8

Matrices and vector spaces

In the previous chapter we defined a *vector* as a geometrical object which has both a magnitude and a direction and which may be thought of as an arrow fixed in our familiar three-dimensional space, a space which, if we need to, we define by reference to, say, the fixed stars. This geometrical definition of a vector is both useful and important since it is *independent* of any coordinate system with which we choose to label points in space.

In most specific applications, however, it is necessary at some stage to choose a coordinate system and to break down a vector into its *component vectors* in the directions of increasing coordinate values. Thus for a particular Cartesian coordinate system (for example) the component vectors of a vector $\mathbf{a}$ will be $a_x\mathbf{i}$, $a_y\mathbf{j}$ and $a_z\mathbf{k}$ and the complete vector will be

$$\mathbf{a} = a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}. \tag{8.1}$$

Although we have so far considered only real three-dimensional space, we may extend our notion of a vector to more abstract spaces, which in general can have an arbitrary number of dimensions N. We may still think of such a vector as an 'arrow' in this abstract space, so that it is again *independent* of any (N-dimensional) coordinate system with which we choose to label the space. As an example of such a space, which, though abstract, has very practical applications, we may consider the description of a mechanical or electrical system. If the state of a system is uniquely specified by assigning values to a set of N variables, which could be angles or currents, for example, then that state can be represented by a vector in an N-dimensional space, the vector having those values as its components.

In this chapter we first discuss general *vector spaces* and their properties. We then go on to discuss the transformation of one vector into another by a linear operator. This leads naturally to the concept of a *matrix*, a two-dimensional array of numbers. The properties of matrices are then discussed and we conclude with

a discussion of how to use these properties to solve systems of linear equations. The application of matrices to the study of oscillations in physical systems is taken up in chapter 9.

8.1 Vector spaces

A set of objects (vectors) **a**, **b**, **c**, ... is said to form a *linear vector space V* if:

(i) the set is closed under commutative and associative addition, so that

$$\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}, \tag{8.2}$$

$$(\mathbf{a} + \mathbf{b}) + \mathbf{c} = \mathbf{a} + (\mathbf{b} + \mathbf{c}); \tag{8.3}$$

(ii) the set is closed under multiplication by a scalar (any complex number) to form a new vector $\lambda\mathbf{a}$, the operation being both distributive and associative so that

$$\lambda(\mathbf{a} + \mathbf{b}) = \lambda\mathbf{a} + \lambda\mathbf{b}, \tag{8.4}$$

$$(\lambda + \mu)\mathbf{a} = \lambda\mathbf{a} + \mu\mathbf{a}, \tag{8.5}$$

$$\lambda(\mu\mathbf{a}) = (\lambda\mu)\mathbf{a}, \tag{8.6}$$

where λ and μ are arbitrary scalars;

(iii) there exists a *null vector* **0** such that $\mathbf{a} + \mathbf{0} = \mathbf{a}$ for all **a**;

(iv) multiplication by unity leaves any vector unchanged, i.e. $1 \times \mathbf{a} = \mathbf{a}$;

(v) all vectors have a corresponding *negative vector* $-\mathbf{a}$ such that $\mathbf{a} + (-\mathbf{a}) = \mathbf{0}$. It follows from (8.5) with $\lambda = 1$ and $\mu = -1$ that $-\mathbf{a}$ is the same vector as $(-1) \times \mathbf{a}$.

We note that if we restrict all scalars to be real then we obtain a *real vector space* (an example of which is our familiar three-dimensional space); otherwise, in general, we obtain a *complex vector space*. We note that it is common to use the terms 'vector space' and 'space', instead of the more formal 'linear vector space'.

The *span* of a set of vectors $\mathbf{a}, \mathbf{b}, \ldots, \mathbf{s}$ is defined as the set of all vectors that may be written as a linear sum of the original set, i.e. all vectors

$$\mathbf{x} = \alpha\mathbf{a} + \beta\mathbf{b} + \cdots + \sigma\mathbf{s} \tag{8.7}$$

that result from the infinite number of possible values of the (in general complex) scalars $\alpha, \beta, \ldots, \sigma$. If **x** in (8.7) is equal to **0** for some choice of $\alpha, \beta, \ldots, \sigma$ (not *all* zero), i.e. if

$$\alpha\mathbf{a} + \beta\mathbf{b} + \cdots + \sigma\mathbf{s} = \mathbf{0}, \tag{8.8}$$

then the set of vectors $\mathbf{a}, \mathbf{b}, \ldots, \mathbf{s}$, is said to be *linearly dependent*. In such a set at least one vector is redundant, since it can be expressed as a linear sum of the others. If, however, (8.8) is not satisfied by *any* set of coefficients (other than

the trivial case in which all the coefficients are zero) then the vectors are *linearly independent*, and no vector in the set can be expressed as a linear sum of the others.

If, in a given vector space, there exist sets of N linearly independent vectors, but no set of $N+1$ linearly independent vectors, then the vector space is said to be N-dimensional. (In this chapter we will limit our discussion to vector spaces of finite dimensionality; spaces of infinite dimensionality are discussed in chapter 17.)

8.1.1 Basis vectors

If V is an N-dimensional vector space then *any* set of N linearly independent vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_N$ forms a *basis* for V. If $\mathbf{x}$ is an arbitrary vector lying in V then the set of $N+1$ vectors $\mathbf{x}, \mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_N$, must be *linearly dependent* and therefore such that

$$\alpha\mathbf{e}_1 + \beta\mathbf{e}_2 + \cdots + \sigma\mathbf{e}_N + \chi\mathbf{x} = \mathbf{0}, \tag{8.9}$$

where the coefficients $\alpha, \beta, \ldots, \chi$ are not all equal to 0, and in particular $\chi \neq 0$. Rearranging (8.9) we may write $\mathbf{x}$ as a linear sum of the vectors $\mathbf{e}_i$ as follows:

$$\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + \cdots + x_N\mathbf{e}_N = \sum_{i=1}^{N} x_i\mathbf{e}_i, \tag{8.10}$$

for some set of coefficients x_i that are simply related to the original coefficients, e.g. $x_1 = -\alpha/\chi$, $x_2 = -\beta/\chi$, etc. Since any $\mathbf{x}$ lying in the span of V can be expressed in terms of the *basis* or *base vectors* $\mathbf{e}_i$, the latter are said to form a *complete* set. The coefficients x_i are the *components* of $\mathbf{x}$ with respect to the $\mathbf{e}_i$-basis. These components are *unique*, since if both

$$\mathbf{x} = \sum_{i=1}^{N} x_i\mathbf{e}_i \qquad \text{and} \qquad \mathbf{x} = \sum_{i=1}^{N} y_i\mathbf{e}_i,$$

then

$$\sum_{i=1}^{N} (x_i - y_i)\mathbf{e}_i = \mathbf{0}, \tag{8.11}$$

which, since the $\mathbf{e}_i$ are linearly independent, has only the solution $x_i = y_i$ for all $i = 1, 2, \ldots, N$.

From the above discussion we see that *any* set of N linearly independent vectors can form a basis for an N-dimensional space. If we choose a different set $\mathbf{e}'_i$, $i = 1, \ldots, N$ then we can write $\mathbf{x}$ as

$$\mathbf{x} = x'_1\mathbf{e}'_1 + x'_2\mathbf{e}'_2 + \cdots + x'_N\mathbf{e}'_N = \sum_{i=1}^{N} x'_i\mathbf{e}'_i. \tag{8.12}$$

We reiterate that the vector $\mathbf{x}$ (a geometrical entity) is independent of the basis – it is only the components of $\mathbf{x}$ that depend on the basis. We note, however, that given a set of vectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_M$, where $M \neq N$, in an N-dimensional vector space, then *either* there exists a vector that cannot be expressed as a linear combination of the $\mathbf{u}_i$ *or*, for some vector that can be so expressed, the components are not unique.

8.1.2 The inner product

We may usefully add to the description of vectors in a vector space by defining the *inner product* of two vectors, denoted in general by $\langle \mathbf{a}|\mathbf{b}\rangle$, which is a scalar function of $\mathbf{a}$ and $\mathbf{b}$. The scalar or dot product, $\mathbf{a} \cdot \mathbf{b} \equiv |\mathbf{a}||\mathbf{b}| \cos\theta$, of vectors in real three-dimensional space (where θ is the angle between the vectors), was introduced in the last chapter and is an example of an inner product. In effect the notion of an inner product $\langle \mathbf{a}|\mathbf{b}\rangle$ is a generalisation of the dot product to more abstract vector spaces. Alternative notations for $\langle \mathbf{a}|\mathbf{b}\rangle$ are $(\mathbf{a}, \mathbf{b})$, or simply $\mathbf{a} \cdot \mathbf{b}$.

The inner product has the following properties:

(i) $\langle \mathbf{a}|\mathbf{b}\rangle = \langle \mathbf{b}|\mathbf{a}\rangle^*$,
(ii) $\langle \mathbf{a}|\lambda\mathbf{b} + \mu\mathbf{c}\rangle = \lambda\langle \mathbf{a}|\mathbf{b}\rangle + \mu\langle \mathbf{a}|\mathbf{c}\rangle$.

We note that in general, for a complex vector space, (i) and (ii) imply that

$$\langle \lambda\mathbf{a} + \mu\mathbf{b}|\mathbf{c}\rangle = \lambda^*\langle \mathbf{a}|\mathbf{c}\rangle + \mu^*\langle \mathbf{b}|\mathbf{c}\rangle, \tag{8.13}$$

$$\langle \lambda\mathbf{a}|\mu\mathbf{b}\rangle = \lambda^*\mu\langle \mathbf{a}|\mathbf{b}\rangle. \tag{8.14}$$

Following the analogy with the dot product in three-dimensional real space, two vectors in a general vector space are defined to be *orthogonal* if $\langle \mathbf{a}|\mathbf{b}\rangle = 0$. Similarly, the *norm* of a vector $\mathbf{a}$ is given by $\|\mathbf{a}\| = \langle \mathbf{a}|\mathbf{a}\rangle^{1/2}$ and is clearly a generalisation of the length or modulus $|\mathbf{a}|$ of a vector $\mathbf{a}$ in three-dimensional space. In a general vector space $\langle \mathbf{a}|\mathbf{a}\rangle$ can be positive or negative; however, we shall be primarily concerned with spaces in which $\langle \mathbf{a}|\mathbf{a}\rangle \geq 0$ and which are thus said to have a *positive semi-definite norm*. In such a space $\langle \mathbf{a}|\mathbf{a}\rangle = 0$ implies $\mathbf{a} = \mathbf{0}$.

Let us now introduce into our N-dimensional vector space a basis $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \ldots, \hat{\mathbf{e}}_N$ that has the desirable property of being *orthonormal* (the basis vectors are mutually orthogonal and each has unit norm), i.e. a basis that has the property

$$\langle \hat{\mathbf{e}}_i|\hat{\mathbf{e}}_j\rangle = \delta_{ij}. \tag{8.15}$$

Here δ_{ij} is the *Kronecker delta* symbol (of which we say more in chapter 26) and has the properties

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases}$$

In the above basis we may express any two vectors $\mathbf{a}$ and $\mathbf{b}$ as

$$\mathbf{a} = \sum_{i=1}^{N} a_i \hat{\mathbf{e}}_i \qquad \text{and} \qquad \mathbf{b} = \sum_{i=1}^{N} b_i \hat{\mathbf{e}}_i.$$

Furthermore, *in such an orthonormal basis* we have, for any $\mathbf{a}$,

$$\langle \hat{\mathbf{e}}_j | \mathbf{a} \rangle = \sum_{i=1}^{N} \langle \hat{\mathbf{e}}_j | a_i \hat{\mathbf{e}}_i \rangle = \sum_{i=1}^{N} a_i \langle \hat{\mathbf{e}}_j | \hat{\mathbf{e}}_i \rangle = a_j. \tag{8.16}$$

Thus the components of $\mathbf{a}$ are given by $a_i = \langle \hat{\mathbf{e}}_i | \mathbf{a} \rangle$. Note that this is *not* true unless the basis is orthonormal. We can write the inner product of $\mathbf{a}$ and $\mathbf{b}$ in terms of their components in an orthonormal basis as

$$\begin{aligned}
\langle \mathbf{a} | \mathbf{b} \rangle &= \langle a_1 \hat{\mathbf{e}}_1 + a_2 \hat{\mathbf{e}}_2 + \cdots + a_N \hat{\mathbf{e}}_N | b_1 \hat{\mathbf{e}}_1 + b_2 \hat{\mathbf{e}}_2 + \cdots + b_N \hat{\mathbf{e}}_N \rangle \\
&= \sum_{i=1}^{N} a_i^* b_i \langle \hat{\mathbf{e}}_i | \hat{\mathbf{e}}_i \rangle + \sum_{i=1}^{N} \sum_{j \neq i}^{N} a_i^* b_j \langle \hat{\mathbf{e}}_i | \hat{\mathbf{e}}_j \rangle \\
&= \sum_{i=1}^{N} a_i^* b_i,
\end{aligned}$$

where the second equality follows from (8.14) and the third from (8.15). This is clearly a generalisation of the expression (7.21) for the dot product of vectors in three-dimensional space.

We may generalise the above to the case where the base vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_N$ are *not* orthonormal (or orthogonal). In general we can define the N^2 numbers

$$G_{ij} = \langle \mathbf{e}_i | \mathbf{e}_j \rangle. \tag{8.17}$$

Then, if $\mathbf{a} = \sum_{i=1}^{N} a_i \mathbf{e}_i$ and $\mathbf{b} = \sum_{i=1}^{N} b_i \mathbf{e}_i$, the inner product of $\mathbf{a}$ and $\mathbf{b}$ is given by

$$\begin{aligned}
\langle \mathbf{a} | \mathbf{b} \rangle &= \left\langle \sum_{i=1}^{N} a_i \mathbf{e}_i \middle| \sum_{j=1}^{N} b_j \mathbf{e}_j \right\rangle \\
&= \sum_{i=1}^{N} \sum_{j=1}^{N} a_i^* b_j \langle \mathbf{e}_i | \mathbf{e}_j \rangle \\
&= \sum_{i=1}^{N} \sum_{j=1}^{N} a_i^* G_{ij} b_j.
\end{aligned} \tag{8.18}$$

We further note that from (8.17) and the properties of the inner product we require $G_{ij} = G_{ji}^*$. This in turn ensures that $\|\mathbf{a}\| = \langle \mathbf{a} | \mathbf{a} \rangle$ is real, since then

$$\langle \mathbf{a} | \mathbf{a} \rangle^* = \sum_{i=1}^{N} \sum_{j=1}^{N} a_i G_{ij}^* a_j^* = \sum_{j=1}^{N} \sum_{i=1}^{N} a_j^* G_{ji} a_i = \langle \mathbf{a} | \mathbf{a} \rangle.$$

8.1.3 Some useful inequalities

For a set of objects (vectors) forming a linear vector space in which $\langle \mathbf{a}|\mathbf{a}\rangle \geq 0$ for all $\mathbf{a}$, the following inequalities are often useful.

(i) *Schwarz's inequality* is the most basic result and states that

$$|\langle \mathbf{a}|\mathbf{b}\rangle| \leq \|\mathbf{a}\|\|\mathbf{b}\|, \tag{8.19}$$

where the equality holds when $\mathbf{a}$ is a scalar multiple of $\mathbf{b}$, i.e. when $\mathbf{a} = \lambda\mathbf{b}$. It is important here to distinguish between the *absolute value* of a scalar, $|\lambda|$, and the *norm* of a vector, $\|\mathbf{a}\|$. Schwarz's inequality may be proved by considering

$$\begin{aligned}\|\mathbf{a} + \lambda\mathbf{b}\|^2 &= \langle \mathbf{a} + \lambda\mathbf{b}|\mathbf{a} + \lambda\mathbf{b}\rangle \\ &= \langle \mathbf{a}|\mathbf{a}\rangle + \lambda\langle \mathbf{a}|\mathbf{b}\rangle + \lambda^*\langle \mathbf{b}|\mathbf{a}\rangle + \lambda\lambda^*\langle \mathbf{b}|\mathbf{b}\rangle.\end{aligned}$$

If we write $\langle \mathbf{a}|\mathbf{b}\rangle$ as $|\langle \mathbf{a}|\mathbf{b}\rangle|e^{i\alpha}$ then

$$\|\mathbf{a} + \lambda\mathbf{b}\|^2 = \|\mathbf{a}\|^2 + |\lambda|^2\|\mathbf{b}\|^2 + \lambda|\langle \mathbf{a}|\mathbf{b}\rangle|e^{i\alpha} + \lambda^*|\langle \mathbf{a}|\mathbf{b}\rangle|e^{-i\alpha}.$$

However, $\|\mathbf{a} + \lambda\mathbf{b}\|^2 \geq 0$ for all λ, so we may choose $\lambda = re^{-i\alpha}$ and require that, for all r,

$$0 \leq \|\mathbf{a} + \lambda\mathbf{b}\|^2 = \|\mathbf{a}\|^2 + r^2\|\mathbf{b}\|^2 + 2r|\langle \mathbf{a}|\mathbf{b}\rangle|.$$

This means that the quadratic equation in r formed by setting the RHS equal to zero must have no real roots. This, in turn, implies that

$$4|\langle \mathbf{a}|\mathbf{b}\rangle|^2 \leq 4\|\mathbf{a}\|^2\|\mathbf{b}\|^2,$$

which, on taking the square root (all factors are necessarily positive) of both sides, gives Schwarz's inequality.

(ii) The *triangle inequality* states that

$$\|\mathbf{a} + \mathbf{b}\| \leq \|\mathbf{a}\| + \|\mathbf{b}\| \tag{8.20}$$

and may be derived from the properties of the inner product and Schwarz's inequality as follows. Let us first consider

$$\|\mathbf{a} + \mathbf{b}\|^2 = \|\mathbf{a}\|^2 + \|\mathbf{b}\|^2 + 2\ \mathrm{Re}\,\langle \mathbf{a}|\mathbf{b}\rangle \leq \|\mathbf{a}\|^2 + \|\mathbf{b}\|^2 + 2|\langle \mathbf{a}|\mathbf{b}\rangle|.$$

Using Schwarz's inequality we then have

$$\|\mathbf{a} + \mathbf{b}\|^2 \leq \|\mathbf{a}\|^2 + \|\mathbf{b}\|^2 + 2\|\mathbf{a}\|\|\mathbf{b}\| = (\|\mathbf{a}\| + \|\mathbf{b}\|)^2,$$

which, on taking the square root, gives the triangle inequality (8.20).

(iii) *Bessel's inequality* requires the introduction of an orthonormal basis $\hat{\mathbf{e}}_i$, $i = 1, 2, \ldots, N$ into the N-dimensional vector space; it states that

$$\|\mathbf{a}\|^2 \geq \sum_i |\langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle|^2, \tag{8.21}$$

where the equality holds if the sum includes all N basis vectors. If not all the basis vectors are included in the sum then the inequality results (though of course the equality remains if those basis vectors omitted all have $a_i = 0$). Bessel's inequality can also be written

$$\langle \mathbf{a}|\mathbf{a}\rangle \geq \sum_i |a_i|^2,$$

where the a_i are the components of $\mathbf{a}$ in the orthonormal basis. From (8.16) these are given by $a_i = \langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle$. The above may be proved by considering

$$\left\| \mathbf{a} - \sum_i \langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle \hat{\mathbf{e}}_i \right\|^2 = \left\langle \mathbf{a} - \sum_i \langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle \hat{\mathbf{e}}_i \middle| \mathbf{a} - \sum_j \langle \hat{\mathbf{e}}_j|\mathbf{a}\rangle \hat{\mathbf{e}}_j \right\rangle.$$

Expanding out the inner product and using $\langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle^* = \langle \mathbf{a}|\hat{\mathbf{e}}_i\rangle$, we obtain

$$\left\| \mathbf{a} - \sum_i \langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle \hat{\mathbf{e}}_i \right\|^2 = \langle \mathbf{a}|\mathbf{a}\rangle - 2\sum_i \langle \mathbf{a}|\hat{\mathbf{e}}_i\rangle\langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle + \sum_i \sum_j \langle \mathbf{a}|\hat{\mathbf{e}}_i\rangle\langle \hat{\mathbf{e}}_j|\mathbf{a}\rangle\langle \hat{\mathbf{e}}_i|\hat{\mathbf{e}}_j\rangle.$$

Now $\langle \hat{\mathbf{e}}_i|\hat{\mathbf{e}}_j\rangle = \delta_{ij}$, since the basis is orthonormal, and so we find

$$0 \leq \left\| \mathbf{a} - \sum_i \langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle \hat{\mathbf{e}}_i \right\|^2 = \|\mathbf{a}\|^2 - \sum_i |\langle \hat{\mathbf{e}}_i|\mathbf{a}\rangle|^2,$$

which is Bessel's inequality.

We take this opportunity to mention also

(iv) the *parallelogram equality*

$$\|\mathbf{a} + \mathbf{b}\|^2 + \|\mathbf{a} - \mathbf{b}\|^2 = 2\left(\|\mathbf{a}\|^2 + \|\mathbf{b}\|^2\right), \tag{8.22}$$

which may be proved straightforwardly from the properties of the inner product.

8.2 Linear operators

We now discuss the action of *linear operators* on vectors in a vector space. A linear operator $\mathcal{A}$ associates with every vector $\mathbf{x}$ another vector

$$\mathbf{y} = \mathcal{A}\,\mathbf{x},$$

in such a way that, for two vectors $\mathbf{a}$ and $\mathbf{b}$,

$$\mathcal{A}\,(\lambda\mathbf{a} + \mu\mathbf{b}) = \lambda\mathcal{A}\,\mathbf{a} + \mu\mathcal{A}\,\mathbf{b},$$

where λ, μ are scalars. We say that $\mathcal{A}$ 'operates' on $\mathbf{x}$ to give the vector $\mathbf{y}$. We note that the action of $\mathcal{A}$ is *independent* of any basis or coordinate system and

may be thought of as 'transforming' one geometrical entity (i.e. a vector) into another.

If we now introduce a basis $\mathbf{e}_i$, $i = 1, 2, \ldots, N$, into our vector space then the action of $\mathcal{A}$ on each of the basis vectors is to produce a linear combination of the latter; this may be written as

$$\mathcal{A}\,\mathbf{e}_j = \sum_{i=1}^{N} A_{ij}\mathbf{e}_i, \tag{8.23}$$

where A_{ij} is the ith component of the vector $\mathcal{A}\,\mathbf{e}_j$ in this basis; collectively the numbers A_{ij} are called the components of the linear operator in the $\mathbf{e}_i$-basis. *In this basis* we can express the relation $\mathbf{y} = \mathcal{A}\,\mathbf{x}$ in component form as

$$\mathbf{y} = \sum_{i=1}^{N} y_i\mathbf{e}_i = \mathcal{A}\left(\sum_{j=1}^{N} x_j\mathbf{e}_j\right) = \sum_{j=1}^{N} x_j \sum_{i=1}^{N} A_{ij}\mathbf{e}_i,$$

and hence, in purely component form, in this basis we have

$$y_i = \sum_{j=1}^{N} A_{ij}x_j. \tag{8.24}$$

If we had chosen a different basis $\mathbf{e}'_i$, in which the components of $\mathbf{x}$, $\mathbf{y}$ and $\mathcal{A}$ are x'_i, y'_i and A'_{ij} respectively then the geometrical relationship $\mathbf{y} = \mathcal{A}\,\mathbf{x}$ would be represented in this new basis by

$$y'_i = \sum_{j=1}^{N} A'_{ij}x'_j.$$

We have so far assumed that the vector $\mathbf{y}$ is in the same vector space as $\mathbf{x}$. If, however, $\mathbf{y}$ belongs to a different vector space, which may in general be M-dimensional ($M \neq N$) then the above analysis needs a slight modification. By introducing a basis set $\mathbf{f}_i$, $i = 1, 2, \ldots, M$, into the vector space to which $\mathbf{y}$ belongs we may generalise (8.23) as

$$\mathcal{A}\,\mathbf{e}_j = \sum_{i=1}^{M} A_{ij}\mathbf{f}_i,$$

where the components A_{ij} of the linear operator $\mathcal{A}$ relate to both of the bases $\mathbf{e}_j$ and $\mathbf{f}_i$.

8.2.1 Properties of linear operators

If $\mathbf{x}$ is a vector and $\mathcal{A}$ and $\mathcal{B}$ are two linear operators then it follows that

$$(\mathcal{A}+\mathcal{B})\mathbf{x} = \mathcal{A}\mathbf{x} + \mathcal{B}\mathbf{x},$$
$$(\lambda\mathcal{A})\mathbf{x} = \lambda(\mathcal{A}\mathbf{x}),$$
$$(\mathcal{A}\mathcal{B})\mathbf{x} = \mathcal{A}(\mathcal{B}\mathbf{x}),$$

where in the last equality we see that the action of two linear operators in succession is associative. The product of two linear operators is not in general commutative, however, so that in general $\mathcal{A}\mathcal{B}\mathbf{x} \neq \mathcal{B}\mathcal{A}\mathbf{x}$. In an obvious way we define the null (or zero) and identity operators by

$$\mathcal{O}\mathbf{x} = \mathbf{0} \qquad \text{and} \qquad \mathcal{I}\mathbf{x} = \mathbf{x},$$

for any vector $\mathbf{x}$ in our vector space. Two operators $\mathcal{A}$ and $\mathcal{B}$ are equal if $\mathcal{A}\mathbf{x} = \mathcal{B}\mathbf{x}$ for all vectors $\mathbf{x}$. Finally, if there exists an operator $\mathcal{A}^{-1}$ such that

$$\mathcal{A}\mathcal{A}^{-1} = \mathcal{A}^{-1}\mathcal{A} = \mathcal{I}$$

then $\mathcal{A}^{-1}$ is the *inverse* of $\mathcal{A}$. Some linear operators do not possess an inverse and are called *singular*, whilst those operators that do have an inverse are termed *non-singular*.

8.3 Matrices

We have seen that in a particular basis $\mathbf{e}_i$ both vectors and linear operators can be described in terms of their components with respect to the basis. These components may be displayed as an array of numbers called a *matrix*. In general, if a linear operator $\mathcal{A}$ transforms vectors from an N-dimensional vector space, for which we choose a basis $\mathbf{e}_j$, $j = 1, 2, \ldots, N$, into vectors belonging to an M-dimensional vector space, with basis $\mathbf{f}_i$, $i = 1, 2, \ldots, M$, then we may represent the operator $\mathcal{A}$ by the matrix

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & \ldots & A_{1N} \\ A_{21} & A_{22} & \ldots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{M1} & A_{M2} & \ldots & A_{MN} \end{pmatrix}. \tag{8.25}$$

The *matrix elements* A_{ij} are the components of the linear operator with respect to the bases $\mathbf{e}_j$ and $\mathbf{f}_i$; the component A_{ij} of the linear operator appears in the ith row and jth column of the matrix. The array has M rows and N columns and is thus called an $M \times N$ matrix. If the dimensions of the two vector spaces are the same, i.e. $M = N$ (for example, if they are the same vector space) then we may represent $\mathcal{A}$ by an $N \times N$ or *square* matrix of *order* N. The component A_{ij}, which in general may be complex, is also denoted by $(\mathsf{A})_{ij}$.

In a similar way we may denote a vector $\mathbf{x}$ in terms of its components x_i in a basis $\mathbf{e}_i$, $i = 1, 2, \ldots, N$, by the array

$$\mathsf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix},$$

which is a special case of (8.25) and is called a *column matrix* (or conventionally, and slightly confusingly, a *column vector* or even just a *vector* – strictly speaking the term 'vector' refers to the geometrical entity $\mathbf{x}$). The column matrix x can also be written as

$$\mathsf{x} = (x_1 \quad x_2 \quad \cdots \quad x_N)^{\mathrm{T}},$$

which is the *transpose* of a *row matrix* (see section 8.6).

We note that in a different basis $\mathbf{e}'_i$ the vector $\mathbf{x}$ would be represented by a *different* column matrix containing the components x'_i in the new basis, i.e.

$$\mathsf{x}' = \begin{pmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_N \end{pmatrix}.$$

Thus, we use x and x' to denote different column matrices which, in different bases $\mathbf{e}_i$ and $\mathbf{e}'_i$, represent the *same* vector $\mathbf{x}$. In many texts, however, this distinction is not made and $\mathbf{x}$ (rather than x) is equated to the corresponding column matrix; if we regard $\mathbf{x}$ as the geometrical entity, however, this can be misleading and so we explicitly make the distinction. A similar argument follows for linear operators; the same linear operator $\mathcal{A}$ is described in different bases by different matrices A and A', containing different matrix elements.

