

Natural Sciences Tripos Part IA Mathematics III (B course), Easter Term

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*These notes have also been previously developed by P O'Donnell, J Papaloizou, M Wingate and R Horgan, among others

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1 Linear Algebra

1.1 Linear vector spaces

The idea of a **linear vector space** is central to the analysis of many problems in physics and mathematics and it is the basic object of study in **linear algebra**. In particular, it applies to the study of

- linear simultaneous equations. This involves the study of matrices and their properties;
- the solutions to linear partial (and ordinary) differential equations abbreviated to PDE (ODE).

Physical problems that can be tackled include

- the harmonic vibrations of a system about an equilibrium and the natural frequencies of oscillation. E.g., molecules and vibrational frequencies of absorption of radiation;
- waves in various media;
- problems in diffusion;
- the electrostatic potential of charge distributions;
- Fourier series;
- quantum mechanics.

In the first part of this course we will concentrate on **linear algebra** applied to matrices but it is important to understand that we are discussing a particular kind of realization, or representation, of a linear vector space and that there are many others. For this reason, it is important to give a formal definition.

1.1.1 Definition of a linear vector space

Notation:

V : a set of elements denoted by bold letters: $\mathbf{x}, \mathbf{y}, \mathbf{u}, \mathbf{v}$ etc..

K : a field consisting of elements called **scalars**, denoted by unbold letters: a, b, c, k etc..
For us these will be real or complex numbers.

Rules:

- **addition**: This is a binary operation denoted "+". To any $x, y \in V$ this rule assigns an element $z \in V$: $z = x + y$.
- **scalar multiplication**: To any $a \in K$ and $x \in V$ this rule assigns an element $z \in V$: $z = ax$.

Definition. V is called a **vector space over K** , and the elements of V are called **vectors**, if the following **axioms** hold:

- A1** For any vectors $u, v, w \in V$, $(u + v) + w = u + (v + w)$. (**Associativity.**)
- A2** For any vectors $u, v \in V$, $u + v = v + u$. (**Commutativity.**)
- A3** There is a vector in V denoted 0 , called the **zero vector** for which $u + 0 = u$
 $\forall u \in V$.
- A4** For each vector $u \in V$ there is a vector in V denoted $-u$ for which $u + (-u) = 0$.
(**Inverse.**)
- A5** For any $a \in K$ and any $u, v \in V$, $a(u + v) = au + av$.
- A6** For any $a, b \in K$ and any $u \in V$, $(a + b)u = au + bu$.
- A7** For any $a, b \in K$ and any $u \in V$, $(ab)u = a(bu)$.
- A8** For the unit scalar $1 \in K$ and any $u \in V$, $1u = u$.

Other results follow from these axioms. E.g.,

$$0u = 0, a0 = 0, (-a)u = -au, au = 0 \\ \implies a = 0 \text{ or } u = 0.$$

1.1.2 Examples of vector spaces

- i) Let K be an arbitrary field. A vector space is the set of all n -tuples of elements of K with vector addition and scalar multiplication defined by

where $a_i, b_i, k \in K$. This space is denoted K^n

- ii) The set of all n -tuples of real numbers (u_1, \dots, u_n) , denoted \mathbb{R}^n , is a vector space over the field \mathbb{R} . This follows as an example of i). Likewise, the set of all n -tuples of complex numbers (z_1, \dots, z_n) , denoted \mathbb{C}^n , is a vector space over the field \mathbb{C} .
Examples of vectors in \mathbb{R}^3 are

The last of these is the zero, or null, vector $\mathbf{0}$.

- iii) V is the set of all polynomials in t of degree $\leq n$

with coefficients a_i from a field K . V is a vector space over K with respect to the usual operations of addition of polynomials and multiplication by a constant.

1.1.3 Linear combinations and linear spans

Let $\mathbf{v}_1, \dots, \mathbf{v}_m \in V$ and $a_1, \dots, a_m \in K$ and let

Then x is called a **linear combination** of v_1, \dots, v_m .

The set of all such linear combinations of v_1, \dots, v_m is a subspace, S , of V . In other words, S contains all vectors of the form of x above that are **generated** by all possible choices of $a_1, \dots, a_m \in K$. This is written

Then we say that the subspace S is **spanned** or **generated** by the v 's, and that the v 's **span** or **generate** S .

1.1.4 Linear independence

Suppose that for some $a_1, \dots, a_m \in K$ we have

Then the vectors v_1, \dots, v_m are said to be **linearly independent** if the only solution is $a_i = 0, \forall i$.

Conversely, if there **is** a solution with at least one of the a 's non-zero then the vectors are **linearly dependent**. Note, that if any of the v 's is the zero vector, $\mathbf{0}$, then the vectors are linearly dependent.

1.1.5 Dimension and basis

A vector space V is said to be of **finite dimension** n or to be **n -dimensional**, written $\dim V = n$, if there exist linearly independent vectors e_1, e_2, \dots, e_n which span V . That is, every $v \in V$ can be written as a linear combination of the e 's. The sequence $\{e_1, e_2, \dots, e_n\}$ is then called a **basis** of V .

Note that a set of vectors might **span** V but they do not necessarily form a basis since they might not be linearly independent. However, given such a set we can systematically reduce the number of elements until we do have an independent set which then will form a basis.

The definition of dimension is well defined because it can be shown that every basis of V has the **same number** of elements.

1.1.6 Examples of bases

1. A basis for K^3 over the field K is

An alternative basis is

2. Let W be the vector space of polynomials in t of degree $\leq n$. The set $\{1, t, t^2, \dots, t^n\}$ is linearly independent and spans W . Thus it is a basis of W and so $\dim W = n + 1$.

A different basis when, e.g., $n = 2$ is

1.1.7 Coordinates

Given a basis $\{e_1, \dots, e_n\}$ for V , then any vector $v \in V$ can be expressed as

Then the n -tuple $\mathbf{x} = (x_1, \dots, x_n)$ are the **coordinates** of \mathbf{v} with respect to the given basis. If we change the basis the coordinates will change but, of course, \mathbf{v} is still the same vector:

with coordinates $\mathbf{y} = (y_1, \dots, y_n)$.

Note that \mathbf{x}, \mathbf{y} are themselves vectors since $\mathbf{x}, \mathbf{y} \in K^n$. K^n is a vector space over the field K defined earlier.

1.1.8 Linear maps

A **mapping** A of a vector space V into a vector space U assigns to any vector $\mathbf{x} \in V$ another vector $\mathbf{y} \in U$. We write either

There might be an inverse (this does not always exist), A^{-1} defined by

$$\mathbf{x} = A^{-1}\mathbf{y} .$$

The map is **linear** if it satisfies the following properties

- (i) $\mathbf{A}(x_1 + x_2) = \mathbf{A}x_1 + \mathbf{A}x_2$ for every $x_1, x_2 \in V$.
- (ii) $\mathbf{A}(\alpha x) = \alpha \mathbf{A}x$ for every $x \in V$ and every scalar α in K .

Examples of linear maps

- $\mathbf{A}x = ax$.
- For position vectors in 3D: $\mathbf{A}x = \mathbf{a} \wedge x$, \mathbf{a} a constant vector, (where “ \wedge ” is vector product).
- For position vectors in 3D: $\mathbf{A}x = \mathbf{a} \cdot x$, \mathbf{a} a constant vector, (where “ \cdot ” is scalar, or dot, product). Note that here \mathbf{A} maps $V = \mathbb{R}^3$ into $U = \mathbb{R}$.

Examples of non-linear maps

- (i) $\mathbf{A}x = x + a$.
- (ii) For position vectors in 3D: $\mathbf{A}x = a|x|x$. ($|x|$ is the length of x .)

1.2 Matrices

A matrix is a rectangular array of real or complex numbers. We shall mainly use real numbers in this course but complex matrices are central to many applications. Some examples are:

Suffix Notation

An $m \times n$ matrix has m rows and n columns. The matrix is usually denoted by a bold upper case letter, \mathbf{A} , say, and then a_{ij} will denote the j th entry in the i th row:

$$\mathbf{A} = (a_{ij}), \quad (\mathbf{A})_{ij} = a_{ij}, \quad \mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2j} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{i1} & a_{i2} & \cdots & a_{ij} & \cdots & a_{in} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mj} & \cdots & a_{mn} \end{pmatrix}$$

Notes

i) An $m \times m$ matrix is called a **square** matrix.

ii) An $m \times 1$ matrix is a **column vector**:

iii) A $1 \times n$ matrix is a **row vector**:

Examples of suffix notation with vectors

Note that un-summed indices should always match on the left and on the right. Summed indices should **always come in pairs** and sum from 1 to the maximum value implied by the dimensions of the object. The *Einsten summation convention* (which we shall not follow here, but which many people do) omits the \sum_i : it is implied whenever one has a pair of repeated indices. We call the sum over pairs of indices a **contraction** of those indices.

In what follows it is often useful to understand a general statement by working through the most simple non-trivial example. E.g., choose the smallest matrices to illustrate the point.

1.2.1 Algebra of matrices

For given n, m the set of all real (complex) $m \times n$ matrices form a vector space over \mathbb{R} (\mathbb{C}). We need a rule of addition (+) and multiplication by a scalar which we make explicit in (a) and (b) below.

