Convex Optimization for Machine Learning

with Mathematica Applications

Chapter 4

Euclidean Space $\mathbb{R}^n$, Hypersurface and Quadratic Form

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4.1 Basic Notations of Vectors and Matrices Using Dirac and Index Notations

Vectors and Matrices with Dirac Notations

In what follows we will distinguish scalars, vectors and matrices by their typeface. We will let $M_{m\times n}$ denote the space of real $n \times m$ matrices with n rows and m columns. Such matrices will be denoted using bold capital letters: **A**, **X**, **Y**, etc. An element of $M_{n\times 1}$ or $M_{1\times n}$, that is, a column or row vector, is denoted with a boldface lowercase letter: **a**, **x**, **y**, etc. An element of $M(1,1)$ is a scalar, denoted with lowercase italic typeface: A, X, Y, a, x, y, etc.

The entities that Dirac called "kets" and "bras" are simply column vectors and row vectors, respectively. Of course, the elements of these vectors are generally complex numbers. In these lectures, for convenience we will express ourselves in terms of vectors and matrices of real numbers. Hence, in the language of matrices these two vectors are related to each other by simply taking the transpose. In summary, Dirac refers to a "bra", which he denoted as $\langle \mathbf{a}|$, a "ket", which he denoted as $|\mathbf{b}\rangle$, and a square matrix **M**, we can associate these with vectors and matrices as follows

$$\langle \mathbf{a}| = (a_1, a_2, a_3), \quad |\mathbf{b}\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}, \quad \mathbf{M} = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix}. \tag{4.1}$$

The product of a bra and a ket, denoted by Dirac as $\langle \mathbf{a}||\mathbf{b}\rangle$ or, more commonly by omitting one of the middle lines, as $\langle \mathbf{a}|\mathbf{b}\rangle$, is simply a number given by multiplying a row vector and a column vector in the usual way, i.e.,

$$\langle \mathbf{a}|\mathbf{b}\rangle = (a_1, a_2, a_3)\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = a_1 b_1 + a_2 b_2 + a_3 b_3 = \sum_{i=1}^{3} a_i b_i. \tag{4.2}$$

We can also form the product of a ket times a bra, which gives a square matrix, as shown below,

$$|\mathbf{b}\rangle\langle \mathbf{a}| = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}(a_1, a_2, a_3) = \begin{pmatrix} b_1 a_1 & b_1 a_2 & b_1 a_3 \\ b_2 a_1 & b_2 a_2 & b_2 a_3 \\ b_3 a_1 & b_3 a_2 & b_3 a_3 \end{pmatrix}. \tag{4.3}$$

The product of a square matrix times a ket corresponds to the product of a square matrix times a column vector, yielding another column vector (i.e., a ket) as follows (row-column multiplication)

$$\begin{aligned} \mathbf{M}|\mathbf{b}\rangle &= \begin{pmatrix} (M_{11} & M_{12} & M_{13}) \\ (M_{21} & M_{22} & M_{23}) \\ (M_{31} & M_{32} & M_{33}) \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \\ &= \begin{pmatrix} M_{11}b_1 + M_{12}b_2 + M_{13}b_3 \\ M_{21}b_1 + M_{22}b_2 + M_{23}b_3 \\ M_{31}b_1 + M_{32}b_2 + M_{33}b_3 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{3} M_{1i} b_i \\ \sum_{i=1}^{3} M_{2i} b_i \\ \sum_{i=1}^{3} M_{3i} b_i \end{pmatrix} = \begin{pmatrix} \langle \mathbf{m}_{(1)}|\mathbf{b}^{(1)}\rangle \\ \langle \mathbf{m}_{(2)}|\mathbf{b}^{(1)}\rangle \\ \langle \mathbf{m}_{(3)}|\mathbf{b}^{(1)}\rangle \end{pmatrix} \end{aligned} \tag{4.4}$$

where

$$\langle \mathbf{m}_{(1)}| = (M_{11} \quad M_{12} \quad M_{13}), \qquad \langle \mathbf{m}_{(2)}| = (M_{21} \quad M_{22} \quad M_{23}), \qquad \langle \mathbf{m}_{(3)}| = (M_{31} \quad M_{32} \quad M_{33}), \tag{4.5}$$

$$|\mathbf{b}^{(1)}\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}. \tag{4.6}$$

However, we have also (column-row multiplication)

$$
\begin{aligned}
\mathbf{M}|\mathbf{b}\rangle &= \left(\begin{pmatrix} M_{11} \\ M_{21} \\ M_{31} \end{pmatrix} \begin{pmatrix} M_{12} \\ M_{22} \\ M_{32} \end{pmatrix} \begin{pmatrix} M_{13} \\ M_{23} \\ M_{33} \end{pmatrix}\right) \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \\
&= \begin{pmatrix} M_{11} \\ M_{21} \\ M_{31} \end{pmatrix} b_1 + \begin{pmatrix} M_{12} \\ M_{22} \\ M_{32} \end{pmatrix} b_2 + \begin{pmatrix} M_{13} \\ M_{23} \\ M_{33} \end{pmatrix} b_3 \\
&= \begin{pmatrix} M_{11}b_1 \\ M_{21}b_1 \\ M_{31}b_1 \end{pmatrix} + \begin{pmatrix} M_{12}b_2 \\ M_{22}b_2 \\ M_{32}b_2 \end{pmatrix} + \begin{pmatrix} M_{13}b_3 \\ M_{23}b_3 \\ M_{33}b_3 \end{pmatrix} \\
&= \begin{pmatrix} M_{11}b_1 + M_{12}b_2 + M_{13}b_3 \\ M_{21}b_1 + M_{22}b_2 + M_{23}b_3 \\ M_{31}b_1 + M_{32}b_2 + M_{33}b_3 \end{pmatrix} \\
&= \left|\mathbf{m}^{(1)}\right\rangle\left\langle\mathbf{b}_{(1)}\right| + \left|\mathbf{m}^{(2)}\right\rangle\left\langle\mathbf{b}_{(2)}\right| + \left|\mathbf{m}^{(3)}\right\rangle\left\langle\mathbf{b}_{(3)}\right| = \sum_{i=1}^{3} \left|\mathbf{m}^{(i)}\right\rangle\left\langle\mathbf{b}_{(i)}\right|
\end{aligned}
\tag{4.7}
$$

where

$$
\left|\mathbf{m}^{(1)}\right\rangle = \begin{pmatrix} M_{11} \\ M_{21} \\ M_{31} \end{pmatrix}, \qquad \left|\mathbf{m}^{(2)}\right\rangle = \begin{pmatrix} M_{12} \\ M_{22} \\ M_{32} \end{pmatrix}, \qquad \left|\mathbf{m}^{(3)}\right\rangle = \begin{pmatrix} M_{13} \\ M_{23} \\ M_{33} \end{pmatrix} \tag{4.8}
$$

$$
\left\langle\mathbf{b}_{(1)}\right| = (b_1), \qquad \left\langle\mathbf{b}_{(2)}\right| = (b_2), \qquad \left\langle\mathbf{b}_{(3)}\right| = (b_3) \tag{4.9}
$$

and the product of a bra times a square matrix corresponds to the product of a row vector times a square matrix, which is again a row vector (i.e., a "bra") as follows

$$
\langle\mathbf{a}|\mathbf{M} = (a_1, a_2, a_3) \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} = \left(\sum\nolimits_{1=1}^{3} a_i M_{i1}\, , \sum\nolimits_{1=1}^{3} a_i M_{i2}\, , \sum\nolimits_{1=1}^{3} a_i M_{i3}\right) \tag{4.10}
$$

or

$$
\begin{aligned}
\langle\mathbf{a}|\mathbf{M} &= (a_1, a_2, a_3) \begin{pmatrix} (M_{11} & M_{12} & M_{13}) \\ (M_{21} & M_{22} & M_{23}) \\ (M_{31} & M_{32} & M_{33}) \end{pmatrix} \\
&= a_1(M_{11} \quad M_{12} \quad M_{13}) + a_2(M_{21} \quad M_{22} \quad M_{23}) + a_3(M_{31} \quad M_{32} \quad M_{33}) \\
&= (a_1M_{11} \quad a_1M_{12} \quad a_1M_{13}) + (a_2M_{21} \quad a_2M_{22} \quad a_2M_{23}) + (a_3M_{31} \quad a_3M_{32} \quad a_3M_{33}) \\
&= \left(\sum\nolimits_{1=1}^{3} a_i M_{i1}\, , \sum\nolimits_{1=1}^{3} a_i M_{i2}\, , \sum\nolimits_{1=1}^{3} a_i M_{i3}\right) = \sum_{i=1}^{3} \left|\mathbf{a}^{(i)}\right\rangle\left\langle\mathbf{m}_{(i)}\right|
\end{aligned}
\tag{4.11}
$$

where

$$
\left|\mathbf{a}^{(1)}\right\rangle = (a_1), \qquad \left|\mathbf{a}^{(2)}\right\rangle = (a_2), \quad \left|\mathbf{a}^{(3)}\right\rangle = (a_3) \tag{4.12}
$$

Obviously, we can form an ordinary (real) number by taking the compound product of a bra, a square matrix, and a ket, which corresponds to forming the product of a row vector times a square matrix times a column vector

$$
\begin{aligned}
\langle\mathbf{a}|\mathbf{M}|\mathbf{b}\rangle &= (a_1, a_2, a_3) \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \\
&= \left(\sum\nolimits_{i=1}^{3} a_i M_{i1}\, , \sum\nolimits_{i=1}^{3} a_i M_{i2}\, , \sum\nolimits_{i=1}^{3} a_i M_{i3}\right) \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \\
&= \sum\nolimits_{i=1}^{3} a_i M_{i1} b_1 + \sum\nolimits_{i=1}^{3} a_i M_{i2} b_2 + \sum\nolimits_{i=1}^{3} a_i M_{i3} b_3 = \sum\nolimits_{j=1}^{3} \sum\nolimits_{i=1}^{3} a_i M_{ij} b_j
\end{aligned}
\tag{4.13}
$$