8.4 Basic matrix algebra

The basic algebra of matrices may be deduced from the properties of the linear operators that they represent. In a given basis the action of two linear operators $\mathcal{A}$ and $\mathcal{B}$ on an arbitrary vector $\mathbf{x}$ (see the beginning of subsection 8.2.1), when written in terms of components using (8.24), is given by

$$\sum_j (\mathsf{A} + \mathsf{B})_{ij} x_j = \sum_j A_{ij} x_j + \sum_j B_{ij} x_j,$$

$$\sum_j (\lambda \mathsf{A})_{ij} x_j = \lambda \sum_j A_{ij} x_j,$$

$$\sum_j (\mathsf{AB})_{ij} x_j = \sum_k A_{ik} (\mathsf{Bx})_k = \sum_j \sum_k A_{ik} B_{kj} x_j.$$

Now, since **x** is arbitrary, we can immediately deduce the way in which matrices are added or multiplied, i.e.

$$(\mathsf{A}+\mathsf{B})_{ij} = A_{ij} + B_{ij}, \tag{8.26}$$

$$(\lambda\mathsf{A})_{ij} = \lambda A_{ij}, \tag{8.27}$$

$$(\mathsf{AB})_{ij} = \sum_k A_{ik}B_{kj}. \tag{8.28}$$

We note that a matrix element may, in general, be complex. We now discuss matrix addition and multiplication in more detail.

8.4.1 Matrix addition and multiplication by a scalar

From (8.26) we see that the sum of two matrices, $\mathsf{S} = \mathsf{A} + \mathsf{B}$, is the matrix whose elements are given by

$$S_{ij} = A_{ij} + B_{ij}$$

for every pair of subscripts i, j, with $i = 1, 2, \ldots, M$ and $j = 1, 2, \ldots, N$. For example, if A and B are 2×3 matrices then $\mathsf{S} = \mathsf{A} + \mathsf{B}$ is given by

$$\begin{aligned}\begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \end{pmatrix} &= \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{pmatrix} + \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \end{pmatrix} \\ &= \begin{pmatrix} A_{11}+B_{11} & A_{12}+B_{12} & A_{13}+B_{13} \\ A_{21}+B_{21} & A_{22}+B_{22} & A_{23}+B_{23} \end{pmatrix}. \end{aligned} \tag{8.29}$$

Clearly, for the sum of two matrices to have any meaning, the matrices must have the same dimensions, i.e. both be $M \times N$ matrices.

From definition (8.29) it follows that $\mathsf{A} + \mathsf{B} = \mathsf{B} + \mathsf{A}$ and that the sum of a number of matrices can be written unambiguously without bracketting, i.e. matrix addition is *commutative* and *associative*.

The difference of two matrices is defined by direct analogy with addition. The matrix $\mathsf{D} = \mathsf{A} - \mathsf{B}$ has elements

$$D_{ij} = A_{ij} - B_{ij}, \qquad \text{for } i = 1, 2, \ldots, M,\ j = 1, 2, \ldots, N. \tag{8.30}$$

From (8.27) the product of a matrix A with a scalar λ is the matrix with elements λA_{ij}, for example

$$\lambda \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{pmatrix} = \begin{pmatrix} \lambda A_{11} & \lambda A_{12} & \lambda A_{13} \\ \lambda A_{21} & \lambda A_{22} & \lambda A_{23} \end{pmatrix}. \tag{8.31}$$

Multiplication by a scalar is distributive and associative.

►*The matrices* A, B *and* C *are given by*

$$\mathsf{A}=\begin{pmatrix}2&-1\\3&1\end{pmatrix},\qquad \mathsf{B}=\begin{pmatrix}1&0\\0&-2\end{pmatrix},\qquad \mathsf{C}=\begin{pmatrix}-2&1\\-1&1\end{pmatrix}.$$

Find the matrix $\mathsf{D}=\mathsf{A}+2\mathsf{B}-\mathsf{C}$.

$$\begin{aligned}\mathsf{D}&=\begin{pmatrix}2&-1\\3&1\end{pmatrix}+2\begin{pmatrix}1&0\\0&-2\end{pmatrix}-\begin{pmatrix}-2&1\\-1&1\end{pmatrix}\\&=\begin{pmatrix}2+2\times1-(-2)&-1+2\times0-1\\3+2\times0-(-1)&1+2\times(-2)-1\end{pmatrix}=\begin{pmatrix}6&-2\\4&-4\end{pmatrix}.\ \blacktriangleleft\end{aligned}$$

From the above considerations we see that the set of all, in general complex, $M\times N$ matrices (with fixed M and N) forms a linear vector space of dimension MN. One basis for the space is the set of $M\times N$ matrices $\mathsf{E}^{(p,q)}$ with the property that $E^{(p,q)}_{ij}=1$ if $i=p$ and $j=q$ whilst $E^{(p,q)}_{ij}=0$ for all other values of i and j, i.e. each matrix has only one non-zero entry, which equals unity. Here the pair (p,q) is simply a label that picks out a particular one of the matrices $E^{(p,q)}$, the total number of which is MN.

8.4.2 Multiplication of matrices

Let us consider again the 'transformation' of one vector into another, $\mathbf{y}=\mathcal{A}\,\mathbf{x}$, which, from (8.24), may be described in terms of components with respect to a particular basis as

$$y_i=\sum_{j=1}^{N}A_{ij}x_j\qquad\text{for } i=1,2,\ldots,M. \tag{8.32}$$

Writing this in matrix form as $\mathsf{y}=\mathsf{A}\mathsf{x}$ we have

$$\begin{pmatrix}y_1\\ \boxed{y_2}\\ \vdots\\ y_M\end{pmatrix}=\begin{pmatrix}A_{11}&A_{12}&\ldots&A_{1N}\\ \boxed{A_{21}&A_{22}&\ldots&A_{2N}}\\ \vdots&\vdots&\ddots&\vdots\\ A_{M1}&A_{M2}&\ldots&A_{MN}\end{pmatrix}\begin{pmatrix}x_1\\x_2\\ \\ \vdots\\ \\ x_N\end{pmatrix} \tag{8.33}$$

where we have highlighted with boxes the components used to calculate the element y_2: using (8.32) for $i=2$,

$$y_2=A_{21}x_1+A_{22}x_2+\cdots+A_{2N}x_N.$$

All the other components y_i are calculated similarly.

If instead we operate with $\mathcal{A}$ on a basis vector $\mathbf{e}_j$ having all components zero

except for the jth, which equals unity, then we find

$$\mathsf{A}\mathbf{e}_j = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1N} \\ \boxed{A_{21} & A_{22} & \dots & A_{2N}} \\ \vdots & \vdots & \ddots & \vdots \\ A_{M1} & A_{M2} & \dots & A_{MN} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} A_{1j} \\ \boxed{A_{2j}} \\ \vdots \\ A_{Mj} \end{pmatrix},$$

and so confirm our identification of the matrix element A_{ij} as the ith component of $\mathsf{A}\mathbf{e}_j$ in this basis.

From (8.28) we can extend our discussion to the product of two matrices $\mathsf{P} = \mathsf{AB}$, where P is the matrix of the quantities formed by the operation of the rows of A on the columns of B, treating each column of B in turn as the vector $\mathbf{x}$ represented in component form in (8.32). It is clear that, for this to be a meaningful definition, the number of columns in A must equal the number of rows in B. Thus the product AB of an $M \times N$ matrix A with an $N \times R$ matrix B is itself an $M \times R$ matrix P, where

$$P_{ij} = \sum_{k=1}^{N} A_{ik} B_{kj} \qquad \text{for } i = 1, 2, \dots, M, \qquad j = 1, 2, \dots, R.$$

For example, $\mathsf{P} = \mathsf{AB}$ may be written in matrix form

$$\begin{pmatrix} \boxed{P_{11}} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} = \begin{pmatrix} \boxed{A_{11} & A_{12} & A_{13}} \\ A_{21} & A_{22} & A_{23} \end{pmatrix} \begin{pmatrix} \boxed{B_{11}} & B_{12} \\ B_{21} & B_{22} \\ B_{31} & B_{32} \end{pmatrix}$$

where

$$\begin{aligned} P_{11} &= A_{11}B_{11} + A_{12}B_{21} + A_{13}B_{31}, \\ P_{21} &= A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}, \\ P_{12} &= A_{11}B_{12} + A_{12}B_{22} + A_{13}B_{32}, \\ P_{22} &= A_{21}B_{12} + A_{22}B_{22} + A_{23}B_{32}. \end{aligned}$$

Multiplication of more than two matrices follows naturally and is associative. So, for example,

$$\mathsf{A}(\mathsf{BC}) \equiv (\mathsf{AB})\mathsf{C}, \tag{8.34}$$

provided, of course, that all the products are defined.

As mentioned above, if A is an $M \times N$ matrix and B is an $N \times M$ matrix then two product matrices are possible, i.e.

$$\mathsf{P} = \mathsf{AB} \qquad \text{and} \qquad \mathsf{Q} = \mathsf{BA}.$$

These are clearly not the same, since P is an $M \times M$ matrix whilst Q is an $N \times N$ matrix. Thus, particular care must be taken to write matrix products in the intended order; $\mathsf{P} = \mathsf{AB}$ but $\mathsf{Q} = \mathsf{BA}$. We note in passing that A^2 means AA, A^3 means $\mathsf{A(AA)} = \mathsf{(AA)A}$ etc. Even if both A and B are square, in general

$$\mathsf{AB} \neq \mathsf{BA}, \tag{8.35}$$

i.e. the multiplication of matrices is not, in general, commutative.

►*Evaluate* $\mathsf{P} = \mathsf{AB}$ *and* $\mathsf{Q} = \mathsf{BA}$ *where*

$$\mathsf{A} = \begin{pmatrix} 3 & 2 & -1 \\ 0 & 3 & 2 \\ 1 & -3 & 4 \end{pmatrix}, \qquad \mathsf{B} = \begin{pmatrix} 2 & -2 & 3 \\ 1 & 1 & 0 \\ 3 & 2 & 1 \end{pmatrix}.$$

As we saw for the 2×2 case above, the element P_{ij} of the matrix $\mathsf{P} = \mathsf{AB}$ is found by mentally taking the 'scalar product' of the ith row of A with the jth column of B. For example, $P_{11} = 3 \times 2 + 2 \times 1 + (-1) \times 3 = 5$, $P_{12} = 3 \times (-2) + 2 \times 1 + (-1) \times 2 = -6$, etc. Thus

$$\mathsf{P} = \mathsf{AB} = \begin{pmatrix} 3 & 2 & -1 \\ 0 & 3 & 2 \\ 1 & -3 & 4 \end{pmatrix} \begin{pmatrix} 2 & -2 & 3 \\ 1 & 1 & 0 \\ 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 5 & -6 & 8 \\ 9 & 7 & 2 \\ 11 & 3 & 7 \end{pmatrix},$$

and, similarly,

$$\mathsf{Q} = \mathsf{BA} = \begin{pmatrix} 2 & -2 & 3 \\ 1 & 1 & 0 \\ 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} 3 & 2 & -1 \\ 0 & 3 & 2 \\ 1 & -3 & 4 \end{pmatrix} = \begin{pmatrix} 9 & -11 & 6 \\ 3 & 5 & 1 \\ 10 & 9 & 5 \end{pmatrix}.$$

These results illustrate that, in general, two matrices do not commute. ◄

The property that matrix multiplication is distributive over addition, i.e. that

$$\mathsf{(A + B)C} = \mathsf{AC} + \mathsf{BC} \tag{8.36}$$

and

$$\mathsf{C(A + B)} = \mathsf{CA} + \mathsf{CB}, \tag{8.37}$$

follows directly from its definition.

8.4.3 The null and identity matrices

Both the null matrix and the identity matrix are frequently encountered, and we take this opportunity to introduce them briefly, leaving their uses until later. The *null* or *zero* matrix $\mathsf{0}$ has all elements equal to zero, and so its properties are

$$\mathsf{A0} = \mathsf{0} = \mathsf{0A},$$

$$\mathsf{A} + \mathsf{0} = \mathsf{0} + \mathsf{A} = \mathsf{A}.$$

The *identity* matrix I has the property

$$\mathsf{AI} = \mathsf{IA} = \mathsf{A}.$$

It is clear that, in order for the above products to be defined, the identity matrix must be square. The $N \times N$ identity matrix (often denoted by I_N) has the form

$$\mathsf{I}_N = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}.$$

8.5 Functions of matrices

If a matrix A is *square* then, as mentioned above, one can define *powers* of A in a straightforward way. For example $\mathsf{A}^2 = \mathsf{AA}$, $\mathsf{A}^3 = \mathsf{AAA}$, or in the general case

$$\mathsf{A}^n = \mathsf{AA}\cdots\mathsf{A} \qquad (n \text{ times}),$$

where n is a positive integer. Having defined powers of a square matrix A, we may construct *functions* of A of the form

$$\mathsf{S} = \sum_n a_n \mathsf{A}^n,$$

where the a_k are simple scalars and the number of terms in the summation may be finite or infinite. In the case where the sum has an infinite number of terms, the sum has meaning only if it converges. A common example of such a function is the *exponential* of a matrix, which is defined by

$$\exp\ \mathsf{A} = \sum_{n=0}^{\infty} \frac{\mathsf{A}^n}{n!}. \tag{8.38}$$

This definition can, in turn, be used to define other functions such as $\sin \mathsf{A}$ and $\cos \mathsf{A}$.

8.6 The transpose of a matrix

We have seen that the components of a linear operator in a given coordinate system can be written in the form of a matrix A. We will also find it useful, however, to consider the different (but clearly related) matrix formed by interchanging the rows and columns of A. The matrix is called the *transpose* of A and is denoted by A^{T}.

►*Find the transpose of the matrix*

$$\mathsf{A} = \begin{pmatrix} 3 & 1 & 2 \\ 0 & 4 & 1 \end{pmatrix}.$$

By interchanging the rows and columns of A we immediately obtain

$$\mathsf{A}^{\mathrm{T}} = \begin{pmatrix} 3 & 0 \\ 1 & 4 \\ 2 & 1 \end{pmatrix}. \blacktriangleleft$$

It is obvious that if A is an $M \times N$ matrix then its transpose A^{T} is a $N \times M$ matrix. As mentioned in section 8.3, the transpose of a column matrix is a row matrix and vice versa. An important use of column and row matrices is in the representation of the inner product of two real vectors in terms of their components in a given basis. This notion is discussed fully in the next section, where it is extended to complex vectors.

The transpose of the product of two matrices, $(\mathsf{AB})^{\mathrm{T}}$, is given by the product of their transposes taken in the reverse order, i.e.

$$(\mathsf{AB})^{\mathrm{T}} = \mathsf{B}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}. \tag{8.39}$$

This is proved as follows:

$$\begin{aligned}(\mathsf{AB})^{\mathrm{T}}_{ij} = (\mathsf{AB})_{ji} &= \sum_k A_{jk}B_{ki} \\ &= \sum_k (\mathsf{A}^{\mathrm{T}})_{kj}(\mathsf{B}^{\mathrm{T}})_{ik} = \sum_k (\mathsf{B}^{\mathrm{T}})_{ik}(\mathsf{A}^{\mathrm{T}})_{kj} = (\mathsf{B}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}})_{ij},\end{aligned}$$

and the proof can be extended to the product of several matrices to give

$$(\mathsf{ABC}\cdots\mathsf{G})^{\mathrm{T}} = \mathsf{G}^{\mathrm{T}}\cdots\mathsf{C}^{\mathrm{T}}\mathsf{B}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}.$$

8.7 The complex and Hermitian conjugates of a matrix

Two further matrices that can be derived from a given general $M \times N$ matrix are the *complex conjugate*, denoted by A^*, and the *Hermitian conjugate*, denoted by $\mathsf{A}^\dagger$.

The complex conjugate of a matrix A is the matrix obtained by taking the complex conjugate of each of the elements of A, i.e.

$$(\mathsf{A}^*)_{ij} = (A_{ij})^*.$$

Obviously if a matrix is *real* (i.e. it contains only real elements) then $\mathsf{A}^* = \mathsf{A}$.

►*Find the complex conjugate of the matrix*

$$\mathsf{A} = \begin{pmatrix} 1 & 2 & 3i \\ 1+i & 1 & 0 \end{pmatrix}.$$

By taking the complex conjugate of each element we obtain immediately

$$\mathsf{A}^* = \begin{pmatrix} 1 & 2 & -3i \\ 1-i & 1 & 0 \end{pmatrix}. \blacktriangleleft$$

The Hermitian conjugate, or *adjoint*, of a matrix A is the transpose of its complex conjugate, or equivalently, the complex conjugate of its transpose, i.e.

$$\mathsf{A}^\dagger = (\mathsf{A}^*)^{\mathrm{T}} = (\mathsf{A}^{\mathrm{T}})^*.$$

We note that if A is real (and so $\mathsf{A}^* = \mathsf{A}$) then $\mathsf{A}^\dagger = \mathsf{A}^{\mathrm{T}}$, and taking the Hermitian conjugate is equivalent to taking the transpose. Following the previous line of argument for the transpose of the product of several matrices, the Hermitian conjugate of such a product can be shown to be given by

$$(\mathsf{AB}\cdots\mathsf{G})^\dagger = \mathsf{G}^\dagger \cdots \mathsf{B}^\dagger \mathsf{A}^\dagger. \tag{8.40}$$

►*Find the Hermitian conjugate of the matrix*

$$\mathsf{A} = \begin{pmatrix} 1 & 2 & 3i \\ 1+i & 1 & 0 \end{pmatrix}.$$

Taking the complex conjugate of A and then forming the transpose we find

$$\mathsf{A}^\dagger = \begin{pmatrix} 1 & 1-i \\ 2 & 1 \\ -3i & 0 \end{pmatrix}.$$

We obtain the same result, of course, if we first take the transpose of A and then take the complex conjugate. ◄

An important use of the Hermitian conjugate (or transpose in the real case) is in connection with the inner product of two vectors. Suppose that in a given orthonormal basis the vectors **a** and **b** may be represented by the column matrices

$$\mathsf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \quad \text{and} \quad \mathsf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}. \tag{8.41}$$

Taking the Hermitian conjugate of a, to give a row matrix, and multiplying (on

the right) by b we obtain

$$\mathsf{a}^\dagger\mathsf{b} = (a_1^* \; a_2^* \; \cdots \; a_N^*) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix} = \sum_{i=1}^{N} a_i^* b_i, \tag{8.42}$$

which is the expression for the inner product $\langle \mathbf{a}|\mathbf{b}\rangle$ in that basis. We note that for real vectors (8.42) reduces to $\mathsf{a}^{\mathrm{T}}\mathsf{b} = \sum_{i=1}^{N} a_i b_i$.

If the basis $\mathbf{e}_i$ is *not* orthonormal, so that, in general,

$$\langle \mathbf{e}_i|\mathbf{e}_j\rangle = G_{ij} \neq \delta_{ij},$$

then, from (8.18), the scalar product of $\mathbf{a}$ and $\mathbf{b}$ in terms of their components with respect to this basis is given by

$$\langle \mathbf{a}|\mathbf{b}\rangle = \sum_{i=1}^{N}\sum_{j=1}^{N} a_i^* G_{ij} b_j = \mathsf{a}^\dagger\mathsf{G}\mathsf{b},$$

where G is the $N \times N$ matrix with elements G_{ij}.

8.8 The trace of a matrix

For a given matrix A, in the previous two sections we have considered various other matrices that can be derived from it. However, sometimes one wishes to derive a single number from a matrix. The simplest example is the *trace* (or *spur*) of a square matrix, which is denoted by $\mathrm{Tr}\,\mathsf{A}$. This quantity is defined as the sum of the diagonal elements of the matrix,

$$\mathrm{Tr}\,\mathsf{A} = A_{11} + A_{22} + \cdots + A_{NN} = \sum_{i=1}^{N} A_{ii}. \tag{8.43}$$

It is clear that taking the trace is a linear operation so that, for example,

$$\mathrm{Tr}(\mathsf{A} \pm \mathsf{B}) = \mathrm{Tr}\,\mathsf{A} \pm \mathrm{Tr}\,\mathsf{B}.$$

A very useful property of traces is that the trace of the product of two matrices is independent of the order of their multiplication; this results holds whether or not the matrices commute and is proved as follows:

$$\mathrm{Tr}\,\mathsf{AB} = \sum_{i=1}^{N}(\mathsf{AB})_{ii} = \sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}B_{ji} = \sum_{i=1}^{N}\sum_{j=1}^{N} B_{ji}A_{ij} = \sum_{j=1}^{N}(\mathsf{BA})_{jj} = \mathrm{Tr}\,\mathsf{BA}. \tag{8.44}$$

The result can be extended to the product of several matrices. For example, from (8.44), we immediately find

$$\mathrm{Tr}\,\mathsf{ABC} = \mathrm{Tr}\,\mathsf{BCA} = \mathrm{Tr}\,\mathsf{CAB},$$

which shows that the trace of a multiple product is invariant under cyclic permutations of the matrices in the product. Other easily derived properties of the trace are, for example, $\mathrm{Tr}\,\mathsf{A}^{\mathrm{T}} = \mathrm{Tr}\,\mathsf{A}$ and $\mathrm{Tr}\,\mathsf{A}^{\dagger} = (\mathrm{Tr}\,\mathsf{A})^{*}$.

8.9 The determinant of a matrix

For a given matrix A, the determinant $\det \mathsf{A}$ (like the trace) is a single number (or algebraic expression) that depends upon the elements of A. Also like the trace, the determinant is defined only for *square* matrices. If, for example, A is a 3×3 matrix then its determinant, of *order* 3, is denoted by

$$\det \mathsf{A} = |\mathsf{A}| = \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix}. \tag{8.45}$$

In order to calculate the value of a determinant, we first need to introduce the notions of the *minor* and the *cofactor* of an element of a matrix. (We shall see that we can use the cofactors to write an order-3 determinant as the weighted sum of three order-2 determinants, thereby simplifying its evaluation.) The minor M_{ij} of the element A_{ij} of an $N \times N$ matrix A is the determinant of the $(N-1) \times (N-1)$ matrix obtained by removing all the elements of the ith row and jth column of A; the associated cofactor, C_{ij}, is found by multiplying the minor by $(-1)^{i+j}$.

►*Find the cofactor of the element A_{23} of the matrix*

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}.$$

Removing all the elements of the second row and third column of A and forming the determinant of the remaining terms gives the minor

$$M_{23} = \begin{vmatrix} A_{11} & A_{12} \\ A_{31} & A_{32} \end{vmatrix}.$$

Multiplying the minor by $(-1)^{2+3} = (-1)^5 = -1$ gives

$$C_{23} = -\begin{vmatrix} A_{11} & A_{12} \\ A_{31} & A_{32} \end{vmatrix}. \blacktriangleleft$$

We now define a determinant as *the sum of the products of the elements of any row or column and their corresponding cofactors*, e.g. $A_{21}C_{21} + A_{22}C_{22} + A_{23}C_{23}$ or $A_{13}C_{13} + A_{23}C_{23} + A_{33}C_{33}$. Such a sum is called a *Laplace expansion*. For example, in the first of these expansions, using the elements of the second row of the

determinant defined by (8.45) and their corresponding cofactors, we write $|\mathsf{A}|$ as the Laplace expansion

$$\begin{aligned}|\mathsf{A}| &= A_{21}(-1)^{(2+1)}M_{21} + A_{22}(-1)^{(2+2)}M_{22} + A_{23}(-1)^{(2+3)}M_{23}\\ &= -A_{21}\begin{vmatrix} A_{12} & A_{13}\\ A_{32} & A_{33}\end{vmatrix} + A_{22}\begin{vmatrix} A_{11} & A_{13}\\ A_{31} & A_{33}\end{vmatrix} - A_{23}\begin{vmatrix} A_{11} & A_{12}\\ A_{31} & A_{32}\end{vmatrix}.\end{aligned}$$

We will see later that the value of the determinant is independent of the row or column chosen. Of course, we have not yet determined the value of $|\mathsf{A}|$ but, rather, written it as the weighted sum of three determinants of order 2. However, applying again the definition of a determinant, we can evaluate each of the order-2 determinants.

►*Evaluate the determinant*

$$\begin{vmatrix} A_{12} & A_{13}\\ A_{32} & A_{33}\end{vmatrix}.$$

By considering the products of the elements of the first row in the determinant, and their corresponding cofactors, we find

$$\begin{aligned}\begin{vmatrix} A_{12} & A_{13}\\ A_{32} & A_{33}\end{vmatrix} &= A_{12}(-1)^{(1+1)}|A_{33}| + A_{13}(-1)^{(1+2)}|A_{32}|\\ &= A_{12}A_{33} - A_{13}A_{32},\end{aligned}$$

where the values of the order-1 determinants $|A_{33}|$ and $|A_{32}|$ are defined to be A_{33} and A_{32} respectively. It must be remembered that the determinant is *not* the same as the modulus, e.g. $\det(-2) = |-2| = -2$, not 2. ◄

We can now combine all the above results to show that the value of the determinant (8.45) is given by

$$\begin{aligned}|\mathsf{A}| &= -A_{21}(A_{12}A_{33} - A_{13}A_{32}) + A_{22}(A_{11}A_{33} - A_{13}A_{31})\\ &\quad - A_{23}(A_{11}A_{32} - A_{12}A_{31}) \qquad (8.46)\\ &= A_{11}(A_{22}A_{33} - A_{23}A_{32}) + A_{12}(A_{23}A_{31} - A_{21}A_{33})\\ &\quad + A_{13}(A_{21}A_{32} - A_{22}A_{31}), \qquad (8.47)\end{aligned}$$

where the final expression gives the form in which the determinant is usually remembered and is the form that is obtained immediately by considering the Laplace expansion using the first row of the determinant. The last equality, which essentially rearranges a Laplace expansion using the second row into one using the first row, supports our assertion that the value of the determinant is unaffected by which row or column is chosen for the expansion.

►*Suppose the rows of a real* 3×3 *matrix* A *are interpreted as the components in a given basis of three (three-component) vectors* $\mathbf{a}$, $\mathbf{b}$ *and* $\mathbf{c}$. *Show that one can write the determinant of* A *as*

$$|\mathsf{A}| = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}).$$

If one writes the rows of A as the components in a given basis of three vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$, we have from (8.47) that

$$|\mathsf{A}| = \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} = a_1(b_2c_3 - b_3c_2) + a_2(b_3c_1 - b_1c_3) + a_3(b_1c_2 - b_2c_1).$$

From expression (7.34) for the scalar triple product given in subsection 7.6.3, it follows that we may write the determinant as

$$|\mathsf{A}| = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}). \tag{8.48}$$

In other words, $|\mathsf{A}|$ is the volume of the parallelepiped defined by the vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$. (One could equally well interpret the *columns* of the matrix A as the components of three vectors, and result (8.48) would still hold.) This result provides a more memorable (and more meaningful) expression than (8.47) for the value of a 3×3 determinant. Indeed, using this geometrical interpretation, we see immediately that, if the vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are not linearly independent then the value of the determinant vanishes: $|\mathsf{A}| = 0$. ◄

The evaluation of determinants of order greater than 3 follows the same general method as that presented above, in that it relies on successively reducing the order of the determinant by writing it as a Laplace expansion. Thus, a determinant of order 4 is first written as a sum of four determinants of order 3, which are then evaluated using the above method. For higher-order determinants, one cannot write down directly a simple geometrical expression for $|\mathsf{A}|$ analogous to that given in (8.48). Nevertheless, it is still true that if the rows or columns of the $N \times N$ matrix A are interpreted as the components in a given basis of N (N-component) vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_N$, then the determinant $|\mathsf{A}|$ vanishes if these vectors are not all linearly independent.

8.9.1 Properties of determinants

A number of properties of determinants follow straightforwardly from the definition of $\det \mathsf{A}$; their use will often reduce the labour of evaluating a determinant. We present them here without specific proofs, though they all follow readily from the alternative form for a determinant, given in equation (26.29) on page 942, and expressed in terms of the Levi–Civita symbol ϵ_{ijk} (see exercise 26.9).

(i) *Determinant of the transpose.* The transpose matrix A^{T} (which, we recall, is obtained by interchanging the rows and columns of A) has the same determinant as A itself, i.e.

$$|\mathsf{A}^{\mathrm{T}}| = |\mathsf{A}|. \tag{8.49}$$

It follows that *any* theorem established for the rows of A will apply to the columns as well, and vice versa.

