3. THE SPECTRAL THEOREM

In the previous chapter we were solely interested in making an invertible change of variable. That is, the change of basis matrix P need only be invertible. When we make an invertible change of variable, *algebraic* properties such as

- determinant, trace, eigenvalues, dimension, rank, invertibility

are all preserved. However geometric properties are not typically preserved such as:

- length, angle, area and volume, scalar product, normal forms of curves and surfaces.

For example the curve with equation

$$x^2 + y^2 = 1,$$

under the invertible change of variable

$$X = 2x, \qquad Y = 3y,$$

takes on the equation

$$\frac{X^2}{4} + \frac{Y^2}{9} = 1.$$

What was a circle with area π has become an ellipse with area 6π.

Should we wish to make changes of variable which preserve geometric properties then we need to make an *orthogonal* change of variable.

Definition 58 *An $n \times n$ matrix P is* ***orthogonal*** *if $P^{-1} = P^T$.*
This is equivalent to the columns (or rows) of P being unit length and mutually perpendicular. That is to say, the columns (or rows) of P form an ***orthonormal basis*** *of $\mathbb{R}^n_{\text{col}}$ (or $\mathbb{R}^n$).*

Proposition 59 *The orthogonal matrices are precisely the matrices which preserve the scalar product. That is*

$$P\mathbf{x} \cdot P\mathbf{y} = \mathbf{x} \cdot \mathbf{y} \ \text{ for all } \mathbf{x}, \mathbf{y} \qquad \Longleftrightarrow \qquad P \text{ is orthogonal.}$$

Proof. Let P be an orthogonal matrix. Then

$$P\mathbf{x} \cdot P\mathbf{y} = (P\mathbf{x})^T P\mathbf{y} = \mathbf{x}^T P^T P\mathbf{y} = \mathbf{x}^T \mathbf{y} = \mathbf{x} \cdot \mathbf{y}.$$

Conversely assume $P\mathbf{x} \cdot P\mathbf{y} = \mathbf{x} \cdot \mathbf{y}$ for all $\mathbf{x}, \mathbf{y}$. If we set $\mathbf{x} = \mathbf{e}_i$ and $\mathbf{y} = \mathbf{e}_j$ then

$$\left[P^T P\right]_{ij} = \mathbf{e}_i^T P^T P \mathbf{e}_j = \mathbf{e}_i^T \mathbf{e}_j = \delta_{ij} = [I]_{ij}\,.$$

As this is true for each i, j then $P^T P = I$ and so P is orthogonal. ■

A first question then is: what matrices can be diagonalized by an orthogonal change of variables? Say that

$$P^{-1}AP = D$$

where D is diagonal and P is orthogonal. Then $A = PDP^{-1} = PDP^T$, so

$$A^T = \left(PDP^T\right)^T = P^{TT}D^TP^T = PDP^T = A.$$

Thus if a matrix A is orthogonally diagonalizable it is necessarily symmetric. The converse is true and known as the *spectral theorem*:

- **Spectral theorem**: Let A be an $n \times n$ symmetric matrix. Then the roots of χ_A are real and A has an eigenbasis consisting of mutually perpendicular unit vectors.

We prove a first result towards the theorem. Recall that eigenvectors associated with distinct eigenvalues are independent – the corresponding result for symmetric matrices is the following.

Proposition 60 *Let A be a real $n \times n$ symmetric matrix. If $\mathbf{v}$ and $\mathbf{w}$ are eigenvectors of A with associated eigenvalues λ and μ, where $\lambda \neq \mu$, then $\mathbf{v} \cdot \mathbf{w} = 0$.*

Proof. We have that $A\mathbf{v} = \lambda\mathbf{v}$ and $A\mathbf{w} = \mu\mathbf{w}$ where $\lambda \neq \mu$. Then, as A is symmetric, we have

$$\lambda\mathbf{v} \cdot \mathbf{w} = \lambda\mathbf{v}^T\mathbf{w} = (\lambda\mathbf{v})^T\mathbf{w} = (A\mathbf{v})^T\mathbf{w} = \mathbf{v}^TA^T\mathbf{w} = \mathbf{v}^TA\mathbf{w} = \mathbf{v}^T\mu\mathbf{w} = \mu\mathbf{v} \cdot \mathbf{w}.$$

As $\lambda \neq \mu$ then $\mathbf{v} \cdot \mathbf{w} = 0$. ■

Example 61 *Let*

$$A = \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}.$$

(a) Find an orthogonal matrix P such that P^TAP is diagonal.
(b) Show that the curve $x^2 + xy + y^2 = 1$ is an ellipse, and find its area. Sketch the curve.

Solution. (a) Note

$$\chi_A(x) = (1-x)^2 - \frac{1}{4} = \left(\frac{1}{2} - x\right)\left(\frac{3}{2} - x\right).$$

When

$$\begin{aligned} \lambda &= \frac{1}{2}: \qquad \ker\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \left\langle \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\rangle; \\ \lambda &= \frac{3}{2}: \qquad \ker\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} = \left\langle \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\rangle. \end{aligned}$$

Note that the $\frac{1}{2}$-eigenvectors and $\frac{3}{2}$-eigenvectors are perpendicular to one another – this was bound to be the case by the previous proposition. The eigenvectors $(1,-1)^T$ and $(1,1)^T$ cannot be the used as the columns of an orthogonal matrix, as they're not unit length, but if we normalize them to unit vectors then they can form the columns of an orthogonal matrix. Thus we set

$$P = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

We then know

$$P^T A P = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{3}{2} \end{pmatrix}.$$

(b) The equation $x^2 + xy + y^2 = 1$ can be rewritten as

$$(x\, y) \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 1.$$

Making the change of variable

$$\begin{pmatrix} x \\ y \end{pmatrix} = P \begin{pmatrix} X \\ Y \end{pmatrix},$$

the equation $1 = (x\, y)\, A\, (x\, y)^T$ becomes

$$1 = (X\, Y)\, P^T A P\, (X\, Y)^T = \frac{1}{2} X^2 + \frac{3}{2} Y^2.$$

This is the equation of an ellipse with semi-axes of length $a = \sqrt{2}$ and $b = \sqrt{2/3}$ with area

$$\pi ab = \frac{2\pi}{\sqrt{3}}.$$

We can say the curve is an ellipse, and calculate its area, as the change of variable is orthogonal. The XY-axes are given by

$$\begin{aligned} X\text{-axis or } Y &= 0 \text{ is in the direction of } P\,(1,0)^T \text{ so is the line } y = x; \\ Y\text{-axis or } X &= 0 \text{ is in the direction of } P\,(0,1)^T \text{ so is the line } x + y = 0. \end{aligned}$$

A sketch of the ellipse, with the XY-axes labelled, is given in Figure 1 below.

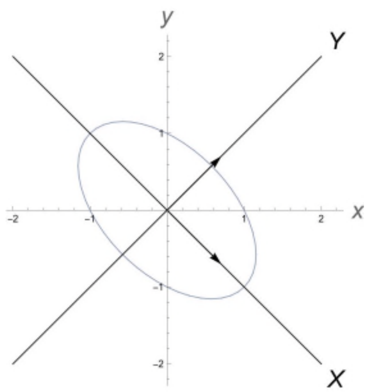


Figure 1: $x^2 + xy + y^2 = 1$

∎

When an $n \times n$ matrix has distinct eigenvalues then we can find n eigenvectors which are independent and so form an eigenbasis; we can create an invertible matrix P with those eigenvectors as the columns of P. Similarly when a symmetric $n \times n$ matrix has distinct eigenvalues then we can find n eigenvectors which are orthogonal (and thus independent) and so form an eigenbasis; the matrix P with those eigenvectors as its columns will not in general be orthogonal, but if we normalize the eigenvectors – scale them to unit length – then the matrix P will be orthogonal as its columns will be mutually perpendicular and unit length.

When an $n \times n$ matrix has repeated eigenvalues then there may not be *any* eigenbasis. This cannot happen when a symmetric square matrix has repeated eigenvalues, but this result is reasonably sophisticated. In particular we will need to prove the following for symmetric matrices:

- The roots of the characteristic polynomial are real.
- The direct sum of the eigenspaces is the entire space.
- Each eigenspace has an orthonormal basis.

We begin by demonstrating the first result.