and

$$
\begin{aligned}
\mathbf{AB} &= \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}\begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} \\
&= \begin{pmatrix}
(A_{11} \quad A_{12} \quad A_{13})\begin{pmatrix} B_{11} \\ B_{21} \\ B_{31} \end{pmatrix} & (A_{11} \quad A_{12} \quad A_{13})\begin{pmatrix} B_{12} \\ B_{22} \\ B_{32} \end{pmatrix} & (A_{11} \quad A_{12} \quad A_{13})\begin{pmatrix} B_{13} \\ B_{23} \\ B_{33} \end{pmatrix} \\
(A_{21} \quad A_{22} \quad A_{23})\begin{pmatrix} B_{11} \\ B_{21} \\ B_{31} \end{pmatrix} & (A_{21} \quad A_{22} \quad A_{23})\begin{pmatrix} B_{12} \\ B_{22} \\ B_{32} \end{pmatrix} & (A_{21} \quad A_{22} \quad A_{23})\begin{pmatrix} B_{13} \\ B_{23} \\ B_{33} \end{pmatrix} \\
(A_{31} \quad A_{32} \quad A_{33})\begin{pmatrix} B_{11} \\ B_{21} \\ B_{31} \end{pmatrix} & (A_{31} \quad A_{32} \quad A_{33})\begin{pmatrix} B_{12} \\ B_{22} \\ B_{32} \end{pmatrix} & (A_{31} \quad A_{32} \quad A_{33})\begin{pmatrix} B_{13} \\ B_{23} \\ B_{33} \end{pmatrix}
\end{pmatrix} \\
&= \begin{pmatrix}
\sum_{p=1}^{3} A_{1p}B_{p1} & \sum_{p=1}^{3} A_{1p}B_{p2} & \sum_{p=1}^{3} A_{1p}B_{p3} \\
\sum_{p=1}^{3} A_{2p}B_{p1} & \sum_{p=1}^{3} A_{2p}B_{p2} & \sum_{p=1}^{3} A_{2p}B_{p3} \\
\sum_{p=1}^{3} A_{3p}B_{p1} & \sum_{p=1}^{3} A_{3p}B_{p2} & \sum_{p=1}^{3} A_{3p}B_{p3}
\end{pmatrix} \\
&= \begin{pmatrix}
\langle \mathbf{a}_{(1)} | \mathbf{b}^{(1)} \rangle & \langle \mathbf{a}_{(1)} | \mathbf{b}^{(2)} \rangle & \langle \mathbf{a}_{(1)} | \mathbf{b}^{(3)} \rangle \\
\langle \mathbf{a}_{(2)} | \mathbf{b}^{(1)} \rangle & \langle \mathbf{a}_{(2)} | \mathbf{b}^{(2)} \rangle & \langle \mathbf{a}_{(2)} | \mathbf{b}^{(3)} \rangle \\
\langle \mathbf{a}_{(3)} | \mathbf{b}^{(1)} \rangle & \langle \mathbf{a}_{(3)} | \mathbf{b}^{(2)} \rangle & \langle \mathbf{a}_{(3)} | \mathbf{b}^{(3)} \rangle
\end{pmatrix}
\end{aligned}
\tag{4.14}
$$

$$
\langle \mathbf{a}_{(1)} | = (A_{11} \quad A_{12} \quad A_{13}), \qquad \langle \mathbf{a}_{(2)} | = (A_{21} \quad A_{22} \quad A_{23}), \qquad \langle \mathbf{a}_{(3)} | = (A_{31} \quad A_{32} \quad A_{33}) \tag{4.15}
$$

$$
| \mathbf{b}^{(1)} \rangle = \begin{pmatrix} B_{11} \\ B_{21} \\ B_{31} \end{pmatrix}, \qquad | \mathbf{b}^{(2)} \rangle = \begin{pmatrix} B_{12} \\ B_{22} \\ B_{32} \end{pmatrix}, \qquad | \mathbf{b}^{(3)} \rangle = \begin{pmatrix} B_{13} \\ B_{23} \\ B_{33} \end{pmatrix} \tag{4.16}
$$

or

$$
\begin{aligned}
\mathbf{AB} &= \begin{pmatrix} A_{11} \\ A_{21} \\ A_{31} \end{pmatrix}(B_{11} \quad B_{12} \quad B_{13}) + \begin{pmatrix} A_{12} \\ A_{22} \\ A_{32} \end{pmatrix}(B_{21} \quad B_{22} \quad B_{23}) + \begin{pmatrix} A_{13} \\ A_{23} \\ A_{33} \end{pmatrix}(B_{31} \quad B_{32} \quad B_{33}) \\
&= \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{11}B_{13} \\ A_{21}B_{11} & A_{21}B_{12} & A_{21}B_{13} \\ A_{31}B_{11} & A_{31}B_{12} & A_{31}B_{13} \end{pmatrix} + \begin{pmatrix} A_{12}B_{21} & A_{12}B_{22} & A_{12}B_{23} \\ A_{22}B_{21} & A_{22}B_{22} & A_{22}B_{23} \\ A_{32}B_{21} & A_{32}B_{22} & A_{32}B_{23} \end{pmatrix} + \begin{pmatrix} A_{13}B_{31} & A_{13}B_{32} & A_{13}B_{33} \\ A_{23}B_{31} & A_{23}B_{32} & A_{23}B_{33} \\ A_{33}B_{31} & A_{33}B_{32} & A_{33}B_{33} \end{pmatrix} \\
&= \begin{pmatrix}
\sum_{p=1}^{3} A_{1p}B_{p1} & \sum_{p=1}^{3} A_{1p}B_{p2} & \sum_{p=1}^{3} A_{1p}B_{p3} \\
\sum_{p=1}^{3} A_{2p}B_{p1} & \sum_{p=1}^{3} A_{2p}B_{p2} & \sum_{p=1}^{3} A_{2p}B_{p3} \\
\sum_{p=1}^{3} A_{3p}B_{p1} & \sum_{p=1}^{3} A_{3p}B_{p2} & \sum_{p=1}^{3} A_{3p}B_{p3}
\end{pmatrix} = \sum_{i=1}^{3} | \mathbf{a}^{(i)} \rangle \langle \mathbf{b}_{(j)} |
\end{aligned}
\tag{4.17}
$$

$$
| \mathbf{a}^{(1)} \rangle = \begin{pmatrix} A_{11} \\ A_{21} \\ A_{31} \end{pmatrix}, \qquad | \mathbf{a}^{(2)} \rangle = \begin{pmatrix} A_{12} \\ A_{22} \\ A_{32} \end{pmatrix}, \qquad | \mathbf{a}^{(3)} \rangle = \begin{pmatrix} A_{13} \\ A_{23} \\ A_{33} \end{pmatrix} \tag{4.18}
$$

$$
\langle \mathbf{b}_{(1)} | = (B_{11} \quad B_{12} \quad B_{13}), \qquad \langle \mathbf{b}_{(2)} | = (B_{21} \quad B_{22} \quad B_{23}), \qquad \langle \mathbf{b}_{(3)} | = (B_{31} \quad B_{32} \quad B_{33}) \tag{4.19}
$$

Vectors and Matrices with Index Notations

Let $A_{ij} \in \mathbb{R}$, $i = 1,2,\dots,m$, $j = 1,2,\dots,n$. Then the ordered rectangular array

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & & A_{1n} \\ A_{21} & A_{22} & & A_{2n} \\ & & & \\ A_{m1} & A_{m2} & & A_{mn} \end{pmatrix} = A_{ij}, \quad i = 1,2,\dots,m; \ j = 1,2,\dots,n, \tag{4.20}$$

Note, the first subscript locates the row in which the typical element lies while the second subscript locates the column. For example, A_{jk} denotes the element lying in the jth row and kth column of the matrix $\mathbf{A}$.

Definition: Let $\mathbf{A}$ and $\mathbf{B}$ are $m \times n$, and let the sum $\mathbf{A} + \mathbf{B}$ be $\mathbf{C} = \mathbf{A} + \mathbf{B}$, then $\mathbf{C}$ is a $m \times n$ matrix, with element (i,j) given by

$$C_{ij} = A_{ij} + B_{ij} \tag{4.21}$$

for all $i = 1,2,\dots,m$, $j = 1,2,\dots,n$.

Definition: Let $\mathbf{A}$ be $m \times n$, and let a is a scalar, then $\mathbf{C} = a\mathbf{A}$ is $m \times n$ matrix, with element (i,j) given by

$$C_{ij} = aA_{ij} \tag{4.22}$$

for all $i = 1,2,\dots,m$, $j = 1,2,\dots,n$.

Definition: Let $\mathbf{A}$ be $m \times n$, then $\mathbf{A}^T$ is $n \times m$ matrix, with element (i,j) given by

$$(A^T)_{ij} = A_{ji} \tag{4.23}$$

for all $i = 1,2,\dots,m$, $j = 1,2,\dots,n$.

Example 4.1

Let us consider also,

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} = A_{ij}, \quad \mathbf{B} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} = B_{ij}$$

We have

$$(A+B)_{ij} = A_{ij} + B_{ij} \rightarrow \mathbf{A} + \mathbf{B} = \begin{pmatrix} A_{11}+B_{11} & A_{12}+B_{12} & A_{13}+B_{13} \\ A_{21}+B_{21} & A_{22}+B_{22} & A_{23}+B_{23} \\ A_{31}+B_{31} & A_{32}+B_{32} & A_{33}+B_{33} \end{pmatrix}$$

$$(c\,A)_{ij} = c\,A_{ij} \rightarrow c\mathbf{A} = \begin{pmatrix} cA_{11} & cA_{12} & cA_{13} \\ cA_{21} & cA_{22} & cA_{23} \\ cA_{31} & cA_{32} & cA_{33} \end{pmatrix}$$

$$(A^T)_{ij} = A_{ji} \rightarrow \mathbf{A}^T = \begin{pmatrix} A_{11} & A_{21} & A_{31} \\ A_{12} & A_{22} & A_{32} \\ A_{13} & A_{23} & A_{33} \end{pmatrix}$$

Definition: Let $\mathbf{A}$ be $m \times n$, and $\mathbf{B}$ be $n \times p$, and let the product $\mathbf{AB}$ be

$$\mathbf{C} = \mathbf{AB} \tag{4.24}$$

then $\mathbf{C}$ is a $m \times p$ matrix, with element (i,j) given by

$$C_{ij} = \sum_{k=1}^{n} A_{ik}B_{kj} \tag{4.25}$$

for all $i = 1,2,\dots,m$, $j = 1,2,\dots,p$.

Definition: Let $\mathbf{A}$ be $m \times n$, and $\mathbf{x}$ be $n \times 1$, then the typical element of the product

$$\mathbf{z} = \mathbf{Ax} \tag{4.26}$$

is given by

$$z_i = \sum_{k=1}^{n} A_{ik}x_k \tag{4.27}$$

for all $i = 1,2,\dots,m$.

Definition: Let $\mathbf{y}$ be $m \times 1$, then the typical element of the product

$$\mathbf{z}^T = \mathbf{y}^T\mathbf{A} \tag{4.28}$$

is given by

$$z_i = \sum_{k=1}^{n} y_k A_{ki} \tag{4.29}$$

for all $i = 1,2,\ldots,n$.