(ii) *Determinant of the complex and Hermitian conjugate*. It is clear that the matrix A^* obtained by taking the complex conjugate of each element of A has the determinant $|\mathsf{A}^*| = |\mathsf{A}|^*$. Combining this result with (8.49), we find that

$$|\mathsf{A}^\dagger| = |(\mathsf{A}^*)^{\mathrm{T}}| = |\mathsf{A}^*| = |\mathsf{A}|^*. \tag{8.50}$$

(iii) *Interchanging two rows or two columns*. If two rows (columns) of A are interchanged, its determinant changes sign but is unaltered in magnitude.

(iv) *Removing factors*. If all the elements of a single row (column) of A have a common factor, λ, then this factor may be removed; the value of the determinant is given by the product of the remaining determinant and λ. Clearly this implies that if all the elements of any row (column) are zero then $|\mathsf{A}| = 0$. It also follows that if every element of the $N \times N$ matrix A is multiplied by a constant factor λ then

$$|\lambda\mathsf{A}| = \lambda^N|\mathsf{A}|. \tag{8.51}$$

(v) *Identical rows or columns*. If any two rows (columns) of A are identical or are multiples of one another, then it can be shown that $|\mathsf{A}| = 0$.

(vi) *Adding a constant multiple of one row (column) to another*. The determinant of a matrix is unchanged in value by adding to the elements of one row (column) any fixed multiple of the elements of another row (column).

(vii) *Determinant of a product*. If A and B are square matrices of the same order then

$$|\mathsf{AB}| = |\mathsf{A}||\mathsf{B}| = |\mathsf{BA}|. \tag{8.52}$$

A simple extension of this property gives, for example,

$$|\mathsf{AB}\cdots\mathsf{G}| = |\mathsf{A}||\mathsf{B}|\cdots|\mathsf{G}| = |\mathsf{A}||\mathsf{G}|\cdots|\mathsf{B}| = |\mathsf{A}\cdots\mathsf{GB}|,$$

which shows that the determinant is invariant under permutation of the matrices in a multiple product.

There is no explicit procedure for using the above results in the evaluation of any given determinant, and judging the quickest route to an answer is a matter of experience. A general guide is to try to reduce all terms but one in a row or column to zero and hence in effect to obtain a determinant of smaller size. The steps taken in evaluating the determinant in the example below are certainly not the fastest, but they have been chosen in order to illustrate the use of most of the properties listed above.

►*Evaluate the determinant*

$$|\mathsf{A}| = \begin{vmatrix} 1 & 0 & 2 & 3 \\ 0 & 1 & -2 & 1 \\ 3 & -3 & 4 & -2 \\ -2 & 1 & -2 & -1 \end{vmatrix}.$$

Taking a factor 2 out of the third column and then adding the second column to the third gives

$$|\mathsf{A}| = 2\begin{vmatrix} 1 & 0 & 1 & 3 \\ 0 & 1 & -1 & 1 \\ 3 & -3 & 2 & -2 \\ -2 & 1 & -1 & -1 \end{vmatrix} = 2\begin{vmatrix} 1 & 0 & 1 & 3 \\ 0 & 1 & 0 & 1 \\ 3 & -3 & -1 & -2 \\ -2 & 1 & 0 & -1 \end{vmatrix}.$$

Subtracting the second column from the fourth gives

$$|\mathsf{A}| = 2\begin{vmatrix} 1 & 0 & 1 & 3 \\ 0 & 1 & 0 & 0 \\ 3 & -3 & -1 & 1 \\ -2 & 1 & 0 & -2 \end{vmatrix}.$$

We now note that the second row has only one non-zero element and so the determinant may conveniently be written as a Laplace expansion, i.e.

$$|\mathsf{A}| = 2 \times 1 \times (-1)^{2+2}\begin{vmatrix} 1 & 1 & 3 \\ 3 & -1 & 1 \\ -2 & 0 & -2 \end{vmatrix} = 2\begin{vmatrix} 4 & 0 & 4 \\ 3 & -1 & 1 \\ -2 & 0 & -2 \end{vmatrix},$$

where the last equality follows by adding the second row to the first. It can now be seen that the first row is minus twice the third, and so the value of the determinant is zero, by property (v) above. ◄

8.10 The inverse of a matrix

Our first use of determinants will be in defining the *inverse* of a matrix. If we were dealing with ordinary numbers we would consider the relation $\mathsf{P} = \mathsf{AB}$ as equivalent to $\mathsf{B} = \mathsf{P}/\mathsf{A}$, provided that $\mathsf{A} \neq 0$. However, if A, B and P are matrices then this notation does not have an obvious meaning. What we really want to know is whether an explicit formula for B can be obtained in terms of A and P. It will be shown that this is possible for those cases in which $|\mathsf{A}| \neq 0$. A square matrix whose determinant is zero is called a *singular* matrix; otherwise it is *non-singular*. We will show that if A is non-singular we can define a matrix, denoted by A^{-1} and called the *inverse* of A, which has the property that if $\mathsf{AB} = \mathsf{P}$ then $\mathsf{B} = \mathsf{A}^{-1}\mathsf{P}$. In words, B can be obtained by multiplying P from the left by A^{-1}. Analogously, if B is non-singular then, by multiplication from the right, $\mathsf{A} = \mathsf{PB}^{-1}$.

It is clear that

$$\mathsf{AI} = \mathsf{A} \quad \Rightarrow \quad \mathsf{I} = \mathsf{A}^{-1}\mathsf{A}, \tag{8.53}$$

where I is the unit matrix, and so $\mathsf{A}^{-1}\mathsf{A} = \mathsf{I} = \mathsf{AA}^{-1}$. These statements are

equivalent to saying that if we first multiply a matrix, B say, by A and then multiply by the inverse A^{-1}, we end up with the matrix we started with, i.e.

$$\mathsf{A}^{-1}\mathsf{AB} = \mathsf{B}. \tag{8.54}$$

This justifies our use of the term inverse. It is also clear that the inverse is only defined for square matrices.

So far we have only defined what we mean by the inverse of a matrix. Actually finding the inverse of a matrix A may be carried out in a number of ways. We will show that one method is to construct first the matrix C containing the cofactors of the elements of A, as discussed in the last subsection. Then the required inverse A^{-1} can be found by forming the transpose of C and dividing by the determinant of A. Thus the elements of the inverse A^{-1} are given by

$$(\mathsf{A}^{-1})_{ik} = \frac{(\mathsf{C})^{\mathrm{T}}_{ik}}{|\mathsf{A}|} = \frac{C_{ki}}{|\mathsf{A}|}. \tag{8.55}$$

That this procedure does indeed result in the inverse may be seen by considering the components of $\mathsf{A}^{-1}\mathsf{A}$, i.e.

$$(\mathsf{A}^{-1}\mathsf{A})_{ij} = \sum_k (\mathsf{A}^{-1})_{ik}(\mathsf{A})_{kj} = \sum_k \frac{C_{ki}}{|\mathsf{A}|}A_{kj} = \frac{|\mathsf{A}|}{|\mathsf{A}|}\delta_{ij}. \tag{8.56}$$

The last equality in (8.56) relies on the property

$$\sum_k C_{ki}A_{kj} = |\mathsf{A}|\delta_{ij}; \tag{8.57}$$

this can be proved by considering the matrix A' obtained from the original matrix A when the ith column of A is replaced by one of the other columns, say the jth. Thus A' is a matrix with two identical columns and so has zero determinant. However, replacing the ith column by another does not change the cofactors C_{ki} of the elements in the ith column, which are therefore the same in A and A'. Recalling the Laplace expansion of a determinant, i.e.

$$|\mathsf{A}| = \sum_k A_{ki}C_{ki},$$

we obtain

$$0 = |\mathsf{A}'| = \sum_k A'_{ki}C'_{ki} = \sum_k A_{kj}C_{ki}, \qquad i \neq j,$$

which together with the Laplace expansion itself may be summarised by (8.57).

It is immediately obvious from (8.55) that the inverse of a matrix is not defined if the matrix is singular (i.e. if $|\mathsf{A}| = 0$).

►*Find the inverse of the matrix*

$$\mathsf{A} = \begin{pmatrix} 2 & 4 & 3 \\ 1 & -2 & -2 \\ -3 & 3 & 2 \end{pmatrix}.$$

We first determine $|\mathsf{A}|$:

$$\begin{aligned} |\mathsf{A}| &= 2[-2(2) - (-2)3] + 4[(-2)(-3) - (1)(2)] + 3[(1)(3) - (-2)(-3)] \\ &= 11. \end{aligned} \tag{8.58}$$

This is non-zero and so an inverse matrix can be constructed. To do this we need the matrix of the cofactors, C, and hence C^{T}. We find

$$\mathsf{C} = \begin{pmatrix} 2 & 4 & -3 \\ 1 & 13 & -18 \\ -2 & 7 & -8 \end{pmatrix} \quad \text{and} \quad \mathsf{C}^{\mathrm{T}} = \begin{pmatrix} 2 & 1 & -2 \\ 4 & 13 & 7 \\ -3 & -18 & -8 \end{pmatrix},$$

and hence

$$\mathsf{A}^{-1} = \frac{\mathsf{C}^{\mathrm{T}}}{|\mathsf{A}|} = \frac{1}{11}\begin{pmatrix} 2 & 1 & -2 \\ 4 & 13 & 7 \\ -3 & -18 & -8 \end{pmatrix}. \blacktriangleleft \tag{8.59}$$

For a 2×2 matrix, the inverse has a particularly simple form. If the matrix is

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

then its determinant $|\mathsf{A}|$ is given by $|\mathsf{A}| = A_{11}A_{22} - A_{12}A_{21}$, and the matrix of cofactors is

$$\mathsf{C} = \begin{pmatrix} A_{22} & -A_{21} \\ -A_{12} & A_{11} \end{pmatrix}.$$

Thus the inverse of A is given by

$$\mathsf{A}^{-1} = \frac{\mathsf{C}^{\mathrm{T}}}{|\mathsf{A}|} = \frac{1}{A_{11}A_{22} - A_{12}A_{21}}\begin{pmatrix} A_{22} & -A_{12} \\ -A_{21} & A_{11} \end{pmatrix}. \tag{8.60}$$

It can be seen that the transposed matrix of cofactors for a 2×2 matrix is the same as the matrix formed by swapping the elements on the leading diagonal (A_{11} and A_{22}) and changing the signs of the other two elements (A_{12} and A_{21}). This is completely general for a 2×2 matrix and is easy to remember.

The following are some further useful properties related to the inverse matrix

and may be straightforwardly derived.

$$\begin{aligned}
&\text{(i)}\ \ (\mathsf{A}^{-1})^{-1} = \mathsf{A}.\\
&\text{(ii)}\ \ (\mathsf{A}^{\mathrm{T}})^{-1} = (\mathsf{A}^{-1})^{\mathrm{T}}.\\
&\text{(iii)}\ \ (\mathsf{A}^{\dagger})^{-1} = (\mathsf{A}^{-1})^{\dagger}.\\
&\text{(iv)}\ \ (\mathsf{AB})^{-1} = \mathsf{B}^{-1}\mathsf{A}^{-1}.\\
&\text{(v)}\ \ (\mathsf{AB}\cdots\mathsf{G})^{-1} = \mathsf{G}^{-1}\cdots\mathsf{B}^{-1}\mathsf{A}^{-1}.
\end{aligned}$$

►*Prove the properties* (i)–(v) *stated above.*

We begin by writing down the fundamental expression defining the inverse of a non-singular square matrix A:

$$\mathsf{A}\mathsf{A}^{-1} = \mathsf{I} = \mathsf{A}^{-1}\mathsf{A}. \tag{8.61}$$

Property (i). This follows immediately from the expression (8.61).

Property (ii). Taking the transpose of each expression in (8.61) gives

$$(\mathsf{A}\mathsf{A}^{-1})^{\mathrm{T}} = \mathsf{I}^{\mathrm{T}} = (\mathsf{A}^{-1}\mathsf{A})^{\mathrm{T}}.$$

Using the result (8.39) for the transpose of a product of matrices and noting that $\mathsf{I}^{\mathrm{T}} = \mathsf{I}$, we find

$$(\mathsf{A}^{-1})^{\mathrm{T}}\mathsf{A}^{\mathrm{T}} = \mathsf{I} = \mathsf{A}^{\mathrm{T}}(\mathsf{A}^{-1})^{\mathrm{T}}.$$

However, from (8.61), this implies $(\mathsf{A}^{-1})^{\mathrm{T}} = (\mathsf{A}^{\mathrm{T}})^{-1}$ and hence proves result (ii) above.

Property (iii). This may be proved in an analogous way to property (ii), by replacing the transposes in (ii) by Hermitian conjugates and using the result (8.40) for the Hermitian conjugate of a product of matrices.

Property (iv). Using (8.61), we may write

$$(\mathsf{AB})(\mathsf{AB})^{-1} = \mathsf{I} = (\mathsf{AB})^{-1}(\mathsf{AB}),$$

From the left-hand equality it follows, by multiplying on the left by A^{-1}, that

$$\mathsf{A}^{-1}\mathsf{AB}(\mathsf{AB})^{-1} = \mathsf{A}^{-1}\mathsf{I} \qquad \text{and hence} \qquad \mathsf{B}(\mathsf{AB})^{-1} = \mathsf{A}^{-1}.$$

Now multiplying on the left by B^{-1} gives

$$\mathsf{B}^{-1}\mathsf{B}(\mathsf{AB})^{-1} = \mathsf{B}^{-1}\mathsf{A}^{-1},$$

and hence the stated result.

Property (v). Finally, result (iv) may extended to case (v) in a straightforward manner. For example, using result (iv) twice we find

$$(\mathsf{ABC})^{-1} = (\mathsf{BC})^{-1}\mathsf{A}^{-1} = \mathsf{C}^{-1}\mathsf{B}^{-1}\mathsf{A}^{-1}.\ \blacktriangleleft$$

We conclude this section by noting that the determinant $|\mathsf{A}^{-1}|$ of the inverse matrix can be expressed very simply in terms of the determinant $|\mathsf{A}|$ of the matrix itself. Again we start with the fundamental expression (8.61). Then, using the property (8.52) for the determinant of a product, we find

$$|\mathsf{A}\mathsf{A}^{-1}| = |\mathsf{A}||\mathsf{A}^{-1}| = |\mathsf{I}|.$$

It is straightforward to show by Laplace expansion that $|\mathsf{I}| = 1$, and so we arrive at the useful result

$$|\mathsf{A}^{-1}| = \frac{1}{|\mathsf{A}|}. \tag{8.62}$$

8.11 The rank of a matrix

The *rank* of a general $M \times N$ matrix is an important concept, particularly in the solution of sets of simultaneous linear equations, to be discussed in the next section, and we now discuss it in some detail. Like the trace and determinant, the rank of matrix A is a single number (or algebraic expression) that depends on the elements of A. Unlike the trace and determinant, however, the rank of a matrix can be defined even when A is not square. As we shall see, there are two *equivalent* definitions of the rank of a general matrix.

Firstly, the rank of a matrix may be defined in terms of the *linear independence* of vectors. Suppose that the columns of an $M \times N$ matrix are interpreted as the components in a given basis of N (M-component) vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$, as follows:

$$\mathsf{A} = \begin{pmatrix} \uparrow & \uparrow & & \uparrow \\ \mathsf{v}_1 & \mathsf{v}_2 & \ldots & \mathsf{v}_N \\ \downarrow & \downarrow & & \downarrow \end{pmatrix}.$$

Then the *rank* of A, denoted by rank A or by $R(\mathsf{A})$, is defined as the number of *linearly independent* vectors in the set $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$, and equals the dimension of the vector space spanned by those vectors. Alternatively, we may consider the rows of A to contain the components in a given basis of the M (N-component) vectors $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_M$ as follows:

$$\mathsf{A} = \begin{pmatrix} \leftarrow & \mathsf{w}_1 & \rightarrow \\ \leftarrow & \mathsf{w}_2 & \rightarrow \\ & \vdots & \\ \leftarrow & \mathsf{w}_M & \rightarrow \end{pmatrix}.$$

It may then be shown[§] that the rank of A is also equal to the number of linearly independent vectors in the set $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_M$. From this definition it is should be clear that the rank of A is unaffected by the exchange of two rows (or two columns) or by the multiplication of a row (or column) by a constant. Furthermore, suppose that a constant multiple of one row (column) is added to another row (column): for example, we might replace the row w_i by $\mathsf{w}_i + c\mathsf{w}_j$. This also has no effect on the number of linearly independent rows and so leaves the rank of A unchanged. We may use these properties to evaluate the rank of a given matrix.

A second (equivalent) definition of the rank of a matrix may be given and uses the concept of *submatrices*. A submatrix of A is any matrix that can be formed from the elements of A by ignoring one, or more than one, row or column. It

[§] For a fuller discussion, see, for example, C. D. Cantrell, *Modern Mathematical Methods for Physicists and Engineers* (Cambridge: Cambridge University Press, 2000), chapter 6.

may be shown that the rank of a general $M \times N$ matrix is equal to the size of the largest square submatrix of A whose determinant is non-zero. Therefore, if a matrix A has an $r \times r$ submatrix S with $|\mathsf{S}| \neq 0$, but no $(r+1) \times (r+1)$ submatrix with non-zero determinant then the rank of the matrix is r. From either definition it is clear that the rank of A is less than or equal to the smaller of M and N.

►*Determine the rank of the matrix*

$$\mathsf{A} = \begin{pmatrix} 1 & 1 & 0 & -2 \\ 2 & 0 & 2 & 2 \\ 4 & 1 & 3 & 1 \end{pmatrix}.$$

The largest possible square submatrices of A must be of dimension 3×3. Clearly, A possesses four such submatrices, the determinants of which are given by

$$\begin{vmatrix} 1 & 1 & 0 \\ 2 & 0 & 2 \\ 4 & 1 & 3 \end{vmatrix} = 0, \qquad \begin{vmatrix} 1 & 1 & -2 \\ 2 & 0 & 2 \\ 4 & 1 & 1 \end{vmatrix} = 0,$$

$$\begin{vmatrix} 1 & 0 & -2 \\ 2 & 2 & 2 \\ 4 & 3 & 1 \end{vmatrix} = 0, \qquad \begin{vmatrix} 1 & 0 & -2 \\ 0 & 2 & 2 \\ 1 & 3 & 1 \end{vmatrix} = 0.$$

(In each case the determinant may be evaluated as described in subsection 8.9.1.)

The next largest square submatrices of A are of dimension 2×2. Consider, for example, the 2×2 submatrix formed by ignoring the third row and the third and fourth columns of A; this has determinant

$$\begin{vmatrix} 1 & 1 \\ 2 & 0 \end{vmatrix} = 1 \times 0 - 2 \times 1 = -2.$$

Since its determinant is non-zero, A is of rank 2 and we need not consider any other 2×2 submatrix. ◄

In the special case in which the matrix A is a *square* $N \times N$ matrix, by comparing either of the above definitions of rank with our discussion of determinants in section 8.9, we see that $|\mathsf{A}| = 0$ unless the rank of A is N. In other words, A is *singular* unless $R(\mathsf{A}) = N$.

8.12 Special types of square matrix

Matrices that are square, i.e. $N \times N$, are very common in physical applications. We now consider some special forms of square matrix that are of particular importance.

8.12.1 Diagonal matrices

The unit matrix, which we have already encountered, is an example of a *diagonal* matrix. Such matrices are characterised by having non-zero elements only on the

leading diagonal, i.e. only elements A_{ij} with $i = j$ may be non-zero. For example,

$$\mathsf{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -3 \end{pmatrix},$$

is a 3×3 diagonal matrix. Such a matrix is often denoted by $\mathsf{A} = \text{diag}\,(1, 2, -3)$. By performing a Laplace expansion, it is easily shown that the determinant of an $N \times N$ diagonal matrix is equal to the product of the diagonal elements. Thus, if the matrix has the form $\mathsf{A} = \text{diag}(A_{11}, A_{22}, \ldots, A_{NN})$ then

$$|\mathsf{A}| = A_{11}A_{22} \cdots A_{NN}. \tag{8.63}$$

Moreover, it is also straightforward to show that the inverse of A is also a diagonal matrix given by

$$\mathsf{A}^{-1} = \text{diag}\left(\frac{1}{A_{11}}, \frac{1}{A_{22}}, \ldots, \frac{1}{A_{NN}}\right).$$

Finally, we note that, if two matrices A and B are *both* diagonal then they have the useful property that their product is commutative:

$$\mathsf{AB} = \mathsf{BA}.$$

This is *not* true for matrices in general.

8.12.2 Lower and upper triangular matrices

A square matrix A is called *lower triangular* if all the elements *above* the principal diagonal are zero. For example, the general form for a 3×3 lower triangular matrix is

$$\mathsf{A} = \begin{pmatrix} A_{11} & 0 & 0 \\ A_{21} & A_{22} & 0 \\ A_{31} & A_{32} & A_{33} \end{pmatrix},$$

where the elements A_{ij} may be zero or non-zero. Similarly an *upper triangular* square matrix is one for which all the elements *below* the principal diagonal are zero. The general 3×3 form is thus

$$\mathsf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A_{22} & A_{23} \\ 0 & 0 & A_{33} \end{pmatrix}.$$

By performing a Laplace expansion, it is straightforward to show that, in the general $N \times N$ case, the determinant of an upper or lower triangular matrix is equal to the product of its diagonal elements,

$$|\mathsf{A}| = A_{11}A_{22} \cdots A_{NN}. \tag{8.64}$$

Clearly result (8.63) for diagonal matrices is a special case of this result. Moreover, it may be shown that the inverse of a non-singular lower (upper) triangular matrix is also lower (upper) triangular.

8.12.3 Symmetric and antisymmetric matrices

A square matrix A of order N with the property $\mathsf{A} = \mathsf{A}^{\mathrm{T}}$ is said to be *symmetric*. Similarly a matrix for which $\mathsf{A} = -\mathsf{A}^{\mathrm{T}}$ is said to be *anti-* or *skew*-symmetric and its diagonal elements $a_{11}, a_{22}, \ldots, a_{NN}$ are necessarily zero. Moreover, if A is (anti-)symmetric then so too is its inverse A^{-1}. This is easily proved by noting that if $\mathsf{A} = \pm\mathsf{A}^{\mathrm{T}}$ then

$$(\mathsf{A}^{-1})^{\mathrm{T}} = (\mathsf{A}^{\mathrm{T}})^{-1} = \pm\mathsf{A}^{-1}.$$

Any $N \times N$ matrix A can be written as the sum of a symmetric and an antisymmetric matrix, since we may write

$$\mathsf{A} = \tfrac{1}{2}(\mathsf{A} + \mathsf{A}^{\mathrm{T}}) + \tfrac{1}{2}(\mathsf{A} - \mathsf{A}^{\mathrm{T}}) = \mathsf{B} + \mathsf{C},$$

where clearly $\mathsf{B} = \mathsf{B}^{\mathrm{T}}$ and $\mathsf{C} = -\mathsf{C}^{\mathrm{T}}$. The matrix B is therefore called the symmetric part of A, and C is the antisymmetric part.

►*If* A *is an* $N \times N$ *antisymmetric matrix, show that* $|\mathsf{A}| = 0$ *if* N *is odd.*

If A is antisymmetric then $\mathsf{A}^{\mathrm{T}} = -\mathsf{A}$. Using the properties of determinants (8.49) and (8.51), we have

$$|\mathsf{A}| = |\mathsf{A}^{\mathrm{T}}| = |-\mathsf{A}| = (-1)^N|\mathsf{A}|.$$

Thus, if N is odd then $|\mathsf{A}| = -|\mathsf{A}|$, which implies that $|\mathsf{A}| = 0$. ◄

8.12.4 Orthogonal matrices

A non-singular matrix with the property that its transpose is also its inverse,

$$\mathsf{A}^{\mathrm{T}} = \mathsf{A}^{-1}, \tag{8.65}$$

is called an *orthogonal matrix*. It follows immediately that the inverse of an orthogonal matrix is also orthogonal, since

$$(\mathsf{A}^{-1})^{\mathrm{T}} = (\mathsf{A}^{\mathrm{T}})^{-1} = (\mathsf{A}^{-1})^{-1}.$$

Moreover, since for an orthogonal matrix $\mathsf{A}^{\mathrm{T}}\mathsf{A} = \mathsf{I}$, we have

$$|\mathsf{A}^{\mathrm{T}}\mathsf{A}| = |\mathsf{A}^{\mathrm{T}}||\mathsf{A}| = |\mathsf{A}|^2 = |\mathsf{I}| = 1.$$

Thus the determinant of an orthogonal matrix must be $|\mathsf{A}| = \pm 1$.

An orthogonal matrix represents, in a particular basis, a linear operator that leaves the norms (lengths) of real vectors unchanged, as we will now show.

Suppose that $\mathbf{y} = \mathcal{A}\mathbf{x}$ is represented in some coordinate system by the matrix equation $\mathsf{y} = \mathsf{A}\mathsf{x}$; then $\langle \mathbf{y}|\mathbf{y}\rangle$ is given in this coordinate system by

$$\mathsf{y}^{\mathrm{T}}\mathsf{y} = \mathsf{x}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}\mathsf{A}\mathsf{x} = \mathsf{x}^{\mathrm{T}}\mathsf{x}.$$

Hence $\langle \mathbf{y}|\mathbf{y}\rangle = \langle \mathbf{x}|\mathbf{x}\rangle$, showing that the action of a linear operator represented by an orthogonal matrix does not change the norm of a real vector.

8.12.5 Hermitian and anti-Hermitian matrices

An *Hermitian* matrix is one that satisfies $\mathsf{A} = \mathsf{A}^{\dagger}$, where $\mathsf{A}^{\dagger}$ is the Hermitian conjugate discussed in section 8.7. Similarly if $\mathsf{A}^{\dagger} = -\mathsf{A}$, then A is called *anti-Hermitian*. A real (anti-)symmetric matrix is a special case of an (anti-)Hermitian matrix, in which all the elements of the matrix are real. Also, if A is an (anti-)Hermitian matrix then so too is its inverse A^{-1}, since

$$(\mathsf{A}^{-1})^{\dagger} = (\mathsf{A}^{\dagger})^{-1} = \pm\mathsf{A}^{-1}.$$

Any $N \times N$ matrix A can be written as the sum of an Hermitian matrix and an anti-Hermitian matrix, since

$$\mathsf{A} = \tfrac{1}{2}(\mathsf{A} + \mathsf{A}^{\dagger}) + \tfrac{1}{2}(\mathsf{A} - \mathsf{A}^{\dagger}) = \mathsf{B} + \mathsf{C},$$

where clearly $\mathsf{B} = \mathsf{B}^{\dagger}$ and $\mathsf{C} = -\mathsf{C}^{\dagger}$. The matrix B is called the Hermitian part of A, and C is called the anti-Hermitian part.

8.12.6 Unitary matrices

A *unitary* matrix A is defined as one for which

$$\mathsf{A}^{\dagger} = \mathsf{A}^{-1}. \tag{8.66}$$

Clearly, if A is real then $\mathsf{A}^{\dagger} = \mathsf{A}^{\mathrm{T}}$, showing that a real orthogonal matrix is a special case of a unitary matrix, one in which all the elements are real. We note that the inverse A^{-1} of a unitary is also unitary, since

$$(\mathsf{A}^{-1})^{\dagger} = (\mathsf{A}^{\dagger})^{-1} = (\mathsf{A}^{-1})^{-1}.$$

Moreover, since for a unitary matrix $\mathsf{A}^{\dagger}\mathsf{A} = \mathsf{I}$, we have

$$|\mathsf{A}^{\dagger}\mathsf{A}| = |\mathsf{A}^{\dagger}||\mathsf{A}| = |\mathsf{A}|^{*}|\mathsf{A}| = |\mathsf{I}| = 1.$$

Thus the determinant of a unitary matrix has unit modulus.

A unitary matrix represents, in a particular basis, a linear operator that leaves the norms (lengths) of complex vectors unchanged. If $\mathbf{y} = \mathcal{A}\mathbf{x}$ is represented in some coordinate system by the matrix equation $\mathsf{y} = \mathsf{A}\mathsf{x}$ then $\langle \mathbf{y}|\mathbf{y}\rangle$ is given in this coordinate system by

$$\mathsf{y}^{\dagger}\mathsf{y} = \mathsf{x}^{\dagger}\mathsf{A}^{\dagger}\mathsf{A}\mathsf{x} = \mathsf{x}^{\dagger}\mathsf{x}.$$

Hence $\langle \mathbf{y}|\mathbf{y}\rangle = \langle \mathbf{x}|\mathbf{x}\rangle$, showing that the action of the linear operator represented by a unitary matrix does not change the norm of a complex vector. The action of a unitary matrix on a complex column matrix thus parallels that of an orthogonal matrix acting on a real column matrix.