Proposition 62 *Let A be a real $n \times n$ symmetric matrix. The roots of $\chi_A(x) = \det(xI - A)$ are real.*

Proof. Let λ be a (potentially complex) root of χ_A. Then by (an appropriate complex version of) Proposition 41(a), there is a non-zero complex vector $\mathbf{v}$ in $\mathbb{C}^n_{\text{col}}$ such that $A\mathbf{v} = \lambda\mathbf{v}$. As the entries of A are real, when we conjugate this equation we obtain $A\bar{\mathbf{v}} = \bar{\lambda}\bar{\mathbf{v}}$. As $A = A^T$, and by the product rule for transposes, we see

$$\bar{\lambda}\bar{\mathbf{v}}^T\mathbf{v} = (\bar{\lambda}\bar{\mathbf{v}})^T\mathbf{v} = (A\bar{\mathbf{v}})^T\mathbf{v} = \bar{\mathbf{v}}^T A^T\mathbf{v} = \bar{\mathbf{v}}^T A\mathbf{v} = \bar{\mathbf{v}}^T\lambda\mathbf{v} = \lambda\bar{\mathbf{v}}^T\mathbf{v}.$$

Now for any non-zero *complex* vector $\mathbf{v} = (v_1, v_2, \ldots, v_n)^T$ we have

$$\bar{\mathbf{v}}^T\mathbf{v} = \bar{\mathbf{v}} \cdot \mathbf{v} = \overline{v_1}v_1 + \cdots + \overline{v_n}v_n = |v_1|^2 + \cdots + |v_n|^2 > 0.$$

As $(\bar{\lambda} - \lambda)\bar{\mathbf{v}}^T\mathbf{v} = 0$ then $\lambda = \bar{\lambda}$ and so λ is real. ■

We now move on to the third bullet point. We will demonstrate that any subspace has an orthonormal basis. This result then applies to eigenspaces as they are subspaces. Our first result is to show how an orthonormal set can be constructed from a linearly independent one.

Say that $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k$ is an independent set in $\mathbb{R}^n$; we shall construct an orthonormal basis $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_k$ such that

$$\langle \mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_i \rangle = \langle \mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_i \rangle \qquad \text{for } 1 \leqslant i \leqslant k.$$

There are, in fact, only limited ways of doing this. As $\langle \mathbf{w}_1 \rangle = \langle \mathbf{v}_1 \rangle$ then $\mathbf{w}_1$ is a scalar multiple of $\mathbf{v}_1$. But as $\mathbf{w}_1$ is a unit vector then $\mathbf{w}_1 = \pm\mathbf{v}_1/|\mathbf{v}_1|$. So there are only two choices for $\mathbf{w}_1$ and it seems most natural to take $\mathbf{w}_1 = \mathbf{v}_1/|\mathbf{v}_1|$ (rather than needlessly introducing a negative sign). With this choice of $\mathbf{w}_1$ we then need to find a unit vector $\mathbf{w}_2$ perpendicular to $\mathbf{w}_1$ and such that $\langle \mathbf{w}_1, \mathbf{w}_2 \rangle = \langle \mathbf{v}_1, \mathbf{v}_2 \rangle$. In particular, we have

$$\mathbf{v}_2 = \alpha \mathbf{w}_1 + \beta \mathbf{w}_2 \qquad \text{for some scalars } \alpha, \beta.$$

We require $\mathbf{w}_2$ to be perpendicular to $\mathbf{w}_1$ and so $\alpha = \mathbf{v}_2 \cdot \mathbf{w}_1$. Note that

$$\mathbf{y}_2 = \beta \mathbf{w}_2 = \mathbf{v}_2 - (\mathbf{v}_2 \cdot \mathbf{w}_1)\, \mathbf{w}_1 \neq \mathbf{0}$$

is the component of $\mathbf{v}_2$ perpendicular to $\mathbf{v}_1$. We then have $\mathbf{w}_2 = \pm \mathbf{y}_2 / |\mathbf{y}_2|$. Again we have two choices of $\mathbf{w}_2$ but again there is no particular reason to choose the negative option.

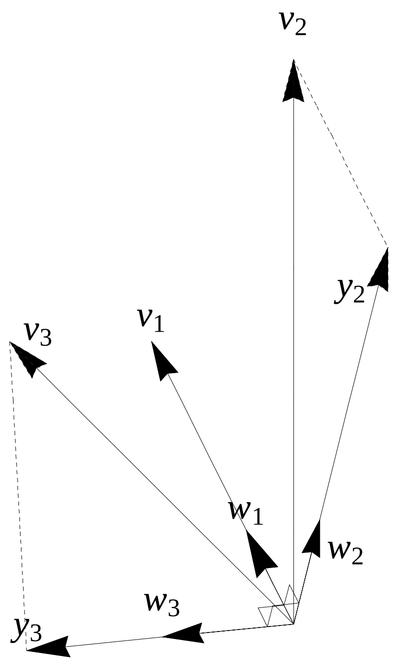


Figure 2: GSOP example

Figure 2 above hopefully captures the geometric nature of this process. $\mathbf{v}_1$ spans a line and so there are only two unit vectors parallel to it with $\mathbf{w}_1 = \mathbf{v}_1 / |\mathbf{v}_1|$ being a more natural choice than its negative. $\langle \mathbf{v}_1, \mathbf{v}_2 \rangle$ is a plane divided into two half-planes by the line $\langle \mathbf{v}_1 \rangle$ and there are two choices of unit vector in this plane which are perpendicular to this line. We choose $\mathbf{w}_2$ to be that unit vector pointing into the same half-plane as $\mathbf{v}_2$ does. Continuing, $\langle \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \rangle$ is a three-dimensional space divided it into two half-spaces by the plane $\langle \mathbf{v}_1, \mathbf{v}_2 \rangle$. There are two choices of unit vector in this space which are perpendicular to the plane. We choose $\mathbf{w}_3$ to be that unit vector pointing into the same half-space as $\mathbf{v}_3$ does. This process is known as the *Gram-Schmidt orthogonalization process* (GSOP)[1], with the rigorous details appearing below.

[1] Named after the Danish mathematician Jorgen Pedersen Gram (1850-1916) and the German mathematician Erhard Schmidt (1876-1959). The orthogonalization process was employed by Gram in a paper of 1883 and by Schmidt, with acknowledgements to Gram, in a 1907 paper, but in fact the process had also been used by Laplace as early as 1812.

Theorem 63 *(Gram-Schmidt Orthogonalization Process (GSOP)) Let* $\mathbf{v}_1, \ldots, \mathbf{v}_k$ *be independent vectors in* $\mathbb{R}^n_{\text{col}}$ *(or* $\mathbb{R}^n$*). Then there are orthonormal vectors* $\mathbf{w}_1, \ldots, \mathbf{w}_k$ *such that, for each* $1 \leqslant i \leqslant k$*, we have*

$$\langle \mathbf{w}_1, \ldots, \mathbf{w}_i \rangle = \langle \mathbf{v}_1, \ldots, \mathbf{v}_i \rangle. \tag{3.1}$$

Proof. We will prove this by induction on i. The result is seen to be true for $i = 1$ by taking $\mathbf{w}_1 = \mathbf{v}_1 / |\mathbf{v}_1|$. Suppose now that $1 \leqslant I < k$ and that we have so far produced orthonormal vectors $\mathbf{w}_1, \ldots, \mathbf{w}_I$ such that (3.1) is true for $1 \leqslant i \leqslant I$. We then set

$$\mathbf{y}_{I+1} = \mathbf{v}_{I+1} - \sum_{j=1}^{I} (\mathbf{v}_{I+1} \cdot \mathbf{w}_j) \mathbf{w}_j.$$

Note that, for $1 \leqslant i \leqslant I$,

$$\mathbf{y}_{I+1} \cdot \mathbf{w}_i = \mathbf{v}_{I+1} \cdot \mathbf{w}_i - \sum_{j=1}^{I} (\mathbf{v}_{I+1} \cdot \mathbf{w}_j) \delta_{ij} = \mathbf{v}_{I+1} \cdot \mathbf{w}_i - \mathbf{v}_{I+1} \cdot \mathbf{w}_i = 0. \tag{3.2}$$