Definition: The scalar resulting from the product

$$\alpha = \mathbf{y}^T\mathbf{A}\mathbf{x} \tag{4.30}$$

is given by

$$\alpha = \sum_{j=1}^{m}\sum_{k=1}^{n} y_j A_{jk} x_k \tag{4.31}$$

Definition: The trace of an $n \times n$ square matrix $\mathbf{A}$ is defined as

$$tr(\mathbf{A}) = \sum_{i=1}^{n} A_{ii} = A_{11} + A_{22} + \cdots + A_{nn} \tag{4.32}$$

Example 4.2

Let $\mathbf{A}$ be a matrix, $\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$, then $\mathrm{tr}(\mathbf{A}) = 1 + 5 + 9 = 15$.

Theorem 4.1:

1- The trace is a linear mapping. That is,

$$\mathrm{tr}(\mathbf{A} + \mathbf{B}) = \mathrm{tr}(\mathbf{A}) + \mathrm{tr}(\mathbf{B}) \tag{4.33}$$

$$\mathrm{tr}(c\ \mathbf{A}) = c\ \mathrm{tr}(\mathbf{A}) \tag{4.34}$$

$$\mathrm{tr}(\mathbf{A}) = \mathrm{tr}(\mathbf{A}^T) \tag{4.35}$$

for all square matrices $\mathbf{A}$ and $\mathbf{B}$, and all scalars c.

2- If $\mathbf{A}$ and $\mathbf{B}$ are $m \times n$ and $n \times m$ real matrices, respectively, then

$$\mathrm{tr}(\mathbf{AB}) = \mathrm{tr}(\mathbf{BA}) \tag{4.36}$$

More generally, the trace is invariant under cyclic permutations, that is,

$$\mathrm{tr}(\mathbf{ABC}) = \mathrm{tr}(\mathbf{BCA}) = \mathrm{tr}(\mathbf{CAB}) \tag{4.37}$$

Proof:

$$\mathrm{tr}(\mathbf{A} + \mathbf{B}) = \sum_{i=1}^{n} A_{ii} + B_{ii} = \sum_{i=1}^{n} A_{ii} + \sum_{i=1}^{n} B_{ii} = \mathrm{tr}(\mathbf{A}) + \mathrm{tr}(\mathbf{B})$$

$$\mathrm{tr}(c\mathbf{A}) = \sum_{i=1}^{n} cA_{ii} = c\sum_{i=1}^{n} A_{ii} = \mathrm{c\ tr}(\mathbf{A})$$

$$\mathrm{tr}(\mathbf{A}) = \sum_{i=1}^{n} A_{ii} = \mathrm{tr}(\mathbf{A}^T)$$

The trace of a matrix is the sum of its diagonal elements, but transposition leaves the diagonal elements unchanged.

$$\mathrm{tr}(\mathbf{AB}) = \sum_{i=1}^{n}\sum_{j=1}^{m} A_{ij}B_{ji} = \sum_{j=1}^{m}\sum_{i=1}^{n} B_{ji}A_{ij} = \mathrm{tr}(\mathbf{BA})$$

$$\mathrm{tr}(\mathbf{ABC}) = \sum_{i=1}^{n}\sum_{j=1}^{m}\sum_{k=1}^{l} A_{ij}B_{jk}C_{ki} = \sum_{i=1}^{n}\sum_{j=1}^{m}\sum_{k=1}^{l} B_{jk}C_{ki}A_{ij} = \mathrm{tr}(\mathbf{BCA})$$

■

Now, let us consider the following types of matrices.

Definition (Identity matrix): The identity matrix of size n is the $n \times n$ square matrix with ones on the main diagonal and zeros elsewhere.

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & \dots & 0 & 1 \end{pmatrix} \tag{4.38}$$

Definition (Real Matrix): The conjugate complex of matrix $\mathbf{M}$ is written as $\mathbf{M}^*$ and the elements of $\mathbf{M}^*$ are the conjugate complexes of the elements of $\mathbf{M}$ i.e.

$$(M^*)_{\mathrm{ij}} = \left(M_{\mathrm{ij}}\right)^*. \tag{4.39}$$

For a real matrix all the elements are real and therefore

$$\mathbf{M} = \mathbf{M}^*, \qquad (M)_{\mathrm{ij}} = M^*_{\mathrm{ij}}. \tag{4.40}$$

Definition (Symmetric Matrix): The transpose of a matrix $\mathbf{M}$ is obtained by changing rows into columns (or vice versa) and is given the symbol $\mathbf{M}^T$. For a symmetric matrix

$$\mathbf{M}^T = \mathbf{M}, \ M_{ij} = M_{ji}. \tag{4.41}$$

Definition (Skew-Symmetric Matrix): The skew-symmetric matrix satisfies

$$\mathbf{M}^T = -\mathbf{M}, \ M_{ij} = -M_{ji}. \tag{4.42}$$

Definition (Orthogonal matrix): An orthogonal matrix satisfies

$$\mathbf{M}\mathbf{M}^T = \mathbf{M}^T\mathbf{M} = \mathbf{I}. \tag{4.43}$$

This leads to the equivalent characterization: a matrix $\mathbf{M}$ is orthogonal if its transpose is equal to its inverse:

$$\mathbf{M}^T = \mathbf{M}^{-1} \tag{4.44}$$

Example 4.3

The matrix $\mathbf{A}$ is symmetric, but the matrix $\mathbf{B}$ is skew- symmetric.

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & -2 \\ 1 & 3 & 0 \\ -2 & 0 & 5 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 & 2 & -45 \\ -2 & 0 & -4 \\ 45 & 4 & 0 \end{pmatrix}.$$

4.2 Vector Spaces

Definition (Vector Space): Let K be a given field and let V be a non-empty set with rules of addition and scalar multiplication which assigns to any $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V$ a sum $|\mathbf{u}\rangle + |\mathbf{v}\rangle \in V$ and to any $|\mathbf{u}\rangle \in V$, $k \in K$ a product $k|\mathbf{u}\rangle \in V$. Then V is called a vector space over K (and the elements of V are called vectors) if the following axioms hold.

1- There is a vector in V, denoted by $|\mathbf{0}\rangle$ and called the zero vector, for which
$$|\mathbf{u}\rangle + |\mathbf{0}\rangle = |\mathbf{u}\rangle, \qquad |\mathbf{u}\rangle \in V. \tag{4.45}$$
2- For each vector $|\mathbf{u}\rangle \in V$ there is a vector in V, denoted by $|-\mathbf{u}\rangle$, for which
$$|\mathbf{u}\rangle + |-\mathbf{u}\rangle = |\mathbf{0}\rangle. \tag{4.46}$$
3- For any vectors $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V$,
$$|\mathbf{u}\rangle + |\mathbf{v}\rangle = |\mathbf{v}\rangle + |\mathbf{u}\rangle. \tag{4.47}$$
4- For any vectors $|\mathbf{u}\rangle, |\mathbf{v}\rangle, |\mathbf{w}\rangle \in V$,
$$(|\mathbf{u}\rangle + |\mathbf{v}\rangle) + |\mathbf{w}\rangle = |\mathbf{u}\rangle + (|\mathbf{v}\rangle + |\mathbf{w}\rangle). \tag{4.48}$$
5- For any scalar $k \in K$ and vectors $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V$,
$$k(|\mathbf{u}\rangle + |\mathbf{v}\rangle) = k|\mathbf{u}\rangle + k|\mathbf{v}\rangle. \tag{4.49}$$
6- For any scalars $a, b \in K$ and any vector $|\mathbf{u}\rangle \in V$,
$$(a + b)|\mathbf{u}\rangle = a|\mathbf{u}\rangle + b|\mathbf{u}\rangle. \tag{4.50}$$
7- For any scalars $a, b \in K$ and any vector $|\mathbf{u}\rangle \in V$,
$$(ab)|\mathbf{u}\rangle = a(b|\mathbf{u}\rangle). \tag{4.51}$$
8- For the unit scalar $1 \in K$, $1|\mathbf{u}\rangle = |\mathbf{u}\rangle$, for any vector $|\mathbf{u}\rangle \in V$.

Let us consider the following two important linear vector spaces:

1- The notation $\mathbb{R}^n$ is frequently used to denote the set of all n-tuples of elements in $\mathbb{R}$. Here $\mathbb{R}^n$ is viewed as a vector space over $\mathbb{R}$ where vector addition and scalar multiplication are defined by

$$(a_1, a_2, \dots, a_n) + (b_1, b_2, \dots, b_n) = (a_1 + b_1, a_2 + b_2, \dots, a_n + b_n), \tag{4.52}$$

and

$$k(a_1, a_2, \dots, a_n) = (ka_1, ka_2, \dots, ka_n). \tag{4.53}$$

The zero vector in $\mathbb{R}^n$ is the n-tuple of zeros,

$$(0,0, \dots ,0), \tag{4.54}$$

and the negative of a vector is defined by

$$-(a_1, a_2, \dots, a_n) = (-a_1, -a_2, \dots, -a_n). \tag{4.55}$$

2- The notation $M_{m\times n}$ or simply M, will be used to denote the set of all $m \times n$ matrices over $\mathbb{R}$. Here $M_{m\times n}$ is viewed as a vector space over $\mathbb{R}$ where matrix addition and scalar multiplication are defined by

$$\begin{pmatrix} a_{11} & a_{11} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \dots & \dots & \cdots & \dots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} + \begin{pmatrix} b_{11} & b_{11} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \dots & \dots & \cdots & \dots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{pmatrix} = \begin{pmatrix} a_{11} + b_{11} & \cdots & \cdots & a_{1n} + b_{1n} \\ a_{21} + a_{21} & \cdots & \cdots & a_{2n} + b_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} + b_{n1} & \cdots & \cdots & a_{nn} + b_{nn} \end{pmatrix}, \tag{4.56}$$

and

$$k\begin{pmatrix} a_{11} & a_{11} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \dots & \dots & \cdots & \dots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} ka_{11} & \cdots & \cdots & ka_{1n} \\ ka_{21} & \cdots & \cdots & ka_{2n} \\ \dots & \dots & \dots & \dots \\ ka_{n1} & \cdots & \cdots & ka_{nn} \end{pmatrix}. \tag{4.57}$$

The zero vector in $M_{m,n}$ is the matrix of zeros,

$$\begin{pmatrix} 0 & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \cdots & \cdots & 0 \end{pmatrix}, \tag{4.58}$$

and the negative of a vector is defined by

$$-\begin{pmatrix} a_{11} & a_{11} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \dots & \dots & \cdots & \dots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} -a_{11} & \cdots & \cdots & -a_{1n} \\ -a_{21} & \cdots & \cdots & -a_{2n} \\ \dots & \dots & \dots & \dots \\ -a_{n1} & \cdots & \cdots & -a_{nn} \end{pmatrix}. \tag{4.59}$$

Definition (Linear Combination): Let V be a vector space over $\mathbb{R}$ and let $|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle \in V$. Any vector in V of the form

$$a_1|\mathbf{u}_1\rangle + a_2|\mathbf{u}_2\rangle + \cdots + a_n|\mathbf{u}_n\rangle, \tag{4.60}$$

where the $a_i \in \mathbb{R}$, is called a linear combination of $|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle$.