(a) Addition of matrices

Let A and B be $m \times n$ matrices. Their sum C is an $m \times n$ matrix defined by

E.g.,

(b) Multiplication by a scalar

Let \mathbf{A} and \mathbf{B} be $m \times n$ matrices.

$$\mathbf{B} = \lambda \mathbf{A} \quad \text{means} \quad b_{ij} = \lambda a_{ij} \quad i = 1 \dots m, j = 1 \dots n.$$

The statement of equality of matrices follows if we set $\lambda = 1$:

$$\mathbf{B} = \mathbf{A} \quad \text{means} \quad b_{ij} = a_{ij} \quad i = 1 \dots m, j = 1 \dots n.$$

(c) Multiplication of matrices

Matrices \mathbf{A} and \mathbf{B} can only be multiplied if \mathbf{A} is $m \times n$ and \mathbf{B} is $n \times p$. Then

is defined by

and the product matrix \mathbf{C} is $m \times p$. Note that, written in suffix notation, the left hand object c_{ij} has a row index i and a column index j , and so the right hand side must do also (k is a dummy index which is summed over): the left-hand side is the ij -th element of a matrix, as is the right-hand side. We have (again) left out the brackets for this matrix, leaving them implicit. It is important to note that although the order matters when we write the equation in matrix form, when we write in suffix

notation, each term in the sum is just the product of two numbers - the ordering of these numbers doesn't matter much.

The product of three matrices $\mathbf{D} = \mathbf{ABE}$ is thus written (where \mathbf{E} is $p \times q$):

An important fact is that the product of two square matrices does not **commute** in general. Suppose \mathbf{A} and \mathbf{B} are both $m \times m$. Then in general $\mathbf{AB} \neq \mathbf{BA}$. If this is the case we say that \mathbf{A} and \mathbf{B} do not **commute**. The **commutator** is defined by:

Of course, \mathbf{C} is also $m \times m$.

Examples of multiplication

Note that the 2×2 matrices here do not commute.

1.2.2 Some definitions and properties

(a) Transpose

The **transpose** of an $m \times n$ matrix M is the $n \times m$ matrix denoted M^T given by the interchange of the rows and columns of M :

Note that

(i) $(M^T)^T = M$.

(ii)

This result generalizes: $(ABC)^T = C^T B^T A^T$ etc.

(b) Symmetric and anti-symmetric matrices

We define a **symmetric** matrix S to be a square matrix which satisfies $S^T = S$.

Thus

We define an **anti-symmetric** (or **skew-symmetric**) matrix A to be a square matrix which satisfies $A^T = -A$. Thus

Given a general $m \times m$ matrix \mathbf{B} we can construct its symmetric and anti-symmetric parts given, respectively, by \mathbf{S} and \mathbf{A} to be

$$\mathbf{S} = \frac{1}{2}(\mathbf{B} + \mathbf{B}^T), \quad \mathbf{A} = \frac{1}{2}(\mathbf{B} - \mathbf{B}^T).$$

Conversely, we may always decompose \mathbf{B} as the sum of a symmetric matrix and an anti-symmetric matrix: $\mathbf{B} = \mathbf{S} + \mathbf{A}$.

(c) **Diagonal matrix**

A square matrix \mathbf{A} with non-zero entries only on the diagonal: $a_{ij} = 0 \quad i \neq j$. E.g.,

(d) **Unit matrix**

The unit or identity matrix is a diagonal matrix denoted $\mathbf{1}$ or \mathbf{I} (for identity) with elements δ_{ij} . δ_{ij} is called **Kronecker delta**, where $\delta_{ii} = 1, \delta_{ij} = 0 \quad i \neq j$. E.g., for $n = 3$

For any matrix \mathbf{A} we have $\mathbf{IA} = \mathbf{AI} = \mathbf{A}$.

(e) Orthogonal matrix

A square matrix O which satisfies $OO^T = O^T O = I$. E.g.,

(f) Complex conjugation

If $A = (a_{ij})$ then the **complex conjugate** is $A^* = (a_{ij}^*)$.

(g) Hermitian conjugation

If $A = (a_{ij})$ then the **hermitian conjugate** is $A^\dagger = (A^T)^* = (A^*)^T = (a_{ji}^*)$.

An **hermitian** matrix satisfies $A^\dagger = A$ (c.f. symmetric matrix) and is important in quantum mechanics.

(h) Trace

The **trace** of a matrix is defined for square matrices. For A being $m \times m$, we have

It is the sum of the elements on the main diagonal of the matrix.

Some properties of **trace** are:

(i)

It is sufficient for its definition that A is $m \times n$ and B is $n \times m$.

(ii)

$$\text{trace}(\mathbf{ABC}) = \text{trace}(\mathbf{CAB})$$

$$\sum_{ijk} a_{ij} b_{jk} c_{ki} = \sum_{kij} c_{ki} a_{ij} b_{jk}$$

(iii) This result can be generalized and holds for any **cyclic** permutation of the order of multiplication. For example

A **cyclic** permutation shifts all elements by a given amount with those elements shifted off one end being inserted at the other. E.g., 12345 \rightarrow 45123). (It's like moving the numbers around a clockface.)

1.2.3 Inner or scalar product

Can introduce a product of two vectors \mathbf{x}, \mathbf{y} called the **inner** or **scalar** product. (It can be defined for many kinds of vector space but it is not part of the axioms defining them; it is an extra optional property.) We now give some well-known examples:

- For real column vectors \mathbf{x}, \mathbf{y}
- For complex column vectors \mathbf{x}, \mathbf{y}

Note: in this case $\mathbf{x} \cdot \mathbf{y} = (\mathbf{y} \cdot \mathbf{x})^*$.

Then $\mathbf{x} \cdot \mathbf{x} = \sum_i |x_i|^2$ is real and positive or zero.

We define the **magnitude** of \mathbf{x} to be $\|\mathbf{x}\| = \sqrt{\mathbf{x} \cdot \mathbf{x}}$.

(i) If $\mathbf{x} \cdot \mathbf{y} = 0$ then \mathbf{x} and \mathbf{y} are said to be **orthogonal**.

(ii) A basis $\mathbf{e}_1, \dots, \mathbf{e}_n$ which satisfies $\mathbf{e}_i \cdot \mathbf{e}_i = 1$, $\mathbf{e}_i \cdot \mathbf{e}_j = 0$, $i \neq j$ is called **orthonormal**.

Write as

E.g., in 2D

1.2.4 Relevance to linear equations

The system of linear algebraic equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= y_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= y_2 \\ &\vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= y_m \end{aligned}$$

can be written compactly using matrix notation as

1. The equations relate an n -dimensional column vector \mathbf{x} to an m -dimensional column vector \mathbf{y} .

2. They may be viewed as defining a linear transformation from an n -dimensional vector space V_n to an m -dimensional vector space V_m .

The problem of solving the equations can be viewed as finding the vector $\mathbf{x} \in V_n$ which is mapped under the transformation \mathbf{A} to the vector $\mathbf{y} \in V_m$. This may not always be possible or there may not always be unique solution for \mathbf{x} . Usually $m = n$, but our interpretation applies more generally.

1.3 Determinants

1.3.1 Definition

The solution of the linear equations

can be written

(provided no denominator vanishes), or more neatly as

where the **determinant** is defined as

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc .$$

Similarly, for 3 equations in 3 unknowns:

$$\begin{array}{c} x_1 \\ \left| \begin{array}{ccc} y_1 & a_{12} & a_{13} \\ y_2 & a_{22} & a_{23} \\ y_3 & a_{32} & a_{33} \end{array} \right| \\ \end{array} = \begin{array}{c} x_2 \\ \left| \begin{array}{ccc} a_{11} & y_1 & a_{13} \\ a_{21} & y_2 & a_{23} \\ a_{31} & y_3 & a_{33} \end{array} \right| \\ \end{array} = \begin{array}{c} x_3 \\ \left| \begin{array}{ccc} a_{11} & a_{12} & y_1 \\ a_{21} & a_{22} & y_2 \\ a_{31} & a_{32} & y_3 \end{array} \right| \\ \end{array} = \begin{array}{c} 1 \\ \left| \begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{array} \right| \\ \end{array} .$$

Spot the rule. The denominator of x_i is the determinant obtained by replacing the i -th column of (a_{ij}) by \mathbf{y} .

The 3×3 determinant is defined by

The general rule is defined recursively and to do this we first define **minors** and **cofactors**.

1.3.2 Minors and cofactors

Consider the square $n \times n$ matrix $\mathbf{A} = (a_{ij})$. Let \mathbf{M}_{ij} be the $(n-1) \times (n-1)$ submatrix of \mathbf{A} obtained by deleting its i th row and j th column. E.g.,

The determinant $|\mathbf{M}_{ij}|$ is called the **minor** of the element a_{ij} of \mathbf{A} .

The **cofactor** of a_{ij} , denoted A_{ij} is the “signed” minor:

The “signs” $(-1)^{i+j}$ form chess-board pattern with +’s on the main diagonal:

The matrix with the cofactors as its elements (*transposed*) is called the **classical adjoint** of \mathbf{A} and is written $\text{adj}\mathbf{A}$. It is defined by $(\text{adj}\mathbf{A})_{ij} = A_{ji}$:

$$\text{adj}\mathbf{A} = \begin{pmatrix} A_{11} & A_{21} & \cdots & A_{j1} & \cdots & A_{n1} \\ A_{12} & A_{22} & \cdots & A_{j2} & \cdots & A_{n2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{1i} & A_{2i} & \cdots & A_{ji} & \cdots & A_{ni} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{1m} & A_{2m} & \cdots & A_{jm} & \cdots & A_{nm} \end{pmatrix}$$

1.3.3 General rule for calculating a determinant

Given the square $n \times n$ matrix \mathbf{A} then the **determinant** of \mathbf{A} , denoted $|\mathbf{A}|$ or $\det \mathbf{A}$, is defined by

or

Examples

Let

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ -1 & 4 & 5 \\ 2 & 7 & 8 \end{pmatrix}.$$

Choosing to fix $i = 1$ then

Or fixing $j = 2$ get

The neat way to do this is to pick a row or column with the most zeros.

