eNote 15

Symmetric Matrices

In this eNote we will consider one of the most used results from linear algebra – the so-called spectral theorem *for symmetric matrices. In short it says that* all *symmetric matrices can be* diagonalized *by a similarity transformation – that is, by change of basis with a suitable substitution matrix.*
The introduction of these concepts and the corresponding method were given in eNotes 10, 13 and 14, which therefore is a necessary basis for the present eNote.
Precisely in that eNote it became clear that not all matrices can be diagonalized. Diagonalization requires a sufficiently large number of eigenvalues (the algebraic multiplicities add up to be as large as possible) and that the corresponding eigenvector spaces actually span all of the vector space (the geometric multiplicities add up to be as large as possible). It is these properties we will consider here, but now for symmetric matrices, which turn out to satisfy the conditions and actually more: the eigenvectors we use in the resulting substitution matrix can be chosen pairwise orthogonal, such that the new basis is the result of a rotation of the old standard basis in $\mathbb{R}^n$.
In order to be able to discuss and apply the spectral theorem most effectively we must first introduce a natural scalar product for vectors in $\mathbb{R}^n$ *in such a way that we will be able to measure angles and lengths in all dimensions. We do this by generalizing the well-known standard scalar product from* $\mathbb{R}^2$ *and* $\mathbb{R}^3$. *As indicated above we will in particular use bases consisting of pairwise orthogonal vectors in order to formulate the spectral theorem, understand it and what use we can make of this important theorem.*

Updated: 20.11.21 David Brander

15.1 Scalar Product

In the vector space $\mathbb{R}^n$ we introduce an inner product, i.e. a scalar product that is a natural generalization of the well-known scalar product from plane geometry and space geometry, see eNote 10.

|||| Definition 15.1 Scalar Product

Let **a** and **b** be two given vectors in $\mathbb{R}^n$ with the coordinates $(a_1, ..., a_n)$ and $(b_1, ..., b_n)$, respectively, with respect to the standard basis shalle in $\mathbb{R}^n$:

$$ {}_{\mathrm{e}}\mathbf{a} = (a_1, ..., a_n) \quad , \quad \text{and} \quad {}_{\mathrm{e}}\mathbf{b} = (b_1, ..., b_n) \quad . \tag{15-1} $$

Then we define the ***scalar product***, the ***inner product***, (also called the *dot product*) of the two vectors in the following way:

$$ \mathbf{a}\cdot\mathbf{b} = a_1 b_1 + a_2 b_2 + \cdots a_n b_n = \sum_{i=1}^{n} a_i b_i \quad . \tag{15-2} $$

When $\mathbb{R}^n$ is equipped with this scalar product $(\mathbb{R}^n, \cdot)$ is thereby an example of a so-called ***Euclidian vector space*** , or a ***vector space with inner product***.

The scalar product can be expressed as a matrix product:

$$ \mathbf{a}\cdot\mathbf{b} = {}_{\mathrm{e}}\mathbf{a}^{\top} \cdot {}_{\mathrm{e}}\mathbf{b} = \begin{bmatrix} a_1 & \cdot & \cdot & \cdot & a_n \end{bmatrix} \cdot \begin{bmatrix} b_1 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{bmatrix} \tag{15-3} $$

For the scalar product introduced above the following arithmetic rules apply:

|||| Theorem 15.2 Arithmetic Rules for the Scalar Product

If $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are vectors in $(\mathbb{R}^n, \cdot)$ and k is an arbitrary real number then:

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a} \tag{15-4}$$

$$\mathbf{a} \cdot (\mathbf{b} + \mathbf{c}) = \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \cdot \mathbf{c} \tag{15-5}$$

$$\mathbf{a} \cdot (k\mathbf{b}) = (k\mathbf{a}) \cdot \mathbf{b} = k(\mathbf{a} \cdot \mathbf{b}) \tag{15-6}$$

A main point about the introduction of a scalar product is that we can now talk about the *lengths of the vectors* in $(\mathbb{R}^n, \cdot)$:

|||| Definition 15.3 The Length of a Vector

Let $\mathbf{a}$ be a vector in $(\mathbb{R}^n, \cdot)$ with the coordinates $(a_1, ..., a_n)$ with respect to the standard e-basis in $\mathbb{R}^n$. Then the ***length of* a** is defined by

$$|\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}} = \sqrt{\sum_{i=1}^{n} a_i^2} \quad . \tag{15-7}$$

The length of $\mathbf{a}$ is also called the ***norm of* a** with respect to the scalar product in $(\mathbb{R}^n, \cdot)$. A vector $\mathbf{a}$ is called a ***proper vector*** if $|\mathbf{a}| > 0$.

It follows from Definition 15.1 that

$$\begin{aligned} &\mathbf{a}\cdot\mathbf{a} \geq 0 \ \text{ for all } \ \mathbf{a} \in (\mathbb{R}^n, \cdot) \ \text{ and} \\ &\mathbf{a}\cdot\mathbf{a} = 0 \Leftrightarrow \mathbf{a} = \mathbf{0}\,. \end{aligned} \tag{15-8}$$

From this we immediately see that

$$\begin{aligned} &|\mathbf{a}| \geq 0, \ \text{ for all } \ \mathbf{a} \in (\mathbb{R}^n, \cdot) \ \text{ and} \\ &|\mathbf{a}| = 0 \Leftrightarrow \mathbf{a} = \mathbf{0}\,. \end{aligned} \tag{15-9}$$

Thus a *proper* vector is a vector that is not the **0**-vector.

Finally it follows from Definition 15.1 and Definition 15.3 that for $\mathbf{a} \in (\mathbb{R}^n, \cdot)$ and an arbitrary real number k we have that

$$|k\mathbf{a}| = |k| \ |\mathbf{a}| \ . \tag{15-10}$$

We can now prove the following important theorem:

|||| Theorem 15.4 Cauchy-Schwarz Inequality

For arbitrary vectors **a** and **b** in $(\mathbb{R}^n, \cdot)$

$$|\mathbf{a}\cdot\mathbf{b}| \leq |\,\mathbf{a}\,|\ |\,\mathbf{b}\,|\ . \tag{15-11}$$

Equality holds if and only if **a** and **b** are linearly dependent.

|||| Proof

If $\mathbf{b} = \mathbf{0}$, both sides of (15-11) are equal to 0 and the inequality is thereby satisfied. We now assume that **b** is a proper vector.

We put $k = \mathbf{b}\cdot\mathbf{b}$ and $\mathbf{e} = \dfrac{1}{\sqrt{k}}\mathbf{b}$. It then follows from (15-6) that

$$\mathbf{e}\cdot\mathbf{e} = \Big(\frac{1}{\sqrt{k}}\mathbf{b}\Big)\cdot\Big(\frac{1}{\sqrt{k}}\mathbf{b}\Big) = \frac{1}{k}\,(\mathbf{b}\cdot\mathbf{b}) = 1$$

and thereby that $|\mathbf{e}| = 1$.

By substituting $\mathbf{b} = \sqrt{k}\,\mathbf{e}$ in the left hand side and the right hand side of (15-11) we get using

(15-6) and (15-10):

$$|\mathbf{a}\cdot\mathbf{b}| = |\,\mathbf{a}\cdot(\sqrt{k}\,\mathbf{e})\,| = \sqrt{k}\,|\mathbf{a}\cdot\mathbf{e}|$$

and

$$|\mathbf{a}|\ |\mathbf{b}| = |\mathbf{a}|\ |\,\sqrt{k}\,\mathbf{e}\,| = \sqrt{k}\,|\mathbf{a}|\ |\mathbf{e}|\ .$$

Therefore we only have to show that for arbitrary $\mathbf{a}$ and $\mathbf{e}$, where $|\mathbf{e}| = 1$,

$$|\mathbf{a}\cdot\mathbf{e}| \leq |\,\mathbf{a}\,| \tag{15-12}$$

where equality holds if and only if $\mathbf{a}$ and $\mathbf{e}$ are linearly dependent.

For an arbitrary $t \in \mathbb{R}$ it follows from (15-8), (15-5) and (15-6) that:

$$0 \leq (\mathbf{a} - t\mathbf{e})\cdot(\mathbf{a} - t\mathbf{e}) = \mathbf{a}\cdot\mathbf{a} + t^2(\mathbf{e}\cdot\mathbf{e}) - 2t(\mathbf{a}\cdot\mathbf{e}) = \mathbf{a}\cdot\mathbf{a} + t^2 - 2t(\mathbf{a}\cdot\mathbf{e})\,.$$

If in particular we choose $t = \mathbf{a}\cdot\mathbf{e}$, we get

$$0 \leq \mathbf{a}\cdot\mathbf{a} - (\mathbf{a}\cdot\mathbf{e})^2 \;\Leftrightarrow\; |\mathbf{a}\cdot\mathbf{e}| \leq \sqrt{\mathbf{a}\cdot\mathbf{a}} = |\mathbf{a}|\ .$$

Since it follows from (15-8) that $(\mathbf{a} - t\mathbf{e})\cdot(\mathbf{a} - t\mathbf{e}) = 0$ if and only if $(\mathbf{a} - t\mathbf{e}) = \mathbf{0}$, we see that $|\mathbf{a}\cdot\mathbf{e}| = |\,\mathbf{a}\,|$ if and only if $\mathbf{a}$ and $\mathbf{e}$ are linearly dependent. The proof is hereby complete.

■

From the Cauchy-Schwarz inequality follows the triangle inequality that is a generalization of the well-known theorem from elementary plane geometry, that a side in a triangle is always less than or equal to the sum of the other sides:

|||| Corollary 15.5 The Triangle Inequality

For arbitrary vectors $\mathbf{a}$ and $\mathbf{b}$ in $(\mathbb{R}^n, \cdot)$

$$|\mathbf{a}+\mathbf{b}| \leq |\mathbf{a}| + |\mathbf{b}|\ . \tag{15-13}$$

|||| Exercise 15.6

Prove Corollary 15.5.

Note that from the Cauchy-Schwarz inequality it follows that:

$$-1 \leq \frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a}| \cdot |\mathbf{b}|} \leq 1 \quad . \tag{15-14}$$

Therefore the *angle between two vectors* in $(\mathbb{R}^n, \cdot)$ can be introduced as follows:

|||| Definition 15.7 The Angle Between Vectors

Let $\mathbf{a}$ and $\mathbf{b}$ be two given proper vectors in $(\mathbb{R}^n, \cdot)$ with the coordinates $(a_1, ..., a_n)$ and $(b_1, ..., b_n)$ with respect to the standard basis in $(\mathbb{R}^n, \cdot)$. Then the ***angle between*** $\mathbf{a}$ ***and*** $\mathbf{b}$ is defined as the value θ in interval $[0, \pi]$ that satisfies

$$\cos(\theta) = \frac{\mathbf{a} \cdot \mathbf{b}}{|\mathbf{a}| \cdot |\mathbf{b}|} \quad . \tag{15-15}$$

If $\mathbf{a} \cdot \mathbf{b} = 0$ we say that the two proper vectors are ***orthogonal*** or ***perpendicular*** with respect to each other. This occurs exactly when $\cos(\theta) = 0$, that is, when $\theta = \pi/2$.

15.2 Symmetric Matrices and the Scalar Product

We know the symmetry concept from square matrices:

|||| Definition 15.8

A square matrix $\mathbf{A}$ is ***symmetric*** if it is equal to its own transpose

$$\mathbf{A} = \mathbf{A}^\top \quad , \tag{15-16}$$

that is if $a_{ij} = a_{ji}$ for all elements in the matrix.

What is the relation between symmetric matrices and the scalar product? This we consider here:

|||| Theorem 15.9

Let $\mathbf{v}$ and $\mathbf{w}$ denote two vectors in the vector space $(\mathbb{R}^n, \cdot)$ with scalar product introduced above. If $\mathbf{A}$ is an arbitrary $(n \times n)-$matrix then

$$(\mathbf{A}\,\mathbf{v})\cdot\mathbf{w} = \mathbf{v}\cdot\left(\mathbf{A}^\top\,\mathbf{w}\right) \quad . \tag{15-17}$$

|||| Proof

We use the fact that the scalar product can be expressed as a matrix product:

$$\begin{aligned}(\mathbf{A}\,\mathbf{v})\cdot\mathbf{w} &= (\mathbf{A}\,\mathbf{v})^\top\cdot\mathbf{w} \\ &= \left(\mathbf{v}^\top\mathbf{A}^\top\right)\cdot\mathbf{w} \\ &= \mathbf{v}^\top\cdot\left(\mathbf{A}^\top\mathbf{w}\right) \\ &= \mathbf{v}\cdot\left(\mathbf{A}^\top\mathbf{w}\right) \quad .\end{aligned} \tag{15-18}$$

■

This we can now use to characterize symmetric matrices:

|||| Theorem 15.10

A matrix $\mathbf{A}$ is a symmetric $(n \times n)-$matrix if and only if

$$(\mathbf{A}\,\mathbf{v})\cdot\mathbf{w} = \mathbf{v}\cdot(\mathbf{A}\,\mathbf{w}) \tag{15-19}$$

for all vectors $\mathbf{v}$ and $\mathbf{w}$ in $(\mathbb{R}^n, \cdot)$.

|||| Proof

If $\mathbf{A}$ is symmetric then we have that $\mathbf{A} = \mathbf{A}^\top$ and therefore Equation (15-19) follows directly from Equation (15-17). Conversely, if we assume that (15-19) applies for all $\mathbf{v}$ and $\mathbf{w}$, we will prove that $\mathbf{A}$ is symmetric. But this follows easily just by *choosing* suitable vectors, e.g. $\mathbf{v} = \mathbf{e}_2 = (0, 1, 0, ..., 0)$ and $\mathbf{w} = \mathbf{e}_3 = (0, 0, 1, ..., 0)$ and substitute these into (15-19) as seen below. Note that $\mathbf{A}\,\mathbf{e}_i$ is the i^{th} column vector in $\mathbf{A}$.

$$\begin{aligned} (\mathbf{A}\,\mathbf{e}_2) \cdot \mathbf{e}_3 &= a_{23} \\ &= \mathbf{e}_2 \cdot (\mathbf{A}\,\mathbf{e}_3) \\ &= (\mathbf{A}\,\mathbf{e}_3) \cdot \mathbf{e}_2 \\ &= a_{32} \quad , \end{aligned} \tag{15-20}$$

such that $a_{23} = a_{32}$. Quite similarly for all other choices of indices i and j we get that $a_{ij} = a_{j\,i}$ – and this is what we had set out to prove.