So $\mathbf{y}_{I+1}$ is perpendicular to each of $\mathbf{w}_1, \ldots, \mathbf{w}_I$. Further $\mathbf{y}_{I+1}$ is non-zero, for if $\mathbf{y}_{I+1} = \mathbf{0}$ then

$$\mathbf{v}_{I+1} = \sum_{j=1}^{I} (\mathbf{v}_{I+1} \cdot \mathbf{w}_j) \mathbf{w}_j \quad \text{is in} \quad \langle \mathbf{w}_1, \ldots, \mathbf{w}_I \rangle = \langle \mathbf{v}_1, \ldots, \mathbf{v}_I \rangle$$

which contradicts the linear independence of $\mathbf{v}_1, \ldots, \mathbf{v}_I, \mathbf{v}_{I+1}$. If we set $\mathbf{w}_{I+1} = \mathbf{y}_{I+1} / |\mathbf{y}_{I+1}|$, it follows from (3.2) that $\mathbf{w}_1, \ldots, \mathbf{w}_{I+1}$ form an orthonormal set. Further

$$\langle \mathbf{w}_1, \ldots, \mathbf{w}_{I+1} \rangle = \langle \mathbf{w}_1, \ldots, \mathbf{w}_I, \mathbf{y}_{I+1} \rangle = \langle \mathbf{w}_1, \ldots, \mathbf{w}_I, \mathbf{v}_{I+1} \rangle = \langle \mathbf{v}_1, \ldots, \mathbf{v}_I, \mathbf{v}_{I+1} \rangle$$

and the proof follows by induction. ■

Corollary 64 *Every subspace of* $\mathbb{R}^n$ *(or* $\mathbb{R}^n_{\text{col}}$*) has an orthonormal basis.*

Proof. If U is a subspace of $\mathbb{R}^n$ then it has a basis $\mathbf{v}_1, \ldots, \mathbf{v}_k$. By applying the GSOP process, an orthonormal set $\mathbf{w}_1, \ldots, \mathbf{w}_k$ can be constructed from them which is a basis for U as

$$\langle \mathbf{w}_1, \ldots, \mathbf{w}_k \rangle = \langle \mathbf{v}_1, \ldots, \mathbf{v}_k \rangle = U.$$

■

Corollary 65 *An orthonormal set can be extended to an orthonormal basis.*

Proof. Let $\mathbf{w}_1, \ldots, \mathbf{w}_k$ be an orthonormal set in $\mathbb{R}^n$. In particular it is linearly independent and so may be extended to a basis $\mathbf{w}_1, \ldots, \mathbf{w}_k, \mathbf{v}_{k+1}, \ldots, \mathbf{v}_n$ for $\mathbb{R}^n$. The GSOP can then be applied to construct an orthonormal basis $\mathbf{x}_1, \ldots, \mathbf{x}_n$ from this basis. The nature of the GSOP means that $\mathbf{x}_i = \mathbf{w}_i$ for $1 \leqslant i \leqslant k$ and so our orthonormal basis is an extension of the original orthonormal set. ■

We now prove the second bullet point above, that the eigenspaces of a symmetric matrix A form a direct sum for the entire space. Eigenvectors from different eigenspaces are automatically orthogonal to one another and via GSOP we now know there exists an orthonormal basis for each eigenspace. The union of the orthonormal bases for the eigenspaces then makes an orthonormal eigenbasis for the whole space. All this is equivalent to showing that there is an orthogonal matrix P such that P^TAP is diagonal – we create P by having the orthonormal eigenbasis as its columns.

Theorem 66 ***(Spectral Theorem***[2]*) Let A be a real symmetric $n \times n$ matrix. Then there exists an orthogonal $n \times n$ matrix P such that P^TAP is diagonal.*

Proof. We shall prove the result by strong induction on n. When $n = 1$ there is nothing to prove as all 1×1 matrices are diagonal and so we can simply take $P = I_1$.

Suppose now that the result holds for $r \times r$ real symmetric matrices where $1 \leqslant r < n$. By the fundamental theorem of algebra, the characteristic polynomial χ_A has a root λ in $\mathbb{C}$, which by Proposition 62 we in fact know to be real. Let X denote the λ-eigenspace, that is

$$X = \{\mathbf{v} \in \mathbb{R}^n_{\text{col}} \mid A\mathbf{v} = \lambda\mathbf{v}\}.$$

Then X is a non-zero subspace as it is $\ker(A - \lambda I)$ and λ is an eigenvalue – so X has an orthonormal basis $\mathbf{v}_1, \dots \mathbf{v}_m$ which we may extend to an orthonormal basis $\mathbf{v}_1, \dots \mathbf{v}_n$ for $\mathbb{R}^n_{\text{col}}$. Let $P = (\mathbf{v}_1 \mid \dots \mid \mathbf{v}_n)$; then P is orthogonal and by the definition of matrix multiplication

$$\left[P^TAP\right]_{ij} = \mathbf{v}_i^T A\mathbf{v}_j = \mathbf{v}_i \cdot (A\mathbf{v}_j).$$

Note that $A\mathbf{v}_i = \lambda\mathbf{v}_i$ for $1 \leqslant i \leqslant m$ and so the first m columns of P^TAP are $\lambda\mathbf{e}_1^T, \dots, \lambda\mathbf{e}_m^T$. Also if $1 \leqslant i \leqslant m$ and $m < j, k \leqslant n$ we have, using $A = A^T$ and the product rule for transposes, that

$$\mathbf{v}_i \cdot (A\mathbf{v}_j) = \mathbf{v}_i^T(A\mathbf{v}_j) = \mathbf{v}_i^T A^T\mathbf{v}_j = (A\mathbf{v}_i)^T\mathbf{v}_j = \lambda\mathbf{v}_i^T\mathbf{v}_j = \lambda(\mathbf{v}_i \cdot \mathbf{v}_j) = 0;$$

so that $\left[P^TAP\right]_{ij} = 0$. Further, as P^TAP is symmetric then $\left[P^TAP\right]_{kj} = \left[P^TAP\right]_{jk}$. Together this means that

$$P^TAP = \begin{pmatrix} \lambda I_m & 0 \\ 0 & M \end{pmatrix},$$

where M is a symmetric $(n - m) \times (n - m)$ matrix. By our inductive hypothesis there is an orthogonal $(n - m) \times (n - m)$ matrix Q such that Q^TMQ is diagonal. If we set

$$R = \begin{pmatrix} I_m & 0 \\ 0 & Q \end{pmatrix}$$

[2] Appreciation of this result, at least in two variables, dates back to Descartes and Fermat. But the equivalent general result was first proven by Cauchy in 1829, though independently of the language of matrices, which were yet to be invented. Rather Cauchy's result was in terms of *quadratic forms* – a quadratic form in two variables is an expression of the form $ax^2 + bxy + cy^2$.

then R is orthogonal, PR is orthogonal and

$$\begin{aligned}(PR)^T A(PR) &= R^T P^T APR \\ &= \begin{pmatrix} I_m & 0 \\ 0 & Q^T \end{pmatrix}^T \begin{pmatrix} \lambda I_m & 0 \\ 0 & M \end{pmatrix} \begin{pmatrix} I_m & 0 \\ 0 & Q \end{pmatrix} \\ &= \begin{pmatrix} \lambda I_m & 0 \\ 0 & Q^T MQ \end{pmatrix}\end{aligned}$$

which is diagonal. This concludes the proof by induction. ■

Corollary 67 *A real symmetric matrix A is said to be:*

- ***positive definite*** *if* $\mathbf{x}^T A\mathbf{x} > 0$ *for all* $\mathbf{x} \neq \mathbf{0}$;
- ***positive semi-definite*** *if* $\mathbf{x}^T A\mathbf{x} \geqslant 0$ *for all* $\mathbf{x}$;
- ***negative definite*** *if* $\mathbf{x}^T A\mathbf{x} < 0$ *for all* $\mathbf{x} \neq \mathbf{0}$;
- ***negative semi-definite*** *if* $\mathbf{x}^T A\mathbf{x} \leqslant 0$ *for all* $\mathbf{x}$;
- ***indefinite*** *otherwise.*

From the spectral theorem we see that these correspond respectively to the eigenvalues of A being (i) all positive, (ii) all non-negative, (iii) all negative, (iv) all non-positive, (v) some positive, some negative and some possibly zero.