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 3 \\ -1 & 0 & 5 \\ 2 & 7 & 8 \end{pmatrix}.$$

Then we choose $j = 2$ and get

It's more work if you choose $j = 3$, for instance.

1.3.4 Permutations and determinants

A notion central to understanding determinants is the idea of a **permutation**. Here we will concentrate on $n = 3$ but the approach can be generalised to any n .

A **permutation** of the numbers $\{1, 2, 3\}$ is a rearrangement (or a sorting) of the numbers into a different order. So

is a permutation which we call $\sigma = 213$. It is understood that we started with 123. In

general there are $n!$ different permutations of n numbers or objects; the permutations simply specify the different orders in which they can be laid out.

A useful operation is to interchange neighbouring numbers. E.g. $213 \rightarrow 123$.

We count the number of pairwise interchange of neighbours that get us back to 123. If this is even (odd) then we say that σ is **even (odd)**. For $n = 3$ then

[This works for any n so, for example, 562341 is odd.]

We now define an important object. This is called the **Levi-Cevita tensor**, the **epsilon tensor** or the **totally antisymmetric tensor**. For $n = 3$ it is defined to be

$$\varepsilon_{j_1 j_2 j_3} = \begin{cases} 0 & \text{if any pair of } j_1 j_2 j_3 \text{ are equal} \\ +1 & \text{if } \sigma = j_1 j_2 j_3 \text{ is even} \\ -1 & \text{if } \sigma = j_1 j_2 j_3 \text{ is odd} \end{cases}$$

Thus

Note that $\varepsilon_{j_1 j_2 j_3}$ is **antisymmetric** under the interchange of **any** pair of indices.

All of these results generalise to n objects and indices. In particular, for $n = 2$ we have

$$\varepsilon_{11} = \varepsilon_{22} = 0, \quad \varepsilon_{12} = 1, \quad \varepsilon_{21} = -1 .$$

An important result is illustrated by the example of 3×3 matrices. It is

The first sum is over $j_i = 1, 2, 3$ for each j_i and in the second sum similarly over the i 's.

Remarks

- A similar result is easily checked for $n = 2$. It can be generalized to arbitrary n .
- The sum on the right-hand side consists of $3! = 6$ terms, corresponding to the number of permutations, each of which is a product of 3 elements from (a_{ij}) ; each term has exactly one element from each row and column.

To get a feel for this expression we illustrate with $n = 3$.

1. let $\mathbf{a}, \mathbf{b}, \mathbf{c}$ be 3-dimensional vectors. Then the well-known **vector product** given by

$$\mathbf{a} = \mathbf{b} \wedge \mathbf{c} \text{ (written also as } \mathbf{b} \times \mathbf{c} \text{) has elements}$$

2. Then by construction we clearly have

The last result follows because $\varepsilon_{ijk} = -\varepsilon_{jik}$; it is anti-symmetric under $i \leftrightarrow j$ whereas $b_i b_j$ is obviously symmetric under this interchange. Similarly, $\mathbf{c} \cdot (\mathbf{b} \wedge \mathbf{c}) = 0$.

3. Consider

$$\mathbf{A} = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}$$

Then

the determinant of a 3×3 matrix is the scalar triple product of its rows (or columns) treated as vectors.

4. One important general result is that if the **same** vector occurs twice anywhere in the sum involving the ε -tensor (i.e., in the **contraction** of vectors with ε) then the answer is zero. E.g.,

The result follows because the permutation needed for $j_2 \leftrightarrow j_3$ is always odd; $\varepsilon_{j_1 j_2 j_3}$ is **anti-symmetric** under interchange of **any** pair of indices.

It also follows immediately that if a matrix has any two rows (or columns) equal then its determinant is **zero**.

5. Consider the 3×3 matrix $\mathbf{A} = (a_{ij})$. Then the cofactors A_{ij} are given by

$$\begin{aligned} A_{1j} &= \sum_{j_2 j_3} \varepsilon_{j j_2 j_3} a_{2j_2} a_{3j_3} = (\mathbf{a}_2 \wedge \mathbf{a}_3)_j, \\ A_{2j} &= \sum_{j_1 j_3} \varepsilon_{j_1 j j_3} a_{1j_1} a_{3j_3} = (\mathbf{a}_3 \wedge \mathbf{a}_1)_j, \\ A_{3j} &= \sum_{j_1 j_2} \varepsilon_{j_1 j_2 j} a_{1j_1} a_{2j_2} = (\mathbf{a}_1 \wedge \mathbf{a}_2)_j. \end{aligned}$$

Here $\mathbf{a}_i = (a_{i1}, a_{i2}, a_{i3})$ – the i -th row of \mathbf{A} written as a (row) vector. It is easy to verify that for each j these are the correct “signed” sub-determinants. Also, we see that, for example,

which recovers our earlier expression for $|\mathbf{A}|$.

We see also that

This follows because

- (a) It is the scalar triple product with two vectors the same.
- (b) It is the determinant of a matrix with two rows the same.
- (c) When we unpack the sums we see that the same vector (either \mathbf{a}_2 or \mathbf{a}_3) occurs twice in the contraction with ε .

The general result for arbitrary n is that

$$\sum_k a_{ik} A_{jk} = \begin{cases} |\mathbf{A}| & i = j \\ 0 & i \neq j \end{cases}.$$

As in (b) above, for $i \neq j$ this is the determinant of a matrix with two rows the same.

In matrix notation we have

1.3.5 Properties of determinants

We collect here properties mentioned above and a few extra ones with examples. Many of these properties can be derived from the equations for determinants of $n \times n$ matrices:

1. Interchanging any two rows or columns of a matrix changes the sign of its determinant.
2. $|\mathbf{A}| = 0$ if any two rows or columns are the same.
3. The matrix obtained by multiplying all the elements of any one row (or column) of \mathbf{A} by λ has determinant $\lambda|\mathbf{A}|$.

4. Adding a multiple of one row (column) to another row (column) leaves the determinant unchanged. This is a useful way of reducing the calculation of $|\mathbf{A}|$. E.g., our 3×3 example from before:

Then easily find $|\mathbf{A}| = 1 \times 6 \times (-2) = -12$.

We have reduced the matrix to **upper triangular form** by performing **row operations**. We could similarly define **lower triangular form** and **column operations**. The determinant is then just the product of the elements on the main diagonal.

This is a much faster method for large matrices. The original definition requires $O(n!)$ mathematical operations (\times , $+$), whereas this new method of reduction to upper (lower) triangular form requires only $O(n^3)$ operations. (Computationally, there can be issues with accuracy depending on the values of the matrix elements.)

5. $\det(\mathbf{AB}) = (\det \mathbf{A})(\det \mathbf{B})$. This follows directly from the definition in terms of the ε -tensor but is fiddly to show. It relies on a useful result that I state for $n = 3$ but is easily generalized:

We can show this by interchanging two i 's on both sides and noting that this is equivalent to interchanging the associated pair of j 's on LHS together with multiplying by (-1) because the ε -tensor is antisymmetric under interchange of j 's.

6. $|\mathbf{A}| = |\mathbf{A}^T|$. Using rows or columns in the formula are equivalent. E.g., consider

This can be proved from the equation in item 5 and is generalisable to $n \times n$ matrices.

7. For ordinary 3D vectors in standard notation:

$$\mathbf{u} \wedge \mathbf{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix}, \quad \text{curl } \mathbf{v} = \nabla \wedge \mathbf{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \partial/\partial x_1 & \partial/\partial x_2 & \partial/\partial x_3 \\ v_1 & v_2 & v_3 \end{vmatrix}.$$

8. The (signed) volume of the parallelepiped in 3D with sides $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is $V(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \mathbf{a} \cdot (\mathbf{b} \wedge \mathbf{c})$. Thus

The general result, which can be proved by induction, is that the (signed) n -dimensional volume of a parallelepiped in n -dimensions with sides $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$ is

Of course, here $\mathbf{A} = (a_{ij})$ as usual. In all examples we can use columns instead of rows.

9. A result that is proved using $\det(\mathbf{AB}) = (\det \mathbf{A})(\det \mathbf{B})$ can be illustrated in 3D. Given two parallelepipeds defined by $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ and $(\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3)$ which are related by

(treating \mathbf{x}_i and \mathbf{y}_i as column vectors), then

We can see that this makes sense in the case that \mathbf{A} is diagonal. With canonical basis vectors the length unit in the e_i direction is scaled by a_{ii} (e.g., the length unit in $(0, 1, 0)$ direction is scaled by a_{22}), and so the volume is scaled by $a_{11}a_{22}a_{33} \equiv |\mathbf{A}|$. This generalizes to $n \times n$ matrices and can be the basis of the general proof.

1.4 Inverse of a matrix

We consider only square matrices from now on.

Suppose we can find a matrix \mathbf{A}^{-1} such that

We then can find the solution to the system of linear algebraic equations

$$\mathbf{Ax} = \mathbf{y},$$

by premultiplying both sides by \mathbf{A}^{-1} to give

and hence we determine x .

The question is whether given A that A^{-1} exists and whether it is unique.

1.4.1 Uniqueness of inverse

If A^{-1} exists, it is unique and is **both** the **left** and **right** inverse. By this we mean

If $LA = I$ then L is the **left inverse** of A

If $AR = I$ then R is the **right inverse** of A .

Suppose that L is not unique, i.e., $L_1A = I$ and $L_2A = I$. Then

Hence, $L_1 = L_2$ and so L (and likewise R) is unique.

Now

and so the left and right inverses are the same.

