrow \mathbb{C}$ given by

$$F(\omega) = \mathcal{F}_{[f]}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-i\omega x} dx$$

whenever the integral exists.

We shall use the notation $F(\omega)$ or $\mathcal{F}_{[f]}(\omega)$ as convenient. The notation $\hat{f}(\omega)$ is also seen widely in the literature.



For functions $f : \mathbb{R} \rightarrow \mathbb{C}$ define the two properties

1. **piecewise continuous**: if f is piecewise continuous on every finite interval. Thus f may have an infinite number of discontinuities but only a finite number in any subinterval.
2. **absolutely integrable**: if

$$\int_{-\infty}^{\infty} |f(x)| dx < \infty$$

Let $G(\mathbb{R})$ be the collection of all functions $f : \mathbb{R} \rightarrow \mathbb{C}$ which are piecewise continuous and absolutely integrable.



Immediate properties

It may be shown $G(\mathbb{R})$ is a linear space over the scalars \mathbb{C} and that for $f \in G(\mathbb{R})$

1. $F(\omega)$ is defined for all $\omega \in \mathbb{R}$
2. F is a continuous function
3. $\lim_{\omega \rightarrow \pm\infty} F(\omega) = 0$



Examples

Let $f(x) = e^{-a|x|}$ then

$$\begin{aligned} F(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-a|x|} e^{-i\omega x} dx \\ &= \frac{1}{2\pi} \left\{ \int_0^{\infty} e^{-ax} e^{-i\omega x} dx + \int_{-\infty}^0 e^{ax} e^{-i\omega x} dx \right\} \\ &= \frac{1}{2\pi} \left\{ - \left[\frac{e^{-(a+i\omega)x}}{a+i\omega} \right]_0^{\infty} + \left[\frac{e^{(a-i\omega)x}}{a-i\omega} \right]_{-\infty}^0 \right\} \\ &= \frac{1}{2\pi} \left\{ \frac{1}{a+i\omega} + \frac{1}{a-i\omega} \right\} \\ &= \frac{a}{\pi(a^2 + \omega^2)}. \end{aligned}$$



Properties

Several properties of the Fourier transform are very helpful in calculations.

First, note that by the linearity of integrals we have that if $f, g \in G(\mathbb{R})$ and $a, b \in \mathbb{C}$ then

$$\mathcal{F}_{[af+bg]}(\omega) = a\mathcal{F}_{[f]}(\omega) + b\mathcal{F}_{[g]}(\omega)$$

and $af + bg \in G(\mathbb{R})$.

Secondly, if f is real-valued only then

$$F(-\omega) = \overline{F(\omega)}.$$



Even and odd real-valued functions

Theorem

If $f \in G(\mathbb{R})$ is an even real-valued function then F is even and real-valued. If f is an odd real-valued function then F is odd and purely imaginary.

Proof.

Suppose that f is even and real-valued then

$$\begin{aligned} F(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x)e^{-i\omega x} dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x)[\cos \omega x - i \sin \omega x] dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) \cos \omega x dx. \end{aligned}$$

Hence, F is real-valued and even (the imaginary part has vanished and both f and $\cos \omega x$ are themselves even functions). The second part follows similarly.



Shift property

Theorem

Let $f \in G(\mathbb{R})$ and $a, b \in \mathbb{R}$ with $a \neq 0$ and define

$$g(x) = f(ax + b)$$

then $g \in G(\mathbb{R})$ and

$$\mathcal{F}_{[g]}(\omega) = \frac{1}{|a|} e^{i\omega b/a} \mathcal{F}_{[f]}\left(\frac{\omega}{a}\right)$$



Proof

Set $y = ax + b$ so for $a > 0$ then

$$\mathcal{F}_{[g]}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(y) e^{-i\omega(\frac{y-b}{a})} \frac{dy}{a}$$

and for $a < 0$

$$\mathcal{F}_{[g]}(\omega) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} f(y) e^{-i\omega(\frac{y-b}{a})} \frac{dy}{a}.$$

Hence,

$$\mathcal{F}_{[g]}(\omega) = \frac{1}{|a|} e^{i\omega b/a} \frac{1}{2\pi} \int_{-\infty}^{\infty} f(y) e^{-i\omega y/a} dy = \frac{1}{|a|} e^{i\omega b/a} \mathcal{F}_{[f]} \left(\frac{\omega}{a} \right).$$

□

Special cases

Two special cases of the shift property are worth highlighting.