■

A basis a in $(\mathbb{R}^n, \cdot)$ consists (as is known from eNote 11) of n linearly independent vectors $(\mathbf{a}_1, ..., \mathbf{a}_n)$. If in addition the vectors are pairwise orthogonal and have length 1 with respect to the scalar product, then $(\mathbf{a}_1, ..., \mathbf{a}_n)$ is an ***orthonormal basis for*** $(\mathbb{R}^n, \cdot)$:

|||| Definition 15.11

A basis $a = (\mathbf{a}_1, ..., \mathbf{a}_n)$ is an *orthonormal basis* if

$$\mathbf{a}_i \cdot \mathbf{a}_j = \begin{cases} 1 & \text{for } i = j \quad , \\ 0 & \text{for } i \neq j \quad . \end{cases} \tag{15-21}$$

|||| Exercise 15.12

Show that if n vectors $(\mathbf{a}_1, ..., \mathbf{a}_n)$ in $(\mathbb{R}^n, \cdot)$ satisfy Equation (15-21) then $a = (\mathbf{a}_1, ..., \mathbf{a}_n)$ is automatically a *basis* for $(\mathbb{R}^n, \cdot)$, i.e. the vectors are linearly independent and span all of $(\mathbb{R}^n, \cdot)$.

|||| Exercise 15.13

Show that the following 3 vectors $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ constitute an orthonormal basis for $(\mathbb{R}^3, \cdot)$ for any given value of $\theta \in \mathbb{R}$:

$$\begin{aligned} \mathbf{a}_1 &= (\cos(\theta), 0, -\sin(\theta)) \\ \mathbf{a}_2 &= (0, 1, 0) \\ \mathbf{a}_3 &= (\sin(\theta), 0, \cos(\theta)) \quad . \end{aligned} \tag{15-22}$$

If we put the vectors from an orthonormal basis into a matrix as columns we get an ***orthogonal matrix***:

|||| Definition 15.14

An $(n \times n)-$matrix $\mathbf{A}$ is said to be *orthogonal* if the column vectors in $\mathbf{A}$ constitute an orthonormal basis for $(\mathbb{R}^n, \cdot)$, that is if the column vectors are pairwise orthogonal and all have length 1 – as is also expressed in Equation (15-21).

Note that *orthogonal matrices* alternatively (and maybe also more descriptively) could be called *orthonormal*, since the columns in the matrix are not only pairwise orthogonal but also normalized such that they all have length 1. We will follow international tradition and call the matrices orthogonal.

It is easy to check whether a given matrix is orthogonal:

|||| Theorem 15.15

An $(n \times n)-$matrix $\mathbf{Q}$ is orthogonal if and only if

$$\mathbf{Q}^\top \cdot \mathbf{Q} = \mathbf{E}_{n \times n} \quad , \tag{15-23}$$

which is equivalent to

$$\mathbf{Q}^\top = \mathbf{Q}^{-1} \quad . \tag{15-24}$$

|||| Proof

See eNote 7 about the computation of the matrix product and then compare with the condition for orthogonality of the column vectors in $\mathbf{Q}$ (Equation (15-21)).

■

We can now explain the geometric significance of an orthogonal matrix: as a linear map it *preserves lengths of, and angles between, vectors*. That is the content of the following theorem, which follows immediately from Theorems 15.9 and Theorem 15.15:

|||| Theorem 15.16

An $n \times n$ matrix $\mathbf{A}$ is orthogonal if and only if the linear mapping $f : \mathbb{R}^n \to \mathbb{R}^n$ given by $f(\mathbf{x}) = \mathbf{A}\mathbf{x}$ preserves the scalar product, i.e.:

$$(\mathbf{A}\mathbf{x})\cdot(\mathbf{A}\mathbf{y}) = \mathbf{x}\cdot\mathbf{y}, \qquad \text{for any } \mathbf{x}, \mathbf{y} \in \mathbb{R}^n.$$

Orthogonal matrices are *regular* and have determinant ± 1:

|||| Exercise 15.17

Show that for a matrix $\mathbf{A}$ to be orthogonal, it is necessary that

$$|\det(\mathbf{A})| = 1 \quad . \tag{15-25}$$

Show that this condition is not sufficient, thus matrices exist that satisfy this determinant-condition but that are not orthogonal.

|||| Definition 15.18

An orthogonal matrix $\mathbf{Q}$ is called ***special orthogonal*** or ***positive orthogonal*** if $\det(\mathbf{Q}) = 1$ and it is called ***negative orthogonal*** if $\det(\mathbf{Q}) = -1$.

In the literature, orthogonal matrices with determinant 1 are called special orthogonal, and those with determinant -1 are usually not given a name.

|||| Exercise 15.19

Given the matrix

$$\mathbf{A} = \begin{bmatrix} 0 & -a & 0 & a \\ a & 0 & a & 0 \\ 0 & -a & 0 & -a \\ -a & 0 & a & 0 \end{bmatrix} \quad , \quad \text{with } a \in \mathbb{R} \quad . \tag{15-26}$$

Determine the values of a for which $\mathbf{A}$ is orthogonal and state in every case whether $\mathbf{A}$ is positive orthogonal or negative orthogonal.

15.3 Gram–Schmidt Orthonormalization

Here we describe a procedure for determining an orthonormal basis for a subspace of the vector space $(\mathbb{R}^n, \cdot)$. Let U be a $p-$dimensional subspace of $(\mathbb{R}^n, \cdot)$; we assume that U is spanned by p given linearly independent vectors $(\mathbf{u}_1, \cdots, \mathbf{u}_p)$, constituting a basis u for U. Gram–Schmidt orthonormalization aims at constructing a new basis v $= (\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p)$ for the subspace of U from the given basis u such that the new vectors $\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_p$ are *pairwise orthogonal and have length* 1.

|||| Method 15.20 Gram–Schmidt Orthonormalization

Orthonormalization of p linearly independent vectors $\mathbf{u}_1, \cdots, \mathbf{u}_p$ in $(\mathbb{R}^n, \cdot)$:

1. Start by normalizing $\mathbf{u}_1$ and call the result $\mathbf{v}_1$, i.e.:

$$\mathbf{v}_1 = \frac{\mathbf{u}_1}{|\mathbf{u}_1|} \quad . \tag{15-27}$$

2. The next vector $\mathbf{v}_2$ in the basis v is now chosen in span$\{\mathbf{u}_1, \mathbf{u}_2\}$ but such that at the same time $\mathbf{v}_2$ is orthogonal to $\mathbf{v}_1$, i.e. $\mathbf{v}_2 \cdot \mathbf{v}_1 = 0$; finally this vector is normalized. First we construct an *auxiliary vector* $\mathbf{w}_2$.

$$\begin{aligned} \mathbf{w}_2 &= \mathbf{u}_2 - (\mathbf{u}_2 \cdot \mathbf{v}_1)\, \mathbf{v}_1 \\ \mathbf{v}_2 &= \frac{\mathbf{w}_2}{|\mathbf{w}_2|} \quad . \end{aligned} \tag{15-28}$$

Note that $\mathbf{w}_2$ (and therefore also $\mathbf{v}_2$) then being orthogonal to $\mathbf{v}_1$:

$$\begin{aligned} \mathbf{w}_2 \cdot \mathbf{v}_1 &= (\mathbf{u}_2 - (\mathbf{u}_2 \cdot \mathbf{v}_1)\, \mathbf{v}_1) \cdot \mathbf{v}_1 \\ &= \mathbf{u}_2 \cdot \mathbf{v}_1 - (\mathbf{u}_2 \cdot \mathbf{v}_1)\, \mathbf{v}_1 \cdot \mathbf{v}_1 \\ &= \mathbf{u}_2 \cdot \mathbf{v}_1 - (\mathbf{u}_2 \cdot \mathbf{v}_1)\, |\mathbf{v}_1|^2 \\ &= \mathbf{u}_2 \cdot \mathbf{v}_1 - (\mathbf{u}_2 \cdot \mathbf{v}_1) \\ &= 0 \quad . \end{aligned} \tag{15-29}$$

3. We continue in this way

$$\begin{aligned} \mathbf{w}_i &= \mathbf{u}_i - (\mathbf{u}_i \cdot \mathbf{v}_1)\, \mathbf{v}_1 - (\mathbf{u}_i \cdot \mathbf{v}_2)\, \mathbf{v}_2 - \cdots - (\mathbf{u}_i \cdot \mathbf{v}_{i-1})\, \mathbf{v}_{i-1} \\ \mathbf{v}_i &= \frac{\mathbf{w}_i}{|\mathbf{w}_i|} \quad . \end{aligned} \tag{15-30}$$

4. Until the last vector $\mathbf{u}_p$ is used:

$$\begin{aligned} \mathbf{w}_p &= \mathbf{u}_p - \left(\mathbf{u}_p \cdot \mathbf{v}_1\right) \mathbf{v}_1 - \left(\mathbf{u}_p \cdot \mathbf{v}_2\right) \mathbf{v}_2 - \cdots - \left(\mathbf{u}_p \cdot \mathbf{v}_{p-1}\right) \mathbf{v}_{p-1} \\ \mathbf{v}_p &= \frac{\mathbf{w}_p}{|\mathbf{w}_p|} \quad . \end{aligned} \tag{15-31}$$

The constructed v-vectors span the same subspace U as the given linearly independent u-vectors, $U = \text{span}\{\mathbf{u}_1, \cdots, \mathbf{u}_p\} = \text{span}\{\mathbf{v}_1, \cdots, \mathbf{v}_p\}$ and $\text{v} = (\mathbf{v}_1, \cdots, \mathbf{v}_p)$ constituting an orthonormal basis for U.

|||| Example 15.21

In $(\mathbb{R}^4, \cdot)$ we will by the use of the Gram–Schmidt orthonormalization method find an orthonormal basis $v = (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$ for the 3−dimensional subspace U that is spanned by the three given linearly independent (!) vectors having the following coordinates with respect to the standard e-basis in $\mathbb{R}^4$:

$$\mathbf{u}_1 = (2,2,4,1) \quad , \quad \mathbf{u}_2 = (0,0,-5,-5) \quad , \quad \mathbf{u}_3 = (5,3,3,-3) \quad .$$

We construct the new basis vectors with respect to the standard e-basis in $\mathbb{R}^4$ by working through the orthonormalization procedure. There are 3 'steps' since there are in this example 3 linearly independent vectors in U :

1.
$$\mathbf{v}_1 = \frac{\mathbf{u}_1}{|\mathbf{u}_1|} = \frac{1}{5}(2,2,4,1) \quad . \tag{15-32}$$

2.
$$\begin{aligned} \mathbf{w}_2 &= \mathbf{u}_2 - (\mathbf{u}_2 \cdot \mathbf{v}_1)\,\mathbf{v}_1 = \mathbf{u}_2 + 5\mathbf{v}_1 = (2,2,-1,-4) \\ \mathbf{v}_2 &= \frac{\mathbf{w}_2}{|\mathbf{w}_2|} = \frac{1}{5}(2,2,-1,-4) \quad . \end{aligned} \tag{15-33}$$

3.
$$\begin{aligned} \mathbf{w}_3 &= \mathbf{u}_3 - (\mathbf{u}_3 \cdot \mathbf{v}_1)\,\mathbf{v}_1 - (\mathbf{u}_3 \cdot \mathbf{v}_2)\,\mathbf{v}_2 = \mathbf{u}_3 - 5\mathbf{v}_1 - 5\mathbf{v}_2 = (1,-1,0,0) \\ \mathbf{v}_3 &= \frac{\mathbf{w}_3}{|\mathbf{w}_3|} = \frac{1}{\sqrt{2}}(1,-1,0,0) \quad . \end{aligned} \tag{15-34}$$

Thus we have constructed an orthonormal basis for the subspace U consisting of those vectors that with respect to the standard basis have the coordinates:

$$\mathbf{v}_1 = \frac{1}{5} \cdot (2,2,4,1) \quad , \quad \mathbf{v}_2 = \frac{1}{5} \cdot (2,2,-1,-4) \quad , \quad \mathbf{v}_3 = \frac{1}{\sqrt{2}} \cdot (1,-1,0,0) \quad .$$

We can check that this is really an orthonormal basis by posing the vectors as columns in a matrix, which then is of the type (4×3). Like this:

$$\mathbf{V} = \begin{bmatrix} 2/5 & 2/5 & 1/\sqrt{2} \\ 2/5 & 2/5 & -1/\sqrt{2} \\ 4/5 & -1/5 & 0 \\ 1/5 & -4/5 & 0 \end{bmatrix} \tag{15-35}$$

The matrix $\mathbf{V}$ cannot be an orthogonal matrix (because of the type), but nevertheless $\mathbf{V}$ can satisfy the following equation, which shows that the three new basis vectors indeed are pairvise orthogonal and all have length 1 !

$$\mathbf{V}^\top \cdot \mathbf{V} = \begin{bmatrix} 2/5 & 2/5 & 4/5 & 1/5 \\ 2/5 & 2/5 & -1/5 & -4/5 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} 2/5 & 2/5 & 1/\sqrt{2} \\ 2/5 & 2/5 & -1/\sqrt{2} \\ 4/5 & -1/5 & 0 \\ 1/5 & -4/5 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad . \tag{15-36}$$

|||| Exercise 15.22

In $(\mathbb{R}^4, \cdot)$ the following vectors are given with respect to the standard basis e:

$$\mathbf{u}_1 = (1,1,1,1) \quad , \quad \mathbf{u}_2 = (3,1,1,3) \quad , \quad \mathbf{u}_3 = (2,0,-2,4) \quad , \quad \mathbf{u}_4 = (1,1,-1,3) \quad .$$

We let U denote the subspace in $(\mathbb{R}^4, \cdot)$ that is spanned by the four given vectors, that is

$$U = \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4\} \quad . \tag{15-37}$$

1. Show that u $= (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$ is a basis for U and find coordinates for $\mathbf{u}_4$ with respect to this basis.