1.4.2 Existence and construction of inverse

Earlier in this course we derived the important result that

$$A(\text{adj}A) = (\det A)I.$$

Thus, if A^{-1} exists, we have a ready-made construction of the right inverse of A and

hence of A^{-1} , namely

The 3×3 case is familiar. Suppose

$$\mathbf{A} = \begin{pmatrix} \mathbf{a} & \longrightarrow & \\ \mathbf{b} & \longrightarrow & \\ \mathbf{c} & \longrightarrow & \end{pmatrix},$$

then

$$\mathbf{A}^{-1} = \frac{1}{\mathbf{a} \cdot (\mathbf{b} \wedge \mathbf{c})} \begin{pmatrix} \mathbf{b} \wedge \mathbf{c} & \mathbf{c} \wedge \mathbf{a} & \mathbf{a} \wedge \mathbf{b} \\ \downarrow & \downarrow & \downarrow \end{pmatrix}.$$

This works because

If $|\mathbf{A}| = 0$ then \mathbf{A}^{-1} does not exist and we say that \mathbf{A} is a **singular matrix**. This is the matrix generalization of the statement that $x \times 0 = 1$ has no solution for x .

However, a matrix whose determinant is zero is still not trivial. Some examples are

These matrices are equivalent under row operations. If $|\mathbf{A}| = 0$ then at least one row

(column) can be reduced to zeros by row (column) operations.

$$\begin{pmatrix} 0 & 4 & 0 & 7 \\ 0 & 3 & 0 & 5 \\ 0 & -1 & 0 & 9 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 15 & 4 & 18 & 7 \\ 11 & 3 & 13 & 5 \\ 7 & -1 & 17 & 9 \\ 2 & 1 & 1 & 0 \end{pmatrix}.$$

These two matrices are equivalent under the column operations $C1 \rightarrow C1 + 2 \times C2 + C4$, $C3 \rightarrow C3 + C2 + 2 \times C4$.

1.4.3 Orthogonal matrices

A square matrix O which satisfies $OO^T = O^T O = I$ is called an **orthogonal matrix**.

Thus, $O^{-1} = O^T$. We have

(i) **Rotations** The rotation of a vector in \mathbb{R}^n is a linear map given by an orthogonal matrix. For $n = 2$:

$$\mathbf{R}(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

$n = 2$ Generally, a rotation of column vector x through angle θ gives a vector y

where

Rotations preserve the length of the vector and so

This property is true for all x and hence we deduce that $\mathbf{R}^T \mathbf{R} = \mathbf{I}$. We may prove that $\mathbf{R} \mathbf{R}^T = \mathbf{I}$ by noting that $x = \mathbf{R}^T y$ and repeating the argument. For rotations, $|\mathbf{R}| = 1$.

(ii) Reflections

The vector x' obtained by reflecting x in a plane with unit normal n is $x' = x - 2(x \cdot n)n$. In matrix notation, writing n as a column vector:

- Note that $O^T = O$; from this and $OO^T = I$ we know that O is its own inverse. This is clear geometrically – two reflections in the same plane get you back to original vector.
- Use $n^T n = 1$ to show $O^T O = I$:

For reflection $|O| = -1$. Check this (without loss of generality) by choosing $n^T = (0, 0, 1)$. Then $O = \text{diag}(1, 1, -1)$ (diagonal matrix with these elements on diagonal).

- Two successive different reflections: O_1 followed by O_2 give a total transformation, or map, $R = O_2 O_1$. Now, R is orthogonal:

and

Thus R is a **rotation**.

1.5 Linear equations

1.5.1 Cramer's rule

If $\mathbf{Ax} = \mathbf{y}$ and $|\mathbf{A}| \neq 0$, then

Then

We can rewrite the RHS and we get

where the y 's replace the i -th column in \mathbf{A} . This is **Cramer's rule**.

1.5.2 Uniqueness of solutions

Consider the set of equations

where \mathbf{A} is $m \times n$, \mathbf{x} is $n \times 1$ and \mathbf{y} is $m \times 1$ (i.e., column vectors). Given \mathbf{y} , we wish to investigate the possible solutions to these m equations for the n unknowns x_1, x_2, \dots, x_n .

- We may have **redundant** equations in this set. A redundant equation is some linear combination of the others and should be omitted. If there are redundant equations the equations will be **linearly dependent**.
- There may be **inconsistent** equations in the set. This is best seen by example:

The first example is more obvious. In the second, on LHS $R3 = 2 \times R1 + R2$ but $7 \neq 2 \times 1 + 3$.

The system of equations is **Inconsistent** if the LHS is **linearly dependent** but the corresponding y -values on RHS do not obey the **same** linear relationship. Then no solution exists.

We can first check linear dependence on the LHS by inspecting the entries in \mathbf{A} and then, if necessary, inspect the entries in \mathbf{y} to check for **redundancy** or **inconsistency**.

- (1) If $m < n$ the system is **underdetermined**; there is not enough information to fix all the x 's. However, unless the equations are inconsistent, it is possible to express some of the x 's in terms of the others. That is, to find a **family** of solutions.

E.g., $m = 1$, $n = 2$:

This defines a straight line in the 2D space of (x_1, x_2) .

In general, the family of solutions will lie in an $(n - m)$ dimensional subspace (or larger if there are redundant equations) of the n -dim space in which \mathbf{x} lies. E.g., in 3 dimensions (and assuming no redundancy) $m = 2$, $n = 3$ is a line, $m = 1$, $n = 3$ is a plane.

- (2) If $m > n$ then the LHS of the equations **must** be linearly dependent since the vectors $\mathbf{a}_1 \cdots \mathbf{a}_m$ lie in an n -dim space. Then, the different cases are

- (i) The equations are **inconsistent** and so there is **no** solution. In this case we say that the system is overdetermined. E.g., 3×2 case

On LHS $R_3 = R_1 + 2 \times R_2$ but on RHS $12 \neq 1 + 2 \times 4$.

- (ii) There are redundant equations and we can discard them and so reduce m . If, after discarding them
- $m > n$: then we are still overdetermined as in (2)(i);
 - $m < n$: then the system is underdetermined as in (1);
 - $m = n$: this is an important case.

- (3) The $n \times n$ case.

- (i) $|\mathbf{A}| \neq 0$. In this case the rows (and columns) of \mathbf{A} are linearly independent and so the equations are neither redundant nor inconsistent. The inverse \mathbf{A}^{-1} exists and is unique. The system of equations has the solution

In the special case $\mathbf{y} = 0$ the **only** solution is $\mathbf{x} = 0$. Thus,

Note, that since the columns of \mathbf{A} treated as vectors $\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_n$ are linearly independent they form a **basis** for \mathbb{R}^n . Thus

$$\mathbf{A} = \begin{pmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_n \\ \downarrow & \downarrow & & \downarrow \end{pmatrix}.$$

The equations are then just

the x_i 's are the **coordinates** of \mathbf{y} in this basis. Hence, if $\mathbf{y} = \mathbf{0}$, the zero vector, we expect all coordinates $x_i = 0, \forall i$.

- In general we can solve the equations $\mathbf{A}\mathbf{x} = \mathbf{y}$ by performing row operations to both sides (i.e., on \mathbf{A} and \mathbf{y}) chosen to reduce \mathbf{A} to upper triangular form. The equations then solve iteratively.

Then operations $R_2 \rightarrow (R_2 - 2 \times R_1)$, $R_3 \rightarrow (R_3 + R_1)$, $R_3 \rightarrow (R_3 - 3 \times R_2)$

give

$$\begin{pmatrix} 1 & 4 & 3 \\ 0 & 1 & -1 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 9 \\ -1 \\ 4 \end{pmatrix}$$

We can now solve, in order, $x_3 = 2$, $x_2 = 1$, $x_1 = -1$. Also, $|\mathbf{A}| = 2$.

This is an example of **Gaussian elimination**.

- (ii) $|\mathbf{A}| = 0$, $\mathbf{y} = \mathbf{0}$. We seek solutions of the **homogeneous** equations

It is now convenient to think of the rows of \mathbf{A} being vectors $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n$:

$$\mathbf{A} = \begin{pmatrix} \mathbf{r}_1 & \longrightarrow \\ \mathbf{r}_2 & \longrightarrow \\ \vdots & \vdots \\ \mathbf{r}_n & \longrightarrow \end{pmatrix}.$$

The \mathbf{r} 's are linearly dependent, and let the greatest number of independent vectors be k . So the \mathbf{r} 's span a subspace S_r of \mathbb{R}^n , with $\dim S_r = k$.

The equations are now written

Consider an example with $n = 3$: suppose that $k = 2$ and so there are two linearly independent vectors in $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$. Choose these to be $\mathbf{r}_1, \mathbf{r}_2$. Then they form a basis for the 2D space S_r ("r" for **row**). The equations to be solved are

$$\mathbf{x} \cdot \mathbf{r}_1 = 0, \quad \mathbf{x} \cdot \mathbf{r}_2 = 0, \quad \mathbf{x} \cdot \mathbf{r}_3 = 0.$$

The trick is to find a vector \mathbf{z} that does **not** lie in S_r , and $\mathbf{z} = \mathbf{r}_1 \wedge \mathbf{r}_2$ is the obvious choice. By construction $\mathbf{z} \cdot \mathbf{r}_i = 0$, $i = 1, 2, 3$. Then clearly

and hence we deduce the solution for \mathbf{x} to be

for any value of λ .

The result for the general case stated above is that there will be $(n - k)$ independent vectors $\mathbf{z}_1, \dots, \mathbf{z}_{n-k}$ that do not lie in S_r so that for any $\mathbf{s} \in S_r$ then $\mathbf{s} \cdot \mathbf{z}_i = 0, \forall i$.

Since

the solution for \mathbf{x} is of the form

for any α_i , $i = 1, 2, \dots, (n - k)$.

(The space spanned by z_1, z_2, \dots, z_{n-k} is called the **kernel** of A .)