Remark 68 *(**Hermitian matrices**) There is a version of the spectral theorem over the complex numbers. The standard inner product on $\mathbb{C}^n$ is given by*

$$\langle \mathbf{z}, \mathbf{w} \rangle = \mathbf{z} \cdot \overline{\mathbf{w}} = z_1\overline{w_1} + \cdots + z_n\overline{w_n}.$$

*So the equivalent of the orthogonal matrices are the **unitary matrices** which satisfy $U^{-1} = \overline{U}^T$. These are precisely the matrices that preserve the complex inner product. And the equivalent of symmetric matrices are the **hermitian matrices**[3] which satisfy $M = \overline{M}^T$. The complex version of the spectral theorem then states that, for any hermitian matrix M there exists a unitary matrix U such that $\overline{U}^T MU$ is diagonal with real entries. Hermitian matrices are important in quantum theory as they represent observables.*

Remark 69 *We saw earlier that the theory of diagonalization applies equally well over any field, mainly because it is part of the theory of vector spaces and linear maps. By contrast the spectral theorem is best set in the context of inner product spaces and so there is a spectral theorem only for symmetric matrices over $\mathbb{R}$ and for Hermitian matrices over $\mathbb{C}$, these being the linear maps which respect the inner product. There is a more detailed comment on this matter at the end of the chapter.*

[3] After the French mathematician, Charles Hermite (1822-1901).

Example 70 *For the matrix A below, find orthogonal P such that $P^T AP$ is diagonal.*

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

Solution. The characteristic polynomial of A is $\chi_A(x) = (x+1)^3(x-3)$. A unit length 3-eigenvector is $\mathbf{v}_1 = (1,1,1,1)^T/2$ and the -1-eigenspace is $x_1 + x_2 + x_3 + x_4 = 0$. So a basis for the -1-eigenspace is

$$(1,-1,0,0)^T, \qquad (0,1,-1,0)^T, \qquad (0,0,1,-1)^T.$$

However to find the last three columns of P, we need an orthonormal basis for the -1-eigenspace. Applying the GSOP to the above three vectors, we arrive at

$$\mathbf{v}_2 = (1,-1,0,0)^T/\sqrt{2}, \qquad \mathbf{v}_3 = (1,1,-2,0)^T/\sqrt{6}, \qquad \mathbf{v}_4 = (1,1,1,-3)^T/\sqrt{12}.$$

Such a required matrix is then $P = (\mathbf{v}_1 \,|\, \mathbf{v}_2 \,|\, \mathbf{v}_3 \,|\, \mathbf{v}_4)$. ■

Algorithm 71 ***(Orthogonal Diagonalization of a Symmetric Matrix)*** *Let M be a symmetric matrix. The spectral theorem shows that M is diagonalizable and so has an eigenbasis. Setting this eigenbasis as the columns of a matrix P will yield an invertible matrix P such that $P^{-1}MP$ is diagonal – in general though this P will not be orthogonal.*

If $\mathbf{v}$ is an eigenvector of M whose eigenvalue is not repeated, then we replace it with $\mathbf{v}/|\mathbf{v}|$. This new eigenvector is of unit length and is necessarily orthogonal to other eigenvectors with different eigenvalues Proposition 60. If none of the eigenvalues is repeated, this is all we need do to the eigenbasis to produce an orthonormal eigenbasis.

If λ is a repeated eigenvalue then we can find a basis for the λ-eigenspace. Applying the GSOP to this basis produces an orthonormal basis for the λ-eigenspace. Again these eigenvectors are orthogonal to all eigenvectors with different eigenvalues. We can see now that the previous non-repeated case is simply a special case of the repeated case, the GSOP for a single eigenvector involving nothing other than normalizing it.

Once the given basis for each eigenspace has had the GSOP applied to it the entire eigenbasis has now been made orthonormal. We may put this orthonormal eigenbasis as the columns of a matrix P which will be orthogonal and such that $P^{-1}MP = P^T MP$ is diagonal.

Example 72 *Find a 2×2 real symmetric matrix M such that $M^2 = A$ where*

$$A = \begin{pmatrix} 3 & \sqrt{3} \\ \sqrt{3} & 5 \end{pmatrix}.$$

Solution. The characteristic polynomial of A is

$$\det(xI - A) = (x-3)(x-5) - (-\sqrt{3})^2 = x^2 - 8x + 12$$

which has roots 2 and 6. Determining the eigenvectors we see

$$\lambda = 2: \qquad \ker\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & 3 \end{pmatrix} = \left\langle \begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix} \right\rangle, \qquad \text{so take } \mathbf{v}_1 = \frac{1}{2}\begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix}.$$

$$\lambda = 6: \qquad \ker\begin{pmatrix} -3 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix} = \left\langle \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \right\rangle, \qquad \text{so take } \mathbf{v}_2 = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}.$$

So with $P = (\mathbf{v}_1 \,|\, \mathbf{v}_2)$ we have $P^T A P = \mathrm{diag}(2, 6)$, which has a clear square root of $\mathrm{diag}(\sqrt{2}, \sqrt{6})$. Thus we might choose

$$M = P\mathrm{diag}\left(\sqrt{2}, \sqrt{6}\right) P^T = \frac{1}{4}\begin{pmatrix} 3\sqrt{2} + \sqrt{6} & 3\sqrt{2} - \sqrt{6} \\ 3\sqrt{2} - \sqrt{6} & \sqrt{2} + 3\sqrt{6} \end{pmatrix}.$$

■

Below are some important examples of symmetric matrices across mathematics and a description of their connection with *quadratic forms*.

Example 73 ***(Gram matrices)*** *The Gram matrix M for an inner product $\langle \quad , \quad \rangle$ on a vector space with basis $\{v_1, \ldots, v_n\}$ has (i, j)th entry*

$$[M]_{ij} = \langle v_i, v_j \rangle .$$

This is a symmetric, positive definite matrix – because of the properties of inner products – and conversely any symmetric, positive definite matrix is the Gram matrix of an inner product.

Example 74 ***(Inertia matrix in dynamics)*** *A rigid body, rotating about a fixed point O with angular velocity $\boldsymbol{\omega}$ has kinetic energy*

$$T = \frac{1}{2}\boldsymbol{\omega}^T I_0 \boldsymbol{\omega},$$

where I_0 is the inertia matrix

$$I_0 = \begin{pmatrix} A & -D & -E \\ -D & B & -F \\ -E & -F & C \end{pmatrix},$$

where

$$\begin{aligned} A &= \iiint_R \rho\left(y^2 + z^2\right) \mathrm{d}V, \quad B = \iiint_R \rho\left(x^2 + z^2\right) \mathrm{d}V, \quad C = \iiint_R \rho\left(x^2 + y^2\right) \mathrm{d}V, \\ D &= \iiint_R \rho yz \,\mathrm{d}V, \quad E = \iiint_R \rho xz \,\mathrm{d}V, \quad F = \iiint_R \rho xy \,\mathrm{d}V, \end{aligned}$$

where ρ denotes density and R is the region that the rigid body occupies. For a spinning top, symmetrical about its axis, the eigenvectors of I_0 are along the axis with two eigenvectors orthogonal to that. Wrt this basis $I_0 = \mathrm{diag}(A, A, C)$, but the spectral theorem applies to any rigid body, however irregular the distribution of matter.

Example 75 ***(Covariance and correlation matrices in probability and statistics)*** *The covariance matrix Σ is a symmetric, positive semi-definite matrix giving the covariance between each pair of elements of a random vector. Given a random vector $\mathbf{X} = (X_1, \ldots, X_n)^T$ the covariance matrix Σ is defined by*

$$[\Sigma]_{i,j} = \operatorname{cov}[X_i, X_j] = \mathbb{E}\left[(X_i - \mathbb{E}(X_i))(Y_j - \mathbb{E}(X_j))\right]$$

or equally

$$\Sigma = \mathbb{E}[\mathbf{X}\mathbf{X}^T] - \mathbb{E}(\mathbf{X})\mathbb{E}(\mathbf{X})^T.$$

It follows from the spectral theorem that every symmetric positive semi-definite matrix is a covariance matrix. This matrix is important in the theory of principal component analysis (PCA).

The correlation matrix C is similarly defined with

$$[C]_{ij} = \frac{\operatorname{cov}[X_i, X_j]}{\sigma(X_i)\,\sigma(X_i)}.$$

C is a symmetric, positive semi-definite matrix with all its diagonal entries equalling 1.

One of the most important applications of the spectral theorem is the classification of quadratic forms.

Definition 76 *A* ***quadratic form*** *in n variables $x_1, x_2, \ldots, x_n$ is a polynomial where each term has degree two. That is, it can be written as a sum*

$$\sum_{i \leqslant j} a_{ij} x_i x_j$$

where the a_{ij} are scalars. Thus a quadratic form in two variables x, y is $ax^2 + bxy + cy^2$ where a, b, c are scalars.