Example 4.4

Let us consider the following set of vectors in $\mathbb{R}^3$

$$S = \{\mathbf{v}_1 = (1,3,1), \mathbf{v}_2 = (0,1,2), \mathbf{v}_3 = (1,0,-5)\}$$

The vector $\mathbf{v}_1$ is a linear combination of $\mathbf{v}_2$ and $\mathbf{v}_3$ because

$$\mathbf{v}_1 = 3\mathbf{v}_2 + \mathbf{v}_3.$$

Definition (Linear Span):
The vectors $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$,…, $|\mathbf{u}_n\rangle$ span V if, for every $|\mathbf{u}\rangle \in V$, there exist scalars a_1, a_2,… a_n such that
$$|\mathbf{u}\rangle = a_1|\mathbf{u}_1\rangle + a_2|\mathbf{u}_2\rangle + \cdots + a_n|\mathbf{u}_n\rangle, \tag{4.61}$$
that is, if $|\mathbf{u}\rangle$ is a linear combination of $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$,…, $|\mathbf{u}_n\rangle$.

Example 4.5

The set of vectors
$$S = \{\mathbf{v}_1 = (1,0,0), \mathbf{v}_2 = (1,0,0), \mathbf{v}_3 = (0,0,1)\}$$
spans $\mathbb{R}^3$ because any vector $\mathbf{u} = (u_1, u_2, u_3)$ in $\mathbb{R}^3$ can be written as
$$\mathbf{u} = u_1(1,0,0) + u_2(1,0,0) + u_3(0,0,1) = (u_1, u_2, u_3)$$
Also, let the field K be the set $\mathbb{R}$ of real numbers and let the vector space V be the Euclidean space $\mathbb{R}^n$. Consider the vectors
$$\langle\mathbf{e}_1| = (1,0, \dots ,0), \langle\mathbf{e}_2| = (0,1, \dots ,0), \dots \langle\mathbf{e}_m| = (0,0, \dots ,1).$$
Actually, any vector $(a_1, a_2, \dots , a_n)$ in $\mathbb{R}^n$ is a linear combination of $\langle\mathbf{e}_1|$, …,$\langle\mathbf{e}_n|$, i.e.,
$$(a_1, a_2, \dots , a_n) = a_1\langle\mathbf{e}_1| + a_2\langle\mathbf{e}_2| + \cdots + a_n\langle\mathbf{e}_n|.$$

Definition (Linear Dependent and Independent): Let V be a vector space over $\mathbb{R}$. The vectors $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$,…, $|\mathbf{u}_n\rangle \in V$ are said to be linearly dependent over $\mathbb{R}$, or simply dependent, if there exist scalars a_1, a_2, ..., $a_m \in \mathbb{R}$ not all of them 0, such that
$$a_1|\mathbf{u}_1\rangle + a_2|\mathbf{u}_2\rangle + \cdots + a_n|\mathbf{u}_n\rangle = |\mathbf{0}\rangle. \tag{4.62}$$
Otherwise, the vectors are said to be linearly independent over $\mathbb{R}$, or simply independent.

For example: The set $S = \{\mathbf{v}_1 = (1,2), \mathbf{v}_2 = (2,4)\}$ in $\mathbb{R}^2$ is linearly dependent because $-2(1,2) + (2,4) = (0,0)$.

Example 4.6

Determine whether the set of vectors in $\mathbb{R}^3$ is linearly independent or linearly dependent.
$$S = \{\mathbf{v}_1 = (1,2,3), \mathbf{v}_2 = (0,1,2), \mathbf{v}_3 = (-2,0,1)\}$$
Solution

To test for linear independence or linear dependence, form the vector equation
$$c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + c_3\mathbf{v}_3 = \mathbf{0}$$
If the only solution of this equation is
$$c_1 = c_2 = c_3 = 0$$
then the set S is linearly independent. Otherwise, S is linearly dependent. We have
$$c_1(1,2,3) + c_2(0,1,2) + c_3(-2,0,1) = (0,0,0)$$
$$(c_1 - 2c_3, 2c_1 + c_2, 3c_1 + 2c_2 + c_3) = (0,0,0)$$
Which yields the homogeneous system of linear equations
$$c_1 - 2c_3 = 0$$
$$2c_1 + c_2 = 0$$
$$3c_1 + 2c_2 + c_3 = 0$$
This implies that the only solution is the trivial solution
$$c_1 = c_2 = c_3 = 0$$
So, S is linearly independent.

Example 4.7

The unit vectors $|\mathbf{e}_1\rangle$, $|\mathbf{e}_2\rangle$,…, $|\mathbf{e}_n\rangle$ in $\mathbb{R}^n$ are linearly independent.

Theorem 4.2: The vectors $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$,…, $|\mathbf{u}_n\rangle$ are linearly dependent if and only if one of them is a linear combination of the others.

Definition (Basis): A set $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ of vectors is a basis of V if the following two conditions hold:

1- $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$,…, $|\mathbf{u}_n\rangle$ are linearly independent.

2- $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$,…, $|\mathbf{u}_n\rangle$ span V.

In other words, a set $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ of vectors is a basis of V if every vector $|\mathbf{u}\rangle \in V$ can be written uniquely as a linear combination of the basis vector.

Example 4.8

Show that $S = \left\{|\mathbf{u}_1\rangle = \begin{pmatrix}1\\-1\end{pmatrix}, |\mathbf{u}_2\rangle = \begin{pmatrix}3\\2\end{pmatrix}\right\}$ is a basis of $\mathbb{R}^2$.

Solution

Suppose that

$$a_1|\mathbf{u}_1\rangle + a_2|\mathbf{u}_2\rangle = \begin{pmatrix}0\\0\end{pmatrix} \Rightarrow \begin{pmatrix}a_1 + 3a_2\\-a_1 + 2a_2\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}.$$

This leads to the equations

$$a_1 + 3a_2 = 0, \quad -a_1 + 2a_2 = 0.$$

Solving the system of equations, we have $a_1 = a_2 = 0$. So that, the vectors $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$ are linearly independent. Next, we show that every vector in $\mathbb{R}^2$ can be written as linear combinations of $|\mathbf{u}_1\rangle$ and $|\mathbf{u}_2\rangle$. Let $|\mathbf{u}\rangle = \begin{pmatrix}x\\y\end{pmatrix} \in \mathbb{R}^2$, we must show that there exist scalars b_1 and b_2 such that

$$|\mathbf{u}\rangle = b_1|\mathbf{u}_1\rangle + b_2|\mathbf{u}_2\rangle \Rightarrow \begin{pmatrix}x\\y\end{pmatrix} = \begin{pmatrix}b_1 + 3b_2\\-b_1 + 2b_2\end{pmatrix}.$$

This leads to the equations

$$b_1 + 3b_2 = x, \quad -b_1 + 2b_2 = y.$$

Therefore, for any values of x and y, we have

$$b_1 = \frac{x+y}{5}, \quad b_2 = \frac{2x-3y}{5}.$$

Example 4.9

For example, $S = \{|\mathbf{e}_1\rangle, |\mathbf{e}_2\rangle, \dots, |\mathbf{e}_n\rangle\}$ is a basis of $\mathbb{R}^n$ and is called the standard basis.

Definition (Dimension): A vector space V is said to be of finite dimension n or to be n dimensional, written

$$\dim V = n, \tag{4.63}$$

if V has such a basis with n elements.

Definition (Coordinates): Let V be an n-dimensional vector space over $\mathbb{R}$, and suppose $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ is a basis of V. Then any vector $|\mathbf{u}\rangle \in V$ can be expressed uniquely as a linear combination of the basis vectors in S; say

$$|\mathbf{u}\rangle = a_1|\mathbf{u}_1\rangle + a_2|\mathbf{u}_2\rangle + \cdots + a_n|\mathbf{u}_n\rangle. \tag{4.64}$$

These n scalars a_1, a_2, …, a_n are called the coordinates of $|\mathbf{u}\rangle$ relative to the basis S; and they form the n-tuple $(a_1, a_2, \dots a_n)$ in $\mathbb{R}^n$, called the coordinate vector of $|\mathbf{u}\rangle$ relative to S. We denote this vector by $[\mathbf{u}]_s$. Thus

$$[\mathbf{u}]_s = (a_1, a_2, \dots a_n). \tag{4.65}$$

4.3 Inner Product

The inner product for a vector space V is a map from $V \times V$ to the real numbers. We can express this more clearly by saying that the inner product is a function on two vectors $|\mathbf{u}\rangle$, $|\mathbf{v}\rangle$ that produces a real number which we represent by $\langle\mathbf{u}|\mathbf{v}\rangle$. A vector space that also has an inner product is referred to as an inner product space.

Definition (Inner Product): Let V be a vector space. Suppose to each pair of vectors $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V$ there is assigned a number, denoted by $\langle\mathbf{u}|\mathbf{v}\rangle$. This function is called an inner product on V if it satisfies the following axioms:

1- $\langle\mathbf{u}|a\mathbf{v}_1 + b\mathbf{v}_2\rangle = a\langle\mathbf{u}|\mathbf{v}_1\rangle + b\langle\mathbf{u}|\mathbf{v}_2\rangle$,

2- $\langle a\mathbf{u}_1 + b\mathbf{u}_2|\mathbf{v}\rangle = a\langle\mathbf{u}_1|\mathbf{v}\rangle + b\langle\mathbf{u}_2|\mathbf{v}\rangle$,

3- $\langle\mathbf{u}|\mathbf{v}\rangle = \langle\mathbf{v}|\mathbf{u}\rangle$,

4- $\langle\mathbf{u}|\mathbf{u}\rangle \geq 0$, and $\langle\mathbf{u}|\mathbf{u}\rangle = 0$ if and only if $|\mathbf{u}\rangle = 0$.