(iii) $|\mathbf{A}| = 0$, $\mathbf{y} \neq \mathbf{0}$.

The column vectors of A , denoted $\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_n$, referred to in (i) are **linearly dependent** and so **do not** form a basis for \mathbb{R}^n but rather only **span** a subspace $S_c \subseteq \mathbb{R}^n$ ("c" for **column**). If the greatest number of independent vectors is k , then S_c has $\dim S_c = k$. (Note, that although S_c and S_r have the same dimension they are generally **not** the same subspace.)

Look again at the equation in the form

- If \mathbf{y} does **not** lie in the subspace S_c ($\mathbf{y} \notin S_c$), there can be **no** solution for \mathbf{x} . (S_c is called the **image** of A since A must map every vector $\mathbf{x} \in \mathbb{R}^n$ into S_c .) Consider an example with $n = 3$:

The columns of the matrix are linearly dependent: $\mathbf{c}_3 = 2 \times \mathbf{c}_1 + \mathbf{c}_2$. One can

choose the basis for the 2 dimensional space S_c to be

In a manner similar to before, consider $\mathbf{w} = \mathbf{c}_1 \wedge \mathbf{c}_2$. Here

$$\mathbf{c}_1 \wedge \mathbf{c}_2 = \begin{pmatrix} 1 \\ -4 \\ 7 \end{pmatrix}.$$

Since $\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_1 \wedge \mathbf{c}_2$ **do** form a basis for \mathbb{R}^3 we can write

The point is that if $p_3 \neq 0$ then \mathbf{y} does not lie in S_c and there is no solution. The condition for \mathbf{y} to lie in S_c is

This is satisfied by \mathbf{y} as given in the example, but it wouldn't be if instead the RHS were $\mathbf{y} = (2, -2, 8)^T$ for example.

The result for the general case stated above is that there will be $(n-k)$ independent vectors $\mathbf{w}_1, \dots, \mathbf{w}_{n-k}$ that **do not** lie in S_c so that for any $\mathbf{s} \in S_c$ then $\mathbf{s} \cdot \mathbf{w}_i = 0, \forall i$. The conditions for a solution for \mathbf{x} to exist are then

$$\mathbf{y} \cdot \mathbf{w}_i = 0 \quad i = 1, 2, \dots, (n-k).$$

Suppose these conditions are satisfied and we find a solution \mathbf{x}_0 : $\mathbf{A}\mathbf{x}_0 = \mathbf{y}$. This solution is **not unique** since we clearly also have

Thus, the most general solution to $\mathbf{Ax} = \mathbf{y}$ in this case is

where the \mathbf{z}_i satisfy $\mathbf{Az}_i = \mathbf{0}$, $i = 1, 2, \dots, (n - k)$ as explained in (ii).

1.6 Eigenvalues and eigenvectors

If

where \mathbf{A} is $n \times n$, λ is a scalar and $\mathbf{v} \neq \mathbf{0}$, then

- λ is an **eigenvalue** of \mathbf{A}
- \mathbf{v} is the **eigenvector** of \mathbf{A} corresponding to the eigenvalue λ .

(i) Acting (or operating) on \mathbf{v} with \mathbf{A} scales it by λ leaving the **direction** unchanged.

(ii) If \mathbf{v} is an eigenvector then so is $\alpha\mathbf{v}$.

We can then write

The only solution is $\mathbf{v} = \mathbf{0}$ **except** for special values of λ for which $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$.

Thus, we seek solutions for λ to

$$\det(\mathbf{A} - \lambda\mathbf{I}) = \begin{vmatrix} a_{11} - \lambda & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} - \lambda & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} - \lambda \end{vmatrix} \equiv P_A(\lambda) = 0.$$

This determinant is a polynomial of degree n in λ and is called the **characteristic polynomial** $P_A(\lambda)$ of \mathbf{A} . It is degree n since

- each term in $P_A(\lambda)$ is n -th order in the elements and contains one element from each row and column.
- The product of a 's on the diagonal is one such term and this contains λ^n .

$P_A(\lambda)$ has n roots and these are the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$. The set of eigenvalues is called the **spectrum** of A . E.g., consider

Here A is symmetric.

The eigenvalues may be **complex** even if the entries in A are real, e.g.

Here A is orthogonal and is a rotation matrix: the eigenvalues give the angle of rotation.

- (i) $\det(\mathbf{A} - \lambda \mathbf{I}) = P_A(\lambda) = (\lambda_1 - \lambda)(\lambda_2 - \lambda) \cdots (\lambda_n - \lambda)$. Evaluate with $\lambda = 0$
and find important result

- (ii) If $|\mathbf{A}| = 0$ then at least one eigenvalue is zero and the corresponding eigenvectors satisfy

This **homogeneous** equation was discussed earlier, and we can see that the set of eigenvectors with $\lambda = 0$ will span the **kernel** of \mathbf{A} ; the space of vectors annihilated by \mathbf{A} .

- (iii) By inspecting the definition of $P_{\mathbf{A}}(\lambda)$ and the coefficient of the λ^{n-1} term we can show that

- (iv) For real matrices the coefficients in $P_{\mathbf{A}}(\lambda)$ are real and so if any λ are complex then they must come in complex-conjugate pairs. The number of real eigenvalues (and eigenvectors) can therefore be less than n ; there are none in the 2×2 rotation example above when $\theta \neq 0, \pi$.

Each eigenvalue λ_a has its corresponding eigenvector \mathbf{v}_a :

Since $\alpha\mathbf{v}$ will also satisfy the eigenvalue equation, we can choose α so that \mathbf{v} is **normalized**, usually to length 1. Using the inner (or scalar) product we can choose the eigenvectors so that $\mathbf{v}_a \cdot \mathbf{v}_a = 1$.

1.6.1 Real symmetric matrices

Defined by $\mathbf{A} = \mathbf{A}^* = \mathbf{A}^T$.

1. A real symmetric matrix has **real eigenvalues**

Since $(\mathbf{v}^*)^T \mathbf{v} \neq 0$ we deduce that $(\lambda - \lambda^*) = 0$ and hence that λ is **real**.

The eigenvector \mathbf{v} is therefore **real** since it solves real equations with real coefficients.

2. The eigenvectors corresponding to different eigenvalues of a symmetric matrix are **orthogonal**. We prove this using a similar procedure to above.

$$\begin{aligned} \mathbf{A}\mathbf{v}_1 &= \lambda_1\mathbf{v}_1 \\ \mathbf{v}_1^T \mathbf{A} &= \lambda_1\mathbf{v}_1^T && \text{transpose} \\ \mathbf{v}_1^T \mathbf{A}\mathbf{v}_2 &= \lambda_1\mathbf{v}_1^T \mathbf{v}_2 && \text{right multiply by } \mathbf{v}_2 \end{aligned} \quad (1)$$

Similarly,

$$\begin{aligned} \mathbf{A}\mathbf{v}_2 &= \lambda_2\mathbf{v}_2 \\ \mathbf{v}_1^T \mathbf{A}\mathbf{v}_2 &= \lambda_2\mathbf{v}_1^T \mathbf{v}_2 && \text{left multiply by } \mathbf{v}_1^T \end{aligned} \quad (2)$$

Subtracting (1) – (2) we get

Since $\lambda_1 \neq \lambda_2$ we deduce that $\mathbf{v}_1^T \mathbf{v}_2 = 0$.

- (i) If some of the λ 's coincide ("degeneracy") there are still n linearly independent eigenvectors which can be made to be orthogonal. This is done by choice of suitable linear combinations of those v 's corresponding to the degenerate eigenvalues.
- (ii) Let us normalise each v_a to unit magnitude. The eigenvectors then comprise an **orthonormal basis** which we now denote e_1, \dots, e_n . So

We learn that if we want to choose a nice basis when working with A we should choose the basis given by its **orthonormal** eigenvectors.

1.6.2 Diagonalization of real symmetric matrices

Consider the $n \times n$ matrix X whose i -th column is e_i :

Now

So

Thus

- $\mathbf{X}^{-1} = \mathbf{X}^T$.
- $\mathbf{X}^T \mathbf{X} = \mathbf{X} \mathbf{X}^T = \mathbf{I}$.
- \mathbf{X} is an **orthogonal** matrix.
- $\det \mathbf{X} = 1$.

Now,

$$\mathbf{A}\mathbf{X} = \mathbf{A} \begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \mathbf{e}_n \\ \downarrow & \downarrow & \downarrow & \downarrow \end{pmatrix} = \begin{pmatrix} \lambda_1 \mathbf{e}_1 & \lambda_2 \mathbf{e}_2 & \cdots & \lambda_n \mathbf{e}_n \\ \downarrow & \downarrow & \downarrow & \downarrow \end{pmatrix}.$$

Thus

is a diagonal matrix with diagonal elements given by the eigenvalues of \mathbf{A} .

Clearly, \mathbf{A}' has the **same** eigenvalues as \mathbf{A} but its eigenvectors are the **canonical** basis:

$$\mathbf{e}'_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \mathbf{e}'_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \text{etc.}$$

1. Given $\mathbf{A}\mathbf{x} = \mathbf{y}$ we can write

with $\mathbf{x}' = \mathbf{X}^T \mathbf{x}$, $\mathbf{y}' = \mathbf{X}^T \mathbf{y}$. Clearly, in the special case of the eigenvectors:

$$\mathbf{e}'_i = \mathbf{X}^T \mathbf{e}_i.$$

2. What are the **coordinates** of \mathbf{x} in the basis of the eigenvectors $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$?

Then

$$\mathbf{x}' = \mathbf{X}^T \mathbf{x} = \sum_{i=1}^n x_i \mathbf{X}^T \mathbf{e}_i = \sum_{i=1}^n x_i \mathbf{e}'_i = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}.$$

The required coordinates x_i , $i = 1 \dots n$ are simply the entries in \mathbf{x}' .