8.12.7 Normal matrices

A final important set of special matrices consists of the *normal* matrices, for which

$$\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A},$$

i.e. a normal matrix is one that commutes with its Hermitian conjugate.

We can easily show that Hermitian matrices and unitary matrices (or symmetric matrices and orthogonal matrices in the real case) are examples of normal matrices. For an Hermitian matrix, $\mathsf{A} = \mathsf{A}^\dagger$ and so

$$\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}\mathsf{A} = \mathsf{A}^\dagger\mathsf{A}.$$

Similarly, for a unitary matrix, $\mathsf{A}^{-1} = \mathsf{A}^\dagger$ and so

$$\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}\mathsf{A}^{-1} = \mathsf{A}^{-1}\mathsf{A} = \mathsf{A}^\dagger\mathsf{A}.$$

Finally, we note that, if A is normal then so too is its inverse A^{-1}, since

$$\mathsf{A}^{-1}(\mathsf{A}^{-1})^\dagger = \mathsf{A}^{-1}(\mathsf{A}^\dagger)^{-1} = (\mathsf{A}^\dagger\mathsf{A})^{-1} = (\mathsf{A}\mathsf{A}^\dagger)^{-1} = (\mathsf{A}^\dagger)^{-1}\mathsf{A}^{-1} = (\mathsf{A}^{-1})^\dagger\mathsf{A}^{-1}.$$

This broad class of matrices is important in the discussion of eigenvectors and eigenvalues in the next section.

8.13 Eigenvectors and eigenvalues

Suppose that a linear operator $\mathcal{A}$ transforms vectors $\mathbf{x}$ in an N-dimensional vector space into other vectors $\mathcal{A}\mathbf{x}$ in the same space. The possibility then arises that there exist vectors $\mathbf{x}$ each of which is transformed by $\mathcal{A}$ into a multiple of itself. Such vectors would have to satisfy

$$\mathcal{A}\mathbf{x} = \lambda\mathbf{x}. \tag{8.67}$$

Any non-zero vector $\mathbf{x}$ that satisfies (8.67) for some value of λ is called an *eigenvector* of the linear operator $\mathcal{A}$, and λ is called the corresponding *eigenvalue*. As will be discussed below, in general the operator $\mathcal{A}$ has N independent eigenvectors $\mathbf{x}^i$, with eigenvalues λ_i. The λ_i are not necessarily all distinct.

If we choose a particular basis in the vector space, we can write (8.67) in terms of the components of $\mathcal{A}$ and $\mathbf{x}$ with respect to this basis as the matrix equation

$$\mathsf{A}\mathsf{x} = \lambda\mathsf{x}, \tag{8.68}$$

where A is an $N \times N$ matrix. The column matrices x that satisfy (8.68) obviously

represent the eigenvectors $\mathbf{x}$ of $\mathcal{A}$ in our chosen coordinate system. Conventionally, these column matrices are also referred to as the *eigenvectors of the matrix* A.[§] Clearly, if x is an eigenvector of A (with some eigenvalue λ) then any scalar multiple $\mu\mathsf{x}$ is also an eigenvector with the same eigenvalue. We therefore often use *normalised* eigenvectors, for which

$$\mathsf{x}^\dagger\mathsf{x} = 1$$

(note that $\mathsf{x}^\dagger\mathsf{x}$ corresponds to the inner product $\langle\mathbf{x}|\mathbf{x}\rangle$ in our basis). Any eigenvector x can be normalised by dividing all its components by the scalar $(\mathsf{x}^\dagger\mathsf{x})^{1/2}$.

As will be seen, the problem of finding the eigenvalues and corresponding eigenvectors of a square matrix A plays an important role in many physical investigations. Throughout this chapter we denote the ith eigenvector of a square matrix A by x^i and the corresponding eigenvalue by λ_i. This superscript notation for eigenvectors is used to avoid any confusion with components.

►*A non-singular matrix* A *has eigenvalues* λ_i *and eigenvectors* x^i. *Find the eigenvalues and eigenvectors of the inverse matrix* A^{-1}.

The eigenvalues and eigenvectors of A satisfy

$$\mathsf{A}\mathsf{x}^i = \lambda_i\mathsf{x}^i.$$

Left-multiplying both sides of this equation by A^{-1}, we find

$$\mathsf{A}^{-1}\mathsf{A}\mathsf{x}^i = \lambda_i\mathsf{A}^{-1}\mathsf{x}^i.$$

Since $\mathsf{A}^{-1}\mathsf{A} = \mathsf{I}$, on rearranging we obtain

$$\mathsf{A}^{-1}\mathsf{x}^i = \frac{1}{\lambda_i}\mathsf{x}^i.$$

Thus, we see that A^{-1} has the *same* eigenvectors $\mathbf{x}^i$ as does A, but the corresponding eigenvalues are $1/\lambda_i$. ◄

In the remainder of this section we will discuss some useful results concerning the eigenvectors and eigenvalues of certain special (though commonly occurring) square matrices. The results will be established for matrices whose elements may be complex; the corresponding properties for real matrices may be obtained as special cases.

8.13.1 Eigenvectors and eigenvalues of a normal matrix

In subsection 8.12.7 we defined a normal matrix A as one that commutes with its Hermitian conjugate, so that

$$\mathsf{A}^\dagger\mathsf{A} = \mathsf{A}\mathsf{A}^\dagger.$$

[§] In this context, when referring to linear combinations of eigenvectors x we will normally use the term 'vector'.

We also showed that both Hermitian and unitary matrices (or symmetric and orthogonal matrices in the real case) are examples of normal matrices. We now discuss the properties of the eigenvectors and eigenvalues of a normal matrix.

If x is an eigenvector of a normal matrix A with corresponding eigenvalue λ then $\mathsf{Ax} = \lambda\mathsf{x}$, or equivalently,

$$(\mathsf{A} - \lambda\mathsf{I})\mathsf{x} = \mathsf{0}. \tag{8.69}$$

Denoting $\mathsf{B} = \mathsf{A} - \lambda\mathsf{I}$, (8.69) becomes $\mathsf{Bx} = \mathsf{0}$ and, taking the Hermitian conjugate, we also have

$$(\mathsf{Bx})^\dagger = \mathsf{x}^\dagger\mathsf{B}^\dagger = \mathsf{0}. \tag{8.70}$$

From (8.69) and (8.70) we then have

$$\mathsf{x}^\dagger\mathsf{B}^\dagger\mathsf{Bx} = \mathsf{0}. \tag{8.71}$$

However, the product $\mathsf{B}^\dagger\mathsf{B}$ is given by

$$\mathsf{B}^\dagger\mathsf{B} = (\mathsf{A} - \lambda\mathsf{I})^\dagger(\mathsf{A} - \lambda\mathsf{I}) = (\mathsf{A}^\dagger - \lambda^*\mathsf{I})(\mathsf{A} - \lambda\mathsf{I}) = \mathsf{A}^\dagger\mathsf{A} - \lambda^*\mathsf{A} - \lambda\mathsf{A}^\dagger + \lambda\lambda^*.$$

Now since A is normal, $\mathsf{A}\mathsf{A}^\dagger = \mathsf{A}^\dagger\mathsf{A}$ and so

$$\mathsf{B}^\dagger\mathsf{B} = \mathsf{A}\mathsf{A}^\dagger - \lambda^*\mathsf{A} - \lambda\mathsf{A}^\dagger + \lambda\lambda^* = (\mathsf{A} - \lambda\mathsf{I})(\mathsf{A} - \lambda\mathsf{I})^\dagger = \mathsf{B}\mathsf{B}^\dagger,$$

and hence B is also normal. From (8.71) we then find

$$\mathsf{x}^\dagger\mathsf{B}^\dagger\mathsf{Bx} = \mathsf{x}^\dagger\mathsf{B}\mathsf{B}^\dagger\mathsf{x} = (\mathsf{B}^\dagger\mathsf{x})^\dagger\mathsf{B}^\dagger\mathsf{x} = \mathsf{0},$$

from which we obtain

$$\mathsf{B}^\dagger\mathsf{x} = (\mathsf{A}^\dagger - \lambda^*\mathsf{I})\mathsf{x} = \mathsf{0}.$$

Therefore, for a normal matrix A, *the eigenvalues of* $\mathsf{A}^\dagger$ *are the complex conjugates of the eigenvalues of* A.

Let us now consider two eigenvectors x^i and x^j of a normal matrix A corresponding to two *different* eigenvalues λ_i and λ_j. We then have

$$\mathsf{A}\mathsf{x}^i = \lambda_i\mathsf{x}^i, \tag{8.72}$$

$$\mathsf{A}\mathsf{x}^j = \lambda_j\mathsf{x}^j. \tag{8.73}$$

Multiplying (8.73) on the left by $(\mathsf{x}^i)^\dagger$ we obtain

$$(\mathsf{x}^i)^\dagger\mathsf{A}\mathsf{x}^j = \lambda_j(\mathsf{x}^i)^\dagger\mathsf{x}^j. \tag{8.74}$$

However, on the LHS of (8.74) we have

$$(\mathsf{x}^i)^\dagger\mathsf{A} = (\mathsf{A}^\dagger\mathsf{x}^i)^\dagger = (\lambda_i^*\mathsf{x}^i)^\dagger = \lambda_i(\mathsf{x}^i)^\dagger, \tag{8.75}$$

where we have used (8.40) and the property just proved for a normal matrix to

write $\mathsf{A}^\dagger \mathsf{x}^i = \lambda_i^* \mathsf{x}^i$. From (8.74) and (8.75) we have

$$(\lambda_i - \lambda_j)(\mathsf{x}^i)^\dagger \mathsf{x}^j = 0. \tag{8.76}$$

Thus, *if* $\lambda_i \neq \lambda_j$ *the eigenvectors* x^i *and* x^j *must be orthogonal*, i.e. $(\mathsf{x}^i)^\dagger \mathsf{x}^j = 0$.

It follows immediately from (8.76) that if all N eigenvalues of a normal matrix A are distinct then all N eigenvectors of A are mutually orthogonal. If, however, two or more eigenvalues are the same then further consideration is required. An eigenvalue corresponding to two or more different eigenvectors (i.e. they are not simply multiples of one another) is said to be *degenerate*. Suppose that λ_1 is k-fold degenerate, i.e.

$$\mathsf{A}\mathsf{x}^i = \lambda_1 \mathsf{x}^i \quad \text{for } i = 1, 2, \ldots, k, \tag{8.77}$$

but that it is different from any of λ_{k+1}, λ_{k+2}, etc. Then any linear combination of these x^i is also an eigenvector with eigenvalue λ_1, since, for $\mathsf{z} = \sum_{i=1}^k c_i \mathsf{x}^i$,

$$\mathsf{A}\mathsf{z} \equiv \mathsf{A} \sum_{i=1}^k c_i \mathsf{x}^i = \sum_{i=1}^k c_i \mathsf{A}\mathsf{x}^i = \sum_{i=1}^k c_i \lambda_1 \mathsf{x}^i = \lambda_1 \mathsf{z}. \tag{8.78}$$

If the x^i defined in (8.77) are not already mutually orthogonal then we can construct new eigenvectors z^i that are orthogonal by the following procedure:

$$\begin{aligned}
\mathsf{z}^1 &= \mathsf{x}^1, \\
\mathsf{z}^2 &= \mathsf{x}^2 - \left[(\hat{\mathsf{z}}^1)^\dagger \mathsf{x}^2\right] \hat{\mathsf{z}}^1, \\
\mathsf{z}^3 &= \mathsf{x}^3 - \left[(\hat{\mathsf{z}}^2)^\dagger \mathsf{x}^3\right] \hat{\mathsf{z}}^2 - \left[(\hat{\mathsf{z}}^1)^\dagger \mathsf{x}^3\right] \hat{\mathsf{z}}^1, \\
&\vdots \\
\mathsf{z}^k &= \mathsf{x}^k - \left[(\hat{\mathsf{z}}^{k-1})^\dagger \mathsf{x}^k\right] \hat{\mathsf{z}}^{k-1} - \cdots - \left[(\hat{\mathsf{z}}^1)^\dagger \mathsf{x}^k\right] \hat{\mathsf{z}}^1.
\end{aligned}$$

In this procedure, known as *Gram–Schmidt orthogonalisation*, each new eigenvector z^i is normalised to give the unit vector $\hat{\mathsf{z}}^i$ before proceeding to the construction of the next one (the normalisation is carried out by dividing each element of the vector z^i by $[(\mathsf{z}^i)^\dagger \mathsf{z}^i]^{1/2}$). Note that each factor in brackets $(\hat{\mathsf{z}}^m)^\dagger \mathsf{x}^n$ is a scalar product and thus only a number. It follows that, as shown in (8.78), each vector z^i so constructed is an eigenvector of A with eigenvalue λ_1 and will remain so on normalisation. It is straightforward to check that, provided the previous new eigenvectors have been normalised as prescribed, each z^i is orthogonal to all its predecessors. (In practice, however, the method is laborious and the example in subsection 8.14.1 gives a less rigorous but considerably quicker way.)

Therefore, even if A has some degenerate eigenvalues we can *by construction* obtain a set of N mutually orthogonal eigenvectors. Moreover, it may be shown (although the proof is beyond the scope of this book) that these eigenvectors are *complete* in that they form a basis for the N-dimensional vector space. As

a result any arbitrary vector y can be expressed as a linear combination of the eigenvectors x^i:

$$\mathsf{y} = \sum_{i=1}^{N} a_i \mathsf{x}^i, \tag{8.79}$$

where $a_i = (\mathsf{x}^i)^\dagger \mathsf{y}$. Thus, the eigenvectors form an orthogonal basis for the vector space. By normalising the eigenvectors so that $(\mathsf{x}^i)^\dagger \mathsf{x}^i = 1$ this basis is made orthonormal.

►*Show that a normal matrix* A *can be written in terms of its eigenvalues* λ_i *and orthonormal eigenvectors* x^i *as*

$$\mathsf{A} = \sum_{i=1}^{N} \lambda_i \mathsf{x}^i (\mathsf{x}^i)^\dagger. \tag{8.80}$$

The key to proving the validity of (8.80) is to show that both sides of the expression give the same result when acting on an arbitary vector y. Since A is normal, we may expand y in terms of the eigenvectors x^i, as shown in (8.79). Thus, we have

$$\mathsf{A}\mathsf{y} = \mathsf{A} \sum_{i=1}^{N} a_i \mathsf{x}^i = \sum_{i=1}^{N} a_i \lambda_i \mathsf{x}^i.$$

Alternatively, the action of the RHS of (8.80) on y is given by

$$\sum_{i=1}^{N} \lambda_i \mathsf{x}^i (\mathsf{x}^i)^\dagger \mathsf{y} = \sum_{i=1}^{N} a_i \lambda_i \mathsf{x}^i,$$

since $a_i = (\mathsf{x}^i)^\dagger \mathsf{y}$. We see that the two expressions for the action of each side of (8.80) on y are identical, which implies that this relationship is indeed correct. ◄

8.13.2 Eigenvectors and eigenvalues of Hermitian and anti-Hermitian matrices

For a normal matrix we showed that if $\mathsf{A}\mathsf{x} = \lambda\mathsf{x}$ then $\mathsf{A}^\dagger\mathsf{x} = \lambda^*\mathsf{x}$. However, if A is also Hermitian, $\mathsf{A} = \mathsf{A}^\dagger$, it follows necessarily that $\lambda = \lambda^*$. Thus, the eigenvalues of an Hermitian matrix are real, a result which may be proved directly.

►*Prove that the eigenvalues of an Hermitian matrix are real.*

For any particular eigenvector x^i, we take the Hermitian conjugate of $\mathsf{A}\mathsf{x}^i = \lambda_i \mathsf{x}^i$ to give

$$(\mathsf{x}^i)^\dagger \mathsf{A}^\dagger = \lambda_i^* (\mathsf{x}^i)^\dagger. \tag{8.81}$$

Using $\mathsf{A}^\dagger = \mathsf{A}$, since A is Hermitian, and multiplying on the right by x^i, we obtain

$$(\mathsf{x}^i)^\dagger \mathsf{A}\mathsf{x}^i = \lambda_i^* (\mathsf{x}^i)^\dagger \mathsf{x}^i. \tag{8.82}$$

But multiplying $\mathsf{A}\mathsf{x}^i = \lambda_i \mathsf{x}^i$ through on the left by $(\mathsf{x}^i)^\dagger$ gives

$$(\mathsf{x}^i)^\dagger \mathsf{A}\mathsf{x}^i = \lambda_i (\mathsf{x}^i)^\dagger \mathsf{x}^i.$$

Subtracting this from (8.82) yields

$$0 = (\lambda_i^* - \lambda_i)(\mathsf{x}^i)^\dagger \mathsf{x}^i.$$

But $(\mathbf{x}^i)^\dagger\mathbf{x}^i$ is the modulus squared of the non-zero vector $\mathbf{x}^i$ and is thus non-zero. Hence λ_i^* must equal λ_i and thus be real. The same argument can be used to show that the eigenvalues of a real symmetric matrix are themselves real. ◄

The importance of the above result will be apparent to any student of quantum mechanics. In quantum mechanics the eigenvalues of operators correspond to measured values of observable quantities, e.g. energy, angular momentum, parity and so on, and these clearly must be real. If we use Hermitian operators to formulate the theories of quantum mechanics, the above property guarantees physically meaningful results.

Since an Hermitian matrix is also a normal matrix, its eigenvectors are orthogonal (or can be made so using the Gram–Schmidt orthogonalisation procedure). Alternatively we can prove the orthogonality of the eigenvectors directly.

►*Prove that the eigenvectors corresponding to different eigenvalues of an Hermitian matrix are orthogonal.*

Consider two unequal eigenvalues λ_i and λ_j and their corresponding eigenvectors satisfying

$$\mathbf{A}\mathbf{x}^i = \lambda_i\mathbf{x}^i, \tag{8.83}$$

$$\mathbf{A}\mathbf{x}^j = \lambda_j\mathbf{x}^j. \tag{8.84}$$

Taking the Hermitian conjugate of (8.83) we find $(\mathbf{x}^i)^\dagger\mathbf{A}^\dagger = \lambda_i^*(\mathbf{x}^i)^\dagger$. Multiplying this on the right by $\mathbf{x}^j$ we obtain

$$(\mathbf{x}^i)^\dagger\mathbf{A}^\dagger\mathbf{x}^j = \lambda_i^*(\mathbf{x}^i)^\dagger\mathbf{x}^j,$$

and similarly multiplying (8.84) through on the left by $(\mathbf{x}^i)^\dagger$ we find

$$(\mathbf{x}^i)^\dagger\mathbf{A}\mathbf{x}^j = \lambda_j(\mathbf{x}^i)^\dagger\mathbf{x}^j.$$

Then, since $\mathbf{A}^\dagger = \mathbf{A}$, the two left-hand sides are equal and, because the λ_i are real, on subtraction we obtain

$$0 = (\lambda_i - \lambda_j)(\mathbf{x}^i)^\dagger\mathbf{x}^j.$$

Finally we note that $\lambda_i \neq \lambda_j$ and so $(\mathbf{x}^i)^\dagger\mathbf{x}^j = 0$, i.e. the eigenvectors $\mathbf{x}^i$ and $\mathbf{x}^j$ are orthogonal. ◄

In the case where some of the eigenvalues are equal, further justification of the orthogonality of the eigenvectors is needed. The Gram–Schmidt orthogonalisation procedure discussed above provides a proof of, and a means of achieving, orthogonality. The general method has already been described and we will not repeat it here.

We may also consider the properties of the eigenvalues and eigenvectors of an anti-Hermitian matrix, for which $\mathbf{A}^\dagger = -\mathbf{A}$ and thus

$$\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}(-\mathbf{A}) = (-\mathbf{A})\mathbf{A} = \mathbf{A}^\dagger\mathbf{A}.$$

Therefore matrices that are anti-Hermitian are also normal and so have mutually orthogonal eigenvectors. The properties of the eigenvalues are also simply deduced, since if $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ then

$$\lambda^*\mathbf{x} = \mathbf{A}^\dagger\mathbf{x} = -\mathbf{A}\mathbf{x} = -\lambda\mathbf{x}.$$

Hence $\lambda^* = -\lambda$ and so λ must be *pure imaginary* (or *zero*). In a similar manner to that used for Hermitian matrices, these properties may be proved directly.

8.13.3 Eigenvectors and eigenvalues of a unitary matrix

A unitary matrix satisfies $\mathsf{A}^\dagger = \mathsf{A}^{-1}$ and is also a normal matrix, with mutually orthogonal eigenvectors. To investigate the eigenvalues of a unitary matrix, we note that if $\mathsf{A}\mathsf{x} = \lambda\mathsf{x}$ then

$$\mathsf{x}^\dagger\mathsf{x} = \mathsf{x}^\dagger\mathsf{A}^\dagger\mathsf{A}\mathsf{x} = \lambda^*\lambda\mathsf{x}^\dagger\mathsf{x},$$

and we deduce that $\lambda\lambda^* = |\lambda|^2 = 1$. Thus, the eigenvalues of a unitary matrix have unit modulus.

8.13.4 Eigenvectors and eigenvalues of a general square matrix

When an $N \times N$ matrix is not normal there are no general properties of its eigenvalues and eigenvectors; in general it is not possible to find any orthogonal set of N eigenvectors or even to find *pairs* of orthogonal eigenvectors (except by chance in some cases). While the N non-orthogonal eigenvectors are usually linearly independent and hence form a basis for the N-dimensional vector space, this is not necessarily so. It may be shown (although we will not prove it) that any $N \times N$ matrix with *distinct* eigenvalues has N linearly independent eigenvectors, which therefore form a basis for the N-dimensional vector space. If a general square matrix has degenerate eigenvalues, however, then it may or may not have N linearly independent eigenvectors. A matrix whose eigenvectors are not linearly independent is said to be *defective*.

8.13.5 Simultaneous eigenvectors

We may now ask under what conditions two different normal matrices can have a common set of eigenvectors. The result – that they do so if, and only if, they commute – has profound significance for the foundations of quantum mechanics.

To prove this important result let A and B be two $N \times N$ normal matrices and x^i be the ith eigenvector of A corresponding to eigenvalue λ_i, i.e.

$$\mathsf{A}\mathsf{x}^i = \lambda_i\mathsf{x}^i \quad \text{for} \quad i = 1, 2, \ldots, N.$$

For the present we assume that the eigenvalues are all different.

(i) First suppose that A and B commute. Now consider

$$\mathsf{A}\mathsf{B}\mathsf{x}^i = \mathsf{B}\mathsf{A}\mathsf{x}^i = \mathsf{B}\lambda_i\mathsf{x}^i = \lambda_i\mathsf{B}\mathsf{x}^i,$$

where we have used the commutativity for the first equality and the eigenvector property for the second. It follows that $\mathsf{A}(\mathsf{B}\mathsf{x}^i) = \lambda_i(\mathsf{B}\mathsf{x}^i)$ and thus that $\mathsf{B}\mathsf{x}^i$ is an

eigenvector of A corresponding to eigenvalue λ_i. But the eigenvector solutions of $(\mathsf{A}-\lambda_i\mathsf{I})\mathsf{x}^i=\mathsf{0}$ are unique to within a scale factor, and we therefore conclude that

$$\mathsf{B}\mathsf{x}^i=\mu_i\mathsf{x}^i$$

for some scale factor μ_i. However, this is just an eigenvector equation for B and shows that x^i is an eigenvector of B, in addition to being an eigenvector of A. By reversing the roles of A and B, it also follows that every eigenvector of B is an eigenvector of A. Thus the two sets of eigenvectors are identical.

(ii) Now suppose that A and B have all their eigenvectors in common, a typical one x^i satisfying both

$$\mathsf{A}\mathsf{x}^i=\lambda_i\mathsf{x}^i \quad \text{and} \quad \mathsf{B}\mathsf{x}^i=\mu_i\mathsf{x}^i.$$

As the eigenvectors span the N-dimensional vector space, any arbitrary vector x in the space can be written as a linear combination of the eigenvectors,

$$\mathsf{x}=\sum_{i=1}^{N}c_i\mathsf{x}^i.$$

Now consider both

$$\mathsf{A}\mathsf{B}\mathsf{x}=\mathsf{A}\mathsf{B}\sum_{i=1}^{N}c_i\mathsf{x}^i=\mathsf{A}\sum_{i=1}^{N}c_i\mu_i\mathsf{x}^i=\sum_{i=1}^{N}c_i\lambda_i\mu_i\mathsf{x}^i,$$

and

$$\mathsf{B}\mathsf{A}\mathsf{x}=\mathsf{B}\mathsf{A}\sum_{i=1}^{N}c_i\mathsf{x}^i=\mathsf{B}\sum_{i=1}^{N}c_i\lambda_i\mathsf{x}^i=\sum_{i=1}^{N}c_i\mu_i\lambda_i\mathsf{x}^i.$$

It follows that $\mathsf{A}\mathsf{B}\mathsf{x}$ and $\mathsf{B}\mathsf{A}\mathsf{x}$ are the same for any arbitrary x and hence that

$$(\mathsf{A}\mathsf{B}-\mathsf{B}\mathsf{A})\mathsf{x}=\mathsf{0}$$

for all x. That is, A and B *commute*.

This completes the proof that a necessary and sufficient condition for two normal matrices to have a set of eigenvectors in common is that they commute. It should be noted that if an eigenvalue of A, say, is degenerate then not all of its possible sets of eigenvectors will also constitute a set of eigenvectors of B. However, provided that by taking linear combinations one set of joint eigenvectors can be found, the proof is still valid and the result still holds.

When extended to the case of Hermitian operators and continuous eigenfunctions (sections 17.2 and 17.3) the connection between commuting matrices and a set of common eigenvectors plays a fundamental role in the postulatory basis of quantum mechanics. It draws the distinction between commuting and non-commuting observables and sets limits on how much information about a system can be known, even in principle, at any one time.

8.14 Determination of eigenvalues and eigenvectors

The next step is to show how the eigenvalues and eigenvectors of a given $N \times N$ matrix A are found. To do this we refer to (8.68) and as in (8.69) rewrite it as

$$\mathsf{Ax} - \lambda\mathsf{Ix} = (\mathsf{A} - \lambda\mathsf{I})\mathsf{x} = \mathsf{0}. \tag{8.85}$$

The slight rearrangement used here is to write x as Ix, where I is the unit matrix of order N. The point of doing this is immediate since (8.85) now has the form of a homogeneous set of simultaneous equations, the theory of which will be developed in section 8.18. What will be proved there is that the equation $\mathsf{Bx} = \mathsf{0}$ only has a non-trivial solution x if $|\mathsf{B}| = 0$. Correspondingly, therefore, we must have in the present case that

$$|\mathsf{A} - \lambda\mathsf{I}| = 0, \tag{8.86}$$

if there are to be non-zero solutions x to (8.85).

Equation (8.86) is known as the *characteristic equation* for A and its LHS as the *characteristic* or *secular determinant* of A. The equation is a polynomial of degree N in the quantity λ. The N roots of this equation λ_i, $i = 1, 2, \ldots, N$, give the eigenvalues of A. Corresponding to each λ_i there will be a column vector x^i, which is the ith eigenvector of A and can be found by using (8.68).

It will be observed that when (8.86) is written out as a polynomial equation in λ, the coefficient of $-\lambda^{N-1}$ in the equation will be simply $A_{11} + A_{22} + \cdots + A_{NN}$ relative to the coefficient of λ^N. As discussed in section 8.8, the quantity $\sum_{i=1}^{N} A_{ii}$ is the *trace* of A and, from the ordinary theory of polynomial equations, will be equal to the sum of the roots of (8.86):

$$\sum_{i=1}^{N} \lambda_i = \mathrm{Tr}\,\mathsf{A}. \tag{8.87}$$

This can be used as one check that a computation of the eigenvalues λ_i has been done correctly. Unless equation (8.87) is satisfied by a computed set of eigenvalues, they have not been calculated correctly. However, that equation (8.87) is satisfied is a necessary, but not sufficient, condition for a correct computation. An alternative proof of (8.87) is given in section 8.16.