For a finite-dimensional vector space, the inner product can be written as a matrix multiplication of a row vector (bra) with a column vector (ket):

$$\langle\mathbf{u}|\mathbf{v}\rangle = u_1\mathrm{v}_1 + u_2\mathrm{v}_2 + \cdots + u_n\mathrm{v}_n = (u_1, u_2, \dots u_n)\begin{pmatrix}\mathrm{v}_1\\ \mathrm{v}_2\\ \dots\\ \mathrm{v}_n\end{pmatrix}. \tag{4.66}$$

Example 4.10

Show that the following function defines an inner product on $\mathbb{R}^2$, where $\mathbf{u} = (u_1, u_2)$ and $\mathbf{v} = (\mathrm{v}_1, \mathrm{v}_2)$.

$$\langle\mathbf{u}|\mathbf{v}\rangle = u_1\mathrm{v}_1 + 2u_2\mathrm{v}_2$$

Solution

Because the product of real numbers is commutative,

$$\langle\mathbf{u}|\mathbf{v}\rangle = u_1\mathrm{v}_1 + 2u_2\mathrm{v}_2 = \mathrm{v}_1u_1 + 2\mathrm{v}_2u_2 = \langle\mathbf{v}|\mathbf{u}\rangle$$

Let $\mathbf{w} = (\mathrm{w}_1, \mathrm{w}_2)$. Then

$$\begin{aligned}\langle\mathbf{u}|\mathbf{v} + \mathbf{w}\rangle &= u_1(\mathrm{v}_1 + \mathrm{w}_1) + 2u_2(\mathrm{v}_2 + \mathrm{w}_2)\\ &= u_1\mathrm{v}_1 + u_1\mathrm{w}_1 + 2u_2\mathrm{v}_2 + 2u_2\mathrm{w}_2\\ &= (u_1\mathrm{v}_1 + 2u_2\mathrm{v}_2) + (u_1\mathrm{w}_1 + 2u_2\mathrm{w}_2)\\ &= \langle\mathbf{u}|\mathbf{v}\rangle + \langle\mathbf{u}|\mathbf{w}\rangle\end{aligned}$$

If c is any scalar, then

$$c\langle\mathbf{u}|\mathbf{v}\rangle = c(u_1\mathrm{v}_1 + 2u_2\mathrm{v}_2) = (cu_1)\mathrm{v}_1 + 2(cu_2)\mathrm{v}_2 = \langle c\mathbf{u}|\mathbf{v}\rangle$$

Because the square of a real number is nonnegative,

$$\langle\mathbf{v}|\mathbf{v}\rangle = \mathrm{v}_1^2 + 2\mathrm{v}_2^2 \geq 0$$

Moreover, this expression is equal to zero if and only if $\mathbf{v} = \mathbf{0}$ (that is, if and only if $\mathrm{v}_1 = \mathrm{v}_2 = 0$).

Definition (Norm): The square root of the inner product of a vector with itself is called the Euclidean norm, or length of $|\mathbf{u}\rangle$ and is designated by:

$$\|\mathbf{u}\| = \sqrt{\langle\mathbf{u}|\mathbf{u}\rangle}. \tag{4.67}$$

Also, a vector $|\mathbf{u}\rangle$ is said to be normalized if

$$\|\mathbf{u}\| = 1. \tag{4.68}$$

Definition (Orthogonal Vectors): Let V be an inner product space. The vectors $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V$ are said to be orthogonal and $|\mathbf{u}\rangle$ is said to be orthogonal to $|\mathbf{v}\rangle$ if

$$\langle\mathbf{u}|\mathbf{v}\rangle = 0. \tag{4.69}$$

Definition (Orthonormal Vectors): A set $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ of vectors in V is called orthogonal if each pair of vectors in S are orthogonal, and S is called orthonormal if S is orthogonal and each vectors in S has unit length. In other words, S is orthogonal if

$$\langle\mathbf{u}_i|\mathbf{u}_j\rangle = 0, \text{ for } i \neq j. \tag{4.70}$$

and S is orthonormal if

$$\langle\mathbf{u}_i|\mathbf{u}_j\rangle = \delta_{ij} = \begin{cases}0 & i \neq j\\ 1 & i = j\end{cases}. \tag{4.71}$$

The completeness, or closure, relation for this basis is given by

$$\textstyle\sum_i |\mathbf{u}_i\rangle\langle\mathbf{u}_i| = \mathbf{I}. \tag{4.72}$$

Definition (Orthogonal and Orthonormal Basis): A basis $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ of a vector space V is called an orthogonal basis or an orthonormal basis according as S is an orthogonal set or an orthonormal set of vectors.

Example 4.11

Show that the following set is an orthonormal basis for $\mathbb{R}^3$

$$S = \{\mathbf{v}_1 = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right), \mathbf{v}_2 = \left(-\frac{\sqrt{2}}{6}, \frac{\sqrt{2}}{6}, \frac{2\sqrt{2}}{3}\right), \mathbf{v}_3 = \left(\frac{2}{3}, -\frac{2}{3}, \frac{1}{3}\right)\}$$

Solution

First, we show that the three vectors are mutually orthogonal

$$\langle \mathbf{v}_1 | \mathbf{v}_2 \rangle = -\frac{1}{6} + \frac{1}{6} + 0 = 0,$$
$$\langle \mathbf{v}_1 | \mathbf{v}_3 \rangle = -\frac{2}{3\sqrt{2}} + \frac{2}{3\sqrt{2}} + 0 = 0,$$
$$\langle \mathbf{v}_2 | \mathbf{v}_3 \rangle = -\frac{\sqrt{2}}{9} - \frac{\sqrt{2}}{9} + 2\frac{\sqrt{2}}{9} = 0.$$

Now, each vector is of length 1 because

$$\|\mathbf{v}_1\| = \sqrt{\langle \mathbf{v}_1 | \mathbf{v}_1 \rangle} = \sqrt{\frac{1}{2} + \frac{1}{2} + 0} = 1,$$
$$\|\mathbf{v}_2\| = \sqrt{\langle \mathbf{v}_2 | \mathbf{v}_2 \rangle} = \sqrt{\frac{2}{36} + \frac{2}{36} + \frac{8}{9}} = 1,$$
$$\|\mathbf{v}_3\| = \sqrt{\langle \mathbf{v}_3 | \mathbf{v}_3 \rangle} = \sqrt{\frac{4}{9} + \frac{4}{9} + \frac{1}{9}} = 1.$$

Theorem 4.3: Suppose $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ is an orthogonal set of nonzero vectors.

1- Then S is linearly independent.

2- For any $|\mathbf{v}\rangle \in V$, we have

$$|\mathbf{v}\rangle = \frac{\langle \mathbf{u}_1 | \mathbf{v} \rangle}{\langle \mathbf{u}_1 | \mathbf{u}_1 \rangle} |\mathbf{u}_1\rangle + \frac{\langle \mathbf{u}_2 | \mathbf{v} \rangle}{\langle \mathbf{u}_2 | \mathbf{u}_2 \rangle} |\mathbf{u}_2\rangle + \cdots + \frac{\langle \mathbf{u}_n | \mathbf{v} \rangle}{\langle \mathbf{u}_n | \mathbf{u}_n \rangle} |\mathbf{u}_n\rangle. \tag{4.73}$$

It's important to note that, if $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ is an orthonormal basis for V. Then, for any $|\mathbf{v}\rangle \in V$, we have

$$|\mathbf{v}\rangle = \langle \mathbf{u}_1 | \mathbf{v} \rangle |\mathbf{u}_1\rangle + \langle \mathbf{u}_2 | \mathbf{v} \rangle |\mathbf{u}_2\rangle + \cdots + \langle \mathbf{u}_n | \mathbf{v} \rangle |\mathbf{u}_n\rangle. \tag{4.74}$$

Proof

Using the completeness relation, we have

$$\begin{aligned} |\mathbf{v}\rangle &= \mathbf{I}|\mathbf{v}\rangle \\ &= \left(\sum_i |\mathbf{u}_i\rangle\langle \mathbf{u}_i|\right)|\mathbf{v}\rangle \\ &= \sum_i \langle \mathbf{u}_i | \mathbf{v} \rangle |\mathbf{u}_i\rangle \\ &= \sum_i a_i |\mathbf{u}_i\rangle \end{aligned}$$

where the coefficient a_i, which is equal to $\langle \mathbf{u}_i | \mathbf{v} \rangle$, represents the projection of $|\mathbf{v}\rangle$ onto $|\mathbf{u}_i\rangle$; a_i is the component of $|\mathbf{v}\rangle$ along the vector $|\mathbf{u}_i\rangle$. So, within the basis $\{|\mathbf{u}_i\rangle\}$, the ket $|\mathbf{v}\rangle$ is represented by the set of its components, a_1, a_2, …, a_n along $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$, …, $|\mathbf{u}_n\rangle$, respectively.

■

Example 4.12

Find the coordinate of $\mathbf{w} = (5, -5, 2)$ relative to the orthonormal basis for $\mathbb{R}^3$ shown below.

$$B = \left\{\mathbf{v}_1 = \left(\frac{3}{5}, \frac{4}{5}, 0\right), \mathbf{v}_2 = \left(-\frac{4}{5}, \frac{3}{5}, 0\right), \mathbf{v}_3 = (0,0,1)\right\}.$$

Solution

Because B is orthonormal, we can use theorem 4.3 to find the required coordinates

$$\langle \mathbf{w}|\mathbf{v}_1\rangle = (5,-5,2)\begin{pmatrix}\frac{3}{5}\\ \frac{4}{5}\\ 0\end{pmatrix} = -1$$

$$\langle \mathbf{w}|\mathbf{v}_2\rangle = (5,-5,2)\begin{pmatrix}-\frac{4}{5}\\ \frac{3}{5}\\ 0\end{pmatrix} = -7$$

$$\langle \mathbf{w}|\mathbf{v}_3\rangle = (5,-5,2)\begin{pmatrix}0\\ 0\\ 1\end{pmatrix} = 2$$

So, the coordinate relative to B is

$$[\mathbf{w}]_B = (-1,-7,2)$$

Change of basis matrix

Suppose $S = \{|\mathbf{v}_1\rangle, |\mathbf{v}_2\rangle, \dots, |\mathbf{v}_n\rangle\}$ is a basis of a vector space V and suppose $\acute{S} = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ is another basis. Since $\acute{S}$ is a basis, each vector in S can be written uniquely as a linear combination of the elements in $\acute{S}$. Say

$$\begin{aligned} |\mathbf{v}_1\rangle &= c_{11}|\mathbf{u}_1\rangle + c_{21}|\mathbf{u}_2\rangle + \cdots + c_{n1}|\mathbf{u}_n\rangle \\ |\mathbf{v}_2\rangle &= c_{12}|\mathbf{u}_1\rangle + c_{22}|\mathbf{u}_2\rangle + \cdots + c_{n2}|\mathbf{u}_n\rangle \\ &\dots\quad \dots\quad \dots \\ |\mathbf{v}_n\rangle &= c_{1n}|\mathbf{u}_1\rangle + c_{2n}|\mathbf{u}_2\rangle + \cdots + c_{nn}|\mathbf{u}_n\rangle \end{aligned} \tag{4.75}$$

Let Q denote the above matrix of coefficients;

$$\mathbf{Q} = \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{pmatrix}. \tag{4.76}$$

That is, $\mathbf{Q} = (c_{ij})$. Then $\mathbf{Q}$ is called the change of basis matrix from the old basis S to the new basis $\acute{S}$. Using the completeness relation, we have

$$\begin{aligned} |\mathbf{v}_j\rangle &= \mathbf{I}|\mathbf{v}_j\rangle \\ &= \left(\sum_i |\mathbf{u}_i\rangle\langle\mathbf{u}_i|\right)|\mathbf{v}_j\rangle \\ &= \sum_i |\mathbf{u}_i\rangle\langle\mathbf{u}_i|\mathbf{v}_j\rangle \\ &= \sum_i c_{ij}\,|\mathbf{u}_i\rangle \end{aligned} \tag{4.77}$$

where $c_{ij} = \langle\mathbf{u}_i|\mathbf{v}_j\rangle$.