2. State an orthonormal basis for U.

|||| Example 15.23

In $(\mathbb{R}^3, \cdot)$ a given first unit vector $\mathbf{v}_1$ is required for the new orthonormal basis v$= (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$ and the task is to find the two other vectors in the basis. Let us assume that the given vector is $\mathbf{v}_1 = (3,0,4)/5$. We see immediately that e.g. $\mathbf{v}_2 = (0,1,0)$ is a unit vector that is orthogonal to $\mathbf{v}_1$. A last vector for the orthonormal basis can then be found directly using the *cross product*: $\mathbf{v}_3 = \mathbf{v}_1 \times \mathbf{v}_2 = \frac{1}{5} \cdot (-4,0,3)$.

15.4 The Orthogonal Complement to a Subspace

Let U be a subspace in $(\mathbb{R}^n, \cdot)$ that is spanned by p given linearly independent vectors, $U = \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_p\}$. The set of those vectors in $(\mathbb{R}^n, \cdot)$ that are all orthogonal to all vectors in U is itself a subspace of $(\mathbb{R}^n, \cdot)$, and it has the dimension $n - p$:

|||| Definition 15.24

The ***orthogonal complement*** to a subspace U of $(\mathbb{R}^n, \cdot)$ is denoted $U^\perp$ and consists of all vectors in $(\mathbb{R}^n, \cdot)$ that are orthogonal to all vectors in U:

$$U^\perp = \{ \mathbf{x} \in \mathbb{R}^n \,|\, \mathbf{x} \cdot \mathbf{u} = 0 \,, \text{ for all } \ \mathbf{u} \in U \} \quad . \tag{15-38}$$

|||| Theorem 15.25

The orthogonal complement $U^\perp$ to a given $p-$dimensional subspace U of $(\mathbb{R}^n, \cdot)$ is itself a subspace in $(\mathbb{R}^n, \cdot)$ and it has dimension $\dim(U^\perp) = n - p$.

|||| Proof

It is easy to check all subspace-properties for $U^\perp$; it is clear that if $\mathbf{a}$ and $\mathbf{b}$ is orthogonal to all vectors in U and k is a real number, then $\mathbf{a} + k\mathbf{b}$ are also orthogonal to all vectors in U. Since the only vector that is orthogonal to itself is $\mathbf{0}$ this is also the only vector in the intersection: $U \cap U^\perp = \{\mathbf{0}\}$. If we let v$=$ $(\mathbf{v}_1, \cdots, \mathbf{v}_p)$ denote an *orthonormal basis* for U and w$=$ $(\mathbf{w}_1, \cdots, \mathbf{w}_r)$ an orthonormal basis for $U^\perp$, then $(\mathbf{v}_1, \cdots, \mathbf{v}_p, \mathbf{w}_1, \cdots, \mathbf{w}_r)$ is an orthonormal basis for the subspace $S = \text{span}\{\mathbf{v}_1, \cdots, \mathbf{v}_p, \mathbf{w}_1, \cdots, \mathbf{w}_r\}$ in $(\mathbb{R}^n, \cdot)$. If we now assume that S is not all of $(\mathbb{R}^n, \cdot)$, then the basis for S can be extended with at least one vector such that the extended system is linearly independent in $(\mathbb{R}^n, \cdot)$; by this we get - through the last step in the Gram–Schmidt method - a new vector that is orthogonal to all vectors in U but which is not an element in $U^\perp$; and thus we get a contradiction, since $U^\perp$ are defined to be *all* those vectors in $(\mathbb{R}^n, \cdot)$ that are orthogonal to every vector in U. Therefore the assumption that S is not all of $(\mathbb{R}^n, \cdot)$ is wrong. I.e. $S = \mathbb{R}^n$ and therefore $r + p = n$, such that $\dim(U^\perp) = r = n - p$; and this is what we had to prove.

■

|||| Example 15.26

The orthogonal complement to $U = \text{span}\{\mathbf{a}, \mathbf{b}\}$ in $\mathbb{R}^3$ (for linearly independent vectors – and therefore proper vectors – $\mathbf{a}$ and $\mathbf{b}$) is $U^\perp = \text{span}\{\mathbf{a} \times \mathbf{b}\}$.

|||| Exercise 15.27

Determine the orthogonal complement to the subspace $U = \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ in $(\mathbb{R}^4, \cdot)$, when the spanning vectors are given by their respective coordinates with respect to the standard basis e in $\mathbb{R}^4$ as:

$$\mathbf{u}_1 = (1,1,1,1) \quad , \quad \mathbf{u}_2 = (3,1,1,3) \quad , \quad \mathbf{u}_3 = (2,0,-2,4) \quad . \tag{15-39}$$

15.5 The Spectral Theorem for Symmetric Matrices

We will now start to formulate the spectral theorem and start with the following non-trivial observation about symmetric matrices:

|||| Theorem 15.28

Let $\mathbf{A}$ denote a symmetric $(n \times n)-$matrix. Then the characteristic polynomial $\mathcal{K}_{\mathbf{A}}(\lambda)$ for $\mathbf{A}$ has exactly n real roots (counted with multiplicity):

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \quad . \tag{15-40}$$

I.e. $\mathbf{A}$ has n real eigenvalues (counted with multiplicity).

If e.g. $\{7,3,3,2,2,2,1\}$ are the roots of $\mathcal{K}_{\mathbf{A}}(\lambda)$ for a $(7 \times 7)-$matrix $\mathbf{A}$, then these roots must be represented *with their respective multiplicity* in the eigenvalue-list:

$$\lambda_1 = 7 \geq \lambda_2 = 3 \geq \lambda_3 = 3 \geq \lambda_4 = 2 \geq \lambda_5 = 2 \geq \lambda_6 = 2 \geq \lambda_7 = 1 \quad .$$

Since Theorem 15.28 expresses a decisive property about symmetric matrices, we will here give a proof of the theorem:

|||| Proof

From the fundamental theorem of algebra we know that $\mathcal{K}_{\mathbf{A}}(\lambda)$ has exactly n complex roots - but we do not know whether the roots are real; this is what we will prove. So we let $\alpha + i\,\beta$ be a complex root of $\mathcal{K}_{\mathbf{A}}(\lambda)$ and we will then show that $\beta = 0$. Note that α and β naturally both are real numbers.

Therefore we have

$$\det\left(\mathbf{A} - (\alpha + i\,\beta)\mathbf{E}\right) = 0 \quad , \tag{15-41}$$

and thus also that

$$\det\left(\mathbf{A} - (\alpha + i\,\beta)\mathbf{E}\right) \cdot \det\left(\mathbf{A} - (\alpha - i\,\beta)\mathbf{E}\right) = 0 \tag{15-42}$$

such that

$$\begin{aligned} \det\left((\mathbf{A} - (\alpha + i\,\beta)\mathbf{E}) \cdot (\mathbf{A} - (\alpha - i\,\beta)\mathbf{E})\right) &= 0 \\ \det\left((\mathbf{A} - \alpha\,\mathbf{E})^2 + \beta^2\,\mathbf{E}\right) &= 0 \quad . \end{aligned} \tag{15-43}$$

The last equation yields that the rank of the real matrix $\left((\mathbf{A} - \alpha\,\mathbf{E})^2 + \beta^2\,\mathbf{E}\right)$ is less than n; this now means (see eNote 6) that proper real solutions $\mathbf{x}$ to the corresponding system of equations must exist.

$$\left((\mathbf{A} - \alpha\,\mathbf{E})^2 + \beta^2\,\mathbf{E}\right)\mathbf{x} = \mathbf{0} \quad . \tag{15-44}$$

Let us choose such a proper real solution $\mathbf{v}$ to (15-44) with $|\mathbf{v}| > 0$. Using the assumption that $\mathbf{A}$ (and therefore $\mathbf{A} - \alpha\mathbf{E}$ also) is assumed to be symmetric, we have:

$$\begin{aligned} 0 &= \left(\left((\mathbf{A} - \alpha\,\mathbf{E})^2 + \beta^2\,\mathbf{E}\right)\mathbf{v}\right) \cdot \mathbf{v} \\ &= \left((\mathbf{A} - \alpha\,\mathbf{E})^2\,\mathbf{v}\right) \cdot \mathbf{v} + \beta^2\,(\mathbf{v} \cdot \mathbf{v}) \\ &= ((\mathbf{A} - \alpha\,\mathbf{E})\,\mathbf{v}) \cdot ((\mathbf{A} - \alpha\,\mathbf{E})\,\mathbf{v}) + \beta^2|\mathbf{v}|^2 \\ &= |\,(\mathbf{A} - \alpha\,\mathbf{E})\,\mathbf{v}|^2 + \beta^2|\mathbf{v}|^2 \quad . \end{aligned} \tag{15-45}$$

Since $|\mathbf{v}| > 0$ we are bound to conclude that $\beta = 0$, because all terms in the last expression are non-negative. And this is what we had to prove.

■

|||| Exercise 15.29

Where was it exactly that we *actually used* the symmetry of $\mathbf{A}$ in the above proof?

To every eigenvalue λ_i for a given matrix **A** is associated an eigenvector space E_{λ_i}, which is subspace of $(\mathbb{R}^n, \cdot)$. If two or more eigenvalues for a given matrix are equal, i.e. if we have a multiple root (e.g. k times) $\lambda_i = \lambda_{i+1} = \cdots \lambda_{thati+k-1}$ of the characteristic polynomial, then the corresponding eigenvector spaces are of course also equal: $E_{\lambda_i} = E_{\lambda_{i+1}} = \cdots E_{\lambda_{i+k-1}}$. We will see below in Theorem 15.31 that for symmetric matrices the dimension of the common eigenvector space E_{λ_i} is exactly equal to the algebraic multiplicity k of the eigenvalue λ_i.

If two eigenvalues λ_i and λ_j for a *symmetric* matrix are *different*, then the two corresponding eigenvector spaces are *orthogonal*, $E_{\lambda_i} \perp E_{\lambda_j}$ in the following sense:

|||| Theorem 15.30

Let **A** be a symmetric matrix and let λ_1 and λ_2 be two different eigenvalues for **A** and let $\mathbf{v}_1$ and $\mathbf{v}_2$ denote two corresponding eigenvectors. Then $\mathbf{v}_1 \cdot \mathbf{v}_2 = 0$, i.e. they are orthogonal.

|||| Proof

Since **A** is symmetric we have from (15-19):

$$\begin{aligned} 0 &= (\mathbf{A}\mathbf{v}_1) \cdot \mathbf{v}_2 - \mathbf{v}_1 \cdot (\mathbf{A}\mathbf{v}_2) \\ &= \lambda_1 \mathbf{v}_1 \cdot \mathbf{v}_2 - \mathbf{v}_1 \cdot (\lambda_2 \mathbf{v}_2) \\ &= \lambda_1 \mathbf{v}_1 \cdot \mathbf{v}_2 - \lambda_2 \mathbf{v}_1 \cdot \mathbf{v}_2 \\ &= (\lambda_1 - \lambda_2)\, \mathbf{v}_1 \cdot \mathbf{v}_2 \quad , \end{aligned} \tag{15-46}$$

and since $\lambda_1 \neq \lambda_2$ we therefore get the following conclusion: $\mathbf{v}_1 \cdot \mathbf{v}_2 = 0$, and this is what we had to prove.

■

We can now formulate one of the most widely applied results for symmetric matrices, the ***spectral theorem for symmetric matrices*** that, with good reason, is also called the theorem about ***diagonalization of symmetric matrices***:

|||| Theorem 15.31

Let $\mathbf{A}$ denote a *symmetric* $(n \times n)-$*matrix*. Then a special orthogonal matrix $\mathbf{Q}$ exists such that

$$\mathbf{\Lambda} = \mathbf{Q}^{-1}\mathbf{A}\mathbf{Q} = \mathbf{Q}^{\top}\mathbf{A}\mathbf{Q} \quad \text{is a diagonal matrix} \quad . \tag{15-47}$$

I.e. that a real symmetric matrix can be diagonalized by application of a positive orthogonal substitution, see eNote 14.

The diagonal matrix can be constructed very simply from the n real eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ of $\mathbf{A}$ as:

$$\mathbf{\Lambda} = \mathbf{diag}(\lambda_1, \lambda_2, ..., \lambda_n) = \begin{bmatrix} \lambda_1 & 0 & \cdot & 0 \\ 0 & \lambda_2 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \lambda_n \end{bmatrix} \quad , \tag{15-48}$$

Remember: A symmetric matrix has exactly n real eigenvalues when we count these with multiplicity.

The special orthogonal matrix $\mathbf{Q}$ is next constructed as columns of the matrix by using the eigenvectors from the corresponding eigenvector-spaces $E_{\lambda_1}, E_{\lambda_2}, \cdots, E_{\lambda_n}$ in the corresponding order:

$$\mathbf{Q} = [\mathbf{v}_1 \; \mathbf{v}_2 \; \cdots \mathbf{v}_n] \quad , \tag{15-49}$$

where $\mathbf{v}_1 \in E_{\lambda_1}$, $\mathbf{v}_2 \in E_{\lambda_2}$, $\cdots$, $\mathbf{v}_n \in E_{\lambda_n}$, and the choice of eigenvectors in the respective eigenvector spaces is made so that

1. Any eigenvectors corresponding to the same eigenvalue are chosen orthogonal (use Gram–Schmidt orthogonalization in every common eigenvector space)

2. The chosen eigenvectors are normalized to have length 1.

3. The resulting matrix $\mathbf{Q}$ has determinant 1 (if not then multiply one of the chosen eigenvectors by -1 to flip the sign of the determinant)

That this is so follows from the results and remarks – we go through a series of enlightening examples below.

15.6 Examples of Diagonalization

Here are some typical examples that show how one diagonalizes some small symmetric matrices, i.e. symmetric matrices of type (2×2) or type (3×3):

|||| Example 15.32 Diagonalization by Orthogonal Substitution

A symmetric $(3 \times 3)-$matrix $\mathbf{A}$ is given as:

$$\mathbf{A} = \begin{bmatrix} 2 & -2 & 1 \\ -2 & 5 & -2 \\ 1 & -2 & 2 \end{bmatrix} \quad . \tag{15-50}$$

We will determine a special orthogonal matrix $\mathbf{Q}$ such that $\mathbf{Q}^{-1}\mathbf{AQ}$ is a diagonal matrix:

$$\mathbf{Q}^{-1}\mathbf{AQ} = \mathbf{Q}^{\top}\mathbf{AQ} = \mathbf{\Lambda} \quad . \tag{15-51}$$

First we determine the eigenvalues for $\mathbf{A}$: The characteristic polynomial for $\mathbf{A}$ is

$$\mathcal{K}_{\mathbf{A}}(\lambda) = \det\left(\begin{bmatrix} 2-\lambda & -2 & 1 \\ -2 & 5-\lambda & -2 \\ 1 & -2 & 2-\lambda \end{bmatrix}\right) = (\lambda - 1)^2 \cdot (7 - \lambda) \quad , \tag{15-52}$$

so $\mathbf{A}$ has the eigenvalues $\lambda_1 = 7$, $\lambda_2 = 1$, and $\lambda_3 = 1$. Because of this we already know through Theorem 15.31 that it is possible to construct a positive orthogonal matrix $\mathbf{Q}$ such that

$$\mathbf{Q}^{-1}\mathbf{AQ} = \mathbf{diag}(7, 1, 1) = \begin{bmatrix} 7 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad . \tag{15-53}$$

The rest of the problem now consists in finding the eigenvectors for $\mathbf{A}$ that can be used as columns in the orthogonal matrix $\mathbf{Q}$.