3. Determinants

since $|\mathbf{X}| = 1$. Then, we have $|\mathbf{A}'| = \prod_{i=1}^n \lambda_i = |\mathbf{A}|$, the result we derived earlier.

Let's look at the earlier example

We now search for e_1 . This satisfies

$$\begin{pmatrix} -2 - \lambda_1 & 6 \\ 6 & 7 - \lambda_1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \equiv \begin{pmatrix} -12 & 6 \\ 6 & -3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \mathbf{0}.$$

These two equations are multiples of each other (by construction). Then

The normalized vector is

e_2 can be derived in a similar fashion, but we also know it is orthogonal to e_1 . Hence,

2 Partial Differential Equations

2.1 Introduction to PDEs

Often, we wish to investigate the behaviour of functions of more than one variable, eg

- The vibrating string where the displacement at position x and time t is $y(x, t)$.
- The amount of a substance at x and t diffusing in a medium measured by its concentration $\Theta(x, t)$, eg an ink drop in water.
- The electrostatic potential $\phi(x, y)$ due to a distribution of charge with charge density $\rho(x, y)$.

Each of these functions satisfies a **partial differential equation** (PDE) characteristic of the physical phenomenon being studied. A PDE is an equation relating a function $f(x, y, \dots)$ of **more than one variable** and its partial derivatives with respect to x, y, \dots

We define the notation

where each suffix denotes partial differentiation with respect to (w.r.t) that variable.

The PDE is then of the form

- The **order** of the PDE is the order of the highest derivative appearing in \mathbb{F} .
- The PDE is **linear** if \mathbb{F} contains no powers of f (or its derivatives) different to one (zero doesn't count).

To define a unique solution to an ordinary differential equation (ODE) we need extra pieces of information in the form of the values of f and/or its derivatives at a number of points to fix the arbitrary constants of integration. These are given by the particular conditions of the system being studied.

To obtain a unique solution to a PDE we need extra information in the form of values of f etc., on surfaces in (x, y, \dots) space. Usually, a solution is sought for (x, y, \dots) in some region \mathbb{D} and the extra information or **boundary conditions** are given on all or part of the **boundary** $\partial\mathbb{D}$ of this region. They fix arbitrary functions arising in the integration. E.g.,

It is generally a hard problem to work out just how much information is needed.

In these lectures we shall study examples of **linear PDEs of second order** in the context of their physical application.

2.2 Physical derivation of important equations

2.2.1 The wave equation

For our first physical example, we take a look at the **vibrating string**. Let the string be under tension T with mass per unit length ρ . The displacement of the string at position x and time t is $y(x, t)$.

Consider element AB of length dx .

- The transverse force F obtained by resolving in the y -direction is (for small displacements)

- The mass of this string element AB is ρdx .

Then Newton's Law is

$$T \frac{\partial^2 y}{\partial x^2} dx = \rho dx \frac{\partial^2 y}{\partial t^2}.$$

This is the **wave equation** for wave motion in the string:

$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 y}{\partial t^2}, \quad \text{Wave equation}$

where $c = \sqrt{T/\rho}$. We shall see that c is the velocity of the waves.

For problems in higher dimensions, such as sound waves, vibrations of a drum membrane etc, the equation becomes

$$\nabla^2 \psi(\mathbf{x}, t) = \frac{1}{c^2} \frac{\partial^2 \psi(\mathbf{x}, t)}{\partial t^2},$$

where $\psi(\mathbf{x}, t)$ is the displacement from equilibrium.

Here, the boundary conditions are the initial conditions for the position and velocity of **each segment** of the string. We need

2.2.2 The heat or diffusion equation

Consider a substance diffusing in 1D and let the concentration (i.e., density) be $\Theta(x, t)$ at position x and time t .

The rate of diffusion from A to B is proportional to the concentration gradient.

Here κ is the constant of diffusion.

Hence the rate of change of substance in region B is

OR

$$\frac{\partial \Theta(x, t)}{\partial t} = \kappa \frac{\partial^2 \Theta(x, t)}{\partial x^2} . \quad \text{Heat/Diffusion equation}$$

A drop of ink in still water spreads out as a cloud with density $\Theta(\mathbf{x}, t)$ at time t . $\Theta(\mathbf{x}, t)$ obeys the 3D **Diffusion equation**

$$\frac{\partial \Theta(\mathbf{x}, t)}{\partial t} = \kappa \nabla^2 \Theta(\mathbf{x}, t) .$$

A closely related equation is the Schrödinger equation for a free particle in quantum mechanics:

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t) .$$

\hbar is Planck's constant and m is the particle mass. The analogy with the heat equation is important.

The boundary condition in this case is to give the initial value of Θ :

This is physically sensible since the spot of ink has an initial shape which is all we need to know to predict how it will spread.

2.2.3 Laplace's equation

Consider the temperature distribution $\phi(x, y)$ in a 2D body in equilibrium: ϕ is independent of time t .

Q_x (Q_y) is the heat-energy flux in the x (y) direction.

The phenomenological physical law giving Q_x and Q_y is

I.e., Q is proportional to minus the temperature gradient and the length of the edge.

The constant of proportionality is the thermal conductivity σ .

The **total** influx of heat-energy is **zero**. Thus

\Rightarrow

$$\frac{\partial Q_x}{\partial x} \Delta x + \frac{\partial Q_y}{\partial y} \Delta y = 0$$

OR

Thus

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0. \quad \text{Laplace's Equation}$$

Another application is to the electrostatic potential $\phi(\mathbf{x})$ due to a distribution of charge density $\rho(\mathbf{x})$. The electric field satisfies

$$\nabla \cdot \mathbf{E}(\mathbf{x}) = \frac{1}{\varepsilon_0} \rho(\mathbf{x}), \quad \text{and} \quad \mathbf{E}(\mathbf{x}) = -\nabla \phi(\mathbf{x}).$$

Hence, we obtain

This reduces to Laplace's equation when $\rho(\mathbf{x}) = 0$.

The boundary conditions are more varied for different problems here. They typically take one of two forms giving data on the whole boundary $\partial\mathbb{D}$ to the region \mathbb{D} where the solution is needed. The two main choices are

(i) **Dirichlet condition**

Give the **value** of ϕ on $\partial\mathbb{D}$. This would be typical if we know the temperature on the boundary and want to know it in the interior.

(ii) **Neumann condition**

Give the **normal derivative** of ϕ on $\partial\mathbb{D}$. This is typical of electrostatic problems where we are given the electric field \mathbf{E} at the boundary and wish to calculate the potential ϕ inside.

$$\mathbf{n}(\mathbf{x}) \cdot \nabla\phi(\mathbf{x}) \equiv \frac{\partial\phi}{\partial n}(\mathbf{x}) = \phi_n(\mathbf{x}) \quad \begin{cases} \mathbf{x} \in \partial\mathbb{D}, \\ \mathbf{n}(\mathbf{x}) \text{ is unit surface normal at } \mathbf{x} \end{cases} .$$

Note that $\mathbf{n}(\mathbf{x}) \cdot \nabla\phi(\mathbf{x}) = -\mathbf{n}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x})$.

It is possible to generalize and give a linear combination $\alpha\phi(\mathbf{x}) + \beta\frac{\partial\phi}{\partial n}$ on $\partial\mathbb{D}$.

2.3 Classification

This is a statement of terminology.

Consider the general form of a linear, 2nd order PDE in 2D

$$a\frac{\partial^2\psi}{\partial x^2} + 2b\frac{\partial^2\psi}{\partial x\partial y} + c\frac{\partial^2\psi}{\partial y^2} + f\frac{\partial\psi}{\partial x} + g\frac{\partial\psi}{\partial y} + h\psi = 0,$$

where a, b , etc. are constants.

(i) **Elliptic**

The equation is **elliptic** if $b^2 < ac$. One example is Laplace's equation

(ii) **Parabolic**

The equation is **parabolic** if $b^2 = ac$. One example is the heat equation in one space dimension, where t is considered to be the second dimension

(iii) Hyperbolic

The equation is **hyperbolic** if $b^2 > ac$. An example is the wave equation

2.4 Methods of solution

2.4.1 Method for some elliptic and hyperbolic equations in 2D

Consider equations of the form

$$a \frac{\partial^2 \psi}{\partial x^2} + 2b \frac{\partial^2 \psi}{\partial x \partial y} + c \frac{\partial^2 \psi}{\partial y^2} = 0.$$

We look for a solution of the form

where p is a constant and $z = x + py$.

Then we use the chain rule:

We substitute these into the original PDE to get

$$a \frac{d^2 f}{dz^2} + 2bp \frac{d^2 f}{dz^2} + cp^2 \frac{d^2 f}{dz^2} = 0.$$

Hence we find

with roots $p = p_+, p_-$ given by

These roots will be **complex** if $b^2 < ac$ i.e., for **elliptic** equations. In this case we see that $p_+ = p_-^*$.

Let $u = x + p_+y$, $v = x + p_-y$ and then, because the equation is **linear** we can take a **linear combination** of independent solutions to be the general solution. So we find

where f and g are arbitrary functions of a single variable. These are the analogues of the arbitrary constants in ordinary differential equations.