Alternatively a co-ordinate-free way of defining quadratic forms on a vector space V is as

$$B(v, v)$$

where $B\colon V \times V \to \mathbb{R}$ is a bilinear map.

The connection with symmetric matrices is that we can write

$$\sum_{i \leqslant j} a_{ij} x_i x_j = \mathbf{x}^T A \mathbf{x}$$

where $\mathbf{x}^T = (x_1, x_2, \ldots, x_n)$ and A is the symmetric matrix

$$[A]_{ij} = \begin{cases} a_{ii} & i = j \\ \frac{1}{2} a_{ij} & i < j \\ \frac{1}{2} a_{ji} & i > j \end{cases}.$$

Thus, for example,

$$ax^2 + bxy + cy^2 = (x\ y)\begin{pmatrix} a & \frac{b}{2} \\ \frac{b}{2} & c \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}.$$

Definition 77 *When the spectral theorem is applied to quadratic forms it is often referred to as the **principal axis theorem**.*

There are many important examples of quadratic forms, some listed below.

Example 78 *(**Conics**) The general degree two equation in two variables has the form*

$$Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0$$

where $A, \ldots, F$ are real scalars and A, B, C are not all zero. This equation can be put into normal forms as follows. Firstly we can rewrite the equation as

$$(x, y)\, M \begin{pmatrix} x \\ y \end{pmatrix} + (D, E) \begin{pmatrix} x \\ y \end{pmatrix} + F = 0, \qquad \textit{where} \quad M = \begin{pmatrix} A & B/2 \\ B/2 & C \end{pmatrix}. \tag{3.3}$$

Note that M is symmetric. By the spectral theorem we know that there is a 2×2 orthogonal matrix P which will diagonalize M. If we set

$$\begin{pmatrix} x \\ y \end{pmatrix} = P \begin{pmatrix} X \\ Y \end{pmatrix},$$

then (3.3) becomes

$$(X, Y)\, P^T M P \begin{pmatrix} X \\ Y \end{pmatrix} + (D, E)\, P \begin{pmatrix} X \\ Y \end{pmatrix} + F = 0,$$

As P is orthogonal then this change of variable will not change any geometric aspects: distances, angles and areas remain unaltered. In these new variables X, Y, and with $P^T M P = \operatorname{diag}(\tilde{A}, \tilde{C})$ and $(D, E)P = (\tilde{D}, \tilde{E})$, our equation now reads as

$$\tilde{A}X^2 + \tilde{C}Y^2 + \tilde{D}X + \tilde{E}Y + F = 0.$$

We can now complete any squares to put this equation into a normal form.

- *Ellipses have normal form*

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \qquad (a \geqslant b > 0)\,.$$

- *Hyperbolae have normal form*

$$\frac{x^2}{a^2} - \frac{y^2}{b^1} = 1 \qquad (a, b > 0)\,.$$

- *Parabolae have normal form*

$$y^2 = 4ax \qquad (a > 0)\,.$$

Each ellipse, hyperbola, parabola can be uniquely put into one of the above forms by an isometry of the plane. The general degree two equation also leads to some degenerate cases such as parallel lines, intersecting lines, repeated lines, points and the empty set.

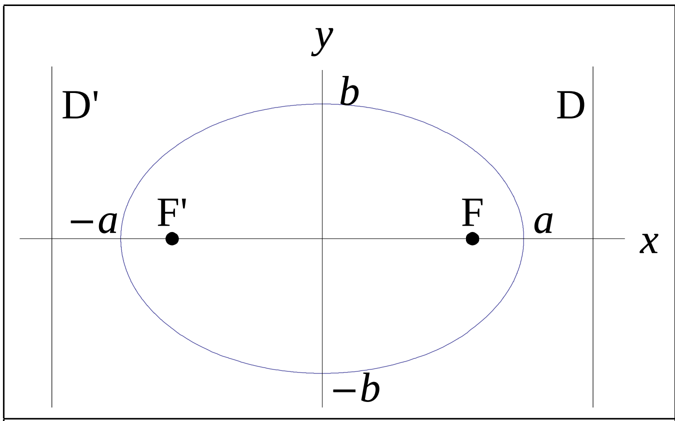


Figure 3a – ellipse

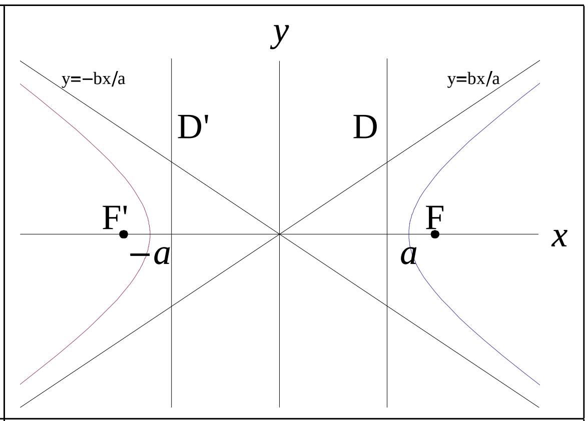


Figure 3b – hyperbola

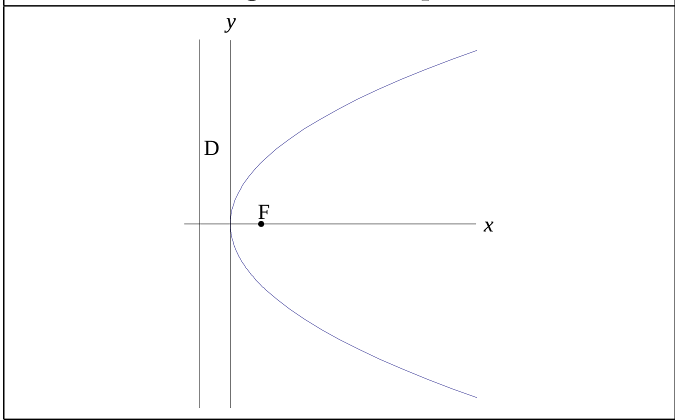


Figure 3c – parabola

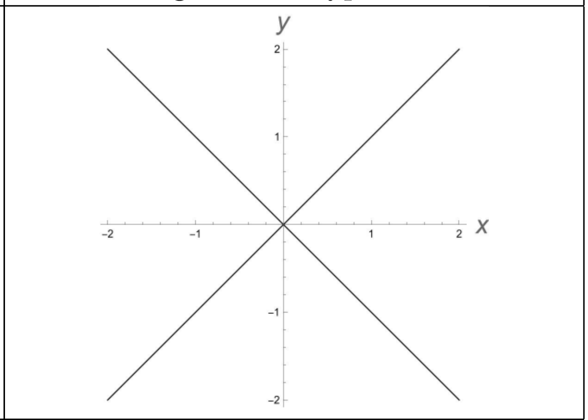


Figure 3d – degenerate case

Example 79 *(**Quadrics**) The spectral theorem applies equally well to the general degree two equation in three variables x, y, z. The normal forms for the non-degenerate cases are*

- *Ellipsoids have normal form*

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1 \qquad (a \geqslant b \geqslant c)\,.$$

- *Hyperboloids of one sheet have normal form*

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = 1 \qquad (a \geqslant b > 0, c > 0)\,.$$

- *Hyperboloids of two sheets have normal form*

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = -1 \qquad (a \geqslant b > 0, c > 0)\,.$$

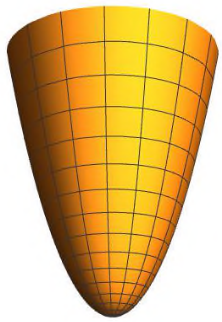
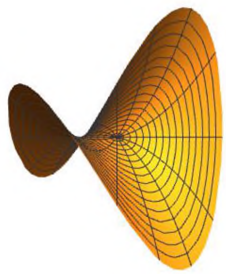
- *Elliptic paraboloids have normal form*

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} - z = 0 \qquad (a \geqslant b > 0)\,.$$

- *Hyperbolic paraboloids have normal form*

$$\frac{x^2}{a^2} - \frac{y^2}{b^2} - z = 0 \qquad (a, b > 0)\,.$$

Each of these non-degenerate cases be uniquely put into one of the above forms by an isometry of the plane. The general degree two equation in three variables also leads to some degenerate cases such as parallel planes, intersecting planes, repeated planes, points, cones, elliptic parabolic and hyperbolic cylinders and the empty set.