Eigenvectors for $\mathbf{A}$ corresponding to the eigenvalue $\lambda_1 = 7$ are found by solving the homogeneous system of equations that has the coefficient matrix

$$\mathbf{K_A}(7) = \mathbf{A} - 7\mathbf{E} = \begin{bmatrix} -5 & -2 & 1 \\ -2 & -2 & -2 \\ 1 & -2 & -5 \end{bmatrix} \quad , \tag{15-54}$$

which by suitable row operations is seen to have

$$\mathrm{rref}(\mathbf{K_A}(7)) = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{bmatrix} \quad . \tag{15-55}$$

The eigenvector solutions to the corresponding homogeneous system of equations are seen to be

$$\mathbf{u} = t \cdot (1,-2,1) \quad , \quad t \in \mathbb{R} \quad , \tag{15-56}$$

such that $E_7 = \text{span}\{(1,-2,1)\}$. The normalized eigenvector $\mathbf{v}_1 = (1/\sqrt{6}) \cdot (1,-2,1)$ is therefore an orthonormal basis for E_7 (and it can also be used as the first column vector in the wanted $\mathbf{Q}$:

$$\mathbf{Q} = \begin{bmatrix} 1/\sqrt{6} & * & * \\ -2/\sqrt{6} & * & * \\ 1/\sqrt{6} & * & * \end{bmatrix} \quad . \tag{15-57}$$

We know from Theorem 15.31 that the two last columns are found by similarly determining all eigenvectors E_1 belonging to the eigenvalue $\lambda_2 = \lambda_3 = 1$ and then choosing two orthonormal eigenvectors from E_1.

The reduction matrix corresponding to the eigenvalue 1 is

$$\mathbf{K_A}(1) = \mathbf{A} - \mathbf{E} = \begin{bmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{bmatrix}, \tag{15-58}$$

which again by suitable row operations is seen to have

$$\text{rref}(\mathbf{K_A}(1)) = \begin{bmatrix} 1 & -2 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad . \tag{15-59}$$

The eigenvector solutions to the corresponding homogeneous system of equations are seen to be

$$\mathbf{u} = t_1 \cdot (2,1,0) + t_2 \cdot (-1,0,1) \quad , \quad t_1 \in \mathbb{R} \quad , \quad t_2 \in \mathbb{R} \quad , \tag{15-60}$$

such that $E_1 = \text{span}\{(-1,0,1),(2,1,0)\}$.

We find an orthonormal basis for E_1 using the Gram–Schmidt orthonormalization of $\text{span}\{(-1,0,1),(2,1,0)\}$ like this: Since we have already defined $\mathbf{v}_1$ we put $\mathbf{v}_2$ to be

$$\mathbf{v}_2 = \frac{(-1,0,1)}{|(-1,0,1)|} = (1/\sqrt{2}) \cdot (-1,0,1) \quad , \tag{15-61}$$

and then as in the Gram–Schmidt process:

$$\mathbf{w}_3 = (2,1,0) - ((2,1,0) \bullet \mathbf{v}_2) \cdot \mathbf{v}_2 = (1,1,1) \quad . \tag{15-62}$$

By normalization we finally get $\mathbf{v}_3 = (1/\sqrt{3}) \cdot (1,1,1)$ and then we finally have all the ingredients to the wanted orthogonal matrix $\mathbf{Q}$:

$$\mathbf{Q} = [\mathbf{v}_1\, \mathbf{v}_2\, \mathbf{v}_3] = \begin{bmatrix} 1/\sqrt{6} & -1/\sqrt{2} & 1/\sqrt{3} \\ -2/\sqrt{6} & 0 & 1/\sqrt{3} \\ 1/\sqrt{6} & 1/\sqrt{2} & 1/\sqrt{3} \end{bmatrix} \quad . \tag{15-63}$$

Finally we investigate whether the chosen eigenvectors give a positive orthogonal matrix. Since

$$\det\left(\begin{bmatrix} 1 & -1 & 1 \\ -2 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix}\right) = -6 < 0 \quad , \tag{15-64}$$

$\mathbf{Q}$ has negative determinant. A special orthogonal matrix is found by multiplying one of the columns of $\mathbf{Q}$ by -1, e.g. the last one. Note that a vector $\mathbf{v}$ is an eigenvector for $\mathbf{A}$ if and only if $-\mathbf{v}$ is also an eigenvector for $\mathbf{A}$. Therefore we have that

$$\mathbf{Q} = \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & (-\mathbf{v}_3) \end{pmatrix} = \begin{bmatrix} 1/\sqrt{6} & -1/\sqrt{2} & -1/\sqrt{3} \\ -2/\sqrt{6} & 0 & -1/\sqrt{3} \\ 1/\sqrt{6} & 1/\sqrt{2} & -1/\sqrt{3} \end{bmatrix} \tag{15-65}$$

is a *positive* orthogonal matrix that diagonalizes $\mathbf{A}$.

This is checked by a direct computation:

$$\begin{aligned} &\mathbf{Q}^{-1}\mathbf{A}\mathbf{Q} = \mathbf{Q}^{\top}\mathbf{A}\mathbf{Q} \\ &= \begin{bmatrix} 1/\sqrt{6} & -2/\sqrt{6} & 1/\sqrt{6} \\ -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ -1/\sqrt{3} & -1/\sqrt{3} & -1/\sqrt{3} \end{bmatrix} \cdot \begin{bmatrix} 2 & -2 & 1 \\ -2 & 5 & -2 \\ 1 & -2 & 3 \end{bmatrix} \cdot \begin{bmatrix} 1/\sqrt{6} & -1/\sqrt{2} & -1/\sqrt{3} \\ -2/\sqrt{6} & 0 & -1/\sqrt{3} \\ 1/\sqrt{6} & 1/\sqrt{2} & -1/\sqrt{3} \end{bmatrix} \\ &= \begin{bmatrix} 7 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad , \end{aligned} \tag{15-66}$$

which we wanted to show.

We should finally remark here that, since we are in three dimensions, instead of using Gram–Schmidt orthonormalization for the determination of $\mathbf{v}_3$ we could have used the cross product $\mathbf{v}_1 \times \mathbf{v}_2$ (see 15.23):

$$\mathbf{v}_3 = \mathbf{v}_1 \times \mathbf{v}_2 = (1/\sqrt{3}) \cdot (-1, -1, -1) \quad . \tag{15-67}$$

|||| Example 15.33 Diagonalization by Orthogonal Substitution

A symmetric $(2 \times 2)-$matrix $\mathbf{A}$ is given as:

$$\mathbf{A} = \begin{bmatrix} 11 & -12 \\ -12 & 4 \end{bmatrix} \quad . \tag{15-68}$$

We will determine a special orthogonal matrix $\mathbf{Q}$ such that $\mathbf{Q}^{-1}\mathbf{A}\mathbf{Q}$ is a diagonal matrix:

$$\mathbf{Q}^{-1}\mathbf{A}\mathbf{Q} = \mathbf{Q}^{\top}\mathbf{A}\mathbf{Q} = \mathbf{\Lambda} \quad . \tag{15-69}$$

First we determine the eigenvalues for $\mathbf{A}$: The characteristic polynomial for $\mathbf{A}$ is

$$\mathcal{K}_{\mathbf{A}}(\lambda) = \det\left(\begin{bmatrix} 11-\lambda & -12 \\ -12 & 4-\lambda \end{bmatrix}\right) = (\lambda - 20)\cdot(\lambda+5) \quad , \tag{15-70}$$

so $\mathbf{A}$ has the eigenvalues $\lambda_1 = 20$ and $\lambda_2 = -5$. Therefore we now have:

$$\mathbf{\Lambda} = \begin{bmatrix} 20 & 0 \\ 0 & -5 \end{bmatrix} \quad . \tag{15-71}$$

The eigenvectors for $\mathbf{A}$ corresponding to the eigenvalue $\lambda_1 = 20$ are found by solving the homogeneous system of equations having the coefficient matrix

$$\mathbf{K}_{\mathbf{A}}(20) = \mathbf{A} - 20\mathbf{E} = \begin{bmatrix} -9 & -12 \\ -12 & -16 \end{bmatrix} \quad , \tag{15-72}$$

which, through suitable row operations, is shown to have the equivalent reduced matrix:

$$\mathrm{rref}(\mathbf{K}_{\mathbf{A}}(20)) = \begin{bmatrix} 3 & 4 \\ 0 & 0 \end{bmatrix} \quad . \tag{15-73}$$

The eigenvector solutions to the corresponding homogeneous system of equations are found to be

$$\mathbf{u} = t\cdot(4,-3) \quad , \quad t \in \mathbb{R} \quad , \tag{15-74}$$

such that $E_{20} = \mathrm{span}\{(4,-3)\}$. The normalized eigenvector $\mathbf{v}_1 = (1/5)\cdot(4,-3)$ is therefore an orthonormal basis for E_{20} (and it can therefore be used as the first column vector in the wanted $\mathbf{Q}$:

$$\mathbf{Q} = \begin{bmatrix} 4/5 & * \\ -3/5 & * \end{bmatrix} \quad . \tag{15-75}$$

The last column in $\mathbf{Q}$ is an eigenvector corresponding to the second eigenvalue $\lambda_2 = -5$ and can therefore be found from the general solution E_{-5} to the homogeneous system of equations having the coefficient matrix

$$\mathbf{K}_{\mathbf{A}}(-5) = \mathbf{A} - 5\cdot\mathbf{E} = \begin{bmatrix} 16 & -12 \\ -12 & 9 \end{bmatrix} \quad , \tag{15-76}$$

but since we know that the wanted eigenvector is orthogonal to the eigenvector $\mathbf{v}_1$ we can just use a vector perpendicular to the first eigenvector, $\mathbf{v}_2 = (1/5)\cdot(3,4)$, evidently a unit vector, that is orthogonal to $\mathbf{v}_1$. It is easy to check that $\mathbf{v}_2$ is an eigenvector for $\mathbf{A}$ corresponding to the eigenvalue -5:

$$\mathbf{K}_{\mathbf{A}}(-5)\cdot\mathbf{v}_2 = \begin{bmatrix} 16 & -12 \\ -12 & 9 \end{bmatrix}\cdot\begin{bmatrix} 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad . \tag{15-77}$$

Therefore we substitute $\mathbf{v}_2$ as the second column in $\mathbf{Q}$ and get

$$\mathbf{Q} = \begin{bmatrix} 4/5 & 3/5 \\ -3/5 & 4/5 \end{bmatrix} \quad . \tag{15-78}$$

This matrix has the determinant $\det(\mathbf{Q}) = 1 > 0$, so $\mathbf{Q}$ is a positive orthogonal substitution matrix satisfying that $\mathbf{Q}^{-1}\mathbf{AQ}$ is a diagonal matrix:

$$\begin{aligned} \mathbf{Q}^{-1}\mathbf{AQ} &= \mathbf{Q}^{\top}\mathbf{AQ} \\ &= \begin{bmatrix} 4/5 & -3/5 \\ 3/5 & 4/5 \end{bmatrix} \cdot \begin{bmatrix} 11 & -12 \\ -12 & 4 \end{bmatrix} \cdot \begin{bmatrix} 4/5 & 3/5 \\ -3/5 & 4/5 \end{bmatrix} \\ &= \begin{bmatrix} 20 & 0 \\ 0 & -5 \end{bmatrix} \\ &= \mathbf{diag}(20, -5) = \mathbf{\Lambda} \quad . \end{aligned} \tag{15-79}$$

|||| Example 15.34 Diagonalization by Orthogonal Substitution

A symmetric $(3 \times 3)-$matrix $\mathbf{A}$ is given like this:

$$\mathbf{A} = \begin{bmatrix} 7 & -2 & 0 \\ -2 & 6 & -2 \\ 0 & -2 & 5 \end{bmatrix} \quad . \tag{15-80}$$

We will determine a positive orthogonal matrix $\mathbf{Q}$ such that $\mathbf{Q}^{-1}\mathbf{AQ}$ is a diagonal matrix:

$$\mathbf{Q}^{-1}\mathbf{AQ} = \mathbf{Q}^{\top}\mathbf{AQ} = \mathbf{\Lambda} \quad . \tag{15-81}$$

First we determine the eigenvalues for $\mathbf{A}$: The characteristic polynomial for $\mathbf{A}$ is

$$\mathcal{K}_{\mathbf{A}}(\lambda) = \det\left(\begin{bmatrix} 7-\lambda & -2 & 1 \\ -2 & 6-\lambda & -2 \\ 1 & -2 & 5-\lambda \end{bmatrix}\right) = -(\lambda-3)\cdot(\lambda-6)\cdot(\lambda-9) \quad , \tag{15-82}$$

from which we read the three different eigenvalues $\lambda_1 = 9$, $\lambda_2 = 6$, and $\lambda_3 = 3$ and then the diagonal matrix we are on the road to describe as $\mathbf{Q}^{-1}\mathbf{AQ}$:

$$\mathbf{\Lambda} = \mathbf{diag}(9,6,3) = \begin{bmatrix} 9 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 3 \end{bmatrix} \tag{15-83}$$

The eigenvectors for $\mathbf{A}$ corresponding to the eigenvalue $\lambda_3 = 3$ are found by solving the homogeneous system of equations having the coefficient matrix

$$\mathbf{K}_{\mathbf{A}}(3) = \mathbf{A} - 3\cdot\mathbf{E} = \begin{bmatrix} 4 & -2 & 0 \\ -2 & 3 & -2 \\ 0 & -2 & 2 \end{bmatrix} \quad , \tag{15-84}$$

which through suitable row operations is seen to have

$$\text{rref}(\mathbf{K_A}(3)) = \begin{bmatrix} 2 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{bmatrix} \quad . \tag{15-85}$$

The eigenvector solutions to the corresponding homogeneous system of equations are found to be

$$\mathbf{u}_3 = t \cdot (1,2,2) \quad , \quad t \in \mathbb{R} \quad , \tag{15-86}$$

such that $E_3 = \text{span}\{(1,2,2)\}$. The normalized eigenvector $\mathbf{v}_1 = (1/3) \cdot (1,2,2)$ is therefore an orthonormal basis for E_3 so it can be used as the *third column vector* in the wanted $\mathbf{Q}$; note that we have just found the eigenvector space to the *third eigenvalue* on the list of eigenvalues for $\mathbf{A}$:

$$\mathbf{Q} = \begin{bmatrix} * & * & 1/3 \\ * & * & 2/3 \\ * & * & 2/3 \end{bmatrix} \quad . \tag{15-87}$$

We know from Theorem 15.31 that the two last columns are found by similarly determining the eigenvector space E_6 corresponding to eigenvalue $\lambda_2 = 6$, and the eigenvector space E_9 corresponding to the eigenvalue $\lambda_1 = 9$.