1. $a \neq 0$ and $b = 0$ so $g(x) = f(ax)$ then

$$\mathcal{F}_{[g]}(\omega) = \frac{1}{|a|} \mathcal{F}_{[f]} \left(\frac{\omega}{a} \right) .$$

2. $a = 1$ so $g(x) = f(x + b)$ then

$$\mathcal{F}_{[g]}(\omega) = e^{i\omega b} \mathcal{F}_{[f]}(\omega) .$$

Theorem

For $f \in G(\mathbb{R})$ and $c \in \mathbb{R}$ then

$$\mathcal{F}_{[e^{icx}f(x)]}(\omega) = \mathcal{F}_{[f]}(\omega - c).$$

Proof.

$$\begin{aligned}\mathcal{F}_{[e^{icx}f(x)]}(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{icx} f(x) e^{-i\omega x} dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-i(\omega-c)x} dx \\ &= \mathcal{F}_{[f]}(\omega - c).\end{aligned}$$



Modulation property

Theorem

For $f \in G(\mathbb{R})$ and $c \in \mathbb{R}$ then

$$\mathcal{F}_{[f(x) \cos cx]}(\omega) = \frac{\mathcal{F}_{[f]}(\omega - c) + \mathcal{F}_{[f]}(\omega + c)}{2}$$
$$\mathcal{F}_{[f(x) \sin cx]}(\omega) = \frac{\mathcal{F}_{[f]}(\omega - c) - \mathcal{F}_{[f]}(\omega + c)}{2i}.$$

Proof.

We have that

$$\begin{aligned}\mathcal{F}_{[f(x) \cos cx]}(\omega) &= \mathcal{F}_{\left[f(x) \frac{e^{icx} + e^{-icx}}{2}\right]}(\omega) \\ &= \frac{1}{2} \mathcal{F}_{[f(x)e^{icx}]}(\omega) + \frac{1}{2} \mathcal{F}_{[f(x)e^{-icx}]}(\omega) \\ &= \frac{\mathcal{F}_{[f]}(\omega - c) + \mathcal{F}_{[f]}(\omega + c)}{2}.\end{aligned}$$

Similarly, for $\mathcal{F}_{[f(x) \sin cx]}(\omega)$.



Derivatives

There are further properties relating to the Fourier transform of derivatives that we shall state here but omit further proofs.

Theorem

If f is a continuous function and $f, f' \in G(\mathbb{R})$ then

$$\mathcal{F}_{[f']}(w) = iw\mathcal{F}_{[f]}(w).$$



Inverse Fourier transform

We have studied the Fourier transform. There is also an inverse operation of recovering a function f given the function $F(\omega) = \mathcal{F}[f](\omega)$ which takes the form

$$f(x) = \int_{-\infty}^{\infty} \mathcal{F}[f](\omega) e^{i\omega x} d\omega.$$

More precisely, and recalling Dirichlet's theorem for Fourier series, the following holds.

Theorem (Inverse Fourier transform)

If $f \in G(\mathbb{R})$ then for every point $x \in \mathbb{R}$ where the one-sided derivatives exist

$$\frac{f(x-) + f(x+)}{2} = \lim_{M \rightarrow \infty} \int_{-M}^M \mathcal{F}[f](\omega) e^{i\omega x} d\omega.$$

Convolution

An important operation between two functions in signal processing applications is **convolution** defined as follows.

Definition (Convolution)

If f and g are two functions $\mathbb{R} \rightarrow \mathbb{C}$ then the **convolution** function, written $f * g$, is given by

$$(f * g)(x) = \int_{-\infty}^{\infty} f(x - y)g(y)dy$$

whenever the integral exists.

It may be shown that the convolution operation is commutative, that is $f * g = g * f$.



Fourier transforms and convolutions

The importance of Fourier transform techniques in signal processing rests, in part, on the following result that leads to much simpler descriptions and mathematical formulae in the Fourier domain.

Theorem (Convolution theorem)

For $f, g \in G(\mathbb{R})$ then

$$\mathcal{F}_{[f * g]}(\omega) = 2\pi \mathcal{F}_{[f]}(\omega) \cdot \mathcal{F}_{[g]}(\omega).$$



Proof

We have that

$$\begin{aligned}\mathcal{F}_{[f*g]}(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} (f * g)(x) e^{-i\omega x} dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} f(x-y)g(y)dy \right) e^{-i\omega x} dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x-y)e^{-i\omega(x-y)}g(y)e^{-i\omega y} dx dy \\ &= \int_{-\infty}^{\infty} \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} f(x-y)e^{-i\omega(x-y)} dx \right) g(y)e^{-i\omega y} dy \\ &= \mathcal{F}_{[f]}(\omega) \int_{-\infty}^{\infty} g(y)e^{-i\omega y} dy \\ &= 2\pi \mathcal{F}_{[f]}(\omega) \cdot \mathcal{F}_{[g]}(\omega).\end{aligned}$$



Some signal processing applications

We first note two types of limitations on functions.