Theorem 4.4: Let $\mathbf{Q}$ be the change of basis matrix from a basis S to a basis $\acute{S}$ in a vector space V. Then, for any vector $|\mathbf{u}\rangle \in V$, we have

$$\mathbf{Q}[\mathbf{u}]_S = [\mathbf{u}]_{\acute{S}}\,. \tag{4.78}$$

Let $\mathbf{P} = \mathbf{Q}^{-1}$ be the change of basis matrix from a basis $\acute{S}$ to a basis S in a vector space V. Then, for any vector $|\mathbf{u}\rangle \in V$, we have

$$\mathbf{Q}^{-1}\mathbf{Q}[\mathbf{u}]_S = [\mathbf{u}]_S = \mathbf{P}[\mathbf{u}]_{\acute{S}}\,. \tag{4.79}$$

Example 4.13

Let $S = \left\{|\mathbf{v}_1\rangle = \begin{pmatrix}1\\1\end{pmatrix}, |\mathbf{v}_2\rangle = \begin{pmatrix}2\\1\end{pmatrix}\right\}$ and $\acute{S} = \left\{|\mathbf{u}_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |\mathbf{u}_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}\right\}$ are bases of $\mathbb{R}^2$.

1- Find the transformation matrix $\mathbf{Q}$.

2- Find $[\mathbf{u}]_{\acute{S}}$, given that $[\mathbf{u}]_S = \begin{pmatrix}-3\\5\end{pmatrix}$.

Solution

It is easy to check that

$$|\mathbf{v}_1\rangle = |\mathbf{u}_1\rangle + |\mathbf{u}_2\rangle, \quad |\mathbf{v}_2\rangle = 2|\mathbf{u}_1\rangle + |\mathbf{u}_2\rangle.$$

Hence, the transformation matrix $\mathbf{Q}$ from S to $\acute{S}$ is the matrix

$$\mathbf{Q} = \begin{pmatrix}1 & 2\\1 & 1\end{pmatrix}.$$

Hence,

$$\begin{pmatrix}1 & 2\\1 & 1\end{pmatrix}\begin{pmatrix}-3\\5\end{pmatrix} = \begin{pmatrix}x\\y\end{pmatrix} \Rightarrow [\mathbf{u}]_{\acute{S}} = \begin{pmatrix}x\\y\end{pmatrix} = \begin{pmatrix}7\\2\end{pmatrix}.$$

4.4 Subspace

Definition (Subspace): Let W be a subset of a vector space V over a field K. W is called a subspace of V if W is itself a vector space over K with respect to the operations of vector addition and scalar multiplication on V.

Theorem 4.5: Suppose W is a subset of a vector space V. Then W is a subspace of V if and only if the following hold:

1- $|\mathbf{0}\rangle \in W$,

2- W is closed under vector addition, that is: for every $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in W$, the sum $|\mathbf{u}\rangle + |\mathbf{v}\rangle \in W$,

3- W is closed under scalar multiplication, that is: for every $|\mathbf{u}\rangle \in W$, $k \in K$, the multiple $k|\mathbf{u}\rangle \in W$.

Definition (Sum of Subsets of Vector Space): Let V be a vector space. Suppose that S_1 and S_2 are non-empty subsets of V. The sum of S_1 and S_2, denoted by $S_1 + S_2$, is

$$S_1 + S_2 = \{|\mathbf{u}\rangle + |\mathbf{v}\rangle; |\mathbf{u}\rangle \in S_1, |\mathbf{v}\rangle \in S_2\}. \tag{4.80}$$

That is, $S_1 + S_2$ is the set of vectors of V that can be obtained by adding a vector in S_1 to a vector in S_2.

Theorem 4.6: Let V be a vector space and suppose W_1 and W_2 are subspaces of V. Then $W_1 + W_2$ is a subspace of V that contains W_1 and W_2.

Definition (Direct Sum of Subspaces): A vector space V is called the direct sum of W_1 and W_2 if W_1 and W_2 are subspaces of V such that

$$W_1 \cap W_2 = \{|\mathbf{0}\rangle\}, \tag{4.81}$$

and

$$W_1 + W_2 = V. \tag{4.82}$$

We denote that V is the direct sum of W_1 and W_2 by writing

$$V = W_1 \oplus W_2. \tag{4.83}$$

Theorem 4.7: Let V be a vector space and suppose W_1 and W_2 are subspaces of V. Then $V = W_1 \oplus W_2$ if and only if each vector $|\mathbf{u}\rangle \in V$ can be written uniquely as

$$|\mathbf{u}\rangle = |\mathbf{u}_1\rangle + |\mathbf{u}_2\rangle, \tag{4.84}$$

where $|\mathbf{u}_1\rangle \in W_1$ and $|\mathbf{u}_2\rangle \in W_2$.

Theorem 4.8: Let V be a vector space and suppose W_1 and W_2 are finite dimensional subspaces of V such that $V = W_1 \oplus W_2$. Then V is a finite dimensional vector space. Moreover, if $\beta = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_k\rangle\}$ is a basis for W_1 and $\gamma = \{|\mathbf{v}_1\rangle, |\mathbf{v}_2\rangle, \dots, |\mathbf{v}_m\rangle\}$ is a basis for W_2, then

$$\alpha = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_k\rangle, |\mathbf{v}_1\rangle, |\mathbf{v}_2\rangle, \dots, |\mathbf{v}_m\rangle\}, \tag{4.85}$$

is a basis for V. Thus, $\dim V = \dim W_1 + \dim W_2$.

Theorem 4.9: Suppose $W_1, W_2, \dots, W_r$ are subspaces of V, and suppose

$$\begin{aligned} B_1 &= \{|\mathbf{u}_{11}\rangle, |\mathbf{u}_{12}\rangle, \dots, |\mathbf{u}_{1n_1}\rangle\} \\ B_2 &= \{|\mathbf{u}_{21}\rangle, |\mathbf{u}_{22}\rangle, \dots, |\mathbf{u}_{2n_2}\rangle\} \\ &\dots \quad \dots \quad \dots \\ B_r &= \{|\mathbf{u}_{r1}\rangle, |\mathbf{u}_{r2}\rangle, \dots, |\mathbf{u}_{rn_r}\rangle\} \end{aligned} \tag{4.86}$$

are bases of $W_1, W_2, \dots, W_r$ respectively. Then V is direct sum of W_i if and only if the union

$$B = B_1 \cup B_2 \cup \dots \cup B_r, \tag{4.87}$$

is a basis of V.

4.5 Linear Operator and Matrix Representation

Definition (Linear Transformation): Let V and U be vector spaces over the same field K. A mapping $\mathbf{T}: V \to U$ is called a linear mapping (or linear transformation) if it satisfies the following two conditions:

1- For any $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V$, $\mathbf{T}(|\mathbf{u}\rangle + |\mathbf{v}\rangle) = \mathbf{T}|\mathbf{u}\rangle + \mathbf{T}|\mathbf{v}\rangle$.

2- For any $k \in K$ and any $|\mathbf{u}\rangle \in V$, $\mathbf{T}(k|\mathbf{u}\rangle) = k\mathbf{T}(\mathbf{u}\rangle)$.

In other words, let V and U be vector spaces over the same field K. A mapping $\mathbf{T}: V \to U$ is called a linear mapping (or linear transformation) if it satisfies the following condition, for any vectors $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V$ and any scalars $a, b \in K$

$$\mathbf{T}(a|\mathbf{u}\rangle + b|\mathbf{v}\rangle) = a\mathbf{T}|\mathbf{u}\rangle + b\mathbf{T}|\mathbf{v}\rangle. \tag{4.88}$$

Definition (Linear Operator): Let V be a vector space over a field K. We now consider the special case of linear mappings $\mathbf{F}: V \to V$, i.e., from V into itself. They are also called linear operators on V.

Let $\mathbf{T}$ be a linear operator on a vector space V over a field K and suppose $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ is a basis of V. Now $\mathbf{T}|\mathbf{u}_1\rangle, \dots, \mathbf{T}|\mathbf{u}_n\rangle$ are vectors in V and so each is a linear combination of the vectors in the basis S; say,

$$\begin{aligned} \mathbf{T}|\mathbf{u}_1\rangle &= a_{11}|\mathbf{u}_1\rangle + a_{21}|\mathbf{u}_2\rangle + \cdots + a_{n1}|\mathbf{u}_n\rangle \\ \mathbf{T}|\mathbf{u}_2\rangle &= a_{12}|\mathbf{u}_1\rangle + a_{22}|\mathbf{u}_2\rangle + \cdots + a_{n2}|\mathbf{u}_n\rangle \\ &\dots \dots \dots \\ \mathbf{T}|\mathbf{u}_n\rangle &= a_{1n}|\mathbf{u}_1\rangle + a_{2n}|\mathbf{u}_2\rangle + \cdots + a_{nn}|\mathbf{u}_n\rangle \end{aligned} \tag{4.89}$$

The following definition applies

Definition (Matrix Representation of an Operator): The above matrix of coefficients, denoted by $[\mathbf{T}]_s$, is called the matrix representation of $\mathbf{T}$ relative to the basis S or simply the matrix of $\mathbf{T}$ in the basis S; that is,

$$[\mathbf{T}]_s = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}. \tag{4.90}$$

Using the completeness relation, we have

$$\begin{aligned} \mathbf{T}|\mathbf{u}_j\rangle &= \mathbf{I}\,\mathbf{T}|\mathbf{u}_j\rangle \\ &= \left(\sum_i |\mathbf{u}_i\rangle\langle\mathbf{u}_i|\right)\mathbf{T}|\mathbf{u}_j\rangle \\ &= \sum_i |\mathbf{u}_i\rangle\langle\mathbf{u}_i|\mathbf{T}|\mathbf{u}_j\rangle = \sum_i a_{ij}|\mathbf{u}_i\rangle \end{aligned} \tag{4.91}$$

where $a_{ij} = \langle\mathbf{u}_i|\mathbf{T}|\mathbf{u}_j\rangle$.