For $\lambda_2 = 6$ we have:

$$\mathbf{K_A}(6) = \mathbf{A} - 6 \cdot \mathbf{E} = \begin{bmatrix} 1 & -2 & 0 \\ -2 & 0 & -2 \\ 0 & -2 & -1 \end{bmatrix} \quad , \tag{15-88}$$

which by suitable row operations is found to have the following equivalent reduced matrix:

$$\text{rref}(\mathbf{K_A}(6)) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad . \tag{15-89}$$

The eigenvector solutions to the corresponding homogeneous system of equations are found to be

$$\mathbf{u}_2 = t \cdot (-2,-1,2) \quad , \quad t \in \mathbb{R} \quad , \tag{15-90}$$

so that $E_6 = \text{span}\{(-2,-1,2)\}$. The normalized eigenvector $\mathbf{v}_2 = (1/3) \cdot (-2,-1,2)$ is therefore an orthonormal basis for E_6 (and it can therefore be used as the *second column vector* in the wanted $\mathbf{Q}$:

$$\mathbf{Q} = \begin{bmatrix} * & -2/3 & 1/3 \\ * & -1/3 & 2/3 \\ * & 2/3 & 2/3 \end{bmatrix} \quad . \tag{15-91}$$

Instead of determining the eigenvector space E_9 for the last eigenvalue $\lambda_1 = 9$ in the same way we use the fact that this eigenvector space is spanned by a vector $\mathbf{v}_1$ that is orthogonal to both $\mathbf{v}_3$ and $\mathbf{v}_2$, so we can use $\mathbf{v}_1 = \mathbf{v}_2 \times \mathbf{v}_3 = (1/3) \cdot (-2, 2, -1)$, and then we finally get

$$\mathbf{Q} = \begin{bmatrix} -2/3 & -2/3 & 1/3 \\ 2/3 & -1/3 & 2/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix} \quad . \tag{15-92}$$

This matrix is positive orthogonal since $\det(\mathbf{Q}) = 1 > 0$, and therefore we have determined a positive orthogonal matrix $\mathbf{Q}$ that diagonalizes $\mathbf{A}$ to the diagonal matrix $\mathbf{\Lambda}$. This is easily proved by direct computation:

$$\begin{aligned} &\mathbf{Q}^{-1}\mathbf{A}\mathbf{Q} = \mathbf{Q}^{\top}\mathbf{A}\mathbf{Q} \\ &= \begin{bmatrix} -2/3 & 2/3 & -1/3 \\ -2/3 & -1/3 & 2/3 \\ 1/3 & 2/3 & 2/3 \end{bmatrix} \cdot \begin{bmatrix} 7 & -2 & 0 \\ -2 & 6 & -2 \\ 0 & -2 & 5 \end{bmatrix} \cdot \begin{bmatrix} -2/3 & -2/3 & 1/3 \\ 2/3 & -1/3 & 2/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix} \\ &= \begin{bmatrix} 9 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 3 \end{bmatrix} \\ &= \mathbf{diag}(9, 6, 3) = \mathbf{\Lambda} \quad . \end{aligned} \tag{15-93}$$

15.7 Controlled Construction of Symmetric Matrices

In the light of the above examples it is clear that if only we can construct all orthogonal (2×2)- and (3×3)-matrices $\mathbf{Q}$ (or for that matter $(n \times n)$-matrices), then we can *produce* all symmetric (2×2)- and (3×3)-matrices $\mathbf{A}$ as $\mathbf{A} = \mathbf{Q} \cdot \mathbf{\Lambda} \cdot \mathbf{Q}^{\top}$. We only have to *choose* the wanted eigenvalues in the diagonal for $\mathbf{\Lambda}$.

Every special orthogonal 2×2-matrix has the following form, which shows that it is a rotation given by a rotation angle φ :

$$\mathbf{Q} = \begin{bmatrix} \cos(\varphi) & -\sin(\varphi) \\ \sin(\varphi) & \cos(\varphi) \end{bmatrix} \quad , \tag{15-94}$$

where φ is an angle in the interval $[-\pi, \pi]$. Note that the column vectors are orthogonal and both have length 1. Furthermore the determinant $\det(\mathbf{Q}) = 1$, so $\mathbf{Q}$ is special orthogonal.

|||| Exercise 15.35

Prove the statement that *every* special orthogonal matrix can be stated in the form (15-94) for a suitable choice of the rotation angle φ.

If $\varphi > 0$ then $\mathbf{Q}$ rotates vectors in the positive direction, i.e. counter-clockwise; if $\varphi < 0$ then $\mathbf{Q}$ rotates vectors in the negative direction, i.e. clockwise.

|||| Definition 15.36 Rotation Matrices

Every special orthogonal (2×2)-matrix is also called a ***rotation matrix***.

Since every positive orthogonal 3×3-matrix similarly can be stated as a product of rotations about the three coordinate axes – see below – we will extend the naming as follows:

|||| Definition 15.37 Rotation Matrices

Every special orthogonal (3×3)-matrix is called a ***rotation matrix***.

A rotation about a coordinate axis, i.e. a rotation by a given angle about one of the coordinate axes, is produced with one of the following special orthogonal matrices:

$$\mathbf{R}_x(u) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(u) & -\sin(u) \\ 0 & \sin(u) & \cos(u) \end{bmatrix}$$

$$\mathbf{R}_y(v) = \begin{bmatrix} \cos(v) & 0 & \sin(v) \\ 0 & 1 & 0 \\ -\sin(v) & 0 & \cos(v) \end{bmatrix} \qquad (15\text{-}95)$$

$$\mathbf{R}_z(w) = \begin{bmatrix} \cos(w) & -\sin(w) & 0 \\ \sin(w) & \cos(w) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad ,$$

where the rotation angles are u, v, and w, respectively.

|||| Exercise 15.38

Show by direct calculation that the three axis-rotation matrices and every product of axis-rotation matrices really *are* special orthogonal matrices, i.e. they satisfy $\mathbf{R}^{-1} = \mathbf{R}^{\top}$ and $\det(\mathbf{R}) = 1$.

|||| Exercise 15.39

Find the image vectors of every one of the given vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ by use of the given mapping matrices $\mathbf{Q}_i$:

$$\begin{aligned}
&\mathbf{Q}_1 = \mathbf{R}_x(\pi/4) \quad , \quad \mathbf{a} = (1,0,0),\ \mathbf{b} = (0,1,0),\ \mathbf{c} = (0,0,1) \\
&\mathbf{Q}_2 = \mathbf{R}_y(\pi/4) \quad , \quad \mathbf{a} = (1,1,1),\ \mathbf{b} = (0,1,0),\ \mathbf{c} = (0,0,1) \\
&\mathbf{Q}_3 = \mathbf{R}_z(\pi/4) \quad , \quad \mathbf{a} = (1,1,0),\ \mathbf{b} = (0,1,0),\ \mathbf{c} = (0,0,1) \\
&\mathbf{Q}_4 = \mathbf{R}_y(\pi/4) \cdot \mathbf{R}_x(\pi/4) \quad , \quad \mathbf{a} = (1,0,0),\ \mathbf{b} = (0,1,0),\ \mathbf{c} = (0,0,1) \\
&\mathbf{Q}_5 = \mathbf{R}_x(\pi/4) \cdot \mathbf{R}_y(\pi/4) \quad , \quad \mathbf{a} = (1,0,0),\ \mathbf{b} = (0,1,0),\ \mathbf{c} = (0,0,1) \quad .
\end{aligned} \tag{15-96}$$

The combination of rotations about the coordinate axes by given rotation angles u, v, and w about the $x-$axis, $y-$axis, and $z-$axis is found by computing the matrix product of the three corresponding rotation matrices.

Here is the complete general expression for the matrix product for all values of u, v and w:

$$\mathbf{R}(u,v,w) \; = \; \mathbf{R}_z(w) \cdot \mathbf{R}_y(v) \cdot \mathbf{R}_x(u)$$

$$= \begin{bmatrix} \cos(w)\cos(v) & -\sin(w)\cos(u) - \cos(w)\sin(v)\sin(u) & \sin(w)\sin(u) - \cos(w)\sin(v)\cos(u) \\ \sin(w)\cos(v) & \cos(w)\cos(u) - \sin(w)\sin(v)\sin(u) & -\cos(w)\sin(u) - \sin(w)\sin(v)\cos(u) \\ \sin(v) & \cos(v)\sin(u) & \cos(v)\cos(u) \end{bmatrix} .$$

As one might suspect, it is possible to prove the following theorem:

|||| Theorem 15.40 Axis Rotation Angles for a Given Rotation Matrix

Every rotation matrix $\mathbf{R}$ (i.e. every special orthogonal matrix $\mathbf{Q}$) can be written as the product of 3 axis-rotation matrices:

$$\mathbf{R} = \mathbf{R}(u,v,w) = \mathbf{R}_z(w) \cdot \mathbf{R}_y(v) \cdot \mathbf{R}_x(u) \quad . \tag{15-97}$$

In other words: the effect of every rotation matrix can be realized by three consecutive rotations about the coordinate axes – with the rotation angles u, v, and w, respectively, as given in the above matrix product.

When a given special orthogonal matrix $\mathbf{R}$ is given (with its matrix elements r_{ij}), it is not difficult to find these axis rotation angles. As is evident from the above matrix product we have e.g. that $\sin(v) = r_{31}$ such that $v = \arcsin(r_{31})$ or $v = \pi - \arcsin(r_{31})$, and $\cos(w)\cos(v) = r_{11}$ such that $w = \arccos(r_{11}/\cos(v))$ or $v = -\arccos(r_{31}/\cos(v))$, if only $\cos(v) \neq 0$ i.e. if only $v \neq \pm\pi/2$.

|||| Exercise 15.41

Show that if $v = \pi/2$ or $v = -\pi/2$ then there exist many values of u and w giving the *same* $\mathbf{R}(u,v,w)$. I.e. not all angle values are uniquely determined in the interval $]-\pi,\pi]$ for every given rotation matrix $\mathbf{R}$.

|||| Exercise 15.42

Show that if $\mathbf{R}$ is a rotation matrix (a positive orthogonal matrix) then $\mathbf{R}^\top$ is also a rotation matrix, and vice versa: if $\mathbf{R}^\top$ is a rotation matrix then $\mathbf{R}$ is also a rotation matrix.

|||| Exercise 15.43

Show that if $\mathbf{R}_1$ and $\mathbf{R}_2$ are rotation matrices then $\mathbf{R}_1 \cdot \mathbf{R}_2$ and $\mathbf{R}_2 \cdot \mathbf{R}_1$ are also rotation matrices. Give examples that show that $\mathbf{R}_1 \cdot \mathbf{R}_2$ is not necesarily the same rotation matrix as $\mathbf{R}_2 \cdot \mathbf{R}_1$.

15.8 Structure of Rotation Matrices

As mentioned above (Exercise 15.35), every 2×2 special orthogonal matrix has the form:

$$\mathbf{Q} = \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix}.$$

This is a rotation of the plane anticlockwise by the angle ϕ. The angle ϕ is related to the eigenvalues of $\mathbf{Q}$:

|||| Exercise 15.44

Show that the eigenvalues of the matrix $\mathbf{Q}$ above are:

$$\lambda_1 = e^{i\phi}, \qquad \lambda_2 = e^{-i\phi}.$$

How about the 3×3 case? We already remarked that any 3×3 special orthogonal matrix can be written as a composition of rotations about the three coordinate matrices: $\mathbf{Q} = \mathbf{R}_z(w) \cdot \mathbf{R}_y(v) \cdot \mathbf{R}_x(u)$. But is $\mathbf{Q}$ itself a rotation about some axis (i.e. some line through the origin)? We can prove this is so, by examining the eigenvalues and eigenvectors of $\mathbf{Q}$.

|||| Theorem 15.45

The eigenvalues of any orthogonal matrix all have absolute value 1.