Definition (Time-limited)

A function f is **time-limited** if

$$f(x) = 0 \quad \text{for all } |x| \geq M$$

for some constant M .

Definition (Band-limited)

A function $f \in G(\mathbb{R})$ is **band-limited** if

$$\mathcal{F}_{[f]}(\omega) = 0 \quad \text{for all } |\omega| \geq L$$

for some constant L .



Let us first calculate the Fourier transform of

$$f(x) = \begin{cases} 1 & a \leq x \leq b \\ 0 & \text{otherwise.} \end{cases}$$

We have that

$$\begin{aligned} F(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x)e^{-i\omega x} dx = \frac{1}{2\pi} \int_a^b e^{-i\omega x} dx \\ &= \left[\frac{1}{2\pi} \frac{e^{-i\omega x}}{-i\omega} \right]_a^b = \frac{e^{-i\omega a} - e^{-i\omega b}}{2\pi i\omega}. \end{aligned}$$

If we set $a = -b$ with $b > 0$ then

$$F(\omega) = \frac{e^{i\omega b} - e^{-i\omega b}}{2\pi i\omega} = \frac{\sin \omega b}{\omega\pi}.$$



Low-pass filters

Suppose that $f \in G(\mathbb{R})$ with Fourier transform $F(\omega)$ and choose a constant $L > 0$. Define

$$F_L(\omega) = \begin{cases} F(\omega) & |\omega| \leq L \\ 0 & |\omega| > L. \end{cases}$$

We wish to find f_L such that $\mathcal{F}_{[f_L]} = F_L$, that is, a function band-limited by L whose Fourier transform equals F in $[-L, L]$.

Rewrite $F_L(\omega) = F(\omega)G_L(\omega)$ where

$$G_L(\omega) = \begin{cases} 1 & |\omega| \leq L \\ 0 & |\omega| > L. \end{cases}$$

We will now use the convolution theorem to find f_L .

By the inverse transform theorem we have that for $|x| \neq L$

$$G_L(x) = \int_{-\infty}^{\infty} \frac{\sin \omega L}{\omega \pi} e^{i\omega x} d\omega$$

But G_L is clearly an even function so

$$G_L(x) = \int_{-\infty}^{\infty} \frac{\sin \omega L}{\omega \pi} e^{-i\omega x} d\omega$$

and if we interchange the variables x and ω we have

$$G_L(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{2 \sin Lx}{x} e^{-i\omega x} dx.$$

This says that if $g_L(x) = \frac{2 \sin Lx}{x}$ then $\mathcal{F}_{[g_L]}(\omega) = G_L(\omega)$.



In terms of convolutions we have

$$\begin{aligned}f_L &= \frac{1}{2\pi}(f * g_L) \\f_L(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f(y) \frac{2 \sin(L(x-y))}{x-y} dy \\&= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(y) \sin(L(x-y))}{x-y} dy\end{aligned}$$

In particular, if $f \in G(\mathbb{R})$ is such that $\mathcal{F}_{[f]}(\omega) = 0$ for $|\omega| \geq L$ then f satisfies

$$f(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(y) \sin(L(x-y))}{x-y} dy.$$



Shannon sampling theorem

Theorem (Shannon sampling theorem)

If $f \in G(\mathbb{R})$ is band-limited by the constant L then

$$f(x) = \sum_{n=-\infty}^{\infty} f\left(\frac{n\pi}{L}\right) \frac{\sin(Lx - n\pi)}{Lx - n\pi}.$$

Proof

Set $F(\omega) = \mathcal{F}_{[L]}(\omega)$ and use the inverse Fourier transform theorem to give

$$f(x) = \int_{-\infty}^{\infty} F(\omega) e^{i\omega x} d\omega = \int_{-L}^L F(\omega) e^{i\omega x} d\omega.$$

So, taking $x = \frac{n\pi}{L}$ for $n \in \mathbb{Z}$ we get

$$f\left(\frac{n\pi}{L}\right) = \int_{-L}^L F(\omega) e^{i\omega n\pi/L} d\omega.$$