		
Fig. 4a: Ellipsoid $\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$	Fig. 4b: Elliptic paraboloid $z = a^2x^2 + b^2y^2$	Fig. 4c: Hyperbolic paraboloid $z = a^2x^2 - b^2y^2$

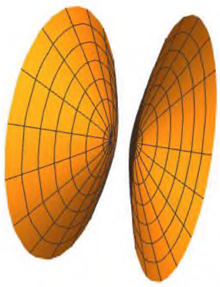
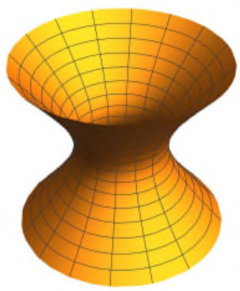
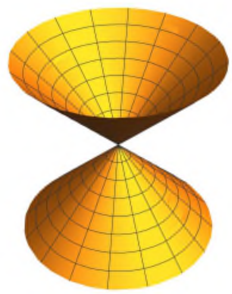

		

Fig. 4d: 2 sheets hyperboloid	Fig. 4e: 1 sheet hyperboloid	Fig. 4f: Double Cone
$\frac{x^2}{a^2} - \frac{y^2}{b^2} - \frac{z^2}{c^2} = 1$	$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = 1$	$z^2 = \frac{x^2}{a^2} + \frac{y^2}{b^2}.$

Example 80 *Show that the equation* $13x^2 + 13y^2 + 10z^2 + 4yz + 4zx + 8xy = 1$ *defines an ellipsoid and find its volume.*

Solution. Let

$$A = \begin{pmatrix} 13 & 4 & 2 \\ 4 & 13 & 2 \\ 2 & 2 & 10 \end{pmatrix}$$

so that $\mathbf{x}^T A\mathbf{x} = 13x^2 + 13y^2 + 10z^2 + 4yz + 4zx + 8xy$. Note that $\chi_A(x)$ equals

$$\begin{vmatrix} x-13 & -4 & -2 \\ -4 & x-13 & -2 \\ -2 & -2 & x-10 \end{vmatrix} = \begin{vmatrix} x-9 & 9-x & 0 \\ -4 & x-13 & -2 \\ -2 & -2 & x-10 \end{vmatrix}$$

$$= (x-9)\begin{vmatrix} 1 & -1 & 0 \\ -4 & x-13 & -2 \\ -2 & -2 & x-10 \end{vmatrix} = (x-9)\begin{vmatrix} 1 & 0 & 0 \\ -4 & x-17 & -2 \\ -2 & -4 & x-10 \end{vmatrix}$$

$$= (x-9)(x^2 - 27x + 162) = (x-9)(x-18)(x-9).$$

This means that there is an orthogonal matrix P such that

$$P^T AP = \operatorname{diag}(9, 9, 18).$$

If we set $\mathbf{x} = P\mathbf{X}$ then we see our quadric now has equation

$$9X^2 + 9Y^2 + 18Z^2 = \mathbf{X}^T P^T AP\mathbf{X} = 1,$$

which is an ellipsoid. Further we have

$$a = \frac{1}{3}, \qquad b = \frac{1}{3}, \qquad c = \frac{1}{3\sqrt{2}}$$

and so by Sheet 4, Question S2, and noting the orthogonal change of variable won't the ellipsoid's volume, we see that volume equals

$$\frac{4\pi}{3} \times \frac{1}{3} \times \frac{1}{3} \times \frac{1}{3\sqrt{2}} = \frac{2\sqrt{2}\pi}{81}.$$

■

Example 81 *(a) Find an orthogonal matrix P such that $P^T AP$ is diagonal where*

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

(b) Consider the real-valued functions f and g defined on $\mathbb{R}^3_{\text{col}}$ by

$$f(\mathbf{x}) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz, \qquad g(\mathbf{x}) = -y^2 + 2z^2 + 2\sqrt{2}xy,$$

where $\mathbf{x} = (x, y, z)^T$. Is there an invertible matrix Q such that $f(Q\mathbf{x}) = g(\mathbf{x})$? Is there an orthogonal Q?
(c) Sketch the surface $f(\mathbf{x}) = 1$.

Solution. (a) The characteristic polynomial $\chi_A(x)$ equals $(x+1)(x-2)^2$ so that the eigenvalues are $-1, 2, 2$. The -1-eigenvectors are multiples of $(1, 1, 1)^T$ and the 2-eigenspace is the plane $x + y + z = 0$. So an orthonormal eigenbasis for A is

$$\frac{(1,1,1)^T}{\sqrt{3}}, \qquad \frac{(1,-1,0)^T}{\sqrt{2}}, \qquad \frac{(1,1,-2)^T}{\sqrt{6}},$$

from which we can form the required

$$P = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{2} & \sqrt{3} & 1 \\ \sqrt{2} & -\sqrt{3} & 1 \\ \sqrt{2} & 0 & -2 \end{pmatrix}.$$

(b) We then have that $f(P\mathbf{x}) = (P\mathbf{x})^T A(P\mathbf{x}) = \mathbf{x}^T P^T AP\mathbf{x} = -x^2+2y^2+2z^2$. Now we similarly have

$$g(\mathbf{x}) = (x, y, z) \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

and this matrix (call it B) has characteristic polynomial $\chi_B(x) = (x+2)(x-1)(x-2)$. This means that there is an orthogonal matrix R such that

$$g(R\mathbf{x}) = -2x^2 + y^2 + 2z^2.$$

We can then see that the (invertible but not orthogonal) map S which sends $(x, y, z)^T$ to $(x/\sqrt{2}, \sqrt{2}y, z)^T$ satisfies

$$g(RS\mathbf{x}) = -2(x/\sqrt{2})^2 = (\sqrt{2}y)^2 + 2z^2 = -x^2 + 2y^2 + 2z^2.$$

That A and B have the same number of eigenvalues of each sign means that there is an invertible change of variables connecting the funvyions f and g, but there is no orthogonal change of variable as that would preserve the eigenvalues.

(c) The quadric surface $f(\mathbf{x}) = 1$ is a hyperboloid of one sheet, as in Figure 4e with the new x-axis being the axis of the hyperboloid. ■

Example 82 ***(Hessian matrix)*** *Let $f(x, y)$ be a function of two variables with partial derivatives of all orders. Taylor's theorem in two variables states*

$$f(a+\delta, b+\varepsilon) = f(a,b)+(f_x(a,b)\delta+f_y(a,b)\varepsilon)+\frac{1}{2}\left(f_{xx}(a,b)\delta^2 + 2f_{xy}(a,b)\,\delta\varepsilon + f_{yy}(a,b)\varepsilon^2\right)+R_3$$

*where R_3 is a remainder term that is at least order three in δ and ε. A **critical point** or **stationary point** (a, b) is one where*

$$f_x(a,b) = 0 = f_y(a,b).$$

Thus, at a critical point, we have

$$f(a+\delta, b+\varepsilon) = f(a,b) + \frac{1}{2}\left(f_{xx}(a,b)\delta^2 + 2f_{xy}(a,b)\,\delta\varepsilon + f_{yy}(a,b)\varepsilon^2\right) + R_3$$

and so the local behaviour of f near a critical point is determined by the quadratic form

$$f_{xx}\delta^2 + 2f_{xy}\delta\varepsilon + f_{yy}\varepsilon^2 = (\delta\ \varepsilon) \begin{pmatrix} f_{xx} & f_{xy} \\ f_{xy} & f_{yy} \end{pmatrix} \begin{pmatrix} \delta \\ \varepsilon \end{pmatrix}.$$

The symmetric matrix

$$H = \begin{pmatrix} f_{xx} & f_{xy} \\ f_{xy} & f_{yy} \end{pmatrix}$$

is known as the ***Hessian***[4]*. As H is symmetric, we know that we can make an orthogonal change of variables $(\delta, \varepsilon) \to (\Delta, E)$ so that the above quadratic form becomes*

$$\lambda \Delta^2 + \mu E^2$$

where λ, μ are the eigenvalues of H. We then see that:

- *there is a (local)* ***minimum*** *at (a, b) if $\lambda, \mu > 0$;*
- *there is a (local)* ***maximum*** *at (a, b) if $\lambda, \mu < 0$;*
- *there is a* ***saddle point*** *at (a, b) if λ, μ have different signs.*

When H is singular then the critical point is said to be degenerate, and its classification depends on the cubic terms (or higher) in Taylor's theorem.