Proof. If λ is an eigenvalue of an orthogonal matrix $\mathbf{Q}$, there is, by definition, a non-zero complex eigenvector $\mathbf{v}$ in $\mathbb{C}^n \setminus \{\mathbf{0}\}$. Writing $\mathbf{v}$ as a column matrix, we then have:

$$\begin{aligned}
\lambda\bar{\lambda}\mathbf{v}^T \cdot \bar{\mathbf{v}} &= (\lambda\mathbf{v})^T \cdot \overline{(\lambda\mathbf{v})} \\
&= (\mathbf{Q}\cdot\mathbf{v})^T \cdot \overline{(\mathbf{Q}\cdot\mathbf{v})} && (\mathbf{Q}\cdot\mathbf{v} = \lambda\mathbf{v}) \\
&= \mathbf{v}^T \cdot \mathbf{Q}^T \cdot \mathbf{Q} \cdot \bar{\mathbf{v}} && (\bar{\mathbf{Q}} = \mathbf{Q}) \\
&= \mathbf{v}^T \cdot \mathbf{E} \cdot \bar{\mathbf{v}} && (\mathbf{Q}^T \cdot \mathbf{Q} = \mathbf{E}) \\
&= \mathbf{v}^T \cdot \bar{\mathbf{v}}.
\end{aligned}$$

Since $\mathbf{v} \neq \mathbf{0}$, it follows that $\mathbf{v}^T \cdot \bar{\mathbf{v}}$ is a non-zero (real) number:

$$\begin{aligned} \mathbf{v}^T \cdot \bar{\mathbf{v}} &= v_1\bar{v}_1 + v_2\bar{v}_2 \ldots v_n\bar{v}_n \\ &= |v_1|^2 + |v_2|^2 + \ldots |v_n|^2 > 0. \end{aligned}$$

Dividing $\lambda\bar{\lambda}\mathbf{v}^T \cdot \bar{\mathbf{v}} = \mathbf{v}^T \cdot \bar{\mathbf{v}}$ by this number we get:

$$|\lambda|^2 = \lambda\bar{\lambda} = 1.$$

□

We can now apply this to the eigenvalues of a 3×3 special orthogonal matrix:

|||| Theorem 15.46

Let $\mathbf{Q}$ be a 3×3 special orthogonal matrix, i.e. $\mathbf{Q}^T\mathbf{Q} = \mathbf{E}$, and $\det \mathbf{Q} = 1$. Then the eigenvalues are:

$$\lambda_1 = 1, \quad \lambda_2 = e^{i\phi}, \quad \lambda_3 = e^{-i\phi},$$

for some $\phi \in]-\pi, \pi]$.

Proof. $\mathbf{Q}$ is a real matrix, so all eigenvalues are either real or come in complex conjugate pairs. There are 3 of them, because $\mathbf{Q}$ is a 3×3 matrix, so the characteristic polynomial has degree 3. Hence there is at least one real eigenvalue:

$$\lambda_1 \in \mathbb{R}.$$

Now there are two possibilities:
Case 1: All roots are real: then, since all eigenvalues have absolute value 1 (by Theorem 15.45), and

$$1 = \det \mathbf{Q} = \lambda_1\lambda_2\lambda_3$$

either one or all three of the eigenvalues are equal to 1.

Case 2: λ_1 is real and the other two are complex conjugate, $\lambda_3 = \bar{\lambda}_2$, so:

$$1 = \det \mathbf{Q} = \lambda_1\lambda_2\bar{\lambda}_2 = \lambda_1|\lambda_2|^2 = \lambda_1,$$

where we used that $|\lambda_2| = 1$. Any complex number λ with absolute value 1 is of the form $e^{i\phi}$, where $\phi = \text{Arg}(\lambda)$, so this gives the claimed form of λ_1, λ_2 and λ_3.

Note that the case $\lambda_2 = \lambda_3 = 1$ or -1 (in Case 1) correspond respectively to $\phi = 0$ and $\phi = \pi$ in the wording of the theorem. □

We can also say something about the eigenvectors corresponding to the eigenvalues.

|||| Theorem 15.47

Let $\mathbf{Q}$ be a special orthogonal matrix, and denote the eigenvalues as in Theorem 15.46. If the eigenvalues are not all real, i.e. $\mathrm{Im}(\lambda_2) \neq 0$, then the eigenvectors corresponding to λ_2 and λ_3 are necessarily of the form:

$$\mathbf{v}_2 = \mathbf{x} + i\mathbf{y}, \qquad \mathbf{v}_3 = \bar{\mathbf{v}}_2 = \mathbf{x} - i\mathbf{y},$$

where $\mathbf{x}$ and $\mathbf{y}$ are respectively the real and imaginary parts of $\mathbf{v}_2$, and

$$\mathbf{x}\cdot\mathbf{y} = 0 \qquad \text{and} \quad |\mathbf{x}| = |\mathbf{y}|.$$

If $\mathbf{v}_1$ is an eigenvector for $\lambda_1 = 1$, then:

$$\mathbf{v}_1\cdot\mathbf{x} = \mathbf{v}_1\cdot\mathbf{y} = 0$$

Proof. We have $\mathbf{Q}\mathbf{v}_2 = \lambda_2\mathbf{v}_2$, and $\mathbf{Q}\bar{\mathbf{v}}_2 = \bar{\lambda}_2\bar{\mathbf{v}}_2$. So clearly a third eigenvector, corresponding to $\bar{\lambda}_2$, is $\mathbf{v}_3 = \bar{\mathbf{v}}_2$. Using $\mathbf{Q}^T\mathbf{Q} = \mathbf{E}$, we have

$$\mathbf{v}_2^T\mathbf{v}_2 = \mathbf{v}_2^T\mathbf{Q}^T\mathbf{Q}\mathbf{v}_2 = (\mathbf{Q}\mathbf{v}_2)^T(\mathbf{Q}\mathbf{v}_2) = \lambda_2^2\mathbf{v}_2^T\mathbf{v}_2.$$

If $\mathbf{v}_2^T\mathbf{v}_2 \neq 0$, then we can divide by this number to get $\lambda_2^2 = 1$. But $\lambda_2 = a + bi$, with $b \neq 0$, so this would mean: $1 = \lambda_2^2 = a^2 - b^2 + 2iab$. The imaginary part is: $ab = 0$, which implies that $a = 0$ and hence $\lambda_2^2 = -b^2$, which cannot be equal to 1. Hence:

$$\mathbf{v}_2^T\mathbf{v}_2 = 0.$$

Writing $\mathbf{v}_2 = \mathbf{x} + i\mathbf{y}$, this is:

$$\begin{aligned} 0 &= (\mathbf{x}^T + i\mathbf{y}^T)(\mathbf{x} + i\mathbf{y}) \\ &= \mathbf{x}^T\mathbf{x} - \mathbf{y}^T\mathbf{y} + i(\mathbf{x}^T\mathbf{y} + \mathbf{y}^T\mathbf{x}). \end{aligned}$$

The real part of this equation is:

$$\mathbf{x}^T\mathbf{x} - \mathbf{y}^T\mathbf{y} = 0, \qquad \text{i.e.,} \quad \mathbf{x}\cdot\mathbf{x} = |\mathbf{x}|^2 = \mathbf{y}\cdot\mathbf{y} = |\mathbf{y}|^2,$$

and the imaginary part is:

$$0 = \mathbf{x}^T\mathbf{y} + \mathbf{y}^T\mathbf{x} = \mathbf{x}\cdot\mathbf{y} + \mathbf{y}\cdot\mathbf{x} = 2\mathbf{x}\cdot\mathbf{y}.$$

Lastly, if $\mathbf{v}_1$ is an eigenvector for $\lambda_1 = 1$, then, by the same argument as above,

$$\mathbf{v}_1^T \mathbf{v}_2 = 1 \cdot \lambda_2 \cdot \mathbf{v}_1^T \mathbf{v}_2,$$

which must be zero, since $\lambda_2 \neq 1$. This is:

$$0 = \mathbf{v}_1^T (\mathbf{x} + i\mathbf{y}) = \mathbf{v}_1 \cdot \mathbf{x} + i\, \mathbf{v}_1 \cdot \mathbf{y}.$$

Since $\mathbf{v}_1$ is real, the real and imaginary parts of this give $\mathbf{v}_1 \cdot \mathbf{x} = \mathbf{v}_1 \cdot \mathbf{y} = 0$.

□

Now we can give a precise description of the geometric effect of a 3×3 rotation matrix:

|||| Theorem 15.48

Let $\mathbf{Q}$ be a 3×3 special orthogonal matrix, and $\lambda_1 = 1$, $\lambda_2 = e^{i\phi}$, $\lambda_3 = e^{-i\phi}$ be its eigenvalues, with corresponding eigenvectors $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3 = \bar{\mathbf{v}}_2$. Then:

1. The map $f : \mathbb{R}^3 \to \mathbb{R}^3$ given by $f(\mathbf{x}) = \mathbf{Q}\mathbf{x}$ is a rotation by angle ϕ around the line spanned by $\mathbf{v}_1$.

2. If λ_2 is not real then an orthonormal basis for $\mathbb{R}^3$ is given by:

$$\mathbf{u}_1 = \frac{\mathbf{v}_1}{|\mathbf{v}_1|}, \quad \mathbf{u}_2 = \frac{\operatorname{Im} \mathbf{v}_2}{|\operatorname{Im} \mathbf{v}_2|}, \quad \mathbf{u}_3 = \frac{\operatorname{Re} \mathbf{v}_2}{|\operatorname{Re} \mathbf{v}_2|},$$

   where $\mathbf{v}_2$ is an eigenvector for $\lambda_2 = e^{i\phi}$. The mapping matrix for f with respect to this basis is:

$${}_u f_u = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{bmatrix}.$$

3. If λ_2 is real then $\mathbf{Q}$ is either the identity map ($\lambda_2 = \lambda_3 = 1$) or a rotation by angle π ($\lambda_2 = \lambda_3 = -1$).

Proof. Statement 1 follows from statements 2 and 3, since these represent rotations by angle ϕ around the $\mathbf{v}_1$ axis.

For statement 2, by Theorem 15.47, if λ_2 is not real, then $u = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$ as defined above are an orthonormal basis for $\mathbb{R}^3$, since they are mutually orthogonal and of length 1.

To find the mapping matrix, we have $f(\mathbf{u}_1) = \mathbf{u}_1 = 1 \cdot \mathbf{u}_1 + 0 \cdot \mathbf{u}_2 + 0 \cdot \mathbf{u}_3$, which gives the first column. For $\mathbf{u}_2$ and $\mathbf{u}_3$, according to Theorem 15.47, the real and imaginary parts of $\mathbf{v}_2$ have the same length, so we can rescale $\mathbf{v}_2$ by dividing by this number to get

$$\mathbf{w} = \mathbf{u}_3 + i\mathbf{u}_2, \qquad \mathbf{u}_2 = \frac{\operatorname{Im} \mathbf{v}_2}{|\operatorname{Im} \mathbf{v}_2|}, \quad \mathbf{u}_3 = \frac{\operatorname{Re} \mathbf{v}_2}{|\operatorname{Re} \mathbf{v}_2|},$$

where $\mathbf{w}$ is an eigenvector for f with eigenvalue $e^{i\phi}$. That is:

$$\begin{aligned} e^{i\phi}\mathbf{w} = (\cos\phi + i\sin\phi)(\mathbf{u}_3 + i\mathbf{u}_2) &= f(\mathbf{u}_3 + i\mathbf{u}_2) \\ (\cos\phi\mathbf{u}_3 - \sin\phi\mathbf{u}_2) + i(\sin\phi\mathbf{u}_3 + \cos\phi\mathbf{u}_2) &= f(\mathbf{u}_3) + if(\mathbf{u}_2). \end{aligned}$$

The imaginary and real parts of this equation give:

$$\begin{aligned} f(\mathbf{u}_2) &= \cos\phi\mathbf{u}_2 + \sin\phi\mathbf{u}_3 \\ f(\mathbf{u}_3) &= -\sin\phi\mathbf{u}_2 + \cos\phi\mathbf{u}_3, \end{aligned}$$

and this gives us the second and third columns of the mapping matrix.

This mapping matrix is precisely the matrix of a rotation by angle ϕ around the $\mathbf{v}_1$ axis (compare ${}_u f_u$ with the matrix $\mathbf{R}_x(u)$ discussed earlier).

For statement 3, the special case that λ_2 is real, if $\lambda_2 = \lambda_3 = 1$, then $\phi = 0$ and $\mathbf{Q}$ is the identity matrix, which can be regarded as a rotation by angle 0 around any axis.

Finally, for the case $\lambda_2 = \lambda_3 = -1$, briefly: let $E_1 = \operatorname{span}\{\mathbf{v}_1\}$. Choose any orthonormal basis for the orthogonal complement $E_1^{\perp}$. Using this, one can show that the restricition of f to $E_1^{\perp}$ is a 2×2 rotation matrix with a repeated eigenvalue -1. This means it is minus the identity matrix on $E_1^{\perp}$, i.e. a rotation by angle π, from which the claim follows. □

|||| Example 15.49

The axis of rotation for a 3×3 rotation matrix is sometimes called the *Euler axis*. Let's find the Euler axis, and the rotation angle for the special orthogonal matrix:

$$\mathbf{Q} = \frac{1}{3}\begin{bmatrix} -2 & -2 & 1 \\ 2 & -1 & 2 \\ -1 & 2 & 2 \end{bmatrix},$$

which was used for a change of basis in Example 15.34.

The eigenvalues are:

$$\lambda_1 = 1, \qquad \lambda_2 = -\frac{2}{3} + i\frac{\sqrt{5}}{3}, \qquad \lambda_3 = -\frac{2}{3} - i\frac{\sqrt{5}}{3},$$

with corresponding eigenvectors:

$$\mathbf{v}_1 = \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix}, \qquad \mathbf{v}_2 = \begin{bmatrix} -i\sqrt{5} \\ -2 \\ 1 \end{bmatrix}, \qquad \mathbf{v}_3 = \overline{\mathbf{v}_2}.$$

So the axis of rotation is the line spanned by $\mathbf{v}_1 = (0, 1, 2)$, and the angle of rotation is:

$$\phi = \operatorname{Arg}(\lambda_2) = -\arctan\left(\frac{\sqrt{5}}{2}\right) + \pi$$

We can set:

$$\mathbf{u}_1 = \mathbf{v}_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix}, \quad \mathbf{u}_2 = \operatorname{Im}\mathbf{v}_2 = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{u}_3 = \operatorname{Re}\mathbf{v}_2 = \frac{1}{\sqrt{5}} \begin{bmatrix} 0 \\ -2 \\ 1 \end{bmatrix},$$

and, setting $U = [\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3]$, the matrix of f in this basis is:

$${}_u f_u = U^T \mathbf{Q} U = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{2}{3} & -\frac{\sqrt{5}}{3} \\ 0 & \frac{\sqrt{5}}{3} & -\frac{2}{3} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{bmatrix}.$$

|||| Exercise 15.50

Find the axis and angle of rotation for the rotation matrix: $\mathbf{Q} = \frac{1}{2} \begin{bmatrix} 0 & -\sqrt{2} & \sqrt{2} \\ \sqrt{2} & 1 & 1 \\ -\sqrt{2} & 1 & 1 \end{bmatrix}$.

Conversely, we can construct a matrix that rotates by any desired angle around any desired axis:

|||| Example 15.51

Problem: Construct the matrix for the linear map $f : \mathbb{R}^3 \to \mathbb{R}^3$ that rotates 3-space around the axis spanned by the vector $\mathbf{a} = (1, 1, 0)$ anti-clockwise by the angle $\pi/2$.