►*Find the eigenvalues and normalised eigenvectors of the real symmetric matrix*

$$\mathsf{A} = \begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix}.$$

Using (8.86),

$$\begin{vmatrix} 1-\lambda & 1 & 3 \\ 1 & 1-\lambda & -3 \\ 3 & -3 & -3-\lambda \end{vmatrix} = 0.$$

Expanding out this determinant gives

$$(1-\lambda)\,[(1-\lambda)(-3-\lambda)-(-3)(-3)]+1\,[(-3)(3)-1(-3-\lambda)] \\ +3\,[1(-3)-(1-\lambda)(3)]=0,$$

which simplifies to give

$$(1-\lambda)(\lambda^2+2\lambda-12)+(\lambda-6)+3(3\lambda-6)=0, \\ \Rightarrow \qquad (\lambda-2)(\lambda-3)(\lambda+6)=0.$$

Hence the roots of the characteristic equation, which are the eigenvalues of A, are $\lambda_1=2$, $\lambda_2=3$, $\lambda_3=-6$. We note that, as expected,

$$\lambda_1+\lambda_2+\lambda_3=-1=1+1-3=A_{11}+A_{22}+A_{33}=\mathrm{Tr}\,\mathsf{A}.$$

For the first root, $\lambda_1=2$, a suitable eigenvector x^1, with elements x_1, x_2, x_3, must satisfy $\mathsf{A}\mathsf{x}^1=2\mathsf{x}^1$ or, equivalently,

$$\begin{aligned} x_1+x_2+3x_3&=2x_1,\\ x_1+x_2-3x_3&=2x_2,\\ 3x_1-3x_2-3x_3&=2x_3. \end{aligned} \tag{8.88}$$

These three equations are consistent (to ensure this was the purpose in finding the particular values of λ) and yield $x_3=0$, $x_1=x_2=k$, where k is any non-zero number. A suitable eigenvector would thus be

$$\mathsf{x}^1=(k \quad k \quad 0)^{\mathrm{T}}.$$

If we apply the normalisation condition, we require $k^2+k^2+0^2=1$ or $k=1/\sqrt{2}$. Hence

$$\mathsf{x}^1=\left(\frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \quad 0\right)^{\mathrm{T}}=\frac{1}{\sqrt{2}}(1 \quad 1 \quad 0)^{\mathrm{T}}.$$

Repeating the last paragraph, but with the factor 2 on the RHS of (8.88) replaced successively by $\lambda_2=3$ and $\lambda_3=-6$, gives two further normalised eigenvectors

$$\mathsf{x}^2=\frac{1}{\sqrt{3}}(1 \quad -1 \quad 1)^{\mathrm{T}}, \qquad \mathsf{x}^3=\frac{1}{\sqrt{6}}(1 \quad -1 \quad -2)^{\mathrm{T}}. \blacktriangleleft$$

In the above example, the three values of λ are all different and A is a real symmetric matrix. Thus we expect, and it is easily checked, that the three eigenvectors are mutually orthogonal, i.e.

$$\left(\mathsf{x}^1\right)^{\mathrm{T}}\mathsf{x}^2=\left(\mathsf{x}^1\right)^{\mathrm{T}}\mathsf{x}^3=\left(\mathsf{x}^2\right)^{\mathrm{T}}\mathsf{x}^3=0.$$

It will be apparent also that, as expected, the normalisation of the eigenvectors has no effect on their orthogonality.

8.14.1 Degenerate eigenvalues

We return now to the case of degenerate eigenvalues, i.e. those that have two or more associated eigenvectors. We have shown already that it is always possible to construct an orthogonal set of eigenvectors for a normal matrix, see subsection 8.13.1, and the following example illustrates one method for constructing such a set.

►*Construct an orthonormal set of eigenvectors for the matrix*

$$\mathsf{A} = \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix}.$$

We first determine the eigenvalues using $|\mathsf{A} - \lambda\mathsf{I}| = 0$:

$$0 = \begin{vmatrix} 1-\lambda & 0 & 3 \\ 0 & -2-\lambda & 0 \\ 3 & 0 & 1-\lambda \end{vmatrix} = -(1-\lambda)^2(2+\lambda) + 3(3)(2+\lambda)$$

$$= (4-\lambda)(\lambda+2)^2.$$

Thus $\lambda_1 = 4$, $\lambda_2 = -2 = \lambda_3$. The eigenvector $\mathsf{x}^1 = (x_1 \quad x_2 \quad x_3)^{\mathrm{T}}$ is found from

$$\begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 4 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \quad \Rightarrow \quad \mathsf{x}^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

A general column vector that is orthogonal to x^1 is

$$\mathsf{x} = (a \quad b \quad -a)^{\mathrm{T}}, \tag{8.89}$$

and it is easily shown that

$$\mathsf{A}\mathsf{x} = \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ -a \end{pmatrix} = -2 \begin{pmatrix} a \\ b \\ -a \end{pmatrix} = -2\mathsf{x}.$$

Thus x is a eigenvector of A with associated eigenvalue -2. It is clear, however, that there is an infinite set of eigenvectors x all possessing the required property; the geometrical analogue is that there are an infinite number of corresponding vectors $\mathbf{x}$ lying in the plane that has $\mathbf{x}^1$ as its normal. We do require that the two remaining eigenvectors are orthogonal to one another, but this still leaves an infinite number of possibilities. For x^2, therefore, let us choose a simple form of (8.89), suitably normalised, say,

$$\mathsf{x}^2 = (0 \quad 1 \quad 0)^{\mathrm{T}}.$$

The third eigenvector is then specified (to within an arbitrary multiplicative constant) by the requirement that it must be orthogonal to x^1 and x^2; thus x^3 may be found by evaluating the vector product of x^1 and x^2 and normalising the result. This gives

$$\mathsf{x}^3 = \frac{1}{\sqrt{2}}(-1 \quad 0 \quad 1)^{\mathrm{T}},$$

to complete the construction of an orthonormal set of eigenvectors. ◄

8.15 Change of basis and similarity transformations

Throughout this chapter we have considered the vector $\mathbf{x}$ as a geometrical quantity that is independent of any basis (or coordinate system). If we introduce a basis $\mathbf{e}_i$, $i = 1, 2, \ldots, N$, into our N-dimensional vector space then we may write

$$\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + \cdots + x_N\mathbf{e}_N,$$

and represent $\mathbf{x}$ in this basis by the column matrix

$$\mathsf{x} = (x_1 \quad x_2 \ \cdots \ x_n)^{\mathrm{T}},$$

having components x_i. We now consider how these components change as a result of a prescribed change of basis. Let us introduce a new basis $\mathbf{e}'_i$, $i = 1, 2, \ldots, N$, which is related to the old basis by

$$\mathbf{e}'_j = \sum_{i=1}^{N} S_{ij}\mathbf{e}_i, \tag{8.90}$$

the coefficient S_{ij} being the ith component of $\mathbf{e}'_j$ with respect to the old (unprimed) basis. For an arbitrary vector $\mathbf{x}$ it follows that

$$\mathbf{x} = \sum_{i=1}^{N} x_i\mathbf{e}_i = \sum_{j=1}^{N} x'_j\mathbf{e}'_j = \sum_{j=1}^{N} x'_j \sum_{i=1}^{N} S_{ij}\mathbf{e}_i.$$

From this we derive the relationship between the components of $\mathbf{x}$ in the two coordinate systems as

$$x_i = \sum_{j=1}^{N} S_{ij}x'_j,$$

which we can write in matrix form as

$$\mathsf{x} = \mathsf{S}\mathsf{x}' \tag{8.91}$$

where S is the *transformation matrix* associated with the change of basis.

Furthermore, since the vectors $\mathbf{e}'_j$ are linearly independent, the matrix S is non-singular and so possesses an inverse S^{-1}. Multiplying (8.91) on the left by S^{-1} we find

$$\mathsf{x}' = \mathsf{S}^{-1}\mathsf{x}, \tag{8.92}$$

which relates the components of $\mathbf{x}$ in the new basis to those in the old basis. Comparing (8.92) and (8.90) we note that the components of $\mathbf{x}$ transform inversely to the way in which the basis vectors $\mathbf{e}_i$ themselves transform. This has to be so, as the vector $\mathbf{x}$ itself must remain unchanged.

We may also find the transformation law for the components of a linear operator under the same change of basis. Now, the operator equation $\mathbf{y} = \mathcal{A}\,\mathbf{x}$ (which is basis independent) can be written as a matrix equation in each of the two bases as

$$\mathsf{y} = \mathsf{A}\mathsf{x}, \qquad \mathsf{y}' = \mathsf{A}'\mathsf{x}'. \tag{8.93}$$

But, using (8.91), we may rewrite the first equation as

$$\mathsf{S}\mathsf{y}' = \mathsf{A}\mathsf{S}\mathsf{x}' \quad \Rightarrow \quad \mathsf{y}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}\mathsf{x}'.$$

Comparing this with the second equation in (8.93) we find that the components of the linear operator $\mathcal{A}$ transform as

$$\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}. \tag{8.94}$$

Equation (8.94) is an example of a *similarity transformation* – a transformation that can be particularly useful in converting matrices into convenient forms for computation.

Given a square matrix A, we may interpret it as representing a linear operator $\mathcal{A}$ in a given basis $\mathbf{e}_i$. From (8.94), however, we may also consider the matrix $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}$, for any non-singular matrix S, as representing the same linear operator $\mathcal{A}$ but in a new basis $\mathbf{e}'_j$, related to the old basis by

$$\mathbf{e}'_j = \sum_i S_{ij}\mathbf{e}_i.$$

Therefore we would expect that any property of the matrix A that represents some (basis-independent) property of the linear operator $\mathcal{A}$ will also be shared by the matrix A'. We list these properties below.

(i) If $\mathsf{A} = \mathsf{I}$ then $\mathsf{A}' = \mathsf{I}$, since, from (8.94),

$$\mathsf{A}' = \mathsf{S}^{-1}\mathsf{I}\mathsf{S} = \mathsf{S}^{-1}\mathsf{S} = \mathsf{I}. \tag{8.95}$$

(ii) The value of the determinant is unchanged:

$$|\mathsf{A}'| = |\mathsf{S}^{-1}\mathsf{A}\mathsf{S}| = |\mathsf{S}^{-1}||\mathsf{A}||\mathsf{S}| = |\mathsf{A}||\mathsf{S}^{-1}||\mathsf{S}| = |\mathsf{A}||\mathsf{S}^{-1}\mathsf{S}| = |\mathsf{A}|. \tag{8.96}$$

(iii) The characteristic determinant and hence the eigenvalues of A' are the same as those of A: from (8.86),

$$\begin{aligned} |\mathsf{A}' - \lambda\mathsf{I}| &= |\mathsf{S}^{-1}\mathsf{A}\mathsf{S} - \lambda\mathsf{I}| = |\mathsf{S}^{-1}(\mathsf{A} - \lambda\mathsf{I})\mathsf{S}| \\ &= |\mathsf{S}^{-1}||\mathsf{S}||\mathsf{A} - \lambda\mathsf{I}| = |\mathsf{A} - \lambda\mathsf{I}|. \end{aligned} \tag{8.97}$$

(iv) The value of the trace is unchanged: from (8.87),

$$\begin{aligned} \operatorname{Tr}\mathsf{A}' &= \sum_i A'_{ii} = \sum_i \sum_j \sum_k (\mathsf{S}^{-1})_{ij} A_{jk} S_{ki} \\ &= \sum_i \sum_j \sum_k S_{ki}(\mathsf{S}^{-1})_{ij} A_{jk} = \sum_j \sum_k \delta_{kj} A_{jk} = \sum_j A_{jj} \\ &= \operatorname{Tr}\mathsf{A}. \end{aligned} \tag{8.98}$$

An important class of similarity transformations is that for which S is a unitary matrix; in this case $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S} = \mathsf{S}^{\dagger}\mathsf{A}\mathsf{S}$. Unitary transformation matrices are particularly important, for the following reason. If the original basis $\mathbf{e}_i$ is

orthonormal and the transformation matrix S is unitary then

$$\begin{aligned}\langle \mathbf{e}'_i|\mathbf{e}'_j\rangle &= \Big\langle \sum_k S_{ki}\mathbf{e}_k \Big| \sum_r S_{rj}\mathbf{e}_r \Big\rangle \\ &= \sum_k S^*_{ki} \sum_r S_{rj}\langle \mathbf{e}_k|\mathbf{e}_r\rangle \\ &= \sum_k S^*_{ki} \sum_r S_{rj}\delta_{kr} = \sum_k S^*_{ki}S_{kj} = (\mathsf{S}^\dagger\mathsf{S})_{ij} = \delta_{ij},\end{aligned}$$

showing that the new basis is also orthonormal.

Furthermore, in addition to the properties of general similarity transformations, for unitary transformations the following hold.

(i) If A is Hermitian (anti-Hermitian) then A' is Hermitian (anti-Hermitian), i.e. if $\mathsf{A}^\dagger = \pm\mathsf{A}$ then

$$(\mathsf{A}')^\dagger = (\mathsf{S}^\dagger\mathsf{A}\mathsf{S})^\dagger = \mathsf{S}^\dagger\mathsf{A}^\dagger\mathsf{S} = \pm\mathsf{S}^\dagger\mathsf{A}\mathsf{S} = \pm\mathsf{A}'. \tag{8.99}$$

(ii) If A is unitary (so that $\mathsf{A}^\dagger = \mathsf{A}^{-1}$) then A' is unitary, since

$$\begin{aligned}(\mathsf{A}')^\dagger\mathsf{A}' &= (\mathsf{S}^\dagger\mathsf{A}\mathsf{S})^\dagger(\mathsf{S}^\dagger\mathsf{A}\mathsf{S}) = \mathsf{S}^\dagger\mathsf{A}^\dagger\mathsf{S}\mathsf{S}^\dagger\mathsf{A}\mathsf{S} = \mathsf{S}^\dagger\mathsf{A}^\dagger\mathsf{A}\mathsf{S} \\ &= \mathsf{S}^\dagger\mathsf{I}\mathsf{S} = \mathsf{I}.\end{aligned} \tag{8.100}$$

8.16 Diagonalisation of matrices

Suppose that a linear operator $\mathcal{A}$ is represented in some basis $\mathbf{e}_i$, $i = 1, 2, \ldots, N$, by the matrix A. Consider a new basis $\mathbf{x}^j$ given by

$$\mathbf{x}^j = \sum_{i=1}^{N} S_{ij}\mathbf{e}_i,$$

where the $\mathbf{x}^j$ are chosen to be the eigenvectors of the linear operator $\mathcal{A}$, i.e.

$$\mathcal{A}\,\mathbf{x}^j = \lambda_j\mathbf{x}^j. \tag{8.101}$$

In the new basis, $\mathcal{A}$ is represented by the matrix $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}$, which has a particularly simple form, as we shall see shortly. The element S_{ij} of S is the ith component, in the old (unprimed) basis, of the jth eigenvector x^j of A, i.e. the columns of S are the eigenvectors of the matrix A:

$$\mathsf{S} = \begin{pmatrix} \uparrow & \uparrow & & \uparrow \\ \mathsf{x}^1 & \mathsf{x}^2 & \cdots & \mathsf{x}^N \\ \downarrow & \downarrow & & \downarrow \end{pmatrix},$$

that is, $S_{ij} = (\mathsf{x}^j)_i$. Therefore A' is given by

$$\begin{aligned}(\mathsf{S}^{-1}\mathsf{AS})_{ij} &= \sum_k \sum_l (\mathsf{S}^{-1})_{ik} A_{kl} S_{lj} \\ &= \sum_k \sum_l (\mathsf{S}^{-1})_{ik} A_{kl} (\mathsf{x}^j)_l \\ &= \sum_k (\mathsf{S}^{-1})_{ik} \lambda_j (\mathsf{x}^j)_k \\ &= \sum_k \lambda_j (\mathsf{S}^{-1})_{ik} S_{kj} = \lambda_j \delta_{ij}.\end{aligned}$$

So the matrix A' is diagonal with the eigenvalues of $\mathcal{A}$ as the diagonal elements, i.e.

$$\mathsf{A}' = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_N \end{pmatrix}.$$

Therefore, given a matrix A, if we construct the matrix S that has the eigenvectors of A as its columns then the matrix $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{AS}$ is diagonal and has the eigenvalues of A as its diagonal elements. Since we require S to be non-singular ($|\mathsf{S}| \neq 0$), the N eigenvectors of A must be linearly independent and form a basis for the N-dimensional vector space. It may be shown that *any matrix with distinct eigenvalues* can be diagonalised by this procedure. If, however, a general square matrix has degenerate eigenvalues then it may, or may not, have N linearly independent eigenvectors. If it does not then it *cannot* be diagonalised.

For normal matrices (which include Hermitian, anti-Hermitian and unitary matrices) the N eigenvectors are indeed linearly independent. Moreover, when normalised, these eigenvectors form an *orthonormal* set (or can be made to do so). Therefore the matrix S with these normalised eigenvectors as columns, i.e. whose elements are $S_{ij} = (\mathsf{x}^j)_i$, has the property

$$(\mathsf{S}^\dagger\mathsf{S})_{ij} = \sum_k (\mathsf{S}^\dagger)_{ik}(\mathsf{S})_{kj} = \sum_k S^*_{ki} S_{kj} = \sum_k (\mathsf{x}^i)^*_k (\mathsf{x}^j)_k = (\mathsf{x}^i)^\dagger \mathsf{x}^j = \delta_{ij}.$$

Hence S is unitary ($\mathsf{S}^{-1} = \mathsf{S}^\dagger$) and the original matrix A can be diagonalised by

$$\mathsf{A}' = \mathsf{S}^{-1}\mathsf{AS} = \mathsf{S}^\dagger\mathsf{AS}.$$

Therefore, any normal matrix A can be diagonalised by a similarity transformation using a *unitary* transformation matrix S.

►*Diagonalise the matrix*

$$\mathsf{A} = \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix}.$$

The matrix A is symmetric and so may be diagonalised by a transformation of the form $\mathsf{A}' = \mathsf{S}^{\dagger}\mathsf{A}\mathsf{S}$, where S has the normalised eigenvectors of A as its columns. We have already found these eigenvectors in subsection 8.14.1, and so we can write straightaway

$$\mathsf{S} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

We note that although the eigenvalues of A are degenerate, its three eigenvectors are linearly independent and so A can still be diagonalised. Thus, calculating $\mathsf{S}^{\dagger}\mathsf{A}\mathsf{S}$ we obtain

$$\begin{aligned} \mathsf{S}^{\dagger}\mathsf{A}\mathsf{S} &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 3 \\ 0 & -2 & 0 \\ 3 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & -1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 4 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \end{aligned}$$

which is diagonal, as required, and has as its diagonal elements the eigenvalues of A. ◄

If a matrix A is diagonalised by the similarity transformation $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}$, so that $\mathsf{A}' = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)$, then we have immediately

$$\mathrm{Tr}\,\mathsf{A}' = \mathrm{Tr}\,\mathsf{A} = \sum_{i=1}^{N} \lambda_i, \tag{8.102}$$

$$|\mathsf{A}'| = |\mathsf{A}| = \prod_{i=1}^{N} \lambda_i, \tag{8.103}$$

since the eigenvalues of the matrix are unchanged by the transformation. Moreover, these results may be used to prove the rather useful *trace formula*

$$|\exp\,\mathsf{A}| = \exp(\mathrm{Tr}\,\mathsf{A}), \tag{8.104}$$

where the exponential of a matrix is as defined in (8.38).

►*Prove the trace formula (8.104).*

At the outset, we note that for the similarity transformation $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}$, we have

$$(\mathsf{A}')^n = (\mathsf{S}^{-1}\mathsf{A}\mathsf{S})(\mathsf{S}^{-1}\mathsf{A}\mathsf{S})\cdots(\mathsf{S}^{-1}\mathsf{A}\mathsf{S}) = \mathsf{S}^{-1}\mathsf{A}^n\mathsf{S}.$$

Thus, from (8.38), we obtain $\exp\,\mathsf{A}' = \mathsf{S}^{-1}(\exp\,\mathsf{A})\mathsf{S}$, from which it follows that $|\exp\,\mathsf{A}'| =$

$|\exp \mathsf{A}|$. Moreover, by choosing the similarity transformation so that it diagonalises A, we have $\mathsf{A}' = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)$, and so

$$|\exp \mathsf{A}| = |\exp \mathsf{A}'| = |\exp[\mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)]| = |\mathrm{diag}(\exp\lambda_1, \exp\lambda_2, \ldots, \exp\lambda_N)| = \prod_{i=1}^{N} \exp\lambda_i.$$

Rewriting the final product of exponentials of the eigenvalues as the exponential of the sum of the eigenvalues, we find

$$|\exp\ \mathsf{A}| = \prod_{i=1}^{N} \exp\ \lambda_i = \exp\left(\sum_{i=1}^{N} \lambda_i\right) = \exp(\mathrm{Tr}\ \mathsf{A}),$$

which gives the trace formula (8.104). ◄

8.17 Quadratic and Hermitian forms

Let us now introduce the concept of quadratic forms (and their complex analogues, Hermitian forms). A quadratic form Q is a scalar function of a real vector $\mathbf{x}$ given by

$$Q(\mathbf{x}) = \langle \mathbf{x} | \mathcal{A}\, \mathbf{x} \rangle, \tag{8.105}$$

for some real linear operator $\mathcal{A}$. In any given basis (coordinate system) we can write (8.105) in matrix form as

$$Q(\mathsf{x}) = \mathsf{x}^{\mathrm{T}} \mathsf{A} \mathsf{x}, \tag{8.106}$$

where A is a real matrix. In fact, as will be explained below, we need only consider the case where A is symmetric, i.e. $\mathsf{A} = \mathsf{A}^{\mathrm{T}}$. As an example in a three-dimensional space,

$$\begin{aligned} Q = \mathsf{x}^{\mathrm{T}} \mathsf{A} \mathsf{x} &= \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ &= x_1^2 + x_2^2 - 3x_3^2 + 2x_1x_2 + 6x_1x_3 - 6x_2x_3. \end{aligned} \tag{8.107}$$

It is reasonable to ask whether a quadratic form $Q = \mathsf{x}^{\mathrm{T}} \mathsf{M} \mathsf{x}$, where M is any (possibly non-symmetric) real square matrix, is a more general definition. That this is not the case may be seen by expressing M in terms of a symmetric matrix $\mathsf{A} = \frac{1}{2}(\mathsf{M} + \mathsf{M}^{\mathrm{T}})$ and an antisymmetric matrix $\mathsf{B} = \frac{1}{2}(\mathsf{M} - \mathsf{M}^{\mathrm{T}})$ such that $\mathsf{M} = \mathsf{A} + \mathsf{B}$. We then have

$$Q = \mathsf{x}^{\mathrm{T}} \mathsf{M} \mathsf{x} = \mathsf{x}^{\mathrm{T}} \mathsf{A} \mathsf{x} + \mathsf{x}^{\mathrm{T}} \mathsf{B} \mathsf{x}. \tag{8.108}$$

However, Q is a scalar quantity and so

$$Q = Q^{\mathrm{T}} = (\mathsf{x}^{\mathrm{T}} \mathsf{A} \mathsf{x})^{\mathrm{T}} + (\mathsf{x}^{\mathrm{T}} \mathsf{B} \mathsf{x})^{\mathrm{T}} = \mathsf{x}^{\mathrm{T}} \mathsf{A}^{\mathrm{T}} \mathsf{x} + \mathsf{x}^{\mathrm{T}} \mathsf{B}^{\mathrm{T}} \mathsf{x} = \mathsf{x}^{\mathrm{T}} \mathsf{A} \mathsf{x} - \mathsf{x}^{\mathrm{T}} \mathsf{B} \mathsf{x}. \tag{8.109}$$

Comparing (8.108) and (8.109) shows that $\mathsf{x}^{\mathrm{T}} \mathsf{B} \mathsf{x} = 0$, and hence $\mathsf{x}^{\mathrm{T}} \mathsf{M} \mathsf{x} = \mathsf{x}^{\mathrm{T}} \mathsf{A} \mathsf{x}$,

i.e. Q is unchanged by considering only the symmetric part of M. Hence, with no loss of generality, we may assume $\mathsf{A} = \mathsf{A}^{\mathrm{T}}$ in (8.106).

From its definition (8.105), Q is clearly a basis- (i.e. coordinate-) independent quantity. Let us therefore consider a new basis related to the old one by an orthogonal transformation matrix S, the components in the two bases of any vector $\mathbf{x}$ being related (as in (8.91)) by $\mathsf{x} = \mathsf{S}\mathsf{x}'$ or, equivalently, by $\mathsf{x}' = \mathsf{S}^{-1}\mathsf{x} = \mathsf{S}^{\mathrm{T}}\mathsf{x}$. We then have

$$Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} = (\mathsf{x}')^{\mathrm{T}}\mathsf{S}^{\mathrm{T}}\mathsf{A}\mathsf{S}\mathsf{x}' = (\mathsf{x}')^{\mathrm{T}}\mathsf{A}'\mathsf{x}',$$

where (as expected) the matrix describing the linear operator $\mathcal{A}$ in the new basis is given by $\mathsf{A}' = \mathsf{S}^{\mathrm{T}}\mathsf{A}\mathsf{S}$ (since $\mathsf{S}^{\mathrm{T}} = \mathsf{S}^{-1}$). But, from the last section, if we choose as S the matrix whose columns are the *normalised* eigenvectors of A then $\mathsf{A}' = \mathsf{S}^{\mathrm{T}}\mathsf{A}\mathsf{S}$ is diagonal with the eigenvalues of A as the diagonal elements. (Since A is symmetric, its normalised eigenvectors are orthogonal, or can be made so, and hence S is orthogonal with $\mathsf{S}^{-1} = \mathsf{S}^{\mathrm{T}}$.)

In the new basis

$$Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} = (\mathsf{x}')^{\mathrm{T}}\Lambda\mathsf{x}' = \lambda_1 x_1'^{\,2} + \lambda_2 x_2'^{\,2} + \cdots + \lambda_N x_N'^{\,2}, \tag{8.110}$$

where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)$ and the λ_i are the eigenvalues of A. It should be noted that Q contains no cross-terms of the form $x_1'x_2'$.

►*Find an orthogonal transformation that takes the quadratic form (8.107) into the form*

$$\lambda_1 x_1'^{\,2} + \lambda_2 x_2'^{\,2} + \lambda_3 x_3'^{\,2}.$$

The required transformation matrix S has the *normalised* eigenvectors of A as its columns. We have already found these in section 8.14, and so we can write immediately

$$\mathsf{S} = \frac{1}{\sqrt{6}}\begin{pmatrix} \sqrt{3} & \sqrt{2} & 1 \\ \sqrt{3} & -\sqrt{2} & -1 \\ 0 & \sqrt{2} & -2 \end{pmatrix},$$

which is easily verified as being orthogonal. Since the eigenvalues of A are $\lambda = 2$, 3, and -6, the general result already proved shows that the transformation $\mathsf{x} = \mathsf{S}\mathsf{x}'$ will carry (8.107) into the form $2x_1'^{\,2} + 3x_2'^{\,2} - 6x_3'^{\,2}$. This may be verified most easily by writing out the inverse transformation $\mathsf{x}' = \mathsf{S}^{-1}\mathsf{x} = \mathsf{S}^{\mathrm{T}}\mathsf{x}$ and substituting. The inverse equations are

$$\begin{aligned} x_1' &= (x_1 + x_2)/\sqrt{2}, \\ x_2' &= (x_1 - x_2 + x_3)/\sqrt{3}, \\ x_3' &= (x_1 - x_2 - 2x_3)/\sqrt{6}. \end{aligned} \tag{8.111}$$

If these are substituted into the form $Q = 2x_1'^{\,2} + 3x_2'^{\,2} - 6x_3'^{\,2}$ then the original expression (8.107) is recovered. ◄

In the definition of Q it was assumed that the components x_1, x_2, x_3 and the matrix A were real. It is clear that in this case the quadratic form $Q \equiv \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}$ is real

also. Another, rather more general, expression that is also real is the *Hermitian form*

$$H(\mathsf{x}) \equiv \mathsf{x}^\dagger \mathsf{A}\mathsf{x}, \tag{8.112}$$

where A is Hermitian (i.e. $\mathsf{A}^\dagger = \mathsf{A}$) and the components of x may now be complex. It is straightforward to show that H is real, since

$$H^* = (H^{\mathrm{T}})^* = \mathsf{x}^\dagger \mathsf{A}^\dagger \mathsf{x} = \mathsf{x}^\dagger \mathsf{A}\mathsf{x} = H.$$

With suitable generalisation, the properties of quadratic forms apply also to Hermitian forms, but to keep the presentation simple we will restrict our discussion to quadratic forms.