Consider the complex Fourier series of F restricted to $[-L, L]$ given by

$$\sum_{n=-\infty}^{\infty} c_n e^{-in\pi\omega/L}$$

where the coefficients are

$$c_n = \frac{1}{2L} \int_{-L}^L F(\omega) e^{in\pi\omega/L} d\omega = \frac{1}{2L} f\left(\frac{n\pi}{L}\right)$$

Thus, since f is band-limited by L

$$F(\omega) = \sum_{n=-\infty}^{\infty} c_n e^{-in\pi\omega/L} G_L(\omega).$$

Hence,

$$F(\omega) = \frac{1}{2L} \sum_{n=-\infty}^{\infty} f\left(\frac{n\pi}{L}\right) e^{-in\pi\omega/L} G_L(\omega).$$

But we have seen that $G_L(\omega) = \mathcal{F}_{\left[\frac{2 \sin Lx}{x}\right]}(\omega)$ hence using the shift formula

$$e^{-in\pi\omega/L} G_L(\omega) = \mathcal{F}_{[g_{L,n}]}(\omega)$$

where

$$g_{L,n}(x) = \frac{2 \sin(Lx - n\pi)}{x - \frac{n\pi}{L}}.$$

Putting this all together we have that

$$F(\omega) = \frac{1}{2L} \sum_{n=-\infty}^{\infty} f\left(\frac{n\pi}{L}\right) \mathcal{F}_{[g_{L,n}]}(\omega)$$

and taking inverse transforms

$$f(x) = \frac{1}{2L} \sum_{n=-\infty}^{\infty} f\left(\frac{n\pi}{L}\right) g_{L,n}(x) = \sum_{n=-\infty}^{\infty} f\left(\frac{n\pi}{L}\right) \frac{\sin(Lx - n\pi)}{Lx - n\pi}.$$



Remarks on Shannon's sampling theorem

- ▶ The theorem says that band-limited functions by a constant L (that is, $\mathcal{F}_{[f]}(\omega) = 0$ for $|\omega| > L$) are completely determined by their values at evenly spaced points a distance $\frac{\pi}{L}$ apart.
- ▶ Moreover, we may recover the function exactly given only its values at this sequence of points.
- ▶ It may be shown that the functions

$$\frac{\sin(Lx - n\pi)}{Lx - n\pi}$$

for $n \in \mathbb{Z}$ form an orthonormal system with inner product

$$\langle f, g \rangle = \frac{L}{\pi} \int_{-\infty}^{\infty} f(x) \overline{g(x)} dx.$$

Discrete Fourier Transforms



We now shift attention from functions defined on intervals or on the whole of \mathbb{R} to sequences of values $f[0], f[1], \dots, f[N-1]$ and consider how we might represent them.

An important result in this area of discrete transforms is that the vectors $\{e_0, e_1, \dots, e_{N-1}\}$ form an orthogonal system in the space \mathbb{C}^N with the usual inner product where the n^{th} component of e_k is given by

$$(e_k)_n = e^{2\pi ink/N} \quad n = 0, 1, 2, \dots, N-1.$$

and $k = 0, 1, 2, \dots, N-1$.



Applying the usual inner product

$$\langle u, v \rangle = \sum_{n=0}^{N-1} u[n] \overline{v[n]}$$

we find that

$$\|e_k\|^2 = \langle e_k, e_k \rangle = N.$$

In fact, using $\{e_0, e_1, \dots, e_{N-1}\}$ we can represent any sequence $f = (f[0], f[1], \dots, f[N-1]) \in \mathbb{C}^N$ by

$$f = \frac{1}{N} \sum_{k=0}^{N-1} \langle f, e_k \rangle e_k.$$



Orthogonality

We shall show orthogonality of the vectors e_k by considering the N distinct complex roots of the equation $z^N = 1$. Put $w = e^{2\pi i/N}$ then the N distinct roots z_j ($j = 0, 1, \dots, N - 1$) of $z^N = 1$ are

$$z_j = e^{2\pi ij/N} = w^j.$$

Now for an arbitrary integer n

$$\begin{aligned} \frac{1}{N} \sum_{k=0}^{N-1} e^{2\pi ink/N} &= \frac{1}{N} \sum_{k=0}^{N-1} w^{nk} \\ &= \begin{cases} 1 & \text{if } n \text{ is an integer multiple of } N \\ \frac{1}{N} \frac{1-w^{nN}}{1-w^n} = 0 & \text{otherwise.} \end{cases} \end{aligned}$$