Solution: Choose any orthonormal basis $(\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$ where $\mathbf{u}_1$ points in the direction of $\mathbf{a}$. For example:

$$\mathbf{u}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{u}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

We have chosen them such that $\det([\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3]) = 1$. This means that the orientation of space is preserved by this change of basis, so we know that the rotation from the following construction will be anti-clockwise around the axis.

The matrix with respect to the u-basis that rotates anti-clockwise around the $\mathbf{u}_1$-axis by the angle $\pi/2$ is:

$$_u f_u = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\pi/2) & -\sin(\pi/2) \\ 0 & \sin(\pi/2) & \cos(\pi/2) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}.$$

The change of basis matrix from u to the standard e-basis is:

$$_e M_u = [\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3] = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix},$$

so the matrix of f with respect to the standard basis is:

$$_e f_e = {_e M_u} \, {_u f_u} \, {_e M_u^T} = \frac{1}{2} \begin{bmatrix} 1 & 1 & \sqrt{2} \\ 1 & 1 & -\sqrt{2} \\ -\sqrt{2} & \sqrt{2} & 0 \end{bmatrix}.$$

Note: for the vectors $\mathbf{u}_1$ and $\mathbf{u}_2$, it would have made no difference what choice we make as long as they are orthogonal to $\mathbf{a}$, and orthonormal. If we rotate them in the plane orthogonal to $\mathbf{a}$, this rotation will cancel in the formula $_e M_u \, {_u f_u} \, {_e M_u^T}$.

|||| Exercise 15.52

Find an orthogonal matrix $\mathbf{Q}$ that, in the standard e-basis for $\mathbb{R}^3$, represents a rotation about the axis spanned by $\mathbf{a} = (1, 1, 1)$ by an angle $\pi/2$.

15.9 Reduction of Quadratic Polynomials

A ***quadratic form*** in $(\mathbb{R}^n, \cdot)$ is a quadratic polynomial in n variables – but without linear and constant terms.

|||| Definition 15.53

Let $\mathbf{A}$ be a symmetric $(n \times n)$-matrix and let $(x_1, x_2, \cdots, x_n)$ denote the coordinates for an arbitrary vector $\mathbf{x}$ in $(\mathbb{R}, \cdot)$ with respect to the standard basis e in $\mathbb{R}^n$.

A ***quadratic form*** in $(\mathbb{R}, \cdot)$ is a function of the n variables $(x_1, x_2, \cdots, x_n)$ in the following form:

$$P_{\mathbf{A}}(\mathbf{x}) = P_{\mathbf{A}}(x_1, x_2, \cdots, x_n) = \begin{bmatrix} x_1 & x_2 & \cdot & \cdot & x_n \end{bmatrix} \cdot \mathbf{A} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \cdot x_i \cdot x_j \quad , \tag{15-98}$$

a_{ij} being the individual elements in $\mathbf{A}$.

|||| Example 15.54 Quadratic Form as Part of a Quadratic Polynomial

Let $f(x, y)$ be the following quadratic polynomial in the two variables x and y.

$$f(x, y) = 11 \cdot x^2 + 4 \cdot y^2 - 24 \cdot x \cdot y - 20 \cdot x + 40 \cdot y - 60 \quad . \tag{15-99}$$

Then we can separate the polynomial in two parts:

$$f(x, y) = P_{\mathbf{A}}(x, y) + (-20 \cdot x + 40 \cdot y - 60) \quad , \tag{15-100}$$

where $P_{\mathbf{A}}(x, y)$ is the quadratic form

$$P_{\mathbf{A}}(x, y) = 11 \cdot x^2 + 4 \cdot y^2 - 24 \cdot x \cdot y \tag{15-101}$$

that is represented by the matrix

$$\mathbf{A} = \begin{bmatrix} 11 & -12 \\ -12 & 4 \end{bmatrix} \tag{15-102}$$

We will now see how the spectral theorem can be used for the description of every quadratic form by use of the eigenvalues for the matrix that represents the quadratic form.

|||| Theorem 15.55 Reduction of Quadratic Forms

Let $\mathbf{A}$ be a symmetric matrix and let $P_{\mathbf{A}}(x_1, \cdots, x_n)$ denote the corresponding quadratic form in $(\mathbb{R}^n, \cdot)$ with respect to standard coordinates. By a change of basis to new coordinates $\widetilde{x}_1, \cdots, \widetilde{x}_n$ given by the positive orthogonal change of basis matrix $\mathbf{Q}$ that diagonalizes $\mathbf{A}$ we get the reduced expression for the quadratic form:

$$P_{\mathbf{A}}(x_1, \cdots, x_n) = \widetilde{P}_{\mathbf{\Lambda}}(\widetilde{x}_1, \cdots, \widetilde{x}_n) = \lambda_1 \cdot \widetilde{x}_1^2 + \cdots + \lambda_n \cdot \widetilde{x}_n^2 \quad , \tag{15-103}$$

where $\lambda_1, \cdots, \lambda_n$ are the n real eigenvalues for the symmetric matrix $\mathbf{A}$.

The *reduction* in the theorem means that the new expression does not contain any product terms of the type $x_i \cdot x_j$ for $i \neq j$.

|||| Proof

Since $\mathbf{A}$ is symmetric it *can* according to the spectral theorem be diagonalized by an orthogonal substitution matrix $\mathbf{Q}$. The gathering of column vectors $(\mathbf{v}_1, \cdots, \mathbf{v}_n)$ in $\mathbf{Q}$ constitutes a new basis v in $(\mathbb{R}^n, \cdot)$.

Let $\mathbf{x}$ be an arbitrary vector in $\mathbb{R}^n$. Then we have the following set of coordinates for $\mathbf{x}$, partly with respect to the standard e-basis and partly with respect to the new basis v

$$\begin{aligned} {}_{\mathrm{e}}\mathbf{x} &= (x_1, \cdots, x_n) \quad , \\ {}_{\mathrm{v}}\mathbf{x} &= (\widetilde{x}_1, \cdots, \widetilde{x}_n) \quad . \end{aligned} \tag{15-104}$$

Then

$$
\begin{aligned}
P_{\mathbf{A}}(\mathbf{x}) &= P_{\mathbf{A}}(x_1, \cdots, x_n) \\
&= \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix} \cdot \mathbf{A} \cdot \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \\
&= \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix} \cdot \mathbf{Q} \cdot \mathbf{\Lambda} \cdot \mathbf{Q}^{-1} \cdot \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \\
&= \left(\begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix} \cdot \mathbf{Q} \right) \cdot \mathbf{\Lambda} \cdot \left(\mathbf{Q}^{\top} \cdot \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \right) \\
&= \begin{bmatrix} \widetilde{x}_1 & \cdots & \widetilde{x}_n \end{bmatrix} \cdot \mathbf{\Lambda} \cdot \begin{bmatrix} \widetilde{x}_1 \\ \cdot \\ \cdot \\ \widetilde{x}_n \end{bmatrix} \\
&= \begin{bmatrix} \widetilde{x}_1 & \cdots & \widetilde{x}_n \end{bmatrix} \cdot \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \lambda_n \end{bmatrix} \cdot \begin{bmatrix} \widetilde{x}_1 \\ \cdot \\ \cdot \\ \widetilde{x}_n \end{bmatrix} \\
&= \widetilde{P}_{\mathbf{\Lambda}}(\widetilde{x}_1, \cdots, \widetilde{x}_n) \quad = \quad \lambda_1 \cdot \widetilde{x}_1^2 + \cdots + \lambda_n \cdot \widetilde{x}_n^2 \quad .
\end{aligned}
\tag{15-105}
$$

■

Note that the matrix that represents the quadratic form in Example 15.54, Equation (15-102), is not much different from the Hessian Matrix $\mathbf{H}f(x, y)$ for $f(x, y)$, which is also a constant matrix, because $f(x, y)$ is a second degree polynomial. See eNote 22. In fact we observe that:

$$
\mathbf{A} = \frac{1}{2} \cdot \mathbf{H}f(x, y) \quad , \tag{15-106}
$$

and this is no coincidence.

|||| Lemma 15.56

Let $f(x_1, x_2, \cdots, x_n)$ denote an arbitrary quadratic polynomial without linear and constant terms. Then $f(x_1, x_2, \cdots, x_n)$ can be expressed as a quadratic form in exactly one way – i.e. there exists exactly one symmetric matrix $\mathbf{A}$ such that:

$$f(\mathbf{x}) = f(x_1, x_2, \cdots, x_n) = P_{\mathbf{A}}(x_1, x_2, \cdots, x_n) \quad . \tag{15-107}$$

The sought matrix is:

$$\mathbf{A} = \frac{1}{2} \cdot \mathbf{H}f(\mathbf{x}) \quad , \tag{15-108}$$

where $\mathbf{H}f(\mathbf{x})$ is (the constant) Hessian matrix for the function $f(\mathbf{x}) = f(x_1, x_2, \cdots, x_n)$.

|||| Proof

We limit ourselves to the case $n = 2$ and refer the analysis to functions of two variables in eNote 22: If $f(x, y)$ is a polynomial in two variables without linear (and constant) terms, i.e. a quadratic form in $(\mathbf{R}^2, \cdot)$, then the wanted $\mathbf{A}$-matrix is exactly the (constant) Hesse-matrix for $f(x, y)$.

■

This applies generally, if we extend the definition of Hessian matrices to functions of more variables as follows: Let $f(x_1, x_2, \cdots, x_n)$ be an arbitrary smooth function of n variables in the obvious meaning for functions of more variables (than two). Then the corresponding Hessian matrices are the following symmetric $(n \times n)$-matrices which contain all the second-order partial derivatives for the function $f(\mathbf{x})$ evaluated at an arbitrary point $\mathbf{x} \in \mathbb{R}^n$:

$$\mathbf{H}f(x_1, x_2, \cdots, x_n) = \begin{bmatrix} f''_{x_1 x_1}(\mathbf{x}) & f''_{x_1 x_2}(\mathbf{x}) & \cdots & f''_{x_1 x_n}(\mathbf{x}) \\ f''_{x_2 x_1}(\mathbf{x}) & f''_{x_2 x_2}(\mathbf{x}) & \cdots & f''_{x_2 x_n}(\mathbf{x}) \\ \vdots & \vdots & \ddots & \vdots \\ f''_{x_n x_1}(\mathbf{x}) & f''_{x_n x_2}(\mathbf{x}) & \ldots & f''_{x_n x_n}(\mathbf{x}) \end{bmatrix} \quad . \tag{15-109}$$

In particular if $f(x, y, z)$ is a smooth function of three variables (as in Example 15.57

below) we get at every point $(x, y, z) \in \mathbb{R}^3$:

$$\mathbf{H}f(x,y,z) = \begin{bmatrix} f''_{xx}(x,y,z) & f''_{xy}(x,y,z) & f''_{xz}(x,y,z) \\ f''_{xy}(x,y,z) & f''_{yy}(x,y,z) & f''_{yz}(x,y,z) \\ f''_{xz}(x,y,z) & f''_{yz}(x,y,z) & f''_{zz}(x,y,z) \end{bmatrix} \quad , \tag{15-110}$$

where we explicitly have used the symmetry of the Hessian matrix, e.g. $f''_{zx}(x,y,z) = f''_{xz}(x,y,z)$.

|||| Example 15.57 Quadratic Form with a Representing Matrix

Let $f(x,y,z)$ denote the following function of three variables:

$$f(x,y,z) = x^2 + 3 \cdot y^2 + z^2 - 8 \cdot x \cdot y + 4 \cdot y \cdot z \quad . \tag{15-111}$$

Then $f(x,y,z)$ is a quadratic form $P_{\mathbf{A}}(x,y,z)$ with

$$\mathbf{A} = \frac{1}{2} \cdot \mathbf{H}f(x,y,z) = \frac{1}{2} \cdot \begin{bmatrix} f''_{xx}(x,y,z) & f''_{xy}(x,y,z) & f''_{xz}(x,y,z) \\ f''_{xy}(x,y,z) & f''_{yy}(x,y,z) & f''_{yz}(x,y,z) \\ f''_{xz}(x,y,z) & f''_{yz}(x,y,z) & f''_{zz}(x,y,z) \end{bmatrix} = \begin{bmatrix} 1 & -4 & 0 \\ -4 & 3 & 2 \\ 0 & 2 & 1 \end{bmatrix} \quad . \tag{15-112}$$

We can prove 15-108 by direct computation:

$$\begin{aligned} P_{\mathbf{A}}(x,y,z) &= \begin{bmatrix} x & y & z \end{bmatrix} \cdot \begin{bmatrix} 1 & -4 & 0 \\ -4 & 3 & 2 \\ 0 & 2 & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} \\ &= \begin{bmatrix} x & y & z \end{bmatrix} \cdot \begin{bmatrix} x - 4 \cdot y \\ 3 \cdot y - 4 \cdot x + 2 \cdot z \\ z + 2 \cdot y \end{bmatrix} \\ &= x \cdot (x - 4 \cdot y) + y \cdot (3 \cdot y - 4 \cdot x + 2 \cdot z) + z \cdot (z + 2 \cdot y) \\ &= x^2 + 3 \cdot y^2 + z^2 - 8 \cdot x \cdot y + 4 \cdot y \cdot z \\ &= f(x,y,z) \quad . \end{aligned} \tag{15-113}$$

As is shown in Section 21.4 in eNote 21 the signs of the eigenvalues for the Hessian matrix play a decisive role when we analyse and inspect a smooth function $f(x, y)$ at and about a stationary point. And since it is again the very same Hessian matrix that appears in the present context we will here tie a pair of definitions to this sign-discussion – now for the general $(n \times n)$ Hessian matrices, and thus also for general quadratic forms represented by symmetric matrices $\mathbf{A}$:

|||| Definition 15.58 Definite and Indefinite Symmetric Matrices

We let $\mathbf{A}$ denote a symmetric matrix. Let $\mathbf{A}$ have the n real eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$. the we say that

1. $\mathbf{A}$ is ***positive definite*** if all eigenvalues λ_i are positive.
2. $\mathbf{A}$ is ***positive semi-definite*** if all eigenvalues λ_i are non-negative (every eigenvalue is greater than or equal to 0).
3. $\mathbf{A}$ is ***negative definite*** if all eigenvalues λ_i are negative.
4. $\mathbf{A}$ is ***negative semi-definite*** if all eigenvalues λ_i are non-positive (every eigenvalue is less than of equal to 0).
5. $\mathbf{A}$ is ***indefinite*** if $\mathbf{A}$ is neither positive semi-definite nor negative semi-definite.