There are two special cases:

(a) The wave equation

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{\tilde{c}^2} \frac{\partial^2 \psi}{\partial t^2},$$

with $u = x - \tilde{c}t$, $v = x + \tilde{c}t$ and solution of the form

Note that here

$$\begin{aligned} \left(\frac{\partial}{\partial x}\right)_t &= \left(\frac{\partial}{\partial u}\right)_v \left(\frac{\partial u}{\partial x}\right)_t + \left(\frac{\partial}{\partial v}\right)_u \left(\frac{\partial v}{\partial x}\right)_t \\ &= \left(\frac{\partial}{\partial u}\right)_v + \left(\frac{\partial}{\partial v}\right)_u \\ \left(\frac{\partial}{\partial t}\right)_x &= \left(\frac{\partial}{\partial u}\right)_v \left(\frac{\partial u}{\partial t}\right)_x + \left(\frac{\partial}{\partial v}\right)_u \left(\frac{\partial v}{\partial t}\right)_x \\ &= -\tilde{c} \left(\frac{\partial}{\partial u}\right)_v + \tilde{c} \left(\frac{\partial}{\partial v}\right)_u \end{aligned}$$

The equation becomes, in terms of u and v :

$$\frac{\partial^2 \psi}{\partial u \partial v} = 0 \quad \Rightarrow \quad \psi(x, t) = f(u) + g(v).$$

An important example of this kind of solution is

with k an arbitrary constant. This is the equation of a wave travelling at velocity \tilde{c} .

More on this shortly.

(b) Laplace's equation

With $u = x + iy$, $v = x - iy$. Then we can write the general form most neatly as

$$\psi(x, y) = f(x + iy) + g(x - iy) \equiv f(z) + g(z^*) \quad \text{where } z = x + iy.$$

It may seem odd that the solution becomes complex when we started out with ψ real. However, because the equation is **linear** with real coefficients it must be that the real and imaginary parts of this solution **separately** satisfy the equation. Thus for our purposes we can restrict our solution to

Some examples are:

2.4.2 Separation of variables

Suppose $b = 0$. The general equation is now

$$a \frac{\partial^2 \psi}{\partial x^2} + c \frac{\partial^2 \psi}{\partial y^2} + f \frac{\partial \psi}{\partial x} + g \frac{\partial \psi}{\partial y} + h\psi = 0.$$

We now try a solution of the **separable** form $\psi(x, y) = X(x)Y(y)$. This will **not** be the most general solution since it would not be separable in this way. However, we will see that this is a very useful move.

We then get

OR, dividing by XY and rearranging slightly

$$\frac{1}{X} \left[a \frac{d^2 X}{dx^2} + f \frac{dX}{dx} + hX \right] = - \frac{1}{Y} \left[c \frac{d^2 Y}{dy^2} + g \frac{dY}{dy} \right] = \lambda \text{ a constant .}$$

This must be true since the LHS depends only on x and the RHS depends only on y and hence they cannot be equal unless they are **independent** of both x and y .

We thus obtain two ODEs which we solve using standard methods:

This is as far as we can go without knowing the specific problem under study and its boundary conditions.

It turns out that not necessarily all values of λ are allowed. Those that are allowed will be determined by the boundary conditions and might be a discrete set. Examples include the allowed frequencies of a plucked string and the values of the allowed energy levels in an atom. They are actually examples of **eigenvalues**.

For each **allowed** value of λ we label the separable solution with λ :

Also, because the equations are linear, then $\alpha\psi_\lambda$ is also a solution, with α being a constant. We then choose the **normalisation** of ψ_λ by some convenient procedure to make life easier. The general solution is the linear combination

where the sum is over the allowed values of λ and the α_λ are constants.

[Note: if $b \neq 0$ in the equation there is a $\partial^2\psi/\partial x\partial y$ term then a change of variables to $w = x + \alpha y, z = x + \beta y$ will give an equation of suitable form (with $b = 0$) for the right choice of constants α, β .]

2.5 Laplace's equation

Q What is the steady-state temperature distribution $\phi(x, y)$ for a region bounded by a square whose boundary, or edges, are maintained at the temperatures shown in the figure? Namely, three edges at $\phi = 0$ and the fourth at $\phi(a, y) = T(y)$. These are Dirichlet conditions. The square has edges of length a .

We use separation of variables and write

We thus have the two ODEs to solve:

$$\begin{aligned}\frac{d^2 X}{dx^2} - \lambda X &= 0, \\ \frac{d^2 Y}{dy^2} + \lambda Y &= 0.\end{aligned}$$

Then for

$$\lambda < 0 \quad \left\{ \begin{array}{l} X \text{ is sinusoidal} \\ Y \text{ is exponential} \end{array} \right., \quad \lambda > 0 \quad \left\{ \begin{array}{l} X \text{ is exponential} \\ Y \text{ is sinusoidal} \end{array} \right.$$

The choice is determined by the **boundary conditions**, and for this example we choose $\lambda > 0$ and set $\lambda = m^2$. The separable solution is then

We need

Hence, we impose

$$\begin{aligned} Y(0) &= Y(a) = 0, & \implies \\ Y(y) &\equiv Y_n(y) = C_n \sin\left(\frac{n\pi}{a}y\right), & n = 1, 2, \dots \end{aligned}$$

So we have that the **allowed** values of m are $m = n\pi/a$ for $n = 1, 2, \dots$. This in turn determines the $X_m(x)$ to have these values of m . Thus, the most **general** solution we can write down subject to these restrictions is

We can do this because the PDE is **linear**. [We have set $C_n = 1$ w.l.o.g. Also note that these solutions are $\text{Imag}(e^{\pm n\pi z/a})$, $z = (x + iy)$.]

We impose the boundary condition that

- $\phi(0, y) = 0$.

This gives

- $\phi(a, y) = T(y)$, some given function of y .

This gives the **Fourier series**

$$\sum_{n=1}^{\infty} 2A_n \sinh(n\pi) \sin\left(\frac{n\pi}{a}y\right) = T(y)$$

and hence that (multiply both sides by the orthogonal function $2\sin(m\pi y/a)/a$ then act on both sides with $\int_0^a dy$ to find A_n):

Suppose $a = 1$ and $T(y) = y$ as an example. Then we have (relabelling $m \rightarrow n$)

Doing this integral

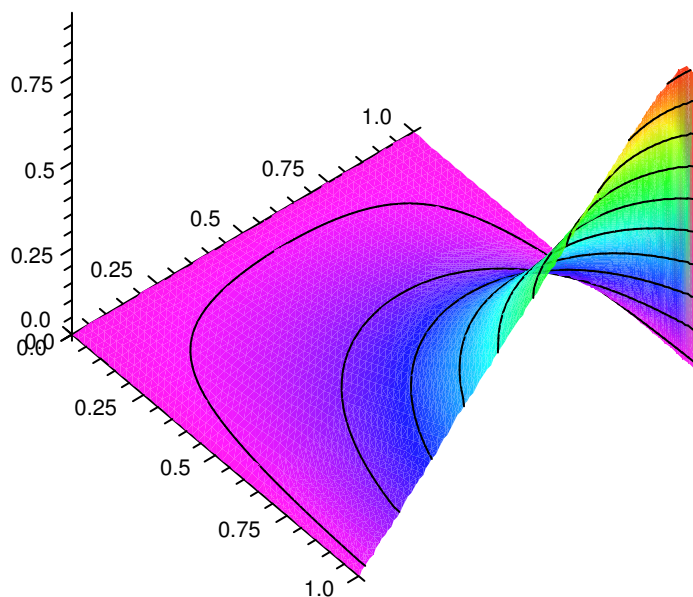
$$\begin{aligned} \int_0^1 dy y \sin(py) &= -\frac{d}{dp} \int_0^1 dy \cos(py) = -\frac{d}{dp} \left(\frac{\sin(p)}{p} \right) \\ &= \frac{1}{p^2} \sin(p) - \frac{1}{p} \cos p. \end{aligned}$$

Setting $p = n\pi$ we find

So

$$\phi(x, y) = \sum_{n=1}^{\infty} 2 \frac{(-1)^{n+1}}{n\pi \sinh(n\pi)} \sinh(n\pi x) \sin(n\pi y).$$

This is a half-range sin series. I used a sum of 100 terms here:



[Note that the set of separable solutions $\psi_n(x, y) = X_n(x)Y_n(y)$, $n = 1, 2, \dots$ form a **basis** for an ∞ -dimensional vector space of which $\phi(x, y)$ is a member given by the **linear combination** of the basis vectors shown in the Fourier series.]

To solve for more complicated boundary conditions we can write the full solution by adding or **superposing** the solutions to related problems that we have already solved.

E.g.,

Another example is the infinitely long strip of width a and with boundary conditions $\phi = 0$ on the upper and lower edges and $\phi \rightarrow 0$ as $x \rightarrow -\infty$. On the edge at $x = a$ we have $\phi(a, y) = T(y)$.

The most general solution is then as before

The condition $\phi \rightarrow 0$ as $x \rightarrow -\infty$ implies that $B_n = 0$.

On the edge at $x = a$ we have

and so again we have a Fourier series. This gives:

$$A_n = \frac{2}{a} e^{-n\pi} \int_0^a dy T(y) \sin\left(\frac{n\pi y}{a}\right).$$

2.6 The wave equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 y}{\partial t^2}.$$

2.6.1 The infinite string

We found a solution in the form

Suppose that the function $g(v)$ is given. Then as t varies $g(x - ct)$ vs x looks like

The shape moves **right** with velocity c .

Likewise, the shape described by $f(u)$, plotted as a function of x , moves **left** with velocity c as t increases.