Example 83 *(**Norms**) Given an inner product space V then the norm squared $\|v\|^2 = \langle v, v \rangle$ is a positive definite quadratic form on V. For a smooth parameterized surface $\mathbf{r}(u, v)$ in $\mathbb{R}^3$ then the tangent space T_p at a point p equals the span of $\mathbf{r}_u$ and $\mathbf{r}_v$. The restriction of $\|v\|^2$ to T_p is the quadratic form*

$$(\alpha, \beta) \mapsto \|\alpha \mathbf{r}_u + \beta \mathbf{r}_v\|^2 = E\alpha^2 + 2F\alpha\beta + G\beta^2$$

where

$$E = \mathbf{r}_u \cdot \mathbf{r}_u, \qquad F = \mathbf{r}_u \cdot \mathbf{r}_v, \qquad G = \mathbf{r}_v \cdot \mathbf{r}_v,$$

and is known as the ***first fundamental form****.*

We conclude this chapter with some comments charting the direction of spectral theory into the second year linear algebra and beyond into third year functional analysis. **You should consider all these remarks – and the subsequent epilogue – to be beyond the Prelims syllabus but they may make interesting further reading to some.**

Remark 84 *(**Adjoints**) As commented earlier, the spectral theorem is most naturally stated in the context of inner product spaces; a more sophisticated version of the theorem appears in the secord year the course A0 Linear Algebra. The version we have met states that a real symmetric matrix (or complex Hermitian matrix) is diagonalizable via an orthogonal change of variable.*

If we seek to extend this theorem to linear maps on vector spaces, our first problem is that there is no well-defined notion of the transpose of a linear map and so no notion of a symmetric linear map. The determinant of a linear map T is well-defined as the determinant is the same

[4] After the German mathematician Ludwig Hesse (1811–1874).

for any matrices A and B representing T. This is because $A = P^{-1}BP$ for some change of basis matrix P and so

$$\det A = \det\left(P^{-1}BP\right) = \frac{1}{\det P}\det B \det P = \det B.$$

However if we wished to define the transpose T^T of T as the linear map defined by A^T wrt the first basis and B^T wrt the second basis we have just defined different linear maps as in general

$$A^T \neq P^{-1}B^T P.$$

This can be gotten around somewhat if we only consider orthogonal changes of variable P. In this case

$$A = P^T BP \quad \Longrightarrow \quad A^T = P^T B^T P.$$

So should we only use orthonormal bases, and orthogonal changes of variable, then we can define the "transpose" of a linear map. But this discussion only makes sense in in an inner product space and not in a general vector space; that "tranpose" is instead referred to a the adjoint of T written T^*.

Given a linear map $T\colon V \to V$ of a finite-dimensional inner product space V, its adjoint $T^*\colon V \to V$ is the unique linear map satisfying

$$\langle Tv, w\rangle = \langle v, T^*w\rangle \qquad \text{for all } v, w \in V.$$

If we choose an orthonormal basis $v_1, \ldots, v_n$ for V and let A and B respectively be the matrices for T and T^* wrt this basis then

$$[A]_{ji} = \langle Tv_i, v_j\rangle = \langle v_i, T^*v_j\rangle = [B]_{ij}\,.$$

*So the matrix for T^* is that of the transpose of the matrix for T. The "symmetric" linear maps are then those satisfying $T = T^*$, the so-called **self-adjoint** linear maps which satisfy*

$$\langle Tv, w\rangle = \langle v, Tw\rangle \qquad \text{for all } v, w \in V.$$

The second year version of the spectral theorem states:

- ***Spectral theorem for self-adjoint maps**. Let $T\colon V \to V$ be a self-adjoint map on a finite-dimensional inner product space. Then all the eigenvalues of T are real and there is an orthonormal eigenbasis of V.*

Example 85 *(See Sheet 4, Exercise P3.) The nth Legendre polynomial $P_n(x)$ satisfies Legendre's equation*

$$\left(1 - x^2\right)\frac{\mathrm{d}^2y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} + n(n+1)y = 0$$

where n is a natural number. This can be rewritten as

$$Ly = -n(n+1)y \qquad \text{where} \qquad L = \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(1 - x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\right].$$

So $P_n(x)$ can be viewed as an $n(n+1)$-eigenvector of the differential operator L. Further it can be shown that

$$\langle P_n(x), P_m(x)\rangle = 0 \qquad \text{when } n \neq m,$$

where the inner product $\langle \quad , \quad \rangle$ *is defined by*

$$\langle f, g\rangle = \int_{-1}^{1} f(x)g(x)\,\mathrm{d}x,$$

so that the Legendre polynomials are in fact orthogonal eigenvectors; further still it is true that

$$\langle Ly_1, y_2\rangle = \langle y_1, Ly_2\rangle\,,$$

showing L *to be self-adjoint.*

Remark 86 ***(Spectral Theory – infinite-dimensional spaces)*** *Whilst the space* $\mathbb{R}[x]$ *of polynomials is infinite dimensional, the above example is not at a great remove from orthogonally diagonalizing a real symmetric matrix – after all any polynomial can be written as a finite linear combination of Legendre polynomials. For contrast,* ***Schrödinger's equation*** *in quantum theory has the form*

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = E\psi, \qquad \psi(0) = \psi(a) = 0.$$

This equation was formulated in 1925 by the Austrian physicist, Erwin Schrödinger (1887-1961). The above is the time-independent equation of a particle in the interval $0 \leqslant x \leqslant a$*. The* ***wave function*** ψ *is a complex-valued function of* x *and* $|\psi(x)|^2$ *can be thought of as the probability density function of the particle's position.* m *is its mass,* $\hbar$ *is the (reduced) Planck constant,* $V(x)$ *denotes potential energy and* E *is the particle's energy.*

A significant, confounding aspect of late nineteenth century experimental physics was the emission spectra of atoms. (By the way, these two uses of the word "spectrum" in mathematics and physics appear to be coincidental.) As an example, experiments showed that only certain discrete, quantized energies could be released by an excited atom of hydrogen. Classical physical theories were unable to explain this phenomenon.

Schrödinger's equation can be rewritten as $H\psi = E\psi$ *with* E *being an eigenvalue of the differential operator* H *known as the Hamiltonian. One can again show that* H *is self-adjoint, that is:*

$$\langle H\psi_1, \psi_2\rangle = \langle \psi_1, H\psi_2\rangle$$

where

$$\langle \varphi, \psi\rangle = \int_0^a \varphi(x)\overline{\psi(x)}\,\mathrm{d}x.$$

And if V *is constant then it's easy to show that the only non-zero solutions of Schrödinger's equation above are*

$$\psi_n(x) = A_n \sin\left(\frac{n\pi x}{a}\right) \qquad \text{where} \qquad E = E_n = V + \frac{n^2\pi^2\hbar^2}{2ma^2},$$

and n *is a positive integer and* A_n *is a constant. If* $|\psi_n(x)|^2$ *is to be a pdf then we need* $A_n = \sqrt{2/a}$*, and again these* ψ_n *are orthonormal with respect to the above inner product. Note above that the energy* E *can only take certain discrete values* E_n*.*

In general though, a wave function need not be one of these eigenstates ψ_n and may be a finite or indeed infinite combination of them. For example we might have

$$\psi(x) = \sqrt{\frac{30}{a^5}}\, x\,(a-x)$$

for which $|\psi(x)|^2$ is a pdf. How might we write such a $\psi(x)$ as a combination of the $\psi_n(x)$? This is an infinite-dimensional version of the problem the spectral theorem solved – how in general to write a vector as a linear combination of orthonormal eigenvectors – and in the infinite dimensional case is the subject of ***Fourier analysis****, named after the French mathematician Joseph Fourier (1768-1830). In this case Fourier analysis shows that*

$$\psi(x) = \sum_0^\infty \alpha_{2n+1}\psi_{2n+1}(x) \qquad \textit{where} \qquad \alpha_n = \frac{8\sqrt{15}}{\pi^3 n^3}.$$

If the particle's energy was measured it would be one of the permitted energies E_n and the effect of measuring this energy is to collapse the above wave function ψ to one of the eigenstates ψ_{2n+1}. It is the case that

$$\sum_0^\infty |\alpha_{2n+1}|^2 = 1$$

(this is Parseval's Identity which is essentially an infinite dimensional version of Pythagoras' Theorem). The probability of the particle having measured energy E_{2n+1} is $|\alpha_{2n+1}|^2$. The role of measurement in quantum theory is very different from that of classical mechanics; the very act of measuring some observable characteristic of the particle actually affects and changes the wave function.