We now formulate an intuitively reasonable result that relates this "definiteness" to the values which the quadratic polynomial $P_{\mathbf{A}}(\mathbf{x})$ assumes for different $\mathbf{x} \in \mathbb{R}^n$.

|||| Theorem 15.59 The Meaning of Positive Definiteness

If $\mathbf{A}$ is a symmetric positive definite matrix then the quadratic form $P_{\mathbf{A}}(\mathbf{x})$ is positive for all $\mathbf{x} \in \mathbb{R}^n - \mathbf{0}$.

|||| Proof

We refer to Theorem 15.55 and from that we can use the reduced expression for the quadratic form:

$$P_{\mathbf{A}}(x_1, \cdots, x_n) = \widetilde{P}_{\mathbf{A}}(\widetilde{x}_1, \cdots, \widetilde{x}_n) = \lambda_1 \cdot \widetilde{x}_1^2 + \cdots + \lambda_n \cdot \widetilde{x}_n^2 \quad , \tag{15-114}$$

from which it is clear to see that since $\mathbf{A}$ is positive definite we get $\lambda_i > 0$ for all $i = 1, \cdots, n$ and then $P_{\mathbf{A}}(\mathbf{x}) > 0$ for all $\mathbf{x} \neq \mathbf{0}$, which corresponds to the fact that none of the sets of coordinates for $\mathbf{x}$ can be $(0, \cdots, 0)$.

∎

Similar theorems can be formulated for negative definite and indefinite matrices, and they are obviously useful in investigations of functions, in particular in investigations of the functional values around stationary points, as shown in eNote 21.

15.10 Reduction of Quadratic Polynomials

By reducing the quadratic form part of a quadratic polynomial we naturally get an equivalently simpler quadratic polynomial – now without product terms. We give a couple of examples.

|||| Example 15.60 Reduction of a Quadratic Polynomial, Two Variables

We consider the following quadratic polynomial in two variables:

$$f(x,y) = 11\cdot x^2 + 4\cdot y^2 - 24\cdot x\cdot y - 20\cdot x + 40\cdot y - 60 \tag{15-115}$$

The part of the polynomial that can be described by a quadratic form is now

$$P_{\mathbf{A}}(x,y) = 11\cdot x^2 + 4\cdot y^2 - 24\cdot x\cdot y \quad , \tag{15-116}$$

where

$$\mathbf{A} = \begin{bmatrix} 11 & -12 \\ -12 & 4 \end{bmatrix} \quad . \tag{15-117}$$

Exactly this matrix is diagonalized by a positive orthogonal substitution $\mathbf{Q}$ in Example 15.32: The eigenvalues for $\mathbf{A}$ are $\lambda_1 = 20$ and $\lambda_2 = -5$ and

$$\mathbf{Q} = \begin{bmatrix} 4/5 & 3/5 \\ -3/5 & 4/5 \end{bmatrix} = \begin{bmatrix} \cos(\varphi) & -\sin(\varphi) \\ \sin(\varphi) & \cos(\varphi) \end{bmatrix} \quad , \quad \text{where} \quad \varphi = -\arcsin(3/5) \quad . \tag{15-118}$$

The change of coordinates $\widetilde{x}, \widetilde{y}$ consequently is a rotation of the standard coordinate system by an angle of $-\arcsin(3/5)$.

We use the reduction theorem 15.55 and get that the quadratic form $P_{\mathbf{A}}(x,y)$ in the new coordinates has the following reduced expression:

$$P_{\mathbf{A}}(x,y) = \widetilde{P}_{\mathbf{\Lambda}}(\widetilde{x},\widetilde{y}) = 20\cdot \widetilde{x}^2 - 5\cdot \widetilde{y}^2 \quad . \tag{15-119}$$

By introducing the reduced expression for the quadratic form in the polynomial $f(x,y)$ we get:

$$f(x,y) = 20\cdot \widetilde{x}^2 - 5\cdot \widetilde{y}^2 + (-20\cdot x + 40\cdot y - 60) \quad , \tag{15-120}$$

where all that remains is to express the last parenthesis by using the new coordinates. This is done using the substitution matrix **Q**. We have the linear relation between the coordinates (x, y) and $(\widetilde{x}, \widetilde{y})$:

$$\begin{bmatrix} x \\ y \end{bmatrix} = \mathbf{Q} \cdot \begin{bmatrix} \widetilde{x} \\ \widetilde{y} \end{bmatrix} = \begin{bmatrix} 4/5 & 3/5 \\ -3/5 & 4/5 \end{bmatrix} \cdot \begin{bmatrix} \widetilde{x} \\ \widetilde{y} \end{bmatrix} \tag{15-121}$$

so that:

$$\begin{aligned} x &= \frac{1}{5} \cdot (4 \cdot \widetilde{x} + 3 \cdot \widetilde{y}) \\ y &= \frac{1}{5} \cdot (-3 \cdot \widetilde{x} + 4 \cdot \widetilde{y}) \quad . \end{aligned} \tag{15-122}$$

We substitute these rewritings of x and y in (15-120) and get:

$$\begin{aligned} f(x, y) &= 20 \cdot \widetilde{x}^2 - 5 \cdot \widetilde{y}^2 + (-4 \cdot (4 \cdot \widetilde{x} + 3 \cdot \widetilde{y}) + 8 \cdot (-3 \cdot \widetilde{x} + 4 \cdot \widetilde{y}) - 60) \\ &= 20 \cdot \widetilde{x}^2 - 5 \cdot \widetilde{y}^2 - 40 \cdot \widetilde{x} + 20 \cdot \widetilde{y} - 60 \quad . \end{aligned} \tag{15-123}$$

Thus we have reduced the expression for $f(x, y)$ to the following expression in new coordinates $\widetilde{x}$ and $\widetilde{y}$, that appears by a suitable rotation of the standard coordinate system:

$$\begin{aligned} f(x, y) &= 11 \cdot x^2 + 4 \cdot y^2 - 24 \cdot x \cdot y - 20 \cdot x + 40 \cdot y - 60 \\ &= 20 \cdot \widetilde{x}^2 - 5 \cdot \widetilde{y}^2 - 40 \cdot \widetilde{x} + 20 \cdot \widetilde{y} - 60 \\ &= \widetilde{f}(\widetilde{x}, \widetilde{y}) \quad . \end{aligned} \tag{15-124}$$

Note again that the *reduction* in Example 15.60 results in the reduced quadratic polynomial $\widetilde{f}(\widetilde{x}, \widetilde{y})$ not containing any product terms of the form $\widetilde{x} \cdot \widetilde{y}$. This reduction technique and the output of the large work becomes somewhat more clear when we consider quadratic polynomials in three variables.

|||| Example 15.61 Reduction of a Quadratic Polynomial, Three Variables

In Example 15.34 we have diagonalized the matrix **A** that represents the quadratic form in the following quadratic polynomial in three variables:

$$f(x, y, z) = 7 \cdot x^2 + 6 \cdot y^2 + 5 \cdot z^2 - 4 \cdot x \cdot y - 4 \cdot y \cdot z - 2 \cdot x + 20 \cdot y - 10 \cdot z - 18 \quad . \tag{15-125}$$

This polynomial is reduced to the following quadratic polynomial in the new variables obtained using the same directives as in Example 15.60:

$$\begin{aligned} f(x, y) &= \widetilde{f}(\widetilde{x}, \widetilde{y}, \widetilde{z}) \\ &= \quad 9 \cdot \widetilde{x}^2 + 6 \cdot \widetilde{y}^2 + 3 \cdot \widetilde{z}^2 + 18 \cdot \widetilde{x} - 12 \cdot \widetilde{y} + 6 \cdot \widetilde{z} - 18 \end{aligned} \tag{15-126}$$

with the positive orthogonal substitution

$$\mathbf{Q} = \begin{bmatrix} -2/3 & -2/3 & 1/3 \\ 2/3 & -1/3 & 2/3 \\ -1/3 & 2/3 & 2/3 \end{bmatrix} \quad . \tag{15-127}$$

The substitution matrix **Q** can be factorized to a product of axis-rotation matrices like this:

$$\mathbf{Q} = \mathbf{R}_z(w) \cdot \mathbf{R}_y(v) \cdot \mathbf{R}_x(u) \quad , \tag{15-128}$$

where the rotation angles are respectively:

$$u = \frac{\pi}{4} \quad , \quad v = -\arcsin\left(\frac{1}{3}\right) \quad , \quad \text{and} \quad w = 3 \cdot \frac{\pi}{4} \quad , \tag{15-129}$$

By rotation of the coordinate system and by using the new coordinates $\widetilde{x}$, $\widetilde{y}$, and $\widetilde{z}$ we obtain a reduction of the polynomial $f(x,y,z)$ to the end that the polynomial $\widetilde{f}(\widetilde{x},\widetilde{y},\widetilde{z})$ does not contain product terms while $f(x,y,z)$ contains two product terms, with $x \cdot y$ and $y \cdot z$, respectively.

15.11 Summary

The main result in this eNote is that symmetric $(n \times n)$-matrices are precisely those matrices that can be diagonalized by a special orthogonal change of basis matrix $\mathbf{Q}$. We have used this theorem for the reduction of quadratic polynomials in n variables – though particularly for $n = 2$ and $n = 3$.

- A symmetric $(n \times n)$-matrix $\mathbf{A}$ has precisely n real eigenvalues $\lambda_1, \cdots, \lambda_n$.
- In the vector space $\mathbb{R}^n$ a scalar product is introduced by extending the standard scalar product of $\mathbb{R}^2$ and $\mathbb{R}^3$, and we refer to this scalar product when we write $(\mathbb{R}^n, \bullet)$. If $\mathbf{a} = (a_1, \cdots, a_n)$ and $\mathbf{b} = (b_1, \cdots, b_n)$ with respect to the standard basis e in $\mathbb{R}^n$, then
$$\mathbf{a} \bullet \mathbf{b} = \sum_{i}^{n} a_i \cdot b_i \quad . \tag{15-130}$$
- The length, the norm, of a vector $\mathbf{a}$ is given by
$$|\mathbf{a}| = \sqrt{\mathbf{a} \bullet \mathbf{a}} = \sqrt{\sum_{i=1}^{n} a_i^2} \quad . \tag{15-131}$$
- The Cauchy-Schwarz inequality is valid for all vectors $\mathbf{a}$ and $\mathbf{b}$ in $(\mathbb{R}^n, \bullet)$
$$|\mathbf{a} \bullet \mathbf{b}| \leq |\,\mathbf{a}\,|\,|\,\mathbf{b}\,|\ , \tag{15-132}$$
and the equality sign applies if and only if $\mathbf{a}$ and $\mathbf{b}$ are linearly dependent.
- The angle $\theta \in [0, \pi]$ between two proper vectors $\mathbf{a}$ and $\mathbf{b}$ in $(\mathbb{R}^n, \bullet)$ is determined by
$$\cos(\theta) = \frac{\mathbf{a} \bullet \mathbf{b}}{|\mathbf{a}| \cdot |\mathbf{b}|} \quad . \tag{15-133}$$
- Two proper vectors $\mathbf{a}$ and $\mathbf{b}$ in $(\mathbb{R}^n, \bullet)$ are orthogonal if $\mathbf{a} \bullet \mathbf{b} = 0$.
- A matrix $\mathbf{Q}$ is orthogonal if the column vectors are pairwise orthogonal and each has length 1 with respect to the scalar product introduced. This corresponds exactly to
$$\mathbf{Q}^\top \cdot \mathbf{Q} = \mathbf{E} \tag{15-134}$$
or equivalently:
$$\mathbf{Q}^{-1} = \mathbf{Q}^\top \quad . \tag{15-135}$$

- The spectral theorem: If $\mathbf{A}$ is symmetric, then a special orthogonal change of basis matrix $\mathbf{Q}$ exists such that

$$\mathbf{A} = \mathbf{Q} \cdot \mathbf{\Lambda} \cdot \mathbf{Q}^{\top} \quad , \tag{15-136}$$

  where $\mathbf{\Lambda} = \mathbf{diag}(\lambda_1, \cdots, \lambda_n)$.

- Every special orthogonal matrix $\mathbf{Q}$ is change of basis matrix that rotates the coordinate-system. It can for $n = 3$ be factorized in three axis-rotation matrices:

$$\mathbf{Q} = \mathbf{R}_z(w) \cdot \mathbf{R}_y(v) \cdot \mathbf{R}_x(u) \quad , \tag{15-137}$$

  for suitable choices of rotation angles u, v, and w.

- For $n = 3$: By rotation of the coordinate-system, i.e. by use of a special orthogonal change of basis matrix $\mathbf{Q}$, the quadratic form $P_{\mathbf{A}}(x, y, z)$ (which is a quadratic polynomial without linear terms and without constant terms) can be expressed by a quadratic form $\widetilde{P}_{\mathbf{\Lambda}}(\widetilde{x}, \widetilde{y}, \widetilde{z})$ in the new coordinates $\widetilde{x}$, $\widetilde{y}$, and $\widetilde{z}$ such that

$$P_{\mathbf{A}}(x, y, z) = \widetilde{P}_{\mathbf{\Lambda}}(\widetilde{x}, \widetilde{y}, \widetilde{z}) \quad \text{for all } (x, y, z), \tag{15-138}$$

  and such that the reduced quadratic form $\widetilde{P}_{\mathbf{\Lambda}}(\widetilde{x}, \widetilde{y}, \widetilde{z})$ does not contain any product term of the type $\widetilde{x} \cdot \widetilde{y}$, $\widetilde{x} \cdot \widetilde{z}$, or $\widetilde{y} \cdot \widetilde{z}$:

$$\widetilde{P}_{\mathbf{\Lambda}}(\widetilde{x}, \widetilde{y}, \widetilde{z}) = \lambda_1 \cdot \widetilde{x}^2 + \lambda_2 \cdot \widetilde{y}^2 + \lambda_3 \cdot \widetilde{z}^2 \quad , \tag{15-139}$$

  where λ_1, λ_2, and λ_3 are the three real eigenvalues for $\mathbf{A}$.