A special case of a quadratic (Hermitian) form is one for which $Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}$ is greater than zero for all column matrices x. By choosing as the basis the eigenvectors of A we have Q in the form

$$Q = \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_3^2.$$

The requirement that $Q > 0$ for all x means that all the eigenvalues λ_i of A must be positive. A symmetric (Hermitian) matrix A with this property is called *positive definite*. If, instead, $Q \geq 0$ for all x then it is possible that some of the eigenvalues are zero, and A is called *positive semi-definite*.

8.17.1 The stationary properties of the eigenvectors

Consider a quadratic form, such as $Q(\mathbf{x}) = \langle \mathbf{x} | \mathcal{A}\,\mathbf{x} \rangle$, equation (8.105), in a fixed basis. As the vector $\mathbf{x}$ is varied, through changes in its three components x_1, x_2 and x_3, the value of the quantity Q also varies. Because of the homogeneous form of Q we may restrict any investigation of these variations to vectors of unit length (since multiplying any vector $\mathbf{x}$ by any scalar k simply multiplies the value of Q by a factor k^2).

Of particular interest are any vectors $\mathbf{x}$ that make the value of the quadratic form a maximum or minimum. A necessary, but not sufficient, condition for this is that Q is stationary with respect to small variations $\Delta\mathbf{x}$ in $\mathbf{x}$, whilst $\langle \mathbf{x} | \mathbf{x} \rangle$ is maintained at a constant value (unity).

In the chosen basis the quadratic form is given by $Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}$ and, using Lagrange undetermined multipliers to incorporate the variational constraints, we are led to seek solutions of

$$\Delta[\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} - \lambda(\mathsf{x}^{\mathrm{T}}\mathsf{x} - 1)] = 0. \tag{8.113}$$

This may be used directly, together with the fact that $(\Delta\mathsf{x}^{\mathrm{T}})\mathsf{A}\mathsf{x} = \mathsf{x}^{\mathrm{T}}\mathsf{A}\,\Delta\mathsf{x}$, since A is symmetric, to obtain

$$\mathsf{A}\mathsf{x} = \lambda\mathsf{x} \tag{8.114}$$

as the necessary condition that x must satisfy. If (8.114) is satisfied for some eigenvector x then the value of $Q(\mathsf{x})$ is given by

$$Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} = \mathsf{x}^{\mathrm{T}}\lambda\mathsf{x} = \lambda. \tag{8.115}$$

However, if x and y are eigenvectors corresponding to different eigenvalues then they are (or can be chosen to be) orthogonal. Consequently the expression $\mathsf{y}^{\mathrm{T}}\mathsf{A}\mathsf{x}$ is necessarily zero, since

$$\mathsf{y}^{\mathrm{T}}\mathsf{A}\mathsf{x} = \mathsf{y}^{\mathrm{T}}\lambda\mathsf{x} = \lambda\mathsf{y}^{\mathrm{T}}\mathsf{x} = 0. \tag{8.116}$$

Summarising, those column matrices x of unit magnitude that make the quadratic form Q stationary are eigenvectors of the matrix A, and the stationary value of Q is then equal to the corresponding eigenvalue. It is straightforward to see from the proof of (8.114) that, conversely, any eigenvector of A makes Q stationary.

Instead of maximising or minimising $Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}$ subject to the constraint $\mathsf{x}^{\mathrm{T}}\mathsf{x} = 1$, an equivalent procedure is to extremise the function

$$\lambda(\mathsf{x}) = \frac{\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}.$$

►*Show that if $\lambda(\mathsf{x})$ is stationary then x is an eigenvector of A and $\lambda(\mathsf{x})$ is equal to the corresponding eigenvalue.*

We require $\Delta\lambda(\mathsf{x}) = 0$ with respect to small variations in x. Now

$$\begin{aligned}\Delta\lambda &= \frac{1}{(\mathsf{x}^{\mathrm{T}}\mathsf{x})^2}\left[(\mathsf{x}^{\mathrm{T}}\mathsf{x})\left(\Delta\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} + \mathsf{x}^{\mathrm{T}}\mathsf{A}\,\Delta\mathsf{x}\right) - \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}\left(\Delta\mathsf{x}^{\mathrm{T}}\mathsf{x} + \mathsf{x}^{\mathrm{T}}\Delta\mathsf{x}\right)\right] \\ &= \frac{2\Delta\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}} - 2\left(\frac{\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\right)\frac{\Delta\mathsf{x}^{\mathrm{T}}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}},\end{aligned}$$

since $\mathsf{x}^{\mathrm{T}}\mathsf{A}\,\Delta\mathsf{x} = (\Delta\mathsf{x}^{\mathrm{T}})\mathsf{A}\mathsf{x}$ and $\mathsf{x}^{\mathrm{T}}\Delta\mathsf{x} = (\Delta\mathsf{x}^{\mathrm{T}})\mathsf{x}$. Thus

$$\Delta\lambda = \frac{2}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}\Delta\mathsf{x}^{\mathrm{T}}[\mathsf{A}\mathsf{x} - \lambda(\mathsf{x})\mathsf{x}].$$

Hence, if $\Delta\lambda = 0$ then $\mathsf{A}\mathsf{x} = \lambda(\mathsf{x})\mathsf{x}$, i.e. x is an eigenvector of A with eigenvalue $\lambda(\mathsf{x})$. ◄

Thus the eigenvalues of a symmetric matrix A are the values of the function

$$\lambda(\mathsf{x}) = \frac{\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}}{\mathsf{x}^{\mathrm{T}}\mathsf{x}}$$

at its stationary points. The eigenvectors of A lie along those directions in space for which the quadratic form $Q = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}$ has stationary values, given a fixed magnitude for the vector x. Similar results hold for Hermitian matrices.

8.17.2 Quadratic surfaces

The results of the previous subsection may be turned round to state that the surface given by

$$\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} = \text{constant} = 1 \text{ (say)} \tag{8.117}$$

and called a *quadratic surface*, has stationary values of its radius (i.e. origin–surface distance) in those directions that are along the eigenvectors of A. More specifically, in three dimensions the quadratic surface $\mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x} = 1$ has its principal axes along the three mutually perpendicular eigenvectors of A, and the squares of the corresponding principal radii are given by λ_i^{-1}, $i = 1, 2, 3$. As well as having this stationary property of the radius, a *principal axis* is characterised by the fact that any section of the surface perpendicular to it has some degree of symmetry about it. If the eigenvalues corresponding to any two principal axes are degenerate then the quadratic surface has rotational symmetry about the third principal axis and the choice of a pair of axes perpendicular to that axis is not uniquely defined.

►*Find the shape of the quadratic surface*

$$x_1^2 + x_2^2 - 3x_3^2 + 2x_1x_2 + 6x_1x_3 - 6x_2x_3 = 1.$$

If, instead of expressing the quadratic surface in terms of x_1, x_2, x_3, as in (8.107), we were to use the new variables x_1', x_2', x_3' defined in (8.111), for which the coordinate axes are along the three mutually perpendicular eigenvector directions $(1, 1, 0)$, $(1, -1, 1)$ and $(1, -1, -2)$, then the equation of the surface would take the form (see (8.110))

$$\frac{x_1'^{\,2}}{(1/\sqrt{2})^2} + \frac{x_2'^{\,2}}{(1/\sqrt{3})^2} - \frac{x_3'^{\,2}}{(1/\sqrt{6})^2} = 1.$$

Thus, for example, a section of the quadratic surface in the plane $x_3' = 0$, i.e. $x_1 - x_2 - 2x_3 = 0$, is an ellipse, with semi-axes $1/\sqrt{2}$ and $1/\sqrt{3}$. Similarly a section in the plane $x_1' = x_1 + x_2 = 0$ is a hyperbola. ◄

Clearly the simplest three-dimensional situation to visualise is that in which all the eigenvalues are positive, since then the quadratic surface is an ellipsoid.

8.18 Simultaneous linear equations

In physical applications we often encounter sets of simultaneous linear equations. In general we may have M equations in N unknowns $x_1, x_2, \ldots, x_N$ of the form

$$\begin{aligned} A_{11}x_1 + A_{12}x_2 + \cdots + A_{1N}x_N &= b_1, \\ A_{21}x_1 + A_{22}x_2 + \cdots + A_{2N}x_N &= b_2, \\ &\vdots \\ A_{M1}x_1 + A_{M2}x_2 + \cdots + A_{MN}x_N &= b_M, \end{aligned} \tag{8.118}$$

where the A_{ij} and b_i have known values. If all the b_i are zero then the system of equations is called *homogeneous*, otherwise it is *inhomogeneous*. Depending on the given values, this set of equations for the N unknowns $x_1, x_2, \ldots, x_N$ may have either a unique solution, no solution or infinitely many solutions. Matrix analysis may be used to distinguish between the possibilities. The set of equations may be expressed as a single matrix equation $\mathsf{A}\mathbf{x} = \mathbf{b}$, or, written out in full, as

$$\begin{pmatrix} A_{11} & A_{12} & \ldots & A_{1N} \\ A_{21} & A_{22} & \ldots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{M1} & A_{M2} & \ldots & A_{MN} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_M \end{pmatrix}.$$

8.18.1 The range and null space of a matrix

As we discussed in section 8.2, we may interpret the matrix equation $\mathsf{A}\mathbf{x} = \mathbf{b}$ as representing, in some basis, the linear transformation $\mathcal{A}\,\mathbf{x} = \mathbf{b}$ of a vector $\mathbf{x}$ in an N-dimensional vector space V into a vector $\mathbf{b}$ in some other (in general different) M-dimensional vector space W.

In general the operator $\mathcal{A}$ will map *any* vector in V into some particular *subspace* of W, which may be the entire space. This subspace is called the *range* of $\mathcal{A}$ (or A) and its dimension is equal to the *rank* of A. Moreover, if $\mathcal{A}$ (and hence A) is *singular* then there exists some subspace of V that is mapped onto the zero vector $\mathbf{0}$ in W; that is, any vector $\mathbf{y}$ that lies in the subspace satisfies $\mathcal{A}\,\mathbf{y} = \mathbf{0}$. This subspace is called the *null space* of A and the dimension of this null space is called the *nullity* of A. We note that the matrix A *must* be singular if $M \neq N$ and *may* be singular even if $M = N$.

The dimensions of the range and the null space of a matrix are related through the fundamental relationship

$$\text{rank } \mathsf{A} + \text{nullity } \mathsf{A} = N, \tag{8.119}$$

where N is the number of original unknowns $x_1, x_2, \ldots, x_N$.

►*Prove the relationship (8.119).*

As discussed in section 8.11, if the columns of an $M \times N$ matrix A are interpreted as the components, in a given basis, of N (M-component) vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ then rank A is equal to the number of linearly independent vectors in this set (this number is also equal to the dimension of the vector space spanned by these vectors). Writing (8.118) in terms of the vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$, we have

$$x_1\mathbf{v}_1 + x_2\mathbf{v}_2 + \cdots + x_N\mathbf{v}_N = \mathbf{b}. \tag{8.120}$$

From this expression, we immediately deduce that the range of A is merely the span of the vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ and hence has dimension $r = \text{rank } \mathsf{A}$.

If a vector $\mathbf{y}$ lies in the null space of A then $\mathcal{A}\,\mathbf{y} = \mathbf{0}$, which we may write as

$$y_1\mathbf{v}_1 + y_2\mathbf{v}_2 + \cdots + y_N\mathbf{v}_N = \mathbf{0}. \tag{8.121}$$

As just shown above, however, only r ($\leq N$) of these vectors are linearly independent. By renumbering, if necessary, we may assume that $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r$ form a linearly independent set; the remaining vectors, $\mathbf{v}_{r+1}, \mathbf{v}_{r+2}, \ldots, \mathbf{v}_N$, can then be written as a linear superposition of $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r$. We are therefore free to choose the $N - r$ coefficients $y_{r+1}, y_{r+2}, \ldots, y_N$ arbitrarily and (8.121) will still be satisfied for some set of r coefficients $y_1, y_2, \ldots, y_r$ (which are not all zero). The dimension of the null space is therefore $N - r$, and this completes the proof of (8.119). ◄

Equation (8.119) has far-reaching consequences for the existence of solutions to sets of simultaneous linear equations such as (8.118). As mentioned previously, these equations may have *no solution*, a *unique solution* or *infinitely many solutions*. We now discuss these three cases in turn.

No solution

The system of equations possesses no solution unless $\mathbf{b}$ lies in the range of $\mathcal{A}$; in this case (8.120) will be satisfied for some $x_1, x_2, \ldots, x_N$. This in turn requires the set of vectors $\mathbf{b}, \mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ to have the same span (see (8.8)) as $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$. In terms of matrices, this is equivalent to the requirement that the matrix A and the *augmented matrix*

$$\mathsf{M} = \begin{pmatrix} A_{11} & A_{12} & \ldots & A_{1N} & b_1 \\ A_{21} & A_{22} & \ldots & A_{2N} & b_1 \\ \vdots & & \ddots & & \vdots \\ A_{M1} & A_{M2} & \ldots & A_{MN} & b_M \end{pmatrix}$$

have the *same* rank r. If this condition is satisfied then $\mathbf{b}$ does lie in the range of $\mathcal{A}$, and the set of equations (8.118) will have either a unique solution or infinitely many solutions. If, however, A and M have different ranks then there will be no solution.

A unique solution

If $\mathbf{b}$ lies in the range of $\mathcal{A}$ and if $r = N$ then all the vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ in (8.120) are linearly independent and the equation has a *unique solution* $x_1, x_2, \ldots, x_N$.

Infinitely many solutions

If $\mathbf{b}$ lies in the range of $\mathcal{A}$ and if $r < N$ then only r of the vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ in (8.120) are linearly independent. We may therefore choose the coefficients of $n - r$ vectors in an arbitrary way, while still satisfying (8.120) for some set of coefficients $x_1, x_2, \ldots, x_N$. There are therefore *infinitely many solutions*, which span an $(n-r)$-dimensional vector space. We may also consider this space of solutions in terms of the null space of A: if $\mathbf{x}$ is some vector satisfying $\mathcal{A}\,\mathbf{x} = \mathbf{b}$ and $\mathbf{y}$ is

any vector in the null space of $\mathcal{A}$ (i.e. $\mathcal{A}\,\mathbf{y} = \mathbf{0}$) then

$$\mathcal{A}\,(\mathbf{x} + \mathbf{y}) = \mathcal{A}\,\mathbf{x} + \mathcal{A}\,\mathbf{y} = \mathcal{A}\,\mathbf{x} + \mathbf{0} = \mathbf{b},$$

and so $\mathbf{x} + \mathbf{y}$ is also a solution. Since the null space is $(n - r)$-dimensional, so too is the space of solutions.

We may use the above results to investigate the special case of the solution of a *homogeneous* set of linear equations, for which $\mathbf{b} = \mathbf{0}$. Clearly the set *always* has the trivial solution $x_1 = x_2 = \cdots = x_n = 0$, and if $r = N$ this will be the only solution. If $r < N$, however, there are infinitely many solutions; they form the null space of A, which has dimension $n - r$. In particular, we note that if $M < N$ (i.e. there are fewer equations than unknowns) then $r < N$ automatically. Hence a set of *homogeneous* linear equations with fewer equations than unknowns *always* has infinitely many solutions.

8.18.2 N simultaneous linear equations in N unknowns

A special case of (8.118) occurs when $M = N$. In this case the matrix A is *square* and we have the same number of equations as unknowns. Since A is square, the condition $r = N$ corresponds to $|\mathsf{A}| \neq 0$ and the matrix A is *non-singular*. The case $r < N$ corresponds to $|\mathsf{A}| = 0$, in which case A is *singular*.

As mentioned above, the equations will have a solution provided b lies in the range of A. If this is true then the equations will possess a unique solution when $|\mathsf{A}| \neq 0$ or infinitely many solutions when $|\mathsf{A}| = 0$. There exist several methods for obtaining the solution(s). Perhaps the most elementary method is *Gaussian elimination*; this method is discussed in subsection 27.3.1, where we also address numerical subtleties such as equation interchange (pivoting). In this subsection, we will outline three further methods for solving a square set of simultaneous linear equations.

Direct inversion

Since A is square it will possess an inverse, provided $|\mathsf{A}| \neq 0$. Thus, if A is non-singular, we immediately obtain

$$\mathsf{x} = \mathsf{A}^{-1}\mathsf{b} \tag{8.122}$$

as the unique solution to the set of equations. However, if $\mathsf{b} = \mathsf{0}$ then we see immediately that the set of equations possesses only the trivial solution $\mathsf{x} = \mathsf{0}$. The direct inversion method has the advantage that, once A^{-1} has been calculated, one may obtain the solutions x corresponding to different vectors b_1, b_2, ... on the RHS, with little further work.

►*Show that the set of simultaneous equations*

$$\begin{aligned} 2x_1 + 4x_2 + 3x_3 &= 4, \\ x_1 - 2x_2 - 2x_3 &= 0, \\ -3x_1 + 3x_2 + 2x_3 &= -7, \end{aligned} \tag{8.123}$$

has a unique solution, and find that solution.

The simultaneous equations can be represented by the matrix equation $\mathsf{A}\mathsf{x} = \mathsf{b}$, i.e.

$$\begin{pmatrix} 2 & 4 & 3 \\ 1 & -2 & -2 \\ -3 & 3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \\ -7 \end{pmatrix}.$$

As we have already shown that A^{-1} exists and have calculated it, see (8.59), it follows that $\mathsf{x} = \mathsf{A}^{-1}\mathsf{b}$ or, more explicitly, that

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \frac{1}{11} \begin{pmatrix} 2 & 1 & -2 \\ 4 & 13 & 7 \\ -3 & -18 & -8 \end{pmatrix} \begin{pmatrix} 4 \\ 0 \\ -7 \end{pmatrix} = \begin{pmatrix} 2 \\ -3 \\ 4 \end{pmatrix}. \tag{8.124}$$

Thus the unique solution is $x_1 = 2$, $x_2 = -3$, $x_3 = 4$. ◄

LU decomposition

Although conceptually simple, finding the solution by calculating A^{-1} can be computationally demanding, especially when N is large. In fact, as we shall now show, it is not necessary to perform the full inversion of A in order to solve the simultaneous equations $\mathsf{A}\mathsf{x} = \mathsf{b}$. Rather, we can perform a *decomposition* of the matrix into the product of a square *lower triangular* matrix L and a square *upper triangular* matrix U, which are such that

$$\mathsf{A} = \mathsf{L}\mathsf{U}, \tag{8.125}$$

and then use the fact that triangular systems of equations can be solved very simply.

We must begin, therefore, by finding the matrices L and U such that (8.125) is satisfied. This may be achieved straightforwardly by writing out (8.125) in component form. For illustration, let us consider the 3×3 case. It is, in fact, always possible, and convenient, to take the diagonal elements of L as unity, so we have

$$\begin{aligned} \mathsf{A} &= \begin{pmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{pmatrix} \\ &= \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ L_{21}U_{11} & L_{21}U_{12} + U_{22} & L_{21}U_{13} + U_{23} \\ L_{31}U_{11} & L_{31}U_{12} + L_{32}U_{22} & L_{31}U_{13} + L_{32}U_{23} + U_{33} \end{pmatrix} \end{aligned} \tag{8.126}$$

The nine unknown elements of L and U can now be determined by equating

the nine elements of (8.126) to those of the 3×3 matrix A. This is done in the particular order illustrated in the example below.

Once the matrices L and U have been determined, one can use the decomposition to solve the set of equations $\mathsf{Ax} = \mathsf{b}$ in the following way. From (8.125), we have $\mathsf{LUx} = \mathsf{b}$, but this can be written as *two* triangular sets of equations

$$\mathsf{Ly} = \mathsf{b} \qquad \text{and} \qquad \mathsf{Ux} = \mathsf{y},$$

where y is another column matrix to be determined. One may easily solve the first triangular set of equations for y, which is then substituted into the second set. The required solution x is then obtained readily from the second triangular set of equations. We note that, as with direct inversion, once the LU decomposition has been determined, one can solve for various RHS column matrices b_1, b_2, ..., with little extra work.

►*Use LU decomposition to solve the set of simultaneous equations (8.123).*

We begin the determination of the matrices L and U by equating the elements of the matrix in (8.126) with those of the matrix

$$\mathsf{A} = \begin{pmatrix} 2 & 4 & 3 \\ 1 & -2 & -2 \\ -3 & 3 & 2 \end{pmatrix}.$$

This is performed in the following order:

1st row:	$U_{11} = 2,$	$U_{12} = 4,$	$U_{13} = 3$
1st column:	$L_{21}U_{11} = 1,$	$L_{31}U_{11} = -3$	$\Rightarrow L_{21} = \frac{1}{2}, L_{31} = -\frac{3}{2}$
2nd row:	$L_{21}U_{12} + U_{22} = -2$	$L_{21}U_{13} + U_{23} = -2$	$\Rightarrow U_{22} = -4, U_{23} = -\frac{7}{2}$
2nd column:	$L_{31}U_{12} + L_{32}U_{22} = 3$		$\Rightarrow L_{32} = -\frac{9}{4}$
3rd row:	$L_{31}U_{13} + L_{32}U_{23} + U_{33} = 2$		$\Rightarrow U_{33} = -\frac{11}{8}$

Thus we may write the matrix A as

$$\mathsf{A} = \mathsf{LU} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ -\frac{3}{2} & -\frac{9}{4} & 1 \end{pmatrix} \begin{pmatrix} 2 & 4 & 3 \\ 0 & -4 & -\frac{7}{2} \\ 0 & 0 & -\frac{11}{8} \end{pmatrix}.$$

We must now solve the set of equations $\mathsf{Ly} = \mathsf{b}$, which read

$$\begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ -\frac{3}{2} & -\frac{9}{4} & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \\ -7 \end{pmatrix}.$$

Since this set of equations is triangular, we quickly find

$$y_1 = 4, \quad y_2 = 0 - (\tfrac{1}{2})(4) = -2, \quad y_3 = -7 - (-\tfrac{3}{2})(4) - (-\tfrac{9}{4})(-2) = -\tfrac{11}{2}.$$

These values must then be substituted into the equations $\mathsf{Ux} = \mathsf{y}$, which read

$$\begin{pmatrix} 2 & 4 & 3 \\ 0 & -4 & -\frac{7}{2} \\ 0 & 0 & -\frac{11}{8} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 4 \\ -2 \\ -\frac{11}{2} \end{pmatrix}.$$

This set of equations is also triangular, and we easily find the solution

$$x_1 = 2, \quad x_2 = -3, \quad x_3 = 4,$$

which agrees with the result found above by direct inversion. ◄

We note, in passing, that one can calculate both the inverse and the determinant of A from its LU decomposition. To find the inverse A^{-1}, one solves the system of equations $\mathsf{Ax} = \mathsf{b}$ repeatedly for the N different RHS column matrices $\mathsf{b} = \mathsf{e}_i$, $i = 1, 2, \ldots, N$, where e_i is the column matrix with its ith element equal to unity and the others equal to zero. The solution x in each case gives the corresponding column of A^{-1}. Evaluation of the determinant $|\mathsf{A}|$ is much simpler. From (8.125), we have

$$|\mathsf{A}| = |\mathsf{LU}| = |\mathsf{L}||\mathsf{U}|. \tag{8.127}$$

Since L and U are triangular, however, we see from (8.64) that their determinants are equal to the products of their diagonal elements. Since $L_{ii} = 1$ for all i, we thus find

$$|\mathsf{A}| = U_{11}U_{22}\cdots U_{NN} = \prod_{i=1}^{N} U_{ii}.$$

As an illustration, in the above example we find $|\mathsf{A}| = (2)(-4)(-11/8) = 11$, which, as it must, agrees with our earlier calculation (8.58).

Finally, we note that if the matrix A is symmetric and positive semi-definite then we can decompose it as

$$\mathsf{A} = \mathsf{LL}^{\dagger}, \tag{8.128}$$

where L is a lower triangular matrix whose diagonal elements are *not*, in general, equal to unity. This is known as a *Cholesky decomposition* (in the special case where A is real, the decomposition becomes $\mathsf{A} = \mathsf{LL}^{\mathrm{T}}$). The reason that we cannot set the diagonal elements of L equal to unity in this case is that we require the same number of independent elements in L as in A. The requirement that the matrix be positive semi-definite is easily derived by considering the Hermitian form (or quadratic form in the real case)

$$\mathsf{x}^{\dagger}\mathsf{Ax} = \mathsf{x}^{\dagger}\mathsf{LL}^{\dagger}\mathsf{x} = (\mathsf{L}^{\dagger}\mathsf{x})^{\dagger}(\mathsf{L}^{\dagger}\mathsf{x}).$$

Denoting the column matrix $\mathsf{L}^{\dagger}\mathsf{x}$ by y, we see that the last term on the RHS is $\mathsf{y}^{\dagger}\mathsf{y}$, which must be greater than or equal to zero. Thus, we require $\mathsf{x}^{\dagger}\mathsf{Ax} \geq 0$ for any arbitrary column matrix x, and so A must be positive semi-definite (see section 8.17).

We recall that the requirement that a matrix be positive semi-definite is equivalent to demanding that all the eigenvalues of A are positive or zero. If one of the eigenvalues of A is zero, however, then from (8.103) we have $|\mathsf{A}| = 0$ and so A is *singular*. Thus, if A is a non-singular matrix, it must be *positive definite* (rather

than just positive semi-definite) in order to perform the Cholesky decomposition (8.128). In fact, in this case, the inability to find a matrix L that satisfies (8.128) implies that A cannot be positive definite.

The Cholesky decomposition can be applied in an analogous way to the LU decomposition discussed above, but we shall not explore it further.

Cramer's rule

An alternative method of solution is to use *Cramer's rule*, which also provides some insight into the nature of the solutions in the various cases. To illustrate this method let us consider a set of three equations in three unknowns,

$$\begin{aligned} A_{11}x_1 + A_{12}x_2 + A_{13}x_3 &= b_1, \\ A_{21}x_1 + A_{22}x_2 + A_{23}x_3 &= b_2, \\ A_{31}x_1 + A_{32}x_2 + A_{33}x_3 &= b_3, \end{aligned} \tag{8.129}$$

which may be represented by the matrix equation $\mathsf{Ax} = \mathsf{b}$. We wish either to find the solution(s) x to these equations or to establish that there are no solutions. From result (vi) of subsection 8.9.1, the determinant $|\mathsf{A}|$ is unchanged by adding to its first column the combination

$$\frac{x_2}{x_1} \times (\text{second column of } |\mathsf{A}|) + \frac{x_3}{x_1} \times (\text{third column of } |\mathsf{A}|).$$

We thus obtain

$$|\mathsf{A}| = \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = \begin{vmatrix} A_{11} + (x_2/x_1)A_{12} + (x_3/x_1)A_{13} & A_{12} & A_{13} \\ A_{21} + (x_2/x_1)A_{22} + (x_3/x_1)A_{23} & A_{22} & A_{23} \\ A_{31} + (x_2/x_1)A_{32} + (x_3/x_1)A_{33} & A_{32} & A_{33} \end{vmatrix},$$

which, on substituting b_i/x_1 for the ith entry in the first column, yields

$$|\mathsf{A}| = \frac{1}{x_1}\begin{vmatrix} b_1 & A_{12} & A_{13} \\ b_2 & A_{22} & A_{23} \\ b_3 & A_{32} & A_{33} \end{vmatrix} = \frac{1}{x_1}\Delta_1.$$

The determinant Δ_1 is known as a *Cramer determinant*. Similar manipulations of the second and third columns of $|\mathsf{A}|$ yield x_2 and x_3, and so the full set of results reads

$$x_1 = \frac{\Delta_1}{|\mathsf{A}|}, \qquad x_2 = \frac{\Delta_2}{|\mathsf{A}|}, \qquad x_3 = \frac{\Delta_3}{|\mathsf{A}|}, \tag{8.130}$$

where

$$\Delta_1 = \begin{vmatrix} b_1 & A_{12} & A_{13} \\ b_2 & A_{22} & A_{23} \\ b_3 & A_{32} & A_{33} \end{vmatrix}, \quad \Delta_2 = \begin{vmatrix} A_{11} & b_1 & A_{13} \\ A_{21} & b_2 & A_{23} \\ A_{31} & b_3 & A_{33} \end{vmatrix}, \quad \Delta_3 = \begin{vmatrix} A_{11} & A_{12} & b_1 \\ A_{21} & A_{22} & b_2 \\ A_{31} & A_{32} & b_3 \end{vmatrix}.$$

It can be seen that each Cramer determinant Δ_i is simply $|\mathsf{A}|$ but with column i replaced by the RHS of the original set of equations. If $|\mathsf{A}| \neq 0$ then (8.130) gives

the unique solution. The proof given here appears to fail if any of the solutions x_i is zero, but it can be shown that result (8.130) is valid even in such a case.