Thus,

$$\begin{aligned}\langle \mathbf{e}_a, \mathbf{e}_b \rangle &= \sum_{k=0}^{N-1} e^{2\pi ika/N} e^{-2\pi ikb/N} \\ &= \sum_{k=0}^{N-1} e^{2\pi ik(a-b)/N} \\ &= \begin{cases} N & \text{if } (a-b) \text{ is a multiple of } N \\ 0 & \text{otherwise.} \end{cases}\end{aligned}$$



Definition (Discrete Fourier Transform/DFT)

The sequence $F[k]$, $k \in \mathbb{Z}$, defined by

$$F[k] = \langle f, e_k \rangle = \sum_{n=0}^{N-1} f[n] e^{-2\pi ink/N}$$

is called the N -point Discrete Fourier Transform of $f[n]$

Thus, for $n = 0, 1, 2, \dots, N - 1$,

$$f[n] = \frac{1}{N} \sum_{k=0}^{N-1} F[k] e^{2\pi ink/N}.$$



Periodicity

Note that the sequence $F[k]$ has period N since

$$F[k + N] = \sum_{n=0}^{N-1} f[n]e^{-2\pi in(k+N)/N} = \sum_{n=0}^{N-1} f[n]e^{-2\pi ink/N} = F[k]$$

using the relation

$$e^{-2\pi in(k+N)/N} = e^{-2\pi ink/N}e^{-2\pi in} = e^{-2\pi ink/N}.$$



Properties of the DFT

The DFT satisfies a range of similar properties to those of the FT relating to linearity, and shifts in either the n or k domain. However, the convolution operation is defined a little differently.

Definition (Cyclical convolution)

The **cyclical convolution** of two periodic sequences $f[n]$ and $g[n]$ of period N is defined as

$$(f * g)[n] = \sum_{m=0}^{N-1} f[m]g[n - m].$$

It can then be shown that the DFT of $f * g$ is the product $F[k]G[k]$ where F and G are the DFTs of f and g , respectively.



Fast Fourier Transforms



Fast Fourier Transform

The Fast Fourier Transform is **not** a new transform but a particular numerical algorithm for computing the DFT.

Since

$$\begin{aligned} F[k] &= \sum_{n=0}^{N-1} f[n]e^{-2\pi ink/N} \\ &= f[0] + f[1]e^{-2\pi ik/N} + \dots + f[N-1]e^{-2\pi ik(N-1)/N} \end{aligned}$$

we can see that in order to compute $F[k]$ we need to do about $2N$ (complex) additions and multiplications. To compute $F[k]$ in this way for all $k = 0, 1, 2, \dots, N-1$ would require about $2N^2$ such operations. In practice, where DFTs are computed for a large number of points N , faster algorithms have been developed. Most approaches are based on the factorization of N into prime factors and are known collectively as **Fast Fourier Transforms**, or **FFT**. In most popular methods N is supposed to be a power of 2.



Fast algorithms for the DFT

In 1965, James W. Cooley and John W. Tukey published a new and substantially faster algorithm for computing the DFT than the direct N^2 approach.

They showed that when N is a composite number with $N = P_1 P_2 \cdots P_m$ then it is possible to reduce the cost of computing the DFT of a vector of length N from

$$N^2 = N(P_1 P_2 \cdots P_m) \quad \text{to} \quad N((P_1 - 1) + (P_2 - 1) + \cdots + (P_m - 1))$$

complex operations. In the case when $P_1 = P_2 = \cdots = P_m = 2$ then this reduces from $N^2 = 2^{2m}$ to $2^m \cdot m = N \log_2 N$.

For example, if $N = 1024 = 2^{10}$ then there is a 100 fold improvement from $N^2 = 1,048,576$ to $N \log_2 N = 10,240$.

See: J.W. Cooley and J.W. Tukey. (1965) An algorithm for the machine computation of complex Fourier series, *Math. Comp.*, 19, 297–301.



We shall not derive any of the details here but instead give an impression of how the method operates.

First, the task of computing the DFT can be represented with matrices as

$$F = Af$$

but where the $N \times N$ matrix, A , has a great deal of internal structure. Cooley and Tukey exploited this structure in the case when $N = 2^m$ to rewrite A as a product of matrices each of which is **sparse**

$$A = M_m M_{m-1} \cdots M_1 B.$$

Since each of these matrices contains only a small number of non-zero entries the effective number of complex operations is much reduced compared to working with A itself.