Example 4.14

Let $\mathbf{T}$ be defined by $\mathbf{T}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x+2y \\ 2x-y \end{pmatrix}$. Let $S = \left\{|\mathbf{e}_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |\mathbf{e}_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\}$ be the standard basis of $\mathbb{R}^2$. Find the matrix representation of $\mathbf{T}$ with respect to S.

Solution

We have the following computation

$$\mathbf{T}|\mathbf{e}_1\rangle = \mathbf{T}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 2\begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\mathbf{e}_1\rangle + 2|\mathbf{e}_2\rangle$$

$$\mathbf{T}|\mathbf{e}_2\rangle = \mathbf{T}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ -1 \end{pmatrix} = 2\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 2|\mathbf{e}_1\rangle - |\mathbf{e}_2\rangle$$

Therefore, the matrix representation of $\mathbf{T}$ is

$$[\mathbf{T}]_S = \begin{pmatrix} 1 & 2 \\ 2 & -1 \end{pmatrix}.$$

Theorem 4.10: Let $S = \{|\mathbf{u}_1\rangle, |\mathbf{u}_2\rangle, \dots, |\mathbf{u}_n\rangle\}$ be a basis for V and let $\mathbf{T}$ be any linear operator on V. Then, for any vector $|\mathbf{u}\rangle \in V$,

$$[\mathbf{T}]_S[\mathbf{u}]_S = [\mathbf{T}|\mathbf{u}\rangle]_S. \tag{4.92}$$

That is, if we multiply the matrix representation of $\mathbf{T}$ by the coordinate vector of $|\mathbf{u}\rangle$, then we obtain the coordinate vector of $\mathbf{T}|\mathbf{u}\rangle$.

The previous discussion shows that we can represent a linear operator by a matrix once we have chosen a basis. We ask the following natural question: How does our representation change if we select another basis?

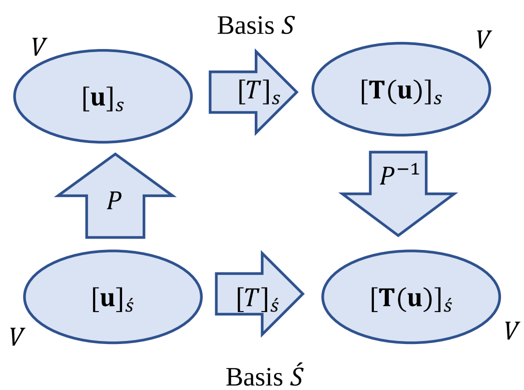


Figure 4.1.

Note that in figure 4.1 there are two ways to get from the coordinate vector $[\mathbf{u}]_{\acute{S}}$ to the coordinate vector $[\mathbf{T}|\mathbf{u}\rangle]_{\acute{S}}$. One way is direct, using the matrix $[\mathbf{T}]_{\acute{S}}$ to obtain

$$[\mathbf{T}]_{\acute{S}}[\mathbf{u}]_{\acute{S}} = [\mathbf{T}|\mathbf{u}\rangle]_{\acute{S}}. \tag{4.93}$$

The other way is indirect, using the matrices $\mathbf{P}$, $[\mathbf{T}]_S$ and $\mathbf{P}^{-1}$ to obtain

$$\mathbf{P}^{-1}[\mathbf{T}]_S\mathbf{P}[\mathbf{u}]_{\acute{S}} = [\mathbf{T}|\mathbf{u}\rangle]_{\acute{S}} \tag{4.94}$$

So that, we get

$$[\mathbf{T}]_{\acute{S}} = \mathbf{P}^{-1}[\mathbf{T}]_S\mathbf{P} \tag{4.95}$$

Theorem 4.11: Let $\mathbf{P}$ be the change of basis matrix from a basis $\acute{S}$ to a basis S in a vector space V. Then, for any linear operator $\mathbf{T}$ on V,

$$[\mathbf{T}]_{\acute{S}} = \mathbf{P}^{-1}[\mathbf{T}]_S\mathbf{P}. \tag{4.96}$$

Example 4.15

Find the matrix representation of $\mathbf{T}\begin{pmatrix}x_1\\x_2\end{pmatrix} = \begin{pmatrix}2x_1-2x_2\\-x_1+3x_2\end{pmatrix}$ with respect to S where $S = \left\{|\mathbf{e}_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |\mathbf{e}_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}\right\}$.

Then, by using the result of the standard basis of $\mathbb{R}^2$, find the matrix $[\mathbf{T}]_{\acute{S}}$, where $\acute{S} = \left\{|\acute{\mathbf{e}}_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |\acute{\mathbf{e}}_2\rangle = \begin{pmatrix}1\\1\end{pmatrix}\right\}$,

Solution

We have the following computation

$$\mathbf{T}|\mathbf{e}_1\rangle = \mathbf{T}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}2\\-1\end{pmatrix} = 2\begin{pmatrix}1\\0\end{pmatrix} - 1\begin{pmatrix}0\\1\end{pmatrix} = 2|\mathbf{e}_1\rangle - 1|\mathbf{e}_2\rangle$$

$$\mathbf{T}|\mathbf{e}_2\rangle = \mathbf{T}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}-2\\3\end{pmatrix} = -2\begin{pmatrix}1\\0\end{pmatrix} + 3\begin{pmatrix}0\\1\end{pmatrix} = -2|\mathbf{e}_1\rangle + 3|\mathbf{e}_2\rangle$$

Therefore, the matrix representation of $\mathbf{T}$ is

$$[\mathbf{T}]_S = \begin{pmatrix}2 & -2\\-1 & 3\end{pmatrix}.$$

It is easy to check that

$$|\acute{\mathbf{e}}_1\rangle = \begin{pmatrix}1\\0\end{pmatrix} = |\mathbf{e}_1\rangle + 0\times|\mathbf{e}_2\rangle$$

$$|\acute{\mathbf{e}}_2\rangle = \begin{pmatrix}1\\1\end{pmatrix} = |\mathbf{e}_1\rangle + |\mathbf{e}_2\rangle$$

The transformation matrix $\mathbf{P}$ is

$$\mathbf{P} = \begin{pmatrix}1 & 1\\0 & 1\end{pmatrix}$$

and the matrix $\mathbf{P}^{-1}$ is

$$\mathbf{P}^{-1} = \begin{pmatrix}1 & -1\\0 & 1\end{pmatrix}$$

Hence, we have

$$[\mathbf{T}]_{\acute{S}} = \mathbf{P}^{-1}[\mathbf{T}]_S\mathbf{P} = \begin{pmatrix}1 & -1\\0 & 1\end{pmatrix}\begin{pmatrix}2 & -2\\-1 & 3\end{pmatrix}\begin{pmatrix}1 & 1\\0 & 1\end{pmatrix} = \begin{pmatrix}3 & -2\\-1 & 2\end{pmatrix}.$$

4.6 Eigenvalues, Eigenvectors and Eigenspaces

Definition (Similar Matrices): If $\mathbf{A}$ and $\mathbf{B}$ are $n\times n$ matrices such that there is an invertible $n\times n$ matrix $\mathbf{P}$ with

$$\mathbf{B} = \mathbf{P}^{-1}\mathbf{AP}, \tag{4.97}$$

then $\mathbf{A}$ and $\mathbf{B}$ are called similar.

Therefore, with $\mathbf{P}$ being the change of basis matrix, similar matrices represent the same linear operator under two different bases,

Definition (Trace): The trace of an $n\times n$ matrix $\mathbf{A}$ is the sum of its diagonal entries:

$$\mathrm{Tr}(\mathbf{A}) = \sum_{i=1}^{n} a_{ii} = a_{11} + a_{22} + \cdots + a_{nn}. \tag{4.98}$$

Remarks:

1- If $\mathbf{B} = \mathbf{P}^{-1}\mathbf{AP}$ then $\mathbf{A} = \mathbf{PBP}^{-1}$, so if $\mathbf{A}$ is similar to $\mathbf{B}$, then $\mathbf{B}$ is similar to $\mathbf{A}$.

2- If $\mathbf{A} = \mathbf{P}_1^{-1}\mathbf{BP}_1$ and $\mathbf{B} = \mathbf{P}_2^{-1}\mathbf{CP}_2$ then

$$\mathbf{A} = \mathbf{P}_1^{-1}(\mathbf{P}_2^{-1}\mathbf{CP}_2)\mathbf{P}_1 = (\mathbf{P}_2\mathbf{P}_1)^{-1}\mathbf{C}(\mathbf{P}_2\mathbf{P}_1). \tag{4.99}$$

So, if $\mathbf{A}$ is similar to $\mathbf{B}$, and $\mathbf{B}$ is similar to $\mathbf{C}$, then $\mathbf{A}$ is similar to $\mathbf{C}$. This allows us to put matrices into families in which all the matrices in a family are similar to each other. Then each family can be represented by a diagonal (or nearly diagonal) matrix.

3- If $\mathbf{B} = \mathbf{P}^{-1}\mathbf{AP}$, then, $\det(\mathbf{A}) = \det(\mathbf{B})$.

4- If $\mathbf{B} = \mathbf{P}^{-1}\mathbf{AP}$, then, $\mathrm{Tr}(\mathbf{A}) = \mathrm{Tr}(\mathbf{B})$.

Consider a polynomial $f(\lambda)$ over a field K; say

$$f(\lambda) = a_n\lambda^n + \cdots + a_1\lambda + a_0. \tag{4.100}$$

Recall that if $\mathbf{A}$ is the square matrix over K, then we define

$$f(\mathbf{A}) = a_n\mathbf{A}^n + \cdots + a_1\mathbf{A} + a_0\mathbf{I}, \tag{4.101}$$

where $\mathbf{I}$ is the identity matrix. In particular, we say that $\mathbf{A}$ is a root or zero of the polynomial $f(\lambda)$ if $f(\mathbf{A}) = 0$.

Definition (Characteristic Matrix): The matrix $\lambda\mathbf{I}_n - \mathbf{A}$, where $\mathbf{I}_n$ is the n-square identity matrix and λ is an indeterminate, is called the characteristic matrix of $\mathbf{A}$:

$$\lambda\mathbf{I}_n - \mathbf{A} = \begin{pmatrix} \lambda - A_{11} & -A_{21} & \cdots & -A_{n1} \\ -A_{12} & \lambda - A_{22} & \cdots & -A_{n2} \\ \cdots & \cdots & \cdots & \cdots \\ -A_{1n} & -A_{2n} & \cdots & \lambda - A_{nn} \end{pmatrix}. \tag{4.102}$$

Its determinant $\Delta_{\mathbf{A}}(\lambda) = \det(\lambda\mathbf{I}_n - \mathbf{A})$ which is a polynomial in λ, is called the characteristic polynomial of $\mathbf{A}$. We also call

$$\Delta_{\mathbf{A}}(\lambda) = \det(\lambda\mathbf{I}_n - \mathbf{A}) = 0, \tag{4.103}$$

the characteristic equation of $\mathbf{A}$.