► *Use Cramer's rule to solve the set of simultaneous equations (8.123).*

Let us again represent these simultaneous equations by the matrix equation $\mathsf{Ax} = \mathsf{b}$, i.e.

$$\begin{pmatrix} 2 & 4 & 3 \\ 1 & -2 & -2 \\ -3 & 3 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \\ -7 \end{pmatrix}.$$

From (8.58), the determinant of A is given by $|\mathsf{A}| = 11$. Following the discussion given above, the three Cramer determinants are

$$\Delta_1 = \begin{vmatrix} 4 & 4 & 3 \\ 0 & -2 & -2 \\ -7 & 3 & 2 \end{vmatrix}, \quad \Delta_2 = \begin{vmatrix} 2 & 4 & 3 \\ 1 & 0 & -2 \\ -3 & -7 & 2 \end{vmatrix}, \quad \Delta_3 = \begin{vmatrix} 2 & 4 & 4 \\ 1 & -2 & 0 \\ -3 & 3 & -7 \end{vmatrix}.$$

These may be evaluated using the properties of determinants listed in subsection 8.9.1 and we find $\Delta_1 = 22$, $\Delta_2 = -33$ and $\Delta_3 = 44$. From (8.130) the solution to the equations (8.123) is given by

$$x_1 = \frac{22}{11} = 2, \qquad x_2 = \frac{-33}{11} = -3, \qquad x_3 = \frac{44}{11} = 4,$$

which agrees with the solution found in the previous example. ◄

At this point it is useful to consider each of the three equations (8.129) as representing a plane in three-dimensional Cartesian coordinates. Using result (7.42) of chapter 7, the sets of components of the vectors normal to the planes are (A_{11}, A_{12}, A_{13}), (A_{21}, A_{22}, A_{23}) and (A_{31}, A_{32}, A_{33}), and using (7.46) the perpendicular distances of the planes from the origin are given by

$$d_i = \frac{b_i}{\left(A_{i1}^2 + A_{i2}^2 + A_{i3}^2\right)^{1/2}} \qquad \text{for } i = 1, 2, 3.$$

Finding the solution(s) to the simultaneous equations above corresponds to finding the point(s) of intersection of the planes.

If there is a unique solution the planes intersect at only a single point. This happens if their normals are linearly independent vectors. Since the rows of A represent the directions of these normals, this requirement is equivalent to $|\mathsf{A}| \neq 0$. If $\mathsf{b} = (0 \quad 0 \quad 0)^{\mathrm{T}} = \mathsf{0}$ then all the planes pass through the origin and, since there is only a single solution to the equations, the origin is that solution.

Let us now turn to the cases where $|\mathsf{A}| = 0$. The simplest such case is that in which all three planes are parallel; this implies that the normals are all parallel and so A is of rank 1. Two possibilities exist:

(i) the planes are coincident, i.e. $d_1 = d_2 = d_3$, in which case there is an infinity of solutions;
(ii) the planes are not all coincident, i.e. $d_1 \neq d_2$ and/or $d_1 \neq d_3$ and/or $d_2 \neq d_3$, in which case there are no solutions.

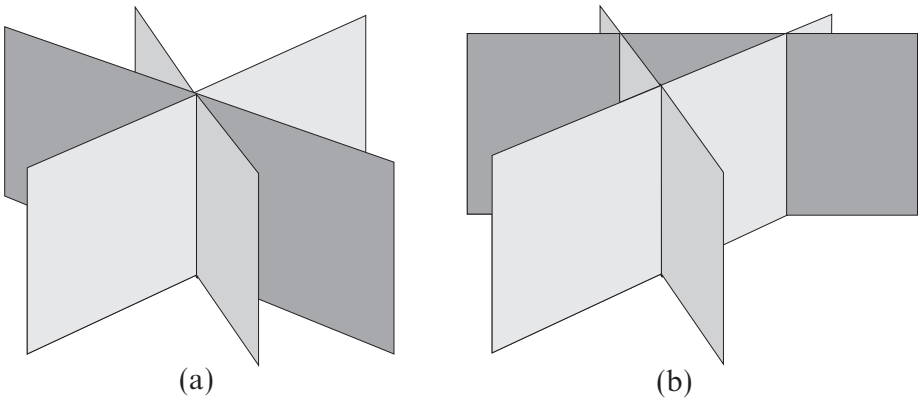

Figure 8.1 The two possible cases when A is of rank 2. In both cases all the normals lie in a horizontal plane but in (a) the planes all intersect on a single line (corresponding to an infinite number of solutions) whilst in (b) there are no common intersection points (no solutions).

It is apparent from (8.130) that case (i) occurs when all the Cramer determinants are zero and case (ii) occurs when at least one Cramer determinant is non-zero.

The most complicated cases with $|\mathsf{A}| = 0$ are those in which the normals to the planes themselves lie in a plane but are not parallel. In this case A has rank 2. Again two possibilities exist and these are shown in figure 8.1. Just as in the rank-1 case, if all the Cramer determinants are zero then we get an infinity of solutions (this time on a line). Of course, in the special case in which $\mathsf{b} = \mathsf{0}$ (and the system of equations is homogeneous), the planes all pass through the origin and so they must intersect on a line through it. If at least one of the Cramer determinants is non-zero, we get no solution.

These rules may be summarised as follows.

(i) $|\mathsf{A}| \neq 0$, $\mathsf{b} \neq \mathsf{0}$: The three planes intersect at a single point that is not the origin, and so there is only one solution, given by both (8.122) and (8.130).

(ii) $|\mathsf{A}| \neq 0$, $\mathsf{b} = \mathsf{0}$: The three planes intersect at the origin only and there is only the trivial solution, $\mathsf{x} = 0$.

(iii) $|\mathsf{A}| = 0$, $\mathsf{b} \neq \mathsf{0}$, Cramer determinants all zero: There is an infinity of solutions either on a line if A is rank 2, i.e. the cofactors are not all zero, or on a plane if A is rank 1, i.e. the cofactors are all zero.

(iv) $|\mathsf{A}| = 0$, $\mathsf{b} \neq \mathsf{0}$, Cramer determinants not all zero: No solutions.

(v) $|\mathsf{A}| = 0$, $\mathsf{b} = \mathsf{0}$: The three planes intersect on a line through the origin giving an infinity of solutions.

8.18.3 Singular value decomposition

There exists a very powerful technique for dealing with a simultaneous set of linear equations $\mathsf{Ax} = \mathsf{b}$, such as (8.118), which may be applied *whether or not*

the number of simultaneous equations M is equal to the number of unknowns N. This technique is known as *singular value decomposition* (SVD) and is the method of choice in analysing *any* set of simultaneous linear equations.

We will consider the general case, in which A is an $M \times N$ (complex) matrix. Let us suppose we can write A as the product[§]

$$\mathsf{A} = \mathsf{USV}^\dagger, \tag{8.131}$$

where the matrices U, S and V have the following properties.

(i) The square matrix U has dimensions $M \times M$ and is *unitary*.
(ii) The matrix S has dimensions $M \times N$ (the same dimensions as those of A) and is *diagonal* in the sense that $S_{ij} = 0$ if $i \neq j$. We denote its diagonal elements by s_i for $i = 1, 2, \ldots, p$, where $p = \min(M, N)$; these elements are termed the *singular values* of A.
(iii) The square matrix V has dimensions $N \times N$ and is *unitary*.

We must now determine the elements of these matrices in terms of the elements of A. From the matrix A, we can construct two square matrices: $\mathsf{A}^\dagger\mathsf{A}$ with dimensions $N \times N$ and $\mathsf{AA}^\dagger$ with dimensions $M \times M$. Both are clearly *Hermitian*. From (8.131), and using the fact that U and V are unitary, we find

$$\mathsf{A}^\dagger\mathsf{A} = \mathsf{VS}^\dagger\mathsf{U}^\dagger\mathsf{USV}^\dagger = \mathsf{VS}^\dagger\mathsf{SV}^\dagger \tag{8.132}$$

$$\mathsf{AA}^\dagger = \mathsf{USV}^\dagger\mathsf{VS}^\dagger\mathsf{U}^\dagger = \mathsf{USS}^\dagger\mathsf{U}^\dagger, \tag{8.133}$$

where $\mathsf{S}^\dagger\mathsf{S}$ and $\mathsf{SS}^\dagger$ are diagonal matrices with dimensions $N \times N$ and $M \times M$ respectively. The first p elements of each diagonal matrix are s_i^2, $i = 1, 2, \ldots, p$, where $p = \min(M, N)$, and the rest (where they exist) are zero.

These two equations imply that both $\mathsf{V}^{-1}\mathsf{A}^\dagger\mathsf{AV}$ $\left(= \mathsf{V}^{-1}\mathsf{A}^\dagger\mathsf{A}(\mathsf{V}^\dagger)^{-1}\right)$ and, by a similar argument, $\mathsf{U}^{-1}\mathsf{AA}^\dagger\mathsf{U}$, must be diagonal. From our discussion of the diagonalisation of Hermitian matrices in section 8.16, we see that the columns of V must therefore be the normalised eigenvectors v^i, $i = 1, 2, \ldots, N$, of the matrix $\mathsf{A}^\dagger\mathsf{A}$ and the columns of U must be the normalised eigenvectors u^j, $j = 1, 2, \ldots, M$, of the matrix $\mathsf{AA}^\dagger$. Moreover, the singular values s_i must satisfy $s_i^2 = \lambda_i$, where the λ_i are the eigenvalues of the smaller of $\mathsf{A}^\dagger\mathsf{A}$ and $\mathsf{AA}^\dagger$. Clearly, the λ_i are also some of the eigenvalues of the larger of these two matrices, the remaining ones being equal to zero. Since each matrix is Hermitian, the λ_i are real and the singular values s_i may be taken as real and non-negative. Finally, to make the decomposition (8.131) unique, it is customary to arrange the singular values in decreasing order of their values, so that $s_1 \geq s_2 \geq \cdots \geq s_p$.

[§] The proof that such a decomposition always exists is beyond the scope of this book. For a full account of SVD one might consult, for example, G. H. Golub and C. F. Van Loan, *Matrix Computations*, 3rd edn (Baltimore MD: Johns Hopkins University Press, 1996).

►*Show that, for* $i = 1, 2, \ldots, p$, $\mathsf{A}\mathsf{v}^i = s_i\mathsf{u}^i$ *and* $\mathsf{A}^\dagger\mathsf{u}^i = s_i\mathsf{v}^i$, *where* $p = \min(M, N)$.

Post-multiplying both sides of (8.131) by V, and using the fact that V is unitary, we obtain

$$\mathsf{A}\mathsf{V} = \mathsf{U}\mathsf{S}.$$

Since the columns of V and U consist of the vectors v^i and u^j respectively and S has only diagonal non-zero elements, we find immediately that, for $i = 1, 2, \ldots, p$,

$$\mathsf{A}\mathsf{v}^i = s_i\mathsf{u}^i. \tag{8.134}$$

Moreover, we note that $\mathsf{A}\mathsf{v}^i = 0$ for $i = p+1, p+2, \ldots, N$.

Taking the Hermitian conjugate of both sides of (8.131) and post-multiplying by U, we obtain

$$\mathsf{A}^\dagger\mathsf{U} = \mathsf{V}\mathsf{S}^\dagger = \mathsf{V}\mathsf{S}^{\mathrm{T}},$$

where we have used the fact that U is unitary and S is real. We then see immediately that, for $i = 1, 2, \ldots, p$,

$$\mathsf{A}^\dagger\mathsf{u}^i = s_i\mathsf{v}^i. \tag{8.135}$$

We also note that $\mathsf{A}^\dagger\mathsf{u}^i = 0$ for $i = p+1, p+2, \ldots, M$. Results (8.134) and (8.135) are useful for investigating the properties of the SVD. ◄

The decomposition (8.131) has some advantageous features for the analysis of sets of simultaneous linear equations. These are best illustrated by writing the decomposition (8.131) in terms of the vectors u^i and v^i as

$$\mathsf{A} = \sum_{i=1}^{p} s_i\mathsf{u}^i(\mathsf{v}^i)^\dagger,$$

where $p = \min(M, N)$. It may be, however, that some of the singular values s_i are *zero*, as a result of degeneracies in the set of M linear equations $\mathsf{A}\mathsf{x} = \mathsf{b}$. Let us suppose that there are r non-zero singular values. Since our convention is to arrange the singular values in order of decreasing size, the non-zero singular values are s_i, $i = 1, 2, \ldots, r$, and the zero singular values are $s_{r+1}, s_{r+2}, \ldots, s_p$. Therefore we can write A as

$$\mathsf{A} = \sum_{i=1}^{r} s_i\mathsf{u}^i(\mathsf{v}^i)^\dagger. \tag{8.136}$$

Let us consider the action of (8.136) on an arbitrary vector x. This is given by

$$\mathsf{A}\mathsf{x} = \sum_{i=1}^{r} s_i\mathsf{u}^i(\mathsf{v}^i)^\dagger\mathsf{x}.$$

Since $(\mathsf{v}^i)^\dagger\mathsf{x}$ is just a number, we see immediately that the vectors u^i, $i = 1, 2, \ldots, r$, must span the *range* of the matrix A; moreover, these vectors form an orthonormal basis for the range. Further, since this subspace is r-dimensional, we have rank $\mathsf{A} = r$, i.e. the rank of A is equal to the number of non-zero singular values.

The SVD is also useful in characterising the null space of A. From (8.119), we already know that the null space must have dimension $N - r$; so, if A has r

non-zero singular values s_i, $i = 1, 2, \ldots, r$, then from the worked example above we have

$$\mathsf{A}\mathsf{v}^i = 0 \qquad \text{for } i = r+1, r+2, \ldots, N.$$

Thus, the $N - r$ vectors v^i, $i = r+1, r+2, \ldots, N$, form an orthonormal basis for the null space of A.

► *Find the singular value decompostion of the matrix*

$$\mathsf{A} = \begin{pmatrix} 2 & 2 & 2 & 2 \\ \frac{17}{10} & \frac{1}{10} & -\frac{17}{10} & -\frac{1}{10} \\ \frac{3}{5} & \frac{9}{5} & -\frac{3}{5} & -\frac{9}{5} \end{pmatrix}. \tag{8.137}$$

The matrix A has dimension 3×4 (i.e. $M = 3$, $N = 4$), and so we may construct from it the 3×3 matrix $\mathsf{A}\mathsf{A}^\dagger$ and the 4×4 matrix $\mathsf{A}^\dagger\mathsf{A}$ (in fact, since A is real, the Hermitian conjugates are just transposes). We begin by finding the eigenvalues λ_i and eigenvectors u^i of the smaller matrix $\mathsf{A}\mathsf{A}^\dagger$. This matrix is easily found to be given by

$$\mathsf{A}\mathsf{A}^\dagger = \begin{pmatrix} 16 & 0 & 0 \\ 0 & \frac{29}{5} & \frac{12}{5} \\ 0 & \frac{12}{5} & \frac{36}{5} \end{pmatrix},$$

and its characteristic equation reads

$$\begin{vmatrix} 16-\lambda & 0 & 0 \\ 0 & \frac{29}{5}-\lambda & \frac{12}{5} \\ 0 & \frac{12}{5} & \frac{36}{5}-\lambda \end{vmatrix} = (16-\lambda)(36 - 13\lambda + \lambda^2) = 0.$$

Thus, the eigenvalues are $\lambda_1 = 16$, $\lambda_2 = 9$, $\lambda_3 = 4$. Since the singular values of A are given by $s_i = \sqrt{\lambda_i}$ and the matrix S in (8.131) has the same dimensions as A, we have

$$\mathsf{S} = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}, \tag{8.138}$$

where we have arranged the singular values in order of decreasing size. Now the matrix U has as its columns the normalised eigenvectors u^i of the 3×3 matrix $\mathsf{A}\mathsf{A}^\dagger$. These normalised eigenvectors correspond to the eigenvalues of $\mathsf{A}\mathsf{A}^\dagger$ as follows:

$$\begin{aligned} \lambda_1 = 16 \quad &\Rightarrow \quad \mathsf{u}^1 = (1 \quad 0 \quad 0)^{\mathrm{T}} \\ \lambda_2 = 9 \quad &\Rightarrow \quad \mathsf{u}^2 = (0 \quad \tfrac{3}{5} \quad \tfrac{4}{5})^{\mathrm{T}} \\ \lambda_3 = 4 \quad &\Rightarrow \quad \mathsf{u}^3 = (0 \quad -\tfrac{4}{5} \quad \tfrac{3}{5})^{\mathrm{T}}, \end{aligned}$$

and so we obtain the matrix

$$\mathsf{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{3}{5} & -\frac{4}{5} \\ 0 & \frac{4}{5} & \frac{3}{5} \end{pmatrix}. \tag{8.139}$$

The columns of the matrix V in (8.131) are the normalised eigenvectors of the 4×4 matrix $\mathsf{A}^\dagger\mathsf{A}$, which is given by

$$\mathsf{A}^\dagger\mathsf{A} = \frac{1}{4}\begin{pmatrix} 29 & 21 & 3 & 11 \\ 21 & 29 & 11 & 3 \\ 3 & 11 & 29 & 21 \\ 11 & 3 & 21 & 29 \end{pmatrix}.$$

We already know from the above discussion, however, that the non-zero eigenvalues of this matrix are *equal* to those of $\mathsf{A}\mathsf{A}^\dagger$ found above, and that the remaining eigenvalue is *zero*. The corresponding normalised eigenvectors are easily found:

$$\begin{aligned}
\lambda_1 = 16 \quad &\Rightarrow \quad \mathsf{v}^1 = \tfrac{1}{2}(1 \quad 1 \quad 1 \quad 1)^{\mathrm{T}} \\
\lambda_2 = 9 \quad &\Rightarrow \quad \mathsf{v}^2 = \tfrac{1}{2}(1 \quad 1 \quad -1 \quad -1)^{\mathrm{T}} \\
\lambda_3 = 4 \quad &\Rightarrow \quad \mathsf{v}^3 = \tfrac{1}{2}(-1 \quad 1 \quad 1 \quad -1)^{\mathrm{T}} \\
\lambda_4 = 0 \quad &\Rightarrow \quad \mathsf{v}^4 = \tfrac{1}{2}(1 \quad -1 \quad 1 \quad -1)^{\mathrm{T}}
\end{aligned}$$

and so the matrix V is given by

$$\mathsf{V} = \frac{1}{2}\begin{pmatrix} 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 \end{pmatrix}. \tag{8.140}$$

Alternatively, we could have found the first three columns of V by using the relation (8.135) to obtain

$$\mathsf{v}^i = \frac{1}{s_i}\mathsf{A}^\dagger \mathsf{u}^i \qquad \text{for } i = 1, 2, 3.$$

The fourth eigenvector could then be found using the Gram–Schmidt orthogonalisation procedure. We note that if there were more than one eigenvector corresponding to a zero eigenvalue then we would need to use this procedure to orthogonalise these eigenvectors before constructing the matrix V.

Collecting our results together, we find the SVD of the matrix A:

$$\mathsf{A} = \mathsf{U}\mathsf{S}\mathsf{V}^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{3}{5} & -\frac{4}{5} \\ 0 & \frac{4}{5} & \frac{3}{5} \end{pmatrix} \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix};$$

this can be verified by direct multiplication. ◄

Let us now consider the use of SVD in solving a set of M simultaneous linear equations in N unknowns, which we write again as $\mathsf{A}\mathsf{x} = \mathsf{b}$. Firstly, consider the solution of a homogeneous set of equations, for which $\mathsf{b} = \mathsf{0}$. As mentioned previously, if A is square and non-singular (and so possesses no zero singular values) then the equations have the unique trivial solution $\mathsf{x} = \mathsf{0}$. Otherwise, *any* of the vectors v^i, $i = r+1, r+2, \ldots, N$, or any linear combination of them, will be a solution.

In the inhomogeneous case, where b is not a zero vector, the set of equations will possess solutions if b lies in the range of A. To investigate these solutions, it is convenient to introduce the $N \times M$ matrix $\overline{\mathsf{S}}$, which is constructed by taking the transpose of S in (8.131) and replacing each non-zero singular value s_i on the diagonal by $1/s_i$. It is clear that, with this construction, $\mathsf{S}\overline{\mathsf{S}}$ is an $M \times M$ diagonal matrix with diagonal entries that equal unity for those values of j for which $s_j \neq 0$, and zero otherwise.

Now consider the vector

$$\hat{\mathsf{x}} = \mathsf{V}\overline{\mathsf{S}}\mathsf{U}^\dagger \mathsf{b}. \tag{8.141}$$

Using the unitarity of the matrices U and V, we find that

$$\mathsf{A}\hat{\mathsf{x}} - \mathsf{b} = \mathsf{U}\mathsf{S}\overline{\mathsf{S}}\mathsf{U}^\dagger\mathsf{b} - \mathsf{b} = \mathsf{U}(\mathsf{S}\overline{\mathsf{S}} - \mathsf{I})\mathsf{U}^\dagger\mathsf{b}. \tag{8.142}$$

The matrix $(\mathsf{S}\overline{\mathsf{S}} - \mathsf{I})$ is diagonal and the jth element on its leading diagonal is non-zero (and equal to -1) only when $s_j = 0$. However, the jth element of the vector $\mathsf{U}^\dagger\mathsf{b}$ is given by the scalar product $(\mathsf{u}^j)^\dagger\mathsf{b}$; if b lies in the range of A, this scalar product can be non-zero only if $s_j \neq 0$. Thus the RHS of (8.142) must equal zero, and so $\hat{\mathsf{x}}$ given by (8.141) is a solution to the equations $\mathsf{A}\mathsf{x} = \mathsf{b}$. We may, however, add to this solution *any* linear combination of the $N - r$ vectors v^i, $i = r+1, r+2, \ldots, N$, that form an orthonormal basis for the null space of A; thus, in general, there exists an infinity of solutions (although it is straightforward to show that (8.141) is the solution vector of shortest length). The only way in which the solution (8.141) can be *unique* is if the rank r equals N, so that the matrix A does not possess a null space; this only occurs if A is square and non-singular.

If b does not lie in the range of A then the set of equations $\mathsf{A}\mathsf{x} = \mathsf{b}$ does not have a solution. Nevertheless, the vector (8.141) provides the closest possible 'solution' in a least-squares sense. In other words, although the vector (8.141) does not exactly solve $\mathsf{A}\mathsf{x} = \mathsf{b}$, it is the vector that minimises the *residual*

$$\epsilon = |\mathsf{A}\mathsf{x} - \mathsf{b}|,$$

where here the vertical lines denote the absolute value of the quantity they contain, not the determinant. This is proved as follows.

Suppose we were to add some arbitrary vector x' to the vector $\hat{\mathsf{x}}$ in (8.141). This would result in the addition of the vector $\mathsf{b}' = \mathsf{A}\mathsf{x}'$ to $\mathsf{A}\hat{\mathsf{x}} - \mathsf{b}$; b' is clearly in the range of A since any part of x' belonging to the null space of A contributes nothing to $\mathsf{A}\mathsf{x}'$. We would then have

$$\begin{aligned} |\mathsf{A}\hat{\mathsf{x}} - \mathsf{b} + \mathsf{b}'| &= |(\mathsf{U}\mathsf{S}\overline{\mathsf{S}}\mathsf{U}^\dagger - \mathsf{I})\mathsf{b} + \mathsf{b}'| \\ &= |\mathsf{U}[(\mathsf{S}\overline{\mathsf{S}} - \mathsf{I})\mathsf{U}^\dagger\mathsf{b} + \mathsf{U}^\dagger\mathsf{b}']| \\ &= |(\mathsf{S}\overline{\mathsf{S}} - \mathsf{I})\mathsf{U}^\dagger\mathsf{b} + \mathsf{U}^\dagger\mathsf{b}'|; \end{aligned} \tag{8.143}$$

in the last line we have made use of the fact that the length of a vector is left unchanged by the action of the unitary matrix U. Now, the jth component of the vector $(\mathsf{S}\overline{\mathsf{S}} - \mathsf{I})\mathsf{U}^\dagger\mathsf{b}$ will only be non-zero when $s_j = 0$. However, the jth element of the vector $\mathsf{U}^\dagger\mathsf{b}'$ is given by the scalar product $(\mathsf{u}^j)^\dagger\mathsf{b}'$, which is non-zero only if $s_j \neq 0$, since b' lies in the range of A. Thus, as these two terms only contribute to (8.143) for two disjoint sets of j-values, its minimum value, as x' is varied, occurs when $\mathsf{b}' = \mathsf{0}$; this requires $\mathsf{x}' = \mathsf{0}$.

►*Find the solution(s) to the set of simultaneous linear equations* $\mathsf{A}\mathsf{x} = \mathsf{b}$*, where* A *is given by (8.137) and* $\mathsf{b} = (1 \quad 0 \quad 0)^{\mathrm{T}}$.

To solve the set of equations, we begin by calculating the vector given in (8.141),

$$\mathsf{x} = \mathsf{V}\overline{\mathsf{S}}\mathsf{U}^\dagger\mathsf{b},$$

where U and V are given by (8.139) and (8.140) respectively and $\overline{\mathsf{S}}$ is obtained by taking the transpose of S in (8.138) and replacing all the non-zero singular values s_i by $1/s_i$. Thus, $\overline{\mathsf{S}}$ reads

$$\overline{\mathsf{S}} = \begin{pmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 \end{pmatrix}.$$

Substituting the appropriate matrices into the expression for x we find

$$\mathsf{x} = \tfrac{1}{8}(1 \quad 1 \quad 1 \quad 1)^{\mathrm{T}}. \tag{8.144}$$

It is straightforward to show that this solves the set of equations $\mathsf{Ax} = \mathsf{b}$ exactly, and so the vector $\mathsf{b} = (1 \quad 0 \quad 0)^{\mathrm{T}}$ must lie in the range of A. This is, in fact, immediately clear, since $\mathsf{b} = \mathsf{u}^1$. The solution (8.144) is *not*, however, unique. There are three non-zero singular values, but $N = 4$. Thus, the matrix A has a one-dimensional null space, which is 'spanned' by v^4, the fourth column of V, given in (8.140). The solutions to our set of equations, consisting of the sum of the exact solution and *any* vector in the null space of A, therefore lie along the line

$$\mathsf{x} = \tfrac{1}{8}(1 \quad 1 \quad 1 \quad 1)^{\mathrm{T}} + \alpha(1 \quad -1 \quad 1 \quad -1)^{\mathrm{T}},$$

where the parameter α can take any real value. We note that (8.144) is the point on this line that is closest to the origin. ◄

8.19 Exercises

8.1 Which of the following statements about linear vector spaces are true? Where a statement is false, give a counter-example to demonstrate this.

(a) Non-singular $N \times N$ matrices form a vector space of dimension N^2.
(b) Singular $N \times N$ matrices form a vector space of dimension N^2.
(c) Complex numbers form a vector space of dimension 2.
(d) Polynomial functions of x form an infinite-dimensional vector space.
(e) Series $\{a_0, a_1, a_2, \ldots, a_N\}$ for which $\sum_{n=0}^{N} |a_n|^2 = 1$ form an N-dimensional vector space.
(f) Absolutely convergent series form an infinite-dimensional vector space.
(g) Convergent series with terms of alternating sign form an infinite-dimensional vector space.

8.2 Evaluate the determinants

$$\text{(a)} \begin{vmatrix} a & h & g \\ h & b & f \\ g & f & c \end{vmatrix}, \qquad \text{(b)} \begin{vmatrix} 1 & 0 & 2 & 3 \\ 0 & 1 & -2 & 1 \\ 3 & -3 & 4 & -2 \\ -2 & 1 & -2 & 1 \end{vmatrix}$$

and

$$\text{(c)} \begin{vmatrix} gc & ge & a+ge & gb+ge \\ 0 & b & b & b \\ c & e & e & b+e \\ a & b & b+f & b+d \end{vmatrix}.$$

8.3 Using the properties of determinants, solve with a minimum of calculation the following equations for x:

$$\text{(a)}\ \begin{vmatrix} x & a & a & 1 \\ a & x & b & 1 \\ a & b & x & 1 \\ a & b & c & 1 \end{vmatrix} = 0, \qquad \text{(b)}\ \begin{vmatrix} x+2 & x+4 & x-3 \\ x+3 & x & x+5 \\ x-2 & x-1 & x+1 \end{vmatrix} = 0.$$

8.4 Consider the matrices

$$\text{(a)}\ \mathsf{B} = \begin{pmatrix} 0 & -i & i \\ i & 0 & -i \\ -i & i & 0 \end{pmatrix}, \qquad \text{(b)}\ \mathsf{C} = \frac{1}{\sqrt{8}} \begin{pmatrix} \sqrt{3} & -\sqrt{2} & -\sqrt{3} \\ 1 & \sqrt{6} & -1 \\ 2 & 0 & 2 \end{pmatrix}.$$

Are they (i) real, (ii) diagonal, (iii) symmetric, (iv) antisymmetric, (v) singular, (vi) orthogonal, (vii) Hermitian, (viii) anti-Hermitian, (ix) unitary, (x) normal?