Wavelet Transforms



Wavelets

Wavelets are a further method of representing functions that has received much interest in applied fields over the last several decades. The approach fits into the general scheme of expansion using orthonormal functions. Here we expand functions $f(x)$ in terms of a doubly-infinite series

$$f(x) = \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} d_{jk} \Psi_{jk}(x)$$

where $\Psi_{jk}(x)$ are the orthonormal functions.

The orthonormal functions arise from **shifting** and **scaling** operations applied to a single function, $\Psi(x)$, known as the **mother wavelet**. The orthonormal functions are given for integers j and k by

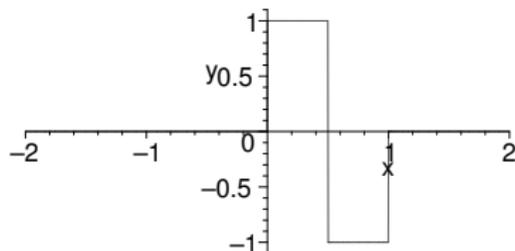
$$\Psi_{jk}(x) = 2^{j/2} \Psi(2^j x - k)$$



The Haar wavelet

A common example is the **Haar wavelet** whose mother function is both **localised** and **oscillatory** defined by

$$\psi(x) = \begin{cases} 1 & \text{if } 0 \leq x < \frac{1}{2}, \\ -1 & \text{if } \frac{1}{2} \leq x < 1, \\ 0 & \text{otherwise.} \end{cases}$$



Wavelet dilations and translations

The Haar mother wavelet oscillates and has a width (or scale) of one. The **dyadic dilates** of $\Psi(x)$, namely,

$$\dots, \Psi(2^{-2}x), \Psi(2^{-1}x), \Psi(x), \Psi(2x), \Psi(2^2x), \dots$$

have widths

$$\dots, 2^2, 2^1, 1, 2^{-1}, 2^{-2}, \dots$$

respectively. Since the dilate $\Psi(2^jx)$ has width 2^{-j} , its translates

$$\Psi(2^jx - k) = \Psi(2^j(x - k2^{-j})), \quad k = 0, \pm 1, \pm 2, \dots$$

will cover the whole x -axis. The collection of coefficients d_{jk} are termed the **Discrete wavelet transform**, or **DWT**, of the function $f(x)$. Just as with Fourier transforms there are fast implementations that exploit structure.

Interpretation of d_{jk}

How should we interpret the values d_{jk} ?

Since the Haar wavelet function $\Psi(2^j x - k)$ vanishes except when

$$0 \leq 2^j x - k < 1, \quad \text{that is} \quad k2^{-j} \leq x < (k+1)2^{-j}$$

we see that d_{jk} gives us information about the behaviour of f near the point $x = k2^{-j}$ measured on the scale of 2^{-j} .

For example, the coefficients $d_{-10,k}$, $k = 0, \pm 1, \pm 2, \dots$ correspond to variations of f that take place over intervals of length $2^{10} = 1024$

while the coefficients $d_{10,k}$, $k = 0, \pm 1, \pm 2, \dots$ correspond to fluctuations of f over intervals of length 2^{-10} .

These observations help explain how the discrete wavelet transform can be an exceptionally efficient scheme for representing functions.



Comparison with Fourier analysis

Some of the practical motivations underlying the use of the orthonormal functions such as Fourier analysis or wavelet analysis are

- ▶ improved understanding,
- ▶ denoising signals, and
- ▶ data compression.

By representation of signals or functions in other forms these tasks become easier or more effective.

The approach taken with Fourier analysis represents signals in terms of trigonometric functions and as such is particularly suited to situations where the signal is relatively smooth and is not of limited extent.



Properties of naturally arising data

Much naturally arising data has been found to be better represented using wavelets which are better able to cope with discontinuities and where the signal is of local extent. Generally, the efficiency of the representation depends on the types of signal involved. If your signal contains

- ▶ discontinuities (in both the signal and its derivatives), or
- ▶ varying frequency behaviour

then wavelets are likely to represent the signal more efficiently than is possible with Fourier analysis.



Other classes of wavelets

- ▶ One of the most useful features of wavelets is the ease with which a scientist can select the wavelet functions adapted for the given problem.
- ▶ In fact, the Haar mother wavelet is perhaps the simplest of a very wide class of possible wavelet systems used in practice today.
- ▶ Many applied fields have started to make use of wavelets including astronomy, acoustics, signal and image processing, neurophysiology, music, magnetic resonance imaging, speech discrimination, optics, fractals, turbulence, earthquake prediction, radar, human vision, etc.