It is sufficient to know $f(x)$ and $g(x)$ for **all** x at $t = 0$ to specify the solution. The shapes are **unchanged**; they do not **disperse** but just move left and right, respectively,

at velocity c : they are travelling waves. To find f and g it is sufficient to know the **initial conditions**

$$y(x, 0) = y_0(x) \quad \text{and} \quad \frac{\partial y}{\partial t}(x, 0) = v_0(x) \quad \text{for all } x.$$

Now, with $u = x + ct$ and $v = x - ct$,

Similarly,

$$\left. \frac{\partial g(v)}{\partial t} \right|_{t=0} = -c \left. \frac{dg}{dx} \right|_{t=0}.$$

The initial conditions are

(i) $f(x) + g(x) = y_0(x)$

(ii) Using the above relations

Thus, solving (i) and (ii),

$$\begin{aligned} f(x) &= \frac{1}{2}y_0(x) + \frac{1}{2c} \int^x dx' v_0(x'), \\ g(x) &= \frac{1}{2}y_0(x) - \frac{1}{2c} \int^x dx' v_0(x'). \end{aligned}$$

So we have

An example is

$$y_0(x) = e^{-x^2/2}, \quad v_0(x) = x^2,$$

for which

$$y(x, t) = \frac{1}{2}[e^{-(x+ct)^2/2} + e^{-(x-ct)^2/2}] + \frac{1}{6c}[(x+ct)^3 - (x-ct)^3].$$

The important special case mentioned earlier is of sinusoidal travelling waves:

$$y(x, t) = A \sin [\omega(x/c + t)] + B \sin [\omega(x/c - t)].$$

Here ω is the **frequency** of the wave.

It is often convenient to use complex exponential notation of the form

and use either the real or imaginary part of y at the end. Here A and B may be complex.

2.6.2 Guitar string (finite string, stopped at the ends)

The boundary conditions are

$$\begin{aligned} y(0, t) &= y(L, t) = 0, \quad \text{for all } t, \\ y(x, 0) &= y_0(x) \quad \text{and} \quad \frac{\partial y}{\partial t}(x, 0) = v_0(x) \quad \text{for } 0 < x < L. \end{aligned}$$

This will be solved by a Fourier series, and so we look for a separable solution:

giving

$$\frac{1}{X} \frac{d^2 X}{dx^2} = \frac{1}{c^2 T} \frac{d^2 T}{dt^2} = \lambda.$$

We shall choose $\lambda = -m^2$ so that we obtain sinusoidal solutions. Then

and we find the separable solution consistent with $y(0, t) = y(L, t) = 0$ to be

$$y_n(x, t) = \left[A_n \cos \left(\frac{n\pi ct}{L} \right) + B_n \sin \left(\frac{n\pi ct}{L} \right) \right] \sin \left(\frac{n\pi x}{L} \right),$$

where $m = n\pi/L$, $n = 1, 2, \dots$. Clearly, the solution vanishes at $x = 0, L \forall t$ by choice of the "sine" solution for $X(x)$.

The general solution is then, as before,

The boundary conditions then impose two Fourier series

1.) $y(x, 0) = y_0(x)$.

Set $t = 0$ to get

which gives

$$A_n = \frac{2}{L} \int_0^L dx y_0(x) \sin \left(\frac{n\pi x}{L} \right) .$$

2.) $\frac{\partial y}{\partial t}(x, 0) = v_0(x)$.

We take the first differential w.r.t. t and then set $t = 0$. We get

which gives

$$B_n = \frac{2}{n\pi c} \int_0^L dx v_0(x) \sin \left(\frac{n\pi x}{L} \right) .$$

The frequency of vibration for the separable solution labelled with n is $\omega_n = n\pi c/L$.

The general solution consists of a superposition of modes, or harmonics, with allowed frequencies ω_n only.

2.7 The heat or diffusion equation

The diffusion equation in 1D is

$$\frac{\partial \Theta}{\partial t} = \kappa \frac{\partial^2 \Theta}{\partial x^2} ,$$

with diffusivity $\kappa > 0$. Here $\Theta(x, t)$ is the concentration, or density, of material at time t . We expect the **total** amount of material to be conserved. I.e.,

To show that this is true, we take the derivative through the \int and use the diffusion equation:

The second step is integration by parts at **fixed** t (or simply integration of a derivative).

For any **physical** distribution we assume

$$\frac{\partial\Theta(\pm\infty, t)}{\partial x} = 0,$$

i.e., there is no outward flux at $x = \pm\infty$. Hence, $\text{RHS} = 0$ and the material is conserved. [This kind of manipulation is also important in quantum mechanics where the total probability is conserved.]

2.7.1 Infinite bar

This state is not in equilibrium, since it changes with time t . Imagine an infinite 1-dimensional bar. Parts of it are held at different temperatures. This temperature distribution at an initial time forms our boundary condition. Let's take an example: suppose that the **initial state** at $t = 0$ is

We look for solutions in terms of a dimensionless variable

Suppose solutions are of the form

We have

$$\begin{aligned}\frac{\partial \Theta}{\partial x} &= F'(u) \frac{\partial u}{\partial x} = F'(u) (4\kappa t)^{-1/2}, \\ \frac{\partial^2 \Theta}{\partial x^2} &= F''(u) (4\kappa t)^{-1}, \\ \frac{\partial \Theta}{\partial t} &= F'(u) \frac{\partial u}{\partial t} = F'(u) \left(\frac{-u}{2t} \right).\end{aligned}$$

The heat/diffusion equation then becomes

or

$$\frac{F''(u)}{F'(u)} = -2u.$$

This is

We thus find that

$$F(u) = A \int_0^u ds e^{-s^2} + B.$$

We define the **error** function $\operatorname{erf}(u)$ by

which satisfies

$$\operatorname{erf}(\pm\infty) = \pm 1 \quad \text{since} \quad \int_0^\infty ds e^{-\alpha s^2} = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}}.$$

Then we have the solution

$$\Theta(x, t) = A\sqrt{\pi}/2 \operatorname{erf}\left(\frac{x}{\sqrt{4\kappa t}}\right) + B.$$

For small t and $x > 0$ ($x < 0$) the argument, u , approaches $u = \infty$ ($-\infty$). Since $\operatorname{erf}(\pm\infty) = \pm 1$, the initial boundary condition imposes that $A = 1/\pi^{1/2}$ and $B = 1/2$.

The solution for $t \geq 0$ as t increases then looks like

2.7.2 Ink drop

Note then that, if $\Theta_1(x, t)$ is a solution to the diffusion equation ie

then so is

and hence taking $\Theta_1(x, t)$ to be the error function solution above we find the new solution

$$\Theta(x, t) = \frac{\partial}{\partial x} \frac{1}{\sqrt{\pi}} \int_0^{x/(4\kappa t)^{1/2}} ds e^{-s^2} = \frac{1}{(4\pi\kappa t)^{1/2}} e^{-x^2/4\kappa t}.$$

For small t , the material is concentrated in a small region around $x = 0$ of width $x \sim (\kappa t)^{1/2}$. The region of high concentration increases in size as the material spreads out: it diffuses. The initial state is therefore a highly concentrated spot at $x = 0$; e.g., an ink drop dropped into water. In fact, this is a normal distribution and as t increases we get

2.7.3 Bar of finite length

Consider a bar that occupies $0 \leq x \leq L$. The distribution of temperature obeys the heat equation.

In this example we give the boundary conditions as

- at $x = 0$ maintain temperature at zero: $\Theta(0, t) = 0 \quad t \geq 0$: a Dirichlet condition;
- at $x = L$ apply insulating boundary condition: there is no flux of heat to $x > L$. Then we have $\frac{\partial \Theta}{\partial x}(L, t) = 0, \quad t \geq 0$: a Neumann condition;
- at $t = 0$ the initial distribution is given: $\Theta(x, 0) = g(x), \quad 0 < x \leq L$: a Dirichlet condition.

We now look for separable solutions $\Theta(x, t) = X(x)T(t)$. Substituting, we find

and so

At this point in general we have different choices for C . These correspond to distinct physical situations and distinct kinds of boundary conditions. In our example it turns out that we need $C < 0$. For convenience, we now set $C = -\kappa\alpha^2$. We have

$$\kappa \frac{X''(x)}{X(x)} = \frac{T'(t)}{T(t)} = -\kappa\alpha^2,$$

with solutions

- The condition $\Theta(0, t) = 0$ is satisfied by taking $B = 0$.
- The condition $\Theta_x(L, t) = 0$ then requires $X'(L) = 0$, and so

Note that not all values of α are allowed.

- We can set $D = 1$ without loss of generality.

The most general solution satisfying the boundary conditions is then the Fourier series

$$\Theta(x, t) = \sum_{n=0}^{\infty} A_n \sin \left[\left(n + \frac{1}{2} \right) \pi x / L \right] \exp \left[-\kappa \left(n + \frac{1}{2} \right)^2 \pi^2 t / L^2 \right] .$$

The initial condition now requires

The functions $\left\{ \sin \left[\left(n + \frac{1}{2} \right) \pi x / L \right], n = 0, 1, \dots \right\}$ are orthogonal. Therefore, multiplying both sides by $\sin \left[\left(m + \frac{1}{2} \right) \pi x / L \right]$ and integrating from 0 to L gives

$$A_m = \frac{2}{L} \int_0^L dx g(x) \sin \left[\left(m + \frac{1}{2} \right) \pi x / L \right] .$$

Remark on other choices for C :

The choice $C > 0$ (real) in the separable solution discussed in the previous example will give solutions which grow exponentially in time and is thus unphysical. However, we **can** choose $C = i\omega$. This leads to **complex** separable solutions whose real and imaginary parts are then taken as the solutions for $\Theta(x, t)$. These are:

where k is an arbitrary constant and $\omega = 2k^2\kappa$. One can verify this by substitution.

Note that they represent **damped** travelling waves, the first two travelling in the **positive** x -direction, and the second two in the **negative** x -direction.

A physical application is to the temperature distribution interior to a bar subject to an oscillating heat source, of frequency ω , applied to one end. This is a simple model for the temperature in the interior of the earth subject to the daily cycle of radiation from the sun on its surface, for example.