8.5 By considering the matrices

$$\mathsf{A} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \mathsf{B} = \begin{pmatrix} 0 & 0 \\ 3 & 4 \end{pmatrix},$$

show that $\mathsf{AB} = \mathsf{0}$ does *not* imply that either A or B is the zero matrix, but that it does imply that at least one of them is singular.

8.6 This exercise considers a crystal whose unit cell has base vectors that are not necessarily mutually orthogonal.

(a) The basis vectors of the unit cell of a crystal, with the origin O at one corner, are denoted by $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$. The matrix G has elements G_{ij}, where $G_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ and H_{ij} are the elements of the matrix $\mathsf{H} \equiv \mathsf{G}^{-1}$. Show that the vectors $\mathbf{f}_i = \sum_j H_{ij}\mathbf{e}_j$ are the reciprocal vectors and that $H_{ij} = \mathbf{f}_i \cdot \mathbf{f}_j$.

(b) If the vectors $\mathbf{u}$ and $\mathbf{v}$ are given by

$$\mathbf{u} = \sum_i u_i \mathbf{e}_i, \qquad \mathbf{v} = \sum_i v_i \mathbf{f}_i,$$

obtain expressions for $|\mathbf{u}|$, $|\mathbf{v}|$, and $\mathbf{u} \cdot \mathbf{v}$.

(c) If the basis vectors are each of length a and the angle between each pair is $\pi/3$, write down G and hence obtain H.

(d) Calculate (i) the length of the normal from O onto the plane containing the points $p^{-1}\mathbf{e}_1$, $q^{-1}\mathbf{e}_2$, $r^{-1}\mathbf{e}_3$, and (ii) the angle between this normal and $\mathbf{e}_1$.

8.7 Prove the following results involving Hermitian matrices:

(a) If A is Hermitian and U is unitary then $\mathsf{U}^{-1}\mathsf{AU}$ is Hermitian.

(b) If A is anti-Hermitian then $i\mathsf{A}$ is Hermitian.

(c) The product of two Hermitian matrices A and B is Hermitian if and only if A and B commute.

(d) If S is a real antisymmetric matrix then $\mathsf{A} = (\mathsf{I} - \mathsf{S})(\mathsf{I} + \mathsf{S})^{-1}$ is orthogonal. If A is given by

$$\mathsf{A} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

then find the matrix S that is needed to express A in the above form.

(e) If K is skew-hermitian, i.e. $\mathsf{K}^\dagger = -\mathsf{K}$, then $\mathsf{V} = (\mathsf{I} + \mathsf{K})(\mathsf{I} - \mathsf{K})^{-1}$ is unitary.

8.8 A and B are real non-zero 3×3 matrices and satisfy the equation

$$(\mathsf{AB})^{\mathrm{T}} + \mathsf{B}^{-1}\mathsf{A} = \mathsf{0}.$$

(a) Prove that if B is orthogonal then A is antisymmetric.

(b) Without assuming that B is orthogonal, prove that A is singular.

8.9 The *commutator* $[\mathsf{X},\mathsf{Y}]$ of two matrices is defined by the equation

$$[\mathsf{X},\mathsf{Y}] = \mathsf{XY} - \mathsf{YX}.$$

Two anticommuting matrices A and B satisfy

$$\mathsf{A}^2 = \mathsf{I}, \qquad \mathsf{B}^2 = \mathsf{I}, \qquad [\mathsf{A},\mathsf{B}] = 2i\mathsf{C}.$$

(a) Prove that $\mathsf{C}^2 = \mathsf{I}$ and that $[\mathsf{B},\mathsf{C}] = 2i\mathsf{A}$.

(b) Evaluate $[[[\mathsf{A},\mathsf{B}],[\mathsf{B},\mathsf{C}]],[\mathsf{A},\mathsf{B}]]$.

8.10 The four matrices S_x, S_y, S_z and I are defined by

$$\mathsf{S}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \mathsf{S}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$
$$\mathsf{S}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \mathsf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

where $i^2 = -1$. Show that $\mathsf{S}_x^2 = \mathsf{I}$ and $\mathsf{S}_x\mathsf{S}_y = i\mathsf{S}_z$, and obtain similar results by permutting x, y and z. Given that $\mathbf{v}$ is a vector with Cartesian components (v_x, v_y, v_z), the matrix $\mathsf{S}(\mathbf{v})$ is defined as

$$\mathsf{S}(\mathbf{v}) = v_x\mathsf{S}_x + v_y\mathsf{S}_y + v_z\mathsf{S}_z.$$

Prove that, for general non-zero vectors $\mathbf{a}$ and $\mathbf{b}$,

$$\mathsf{S}(\mathbf{a})\mathsf{S}(\mathbf{b}) = \mathbf{a}\cdot\mathbf{b}\,\mathsf{I} + i\,\mathsf{S}(\mathbf{a}\times\mathbf{b}).$$

Without further calculation, deduce that $\mathsf{S}(\mathbf{a})$ and $\mathsf{S}(\mathbf{b})$ commute if and only if $\mathbf{a}$ and $\mathbf{b}$ are parallel vectors.

8.11 A general triangle has angles α, β and γ and corresponding opposite sides a, b and c. Express the length of each side in terms of the lengths of the other two sides and the relevant cosines, writing the relationships in matrix and vector form, using the vectors having components a, b, c and $\cos\alpha, \cos\beta, \cos\gamma$. Invert the matrix and hence deduce the cosine-law expressions involving α, β and γ.

8.12 Given a matrix

$$\mathsf{A} = \begin{pmatrix} 1 & \alpha & 0 \\ \beta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

where α and β are non-zero complex numbers, find its eigenvalues and eigenvectors. Find the respective conditions for (a) the eigenvalues to be real and (b) the eigenvectors to be orthogonal. Show that the conditions are jointly satisfied if and only if A is Hermitian.

8.13 Using the Gram–Schmidt procedure:

(a) construct an orthonormal set of vectors from the following:

$$\mathsf{x}_1 = (0 \quad 0 \quad 1 \quad 1)^{\mathrm{T}}, \qquad \mathsf{x}_2 = (1 \quad 0 \quad -1 \quad 0)^{\mathrm{T}},$$
$$\mathsf{x}_3 = (1 \quad 2 \quad 0 \quad 2)^{\mathrm{T}}, \qquad \mathsf{x}_4 = (2 \quad 1 \quad 1 \quad 1)^{\mathrm{T}};$$

(b) find an orthonormal basis, within a four-dimensional Euclidean space, for the subspace spanned by the three vectors $(1 \quad 2 \quad 0 \quad 0)^{\mathrm{T}}$, $(3 \quad -1 \quad 2 \quad 0)^{\mathrm{T}}$ and $(0 \quad 0 \quad 2 \quad 1)^{\mathrm{T}}$.

8.14 If a unitary matrix U is written as $\mathsf{A} + i\mathsf{B}$, where A and B are Hermitian with non-degenerate eigenvalues, show the following:

(a) A and B commute;
(b) $\mathsf{A}^2 + \mathsf{B}^2 = \mathsf{I}$;
(c) The eigenvectors of A are also eigenvectors of B;
(d) The eigenvalues of U have unit modulus (as is necessary for any unitary matrix).

8.15 Determine which of the matrices below are mutually commuting, and, for those that are, demonstrate that they have a complete set of eigenvectors in common:

$$\mathsf{A} = \begin{pmatrix} 6 & -2 \\ -2 & 9 \end{pmatrix}, \qquad \mathsf{B} = \begin{pmatrix} 1 & 8 \\ 8 & -11 \end{pmatrix},$$
$$\mathsf{C} = \begin{pmatrix} -9 & -10 \\ -10 & 5 \end{pmatrix}, \quad \mathsf{D} = \begin{pmatrix} 14 & 2 \\ 2 & 11 \end{pmatrix}.$$

8.16 Find the eigenvalues and a set of eigenvectors of the matrix

$$\begin{pmatrix} 1 & 3 & -1 \\ 3 & 4 & -2 \\ -1 & -2 & 2 \end{pmatrix}.$$

Verify that its eigenvectors are mutually orthogonal.

8.17 Find three real orthogonal column matrices, each of which is a simultaneous eigenvector of

$$\mathsf{A} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \text{and} \qquad \mathsf{B} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

8.18 Use the results of the first worked example in section 8.14 to evaluate, without repeated matrix multiplication, the expression $\mathsf{A}^6\mathsf{x}$, where $\mathsf{x} = (2 \quad 4 \quad -1)^{\mathrm{T}}$ and A is the matrix given in the example.

8.19 Given that A is a real symmetric matrix with normalised eigenvectors e^i, obtain the coefficients α_i involved when column matrix x, which is the solution of

$$\mathsf{A}\mathsf{x} - \mu\mathsf{x} = \mathsf{v}, \qquad (*)$$

is expanded as $\mathsf{x} = \sum_i \alpha_i \mathsf{e}^i$. Here μ is a given constant and v is a given column matrix.

(a) Solve $(*)$ when

$$\mathsf{A} = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix},$$

$\mu = 2$ and $\mathsf{v} = (1 \quad 2 \quad 3)^{\mathrm{T}}$.

(b) Would $(*)$ have a solution if $\mu = 1$ and (i) $\mathsf{v} = (1 \quad 2 \quad 3)^{\mathrm{T}}$, (ii) $\mathsf{v} = (2 \quad 2 \quad 3)^{\mathrm{T}}$?

8.20 Demonstrate that the matrix

$$\mathsf{A} = \begin{pmatrix} 2 & 0 & 0 \\ -6 & 4 & 4 \\ 3 & -1 & 0 \end{pmatrix}$$

is defective, i.e. does not have three linearly independent eigenvectors, by showing the following:

(a) its eigenvalues are degenerate and, in fact, all equal;
(b) any eigenvector has the form $(\mu \quad (3\mu - 2v) \quad v)^{\mathrm{T}}$.
(c) if two pairs of values, μ_1, v_1 and μ_2, v_2, define two independent eigenvectors v_1 and v_2, then *any* third similarly defined eigenvector v_3 can be written as a linear combination of v_1 and v_2, i.e.

$$\mathsf{v}_3 = a\mathsf{v}_1 + b\mathsf{v}_2,$$

where

$$a = \frac{\mu_3 v_2 - \mu_2 v_3}{\mu_1 v_2 - \mu_2 v_1} \quad \text{and} \quad b = \frac{\mu_1 v_3 - \mu_3 v_1}{\mu_1 v_2 - \mu_2 v_1}.$$

Illustrate (c) using the example $(\mu_1, v_1) = (1, 1)$, $(\mu_2, v_2) = (1, 2)$ and $(\mu_3, v_3) = (0, 1)$.

Show further that any matrix of the form

$$\begin{pmatrix} 2 & 0 & 0 \\ 6n-6 & 4-2n & 4-4n \\ 3-3n & n-1 & 2n \end{pmatrix}$$

is defective, with the same eigenvalues and eigenvectors as A.

8.21 By finding the eigenvectors of the Hermitian matrix

$$\mathsf{H} = \begin{pmatrix} 10 & 3i \\ -3i & 2 \end{pmatrix},$$

construct a unitary matrix U such that $\mathsf{U}^{\dagger}\mathsf{H}\mathsf{U} = \Lambda$, where Λ is a real diagonal matrix.

8.22 Use the stationary properties of quadratic forms to determine the maximum and minimum values taken by the expression

$$Q = 5x^2 + 4y^2 + 4z^2 + 2xz + 2xy$$

on the unit sphere, $x^2 + y^2 + z^2 = 1$. For what values of x, y and z do they occur?

8.23 Given that the matrix

$$\mathsf{A} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

has two eigenvectors of the form $(1 \quad y \quad 1)^{\mathrm{T}}$, use the stationary property of the expression $J(\mathsf{x}) = \mathsf{x}^{\mathrm{T}}\mathsf{A}\mathsf{x}/(\mathsf{x}^{\mathrm{T}}\mathsf{x})$ to obtain the corresponding eigenvalues. Deduce the third eigenvalue.

8.24 Find the lengths of the semi-axes of the ellipse

$$73x^2 + 72xy + 52y^2 = 100,$$

and determine its orientation.

8.25 The equation of a particular conic section is

$$Q \equiv 8x_1^2 + 8x_2^2 - 6x_1x_2 = 110.$$

Determine the type of conic section this represents, the orientation of its principal axes, and relevant lengths in the directions of these axes.

8.26 Show that the quadratic surface

$$5x^2 + 11y^2 + 5z^2 - 10yz + 2xz - 10xy = 4$$

is an ellipsoid with semi-axes of lengths 2, 1 and 0.5. Find the direction of its longest axis.

8.27 Find the direction of the axis of symmetry of the quadratic surface

$$7x^2 + 7y^2 + 7z^2 - 20yz - 20xz + 20xy = 3.$$

8.28 For the following matrices, find the eigenvalues and sufficient of the eigenvectors to be able to describe the quadratic surfaces associated with them:

$$\text{(a)} \begin{pmatrix} 5 & 1 & -1 \\ 1 & 5 & 1 \\ -1 & 1 & 5 \end{pmatrix}, \quad \text{(b)} \begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{pmatrix}, \quad \text{(c)} \begin{pmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{pmatrix}.$$

8.29 This exercise demonstrates the reverse of the usual procedure of diagonalising a matrix.

(a) Rearrange the result $\mathsf{A}' = \mathsf{S}^{-1}\mathsf{A}\mathsf{S}$ of section 8.16 to express the original matrix A in terms of the unitary matrix S and the diagonal matrix A'. Hence show how to construct a matrix A that has given eigenvalues and given (orthogonal) column matrices as its eigenvectors.

(b) Find the matrix that has as eigenvectors $(1 \quad 2 \quad 1)^{\mathrm{T}}$, $(1 \quad -1 \quad 1)^{\mathrm{T}}$ and $(1 \quad 0 \quad -1)^{\mathrm{T}}$, with corresponding eigenvalues λ, μ and ν.

(c) Try a particular case, say $\lambda = 3$, $\mu = -2$ and $\nu = 1$, and verify by explicit solution that the matrix so found does have these eigenvalues.

8.30 Find an orthogonal transformation that takes the quadratic form

$$Q \equiv -x_1^2 - 2x_2^2 - x_3^2 + 8x_2x_3 + 6x_1x_3 + 8x_1x_2$$

into the form

$$\mu_1 y_1^2 + \mu_2 y_2^2 - 4y_3^2,$$

and determine μ_1 and μ_2 (see section 8.17).

8.31 One method of determining the nullity (and hence the rank) of an $M \times N$ matrix A is as follows.

- Write down an augmented transpose of A, by adding on the right an $N \times N$ unit matrix and thus producing an $N \times (M + N)$ array B.
- Subtract a suitable multiple of the first row of B from each of the other lower rows so as to make $B_{i1} = 0$ for $i > 1$.
- Subtract a suitable multiple of the second row (or the uppermost row that does not start with M zero values) from each of the other lower rows so as to make $B_{i2} = 0$ for $i > 2$.
- Continue in this way until all remaining rows have zeros in the first M places. The number of such rows is equal to the nullity of A, and the N rightmost entries of these rows are the components of vectors that span the null space. They can be made orthogonal if they are not so already.

Use this method to show that the nullity of

$$\mathsf{A} = \begin{pmatrix} -1 & 3 & 2 & 7 \\ 3 & 10 & -6 & 17 \\ -1 & -2 & 2 & -3 \\ 2 & 3 & -4 & 4 \\ 4 & 0 & -8 & -4 \end{pmatrix}$$

is 2 and that an orthogonal base for the null space of A is provided by any two column matrices of the form $(2+\alpha_i \quad -2\alpha_i \quad 1 \quad \alpha_i)^{\mathrm{T}}$, for which the α_i $(i=1,2)$ are real and satisfy $6\alpha_1\alpha_2 + 2(\alpha_1+\alpha_2) + 5 = 0$.

8.32 Do the following sets of equations have non-zero solutions? If so, find them.

(a) $3x + 2y + z = 0, \qquad x - 3y + 2z = 0, \qquad 2x + y + 3z = 0.$
(b) $2x = b(y+z), \qquad x = 2a(y-z), \qquad x = (6a-b)y - (6a+b)z.$

8.33 Solve the simultaneous equations

$$\begin{aligned} 2x + 3y + z &= 11, \\ x + y + z &= 6, \\ 5x - y + 10z &= 34. \end{aligned}$$

8.34 Solve the following simultaneous equations for x_1, x_2 and x_3, using matrix methods:

$$\begin{aligned} x_1 + 2x_2 + 3x_3 &= 1, \\ 3x_1 + 4x_2 + 5x_3 &= 2, \\ x_1 + 3x_2 + 4x_3 &= 3. \end{aligned}$$

8.35 Show that the following equations have solutions only if $\eta = 1$ or 2, and find them in these cases:

$$\begin{aligned} x + y + z &= 1, \\ x + 2y + 4z &= \eta, \\ x + 4y + 10z &= \eta^2. \end{aligned}$$

8.36 Find the condition(s) on α such that the simultaneous equations

$$\begin{aligned} x_1 + \alpha x_2 &= 1, \\ x_1 - x_2 + 3x_3 &= -1, \\ 2x_1 - 2x_2 + \alpha x_3 &= -2 \end{aligned}$$

have (a) exactly one solution, (b) no solutions, or (c) an infinite number of solutions; give all solutions where they exist.

8.37 Make an LU decomposition of the matrix

$$\mathsf{A} = \begin{pmatrix} 3 & 6 & 9 \\ 1 & 0 & 5 \\ 2 & -2 & 16 \end{pmatrix}$$

and hence solve $\mathsf{Ax} = \mathsf{b}$, where (i) $\mathsf{b} = (21 \quad 9 \quad 28)^{\mathrm{T}}$, (ii) $\mathsf{b} = (21 \quad 7 \quad 22)^{\mathrm{T}}$.

8.38 Make an LU decomposition of the matrix

$$\mathsf{A} = \begin{pmatrix} 2 & -3 & 1 & 3 \\ 1 & 4 & -3 & -3 \\ 5 & 3 & -1 & -1 \\ 3 & -6 & -3 & 1 \end{pmatrix}.$$

Hence solve $\mathsf{Ax} = \mathsf{b}$ for (i) $\mathsf{b} = (-4 \quad 1 \quad 8 \quad -5)^{\mathrm{T}}$, (ii) $\mathsf{b} = (-10 \quad 0 \quad -3 \quad -24)^{\mathrm{T}}$. Deduce that $\det \mathsf{A} = -160$ and confirm this by direct calculation.

8.39 Use the Cholesky separation method to determine whether the following matrices are positive definite. For each that is, determine the corresponding lower diagonal matrix L:

$$\mathsf{A} = \begin{pmatrix} 2 & 1 & 3 \\ 1 & 3 & -1 \\ 3 & -1 & 1 \end{pmatrix}, \qquad \mathsf{B} = \begin{pmatrix} 5 & 0 & \sqrt{3} \\ 0 & 3 & 0 \\ \sqrt{3} & 0 & 3 \end{pmatrix}.$$

8.40 Find the equation satisfied by the squares of the singular values of the matrix associated with the following over-determined set of equations:

$$\begin{aligned} 2x + 3y + z &= 0 \\ x - y - z &= 1 \\ 2x + y &= 0 \\ 2y + z &= -2. \end{aligned}$$

Show that one of the singular values is close to zero. Determine the two larger singular values by an appropriate iteration process and the smallest one by indirect calculation.

8.41 Find the SVD of

$$\mathsf{A} = \begin{pmatrix} 0 & -1 \\ 1 & 1 \\ -1 & 0 \end{pmatrix},$$

showing that the singular values are $\sqrt{3}$ and 1.

8.42 Find the SVD form of the matrix

$$\mathsf{A} = \begin{pmatrix} 22 & 28 & -22 \\ 1 & -2 & -19 \\ 19 & -2 & -1 \\ -6 & 12 & 6 \end{pmatrix}.$$

Use it to determine the best solution x of the equation $\mathsf{Ax} = \mathsf{b}$ when (i) $\mathsf{b} = (6 \quad -39 \quad 15 \quad 18)^{\mathrm{T}}$, (ii) $\mathsf{b} = (9 \quad -42 \quad 15 \quad 15)^{\mathrm{T}}$, showing that (i) has an exact solution, but that the best solution to (ii) has a residual of $\sqrt{18}$.

8.43 Four experimental measurements of particular combinations of three physical variables, x, y and z, gave the following inconsistent results:

$$\begin{aligned} 13x + 22y - 13z &= 4, \\ 10x - 8y - 10z &= 44, \\ 10x - 8y - 10z &= 47, \\ 9x - 18y - 9z &= 72. \end{aligned}$$

Find the SVD best values for x, y and z. Identify the null space of A and hence obtain the general SVD solution.

8.20 Hints and answers

8.1 (a) False. O_N, the $N \times N$ null matrix, is *not* non-singular.

(b) False. Consider the sum of $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

(c) True.

(d) True.

(e) False. Consider $b_n = a_n + a_n$ for which $\sum_{n=0}^{N} |b_n|^2 = 4 \neq 1$, or note that there is no zero vector with unit norm.

(f) True.

(g) False. Consider the two series defined by

$$a_0 = \tfrac{1}{2}, \qquad a_n = 2(-\tfrac{1}{2})^n \quad \text{for} \quad n \geq 1; \qquad b_n = -(-\tfrac{1}{2})^n \quad \text{for} \quad n \geq 0.$$

The series that is the sum of $\{a_n\}$ and $\{b_n\}$ does not have alternating signs and so closure does not hold.

8.3 (a) $x = a$, b or c; (b) $x = -1$; the equation is linear in x.

8.5 Use the property of the determinant of a matrix product.

8.7 (d) $\mathsf{S} = \begin{pmatrix} 0 & -\tan(\theta/2) \\ \tan(\theta/2) & 0 \end{pmatrix}$.

(e) Note that $(\mathsf{I}+\mathsf{K})(\mathsf{I}-\mathsf{K}) = \mathsf{I}-\mathsf{K}^2 = (\mathsf{I}-\mathsf{K})(\mathsf{I}+\mathsf{K})$.

8.9 (b) $32i\mathsf{A}$.

8.11 $a = b\cos\gamma + c\cos\beta$, and cyclic permutations; $a^2 = b^2 + c^2 - 2bc\cos\alpha$, and cyclic permutations.

8.13 (a) $2^{-1/2}(0 \quad 0 \quad 1 \quad 1)^{\mathrm{T}}$, $6^{-1/2}(2 \quad 0 \quad -1 \quad 1)^{\mathrm{T}}$,
$39^{-1/2}(-1 \quad 6 \quad -1 \quad 1)^{\mathrm{T}}$, $13^{-1/2}(2 \quad 1 \quad 2 \quad -2)^{\mathrm{T}}$.
(b) $5^{-1/2}(1 \quad 2 \quad 0 \quad 0)^{\mathrm{T}}$, $(345)^{-1/2}(14 \quad -7 \quad 10 \quad 0)^{\mathrm{T}}$,
$(18\,285)^{-1/2}(-56 \quad 28 \quad 98 \quad 69)^{\mathrm{T}}$.

8.15 C does not commute with the others; A, B and D have $(1 \quad -2)^{\mathrm{T}}$ and $(2 \quad 1)^{\mathrm{T}}$ as common eigenvectors.

8.17 For A : $(1 \quad 0 \quad -1)^{\mathrm{T}}$, $(1 \quad \alpha_1 \quad 1)^{\mathrm{T}}$, $(1 \quad \alpha_2 \quad 1)^{\mathrm{T}}$.
For B : $(1 \quad 1 \quad 1)^{\mathrm{T}}$, $(\beta_1 \quad \gamma_1 \quad -\beta_1-\gamma_1)^{\mathrm{T}}$, $(\beta_2 \quad \gamma_2 \quad -\beta_2-\gamma_2)^{\mathrm{T}}$.
The α_i, β_i and γ_i are arbitrary.
Simultaneous and orthogonal: $(1 \quad 0 \quad -1)^{\mathrm{T}}$, $(1 \quad 1 \quad 1)^{\mathrm{T}}$, $(1 \quad -2 \quad 1)^{\mathrm{T}}$.

8.19 $\alpha_j = (\mathsf{v}\cdot\mathsf{e}^{j*})/(\lambda_j - \mu)$, where λ_j is the eigenvalue corresponding to e^j.

(a) $\mathsf{x} = (2 \quad 1 \quad 3)^{\mathrm{T}}$.
(b) Since μ is equal to one of A's eigenvalues λ_j, the equation only has a solution if $\mathsf{v}\cdot\mathsf{e}^{j*} = 0$; (i) no solution; (ii) $\mathsf{x} = (1 \quad 1 \quad 3/2)^{\mathrm{T}}$.

8.21 $\mathsf{U} = (10)^{-1/2}(1, 3i; 3i, 1)$, $\Lambda = (1, 0; 0, 11)$.

8.23 $J = (2y^2-4y+4)/(y^2+2)$, with stationary values at $y = \pm\sqrt{2}$ and corresponding eigenvalues $2 \mp \sqrt{2}$. From the trace property of A, the third eigenvalue equals 2.

8.25 Ellipse; $\theta = \pi/4$, $a = \sqrt{22}$; $\theta = 3\pi/4$, $b = \sqrt{10}$.

8.27 The direction of the eigenvector having the unrepeated eigenvalue is $(1, 1, -1)/\sqrt{3}$.

8.29 (a) $\mathsf{A} = \mathsf{S}\mathsf{A}'\mathsf{S}^{\dagger}$, where S is the matrix whose columns are the eigenvectors of the matrix A to be constructed, and $\mathsf{A}' = \mathrm{diag}\,(\lambda, \mu, \nu)$.
(b) $\mathsf{A} = (\lambda+2\mu+3\nu,\ 2\lambda-2\mu,\ \lambda+2\mu-3\nu;\ 2\lambda-2\mu,\ 4\lambda+2\mu,\ 2\lambda-2\mu;$
$\lambda+2\mu-3\nu,\ 2\lambda-2\mu,\ \lambda+2\mu+3\nu)$.
(c) $\frac{1}{3}(1, 5, -2; 5, 4, 5; -2, 5, 1)$.

8.31 The null space is spanned by $(2 \quad 0 \quad 1 \quad 0)^{\mathrm{T}}$ and $(1 \quad -2 \quad 0 \quad 1)^{\mathrm{T}}$.

8.33 $x = 3$, $y = 1$, $z = 2$.

8.35 First show that A is singular. $\eta = 1$, $x = 1 + 2z$, $y = -3z$; $\eta = 2$, $x = 2z$, $y = 1 - 3z$.

8.37 $L = (1, 0, 0; \frac{1}{3}, 1, 0; \frac{2}{3}, 3, 1)$, $\quad U = (3, 6, 9; 0, -2, 2; 0, 0, 4)$.

(i) $\mathsf{x} = (-1 \quad 1 \quad 2)^{\mathrm{T}}$. (ii) $\mathsf{x} = (-3 \quad 2 \quad 2)^{\mathrm{T}}$.

8.39 A is not positive definite, as L_{33} is calculated to be $\sqrt{-6}$.
$\mathsf{B} = \mathsf{L}\mathsf{L}^{\mathrm{T}}$, where the non-zero elements of L are
$L_{11} = \sqrt{5}$, $L_{31} = \sqrt{3/5}$, $L_{22} = \sqrt{3}$, $L_{33} = \sqrt{12/5}$.

8.41

$$\mathsf{A}^{\dagger}\mathsf{A} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix},\ \mathsf{U} = \frac{1}{\sqrt{6}}\begin{pmatrix} -1 & \sqrt{3} & \sqrt{2} \\ 2 & 0 & \sqrt{2} \\ -1 & -\sqrt{3} & \sqrt{2} \end{pmatrix},\ \mathsf{V} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

8.43 The singular values are $12\sqrt{6}, 0, 18\sqrt{3}$ and the calculated best solution is $x = 1.71, y = -1.94, z = -1.71$. The null space is the line $x = z, y = 0$ and the general SVD solution is $x = 1.71 + \lambda$, $y = -1.94$, $z = -1.71 + \lambda$.