From the more general point of view, it is important that these wave functions lie not just in an infinite-dimensional complex inner product space, but that this space is a ***Hilbert space****, meaning it is complete – Cauchy sequences are convergent. There is a (somewhat technical) version of the spectral theorem for Hilbert spaces which is the subject of the third year functional analysis courses.*

3.1 Epilogue – Singular Value Decomposition (Off-syllabus)

We conclude with an important related theorem, namely the *singular value decomposition theorem* which applies not just to square matrices and is important in numerial analysis, signal processing, pattern recognition and in particular is used in the Trinity term *Statistics and Data Analysis* course when discussing principal component analysis.

Recall that, given an $m \times n$ matrix A of rank r then there exist an invertibel $m \times m$ matrix P and an invertible $n \times n$ matrix Q such that

$$PAQ = \begin{pmatrix} I_r & 0_{r,n-r} \\ 0_{m-r,r} & 0_{m-r,n-r} \end{pmatrix}.$$

The matrix P results from the elementary matrices used to put A into RRE form, and then the ECOs can be used to move the r leading 1s to the first r columns and clear out the rest of the rows.

A natural question is: what form can A be put into if P and Q are required to be orthogonal instead?

Theorem 87 ***(Singular Value Decomposition)*** *Let A be an $m \times n$ matrix of rank r. Then there exist an orthogonal $m \times m$ matrix P and an orthogonal $n \times n$ matrix Q such that*

$$PAQ = \begin{pmatrix} D & 0_{r,n-r} \\ 0_{m-r,r} & 0_{m-r,n-r} \end{pmatrix} \tag{3.4}$$

where D is an invertible diagonal $r \times r$ matrix with positive entries listed in decreasing order.

Proof. Note that $A^T A$ is a symmetric $n \times n$ matrix. So by the spectral theorem there is an $n \times n$ orthogonal matrix Q such that

$$Q^T A^T A Q = \begin{pmatrix} \Delta & 0_{r,n-r} \\ 0_{n-r,r} & 0_{n-r,n-r} \end{pmatrix},$$

where Δ is a diagonal $r \times r$ matrix with its diagonal entries in decreasing order. Note that $A^T A$ has the same rank r as A and that the eigenvalues of $A^T A$ are non-negative, the positive eigenvalues being the entries of Δ. If we write

$$Q = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix}$$

where Q_1 is $n \times r$ and Q_2 is $n \times (n-r)$ then we have in particular that

$$Q_1^T A^T A Q_1 = \Delta; \qquad Q_2^T A^T A Q_2 = 0; \qquad Q_1^T Q_1 = I_r; \qquad Q_1 Q_1^T + Q_2 Q_2^T = I_n,$$

the last two equations following from Q's orthogonality. From the second equation $AQ_2 = 0_{m,n-r}$.

If $\Delta = \operatorname{diag}(\lambda_1, \ldots, \lambda_r)$ then we may set $D = \operatorname{diag}\left(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_r}\right)$ so that $D^2 = \Delta$. We then define P_1 to be the $m \times r$ matrix

$$P_1 = AQ_1 D^{-1}.$$

Note that

$$P_1 D Q_1^T = AQ_1 Q_1^T = A(I_n - Q_2 Q_2^T) = A - (AQ_2) Q_2^T = A.$$

We are almost done now as, by the transpose product rule and because D is diagonal, we have

$$P_1^T P_1 = \left(AQ_1 D^{-1}\right)^T \left(AQ_1 D^{-1}\right) = D^{-1} Q_1^T A^T A Q_1 D^{-1} = D^{-1} \Delta D^{-1} = I_r$$

and also that

$$P_1^T A Q_1 = P_1^T P_1 D = I_r D = D.$$

That $P_1^T P_1 = I_r$ means the columns of P_1 form an orthonormal set, which may then be extended to an orthonormal basis for $\mathbb{R}_m$. We put these vectors as the columns of an orthogonal $m \times m$ matrix $P^T = \begin{pmatrix} P_1 & P_2 \end{pmatrix}$ and note that

$$P_2^T A Q_1 = P_2^T P_1 D = 0_{m-r,r} D = 0_{m-r,r}$$

as the columns of P are orthogonal. Finally we have that PAQ equals

$$\begin{pmatrix} P_1^T \\ P_2^T \end{pmatrix} A \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} = \begin{pmatrix} P_1^T \\ P_2^T \end{pmatrix} \begin{pmatrix} AQ_1 & 0_{m.n-r} \end{pmatrix} = \begin{pmatrix} P_1^T AQ_1 & 0_{r.n-r} \\ 0_{m-r.r} & 0_{m-r,n-r} \end{pmatrix} = \begin{pmatrix} D & 0_{r.n-r} \\ 0_{m-r.r} & 0_{m-r,n-r} \end{pmatrix}.$$

■

Example 88 *Find the singular value decomposition of*

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

Solution. Firstly

$$A^T A = \begin{pmatrix} 1 & 0 \\ 0 & 2 \\ 2 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 2 & 1 \\ 0 & 2 & 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 2 & 1 \\ 0 & 4 & 2 & -2 \\ 2 & 2 & 5 & 1 \\ 1 & -2 & 1 & 2 \end{pmatrix}.$$

$A^T A$ has characteristic polynomial

$$x^4 - 12x^3 + 35x^2 = x^2(x-5)(x-7).$$

We can then take

$$Q = \begin{pmatrix} \frac{1}{\sqrt{14}} & \frac{1}{\sqrt{10}} & -\frac{2}{3} & -\frac{4}{\sqrt{21}} \\ \frac{2}{\sqrt{14}} & -\frac{2}{\sqrt{10}} & \frac{1}{3} & -\frac{1}{\sqrt{21}} \\ \frac{3}{\sqrt{14}} & \frac{1}{\sqrt{10}} & 0 & \frac{2}{\sqrt{21}} \\ 0 & \frac{2}{\sqrt{10}} & \frac{2}{3} & 0 \end{pmatrix},$$

so that $Q^T A^T AQ = \mathrm{diag}(7, 5, 0, 0)$. We then set $D = \mathrm{diag}(\sqrt{7}, \sqrt{5}, 0, 0)$ and $P_1 = AQ_1 D^{-1}$ to give

$$P_1 = \begin{pmatrix} 1 & 0 & 2 & 1 \\ 0 & 2 & 1 & -1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{14}} & \frac{1}{\sqrt{10}} \\ \frac{2}{\sqrt{14}} & -\frac{2}{\sqrt{10}} \\ \frac{3}{\sqrt{14}} & \frac{1}{\sqrt{10}} \\ 0 & \frac{2}{\sqrt{10}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{7}} & 0 \\ 0 & \frac{1}{\sqrt{5}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

and so

$$P = P_1^T = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

■

Remark 89 *With notation as in Theorem 87, the* ***pseudoinverse*** *(or Moore-Penrose inverse) of A is*

$$A^+ = Q \begin{pmatrix} D^{-1} & 0_{r,m-r} \\ 0_{n-r,r} & 0_{n-r,m-r} \end{pmatrix} P.$$

The following facts are then true of the pseudoinverse.

(a) If A is invertible then $A^{-1} = A^+$.

(b) $\left(A^T\right)^+ = (A^+)^T$.
(c) $(AB)^+ \neq B^+A^+$ *in general.*
(d) The pseudoinverse has the following properties.

$$(I) \quad AA^+A = A; \quad (II) \quad A^+AA^+ = A^+; \quad (III) \quad AA^+ \quad \textit{and} \quad A^+A \quad \textit{are symmetric.}$$

(e) A^+ *is the only matrix to have the properties I, II, III.*
(f) AA^+ *is orthogonal projection onto the column space of* A*.*
(g) If the columns of A *are independent then* $A^+ = (A^TA)^{-1}A^T$.
(h) Let $\mathbf{b}$ *be in* $\mathbb{R}^m_{\text{col}}$ *and set* $\mathbf{x}_0 = A^+\mathbf{b}$*. Then*

$$|A\mathbf{x} - \mathbf{b}| \geqslant |A\mathbf{x}_0 - \mathbf{b}| \qquad \textit{for all } \mathbf{x} \textit{ in } \mathbb{R}^n_{\text{col}}.$$