Theorem 4.12 (Cayley-Hamilton Theorem): Every matrix is a zero of its characteristic polynomial.

Example 4.16

If $\mathbf{A} = \begin{pmatrix} 4 & -1 \\ 2 & 1 \end{pmatrix}$, the characteristic polynomial of A is

$$\Delta_{\mathbf{A}}(\lambda) = \begin{vmatrix} \lambda - 4 & 1 \\ -2 & \lambda - 1 \end{vmatrix} = \lambda^2 - 5\lambda + 6,$$

and $\mathbf{A}$ is a zero of its characteristic polynomial

$$f(\mathbf{A}) = \mathbf{A}^2 - 5\mathbf{A} + 6\mathbf{I} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Theorem 4.13: Similar matrices have the same characteristic polynomial.

Definition (Eigenvalue and Eigenvector): Let $\mathbf{A}$ be an n-square matrix over a field K. A scalar $\lambda \in K$ is called an eigenvalue of $\mathbf{A}$ if there exists a nonzero vector $|\mathbf{u}\rangle \in K^n$ for which

$$\mathbf{A}|\mathbf{u}\rangle = \lambda|\mathbf{u}\rangle. \tag{4.104}$$

Every vector satisfying this relation is then called an eigenvector of A belonging to the eigenvalue λ.

Example 4.17

For the matrix $\mathbf{A} = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}$, verify that $\mathbf{x}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\mathbf{x}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are the eigenvector of $\mathbf{A}$ corresponding to eigenvalues $\lambda_1 = 2, \lambda_2 = -1$.

Solution

$$\mathbf{A}\mathbf{x}_1 = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \end{pmatrix} = 2\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 2\mathbf{x}_1$$

$$\mathbf{A}\mathbf{x}_2 = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\mathbf{x}_2$$

Definition (Eigenspace): The set E_λ of all eigenvectors belonging to λ is a subspace of K^n, called the eigenspace of λ.

Theorem 4.14: Let $\mathbf{A}$ be an n-square matrix over a field K. Then the following are equivalent.

1- A scalar λ is an eigenvalue of $\mathbf{A}$.
2- The matrix $\mathbf{M} = \lambda\mathbf{I}_n - \mathbf{A}$ is singular.
3- The scalar λ is a root of the characteristic polynomial $\Delta_{\mathbf{A}}(\lambda)$ of $\mathbf{A}$.

Remark:

1- An eigenvalue of $\mathbf{A}$ is a scalar λ such that

$$|\lambda \mathbf{I}_n - \mathbf{A}| = 0 \tag{4.105}$$

2- The eigenvectors of $\mathbf{A}$ corresponding to λ are the nonzero solutions of

$$(\lambda \mathbf{I}_n - \mathbf{A})\mathbf{x} = \mathbf{0} \tag{4.106}$$

Example 4.18

Find the eigenvalues and corresponding eigenvectors of $\mathbf{A} = \begin{pmatrix} 2 & -12 \\ 1 & -5 \end{pmatrix}$

Solution

The characteristic polynomial of $\mathbf{A}$ is

$$|\lambda \mathbf{I} - \mathbf{A}| = \begin{vmatrix} \lambda - 2 & 12 \\ -1 & \lambda + 5 \end{vmatrix} = (\lambda - 2)(\lambda + 5) + 12 = (\lambda + 1)(\lambda + 2)$$

So, the characteristic equation is $(\lambda + 1)(\lambda + 2) = 0$, which gives $\lambda_1 = -1, \lambda_2 = -2$ as eigenvalues of $\mathbf{A}$.

For $\lambda_1 = -1$

$$-\mathbf{I} - \mathbf{A} = \begin{pmatrix} -1 - 2 & 12 \\ -1 & -1 + 5 \end{pmatrix} = \begin{pmatrix} -3 & 12 \\ -1 & 4 \end{pmatrix}$$

Let

$$\begin{pmatrix} -3 & 12 \\ -1 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

We get

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = t \begin{pmatrix} 4 \\ 1 \end{pmatrix}, t \neq 0$$

For $\lambda_1 = -2$

$$-2\mathbf{I} - \mathbf{A} = \begin{pmatrix} -2 - 2 & 12 \\ -1 & -2 + 5 \end{pmatrix} = \begin{pmatrix} -4 & 12 \\ -1 & 3 \end{pmatrix}$$

Let

$$\begin{pmatrix} -4 & 12 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

We get

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = t \begin{pmatrix} 3 \\ 1 \end{pmatrix}, t \neq 0$$

Definition (Diagonalizable Matrix): A matrix $\mathbf{A}$ is said to be diagonalizable if there exists a non-singular matrix $\mathbf{P}$ such that $\mathbf{D} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$ is a diagonal matrix, i.e., if $\mathbf{A}$ is similar to a diagonal matrix $\mathbf{D}$.

Example 4.19

The matrix $\mathbf{A} = \begin{pmatrix} 1 & 3 & 0 \\ 3 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$ is diagonalizable because $\mathbf{P} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ has the property

$$\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

Theorem 4.15: An n-square matrix $\mathbf{A}$ is similar to diagonal matrix $\mathbf{D}$ if and only if $\mathbf{A}$ has n linearly independent eigenvectors. In this case, the diagonal elements of $\mathbf{D}$ are the corresponding eigenvalues and $\mathbf{D} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$ where $\mathbf{P}$ is the matrix whose columns are the eigenvectors.

Example 4.20

The matrix $\mathbf{A} = \begin{pmatrix} 1 & 3 & 0 \\ 3 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$ has the eigenvalues and corresponding eigenvectors listed below

$$\lambda_1 = 4, \mathbf{p}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$\lambda_2 = -2, \mathbf{p}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

$$\lambda_3 = -2, \mathbf{p}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The eigenvectors $\mathbf{p}_1$, $\mathbf{p}_2$ and $\mathbf{p}_3$ are linearly independent. The matrix P whose columns correspond to these eigenvectors is

$$\mathbf{P} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Hence, we have

$$\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

Theorem 4.16: Let $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$, …, $|\mathbf{u}_n\rangle$ be nonzero eigenvectors of a matrix $\mathbf{A}$ belonging to distinct eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_n$. Then $|\mathbf{u}_1\rangle$, $|\mathbf{u}_2\rangle$, …, $|\mathbf{u}_n\rangle$ are linearly independent.

Theorem 4.17: Suppose the characteristic polynomial $\Delta_{\mathbf{A}}(\lambda)$ of an n-square matrix $\mathbf{A}$ is a product of n distinct factors, say, $\Delta_{\mathbf{A}}(\lambda) = (\lambda - \lambda_1)(\lambda - \lambda_2) \ldots (\lambda - \lambda_n)$. Then $\mathbf{A}$ is similar to a diagonal matrix whose diagonal elements are the λ_i.

4.7 Symmetric Matrices and Orthogonal Diagonalization

Theorem 4.18: If $\mathbf{A}$ is an $n \times n$ symmetric matrix, then the following properties are true.
1. $\mathbf{A}$ is diagonalizable.
2. All eigenvalues of $\mathbf{A}$ are real.
3. If λ is an eigenvalue of $\mathbf{A}$ with multiplicity k, then λ has k linearly independent eigenvectors. That is, the eigenspace of λ has dimension k.

Theorem 4.11 is called the Real Spectral Theorem, and the set of eigenvalues of $\mathbf{A}$ is called the spectrum of $\mathbf{A}$.

Example 4.21

Prove that a symmetric matrix $\mathbf{A} = \begin{pmatrix} a & c \\ c & b \end{pmatrix}$ is diagonalizable.

Solution

The characteristic polynomial of $\mathbf{A}$ is

$$|\lambda\mathbf{I} - \mathbf{A}| = \begin{vmatrix} \lambda - a & -c \\ -c & \lambda - b \end{vmatrix} = \lambda^2 - (a+b)\lambda + ab - c^2.$$

As a quadratic in λ, this polynomial has a discriminant of

$$\begin{aligned}(a+b)^2 - 4(ab - c^2) &= a^2 + 2ab + b^2 - 4ab + 4c^2 \\ &= a^2 - 2ab + b^2 + 4c^2 \\ &= (a-b)^2 + 4c^2\end{aligned}$$

Because this discriminant is the sum of two squares, it must be either zero or positive. If $(a-b)^2 + 4c^2 = 0$, then $a = b$ and $c = 0$, which implies that is already diagonal.
That is,

$$\mathbf{A} = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$$

On the other hand, if $(a-b)^2 + 4c^2 > 0$then by the Quadratic Formula the characteristic polynomial of **A** has two distinct real roots, which implies that **A** has two distinct real eigenvalues. So, **A** is diagonalizable in this case also.

Theorem 4.19: An $n \times n$ matrix **P** is orthogonal if and only if its column vectors form an orthonormal set.

Proof:

Suppose the column vectors of P form an orthonormal set:

$$\mathbf{P} = \begin{pmatrix} P_{11} & P_{12} & \dots & P_{1n} \\ P_{21} & P_{22} & \dots & P_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ P_{n1} & P_{n2} & \dots & P_{nn} \end{pmatrix} = (\mathbf{p}_1 \vdots \quad \mathbf{p}_2 \vdots \quad \dots \quad \vdots \mathbf{p}_n)$$

Then the product $\mathbf{P}^T\mathbf{P}$ has the form

$$\mathbf{P}^T\mathbf{P} = \begin{pmatrix} P_{11} & P_{21} & \dots & P_{n1} \\ P_{12} & P_{22} & \dots & P_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ P_{1n} & P_{2n} & \dots & P_{nn} \end{pmatrix} \begin{pmatrix} P_{11} & P_{12} & \dots & P_{1n} \\ P_{21} & P_{22} & \dots & P_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ P_{n1} & P_{n2} & \dots & P_{nn} \end{pmatrix} = \begin{pmatrix} \langle \mathbf{p}_1 | \mathbf{p}_1 \rangle & \langle \mathbf{p}_1 | \mathbf{p}_2 \rangle & \dots & \langle \mathbf{p}_1 | \mathbf{p}_n \rangle \\ \langle \mathbf{p}_2 | \mathbf{p}_1 \rangle & \langle \mathbf{p}_2 | \mathbf{p}_2 \rangle & \dots & \langle \mathbf{p}_2 | \mathbf{p}_n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \mathbf{p}_n | \mathbf{p}_1 \rangle & \langle \mathbf{p}_n | \mathbf{p}_2 \rangle & \dots & \langle \mathbf{p}_n | \mathbf{p}_n \rangle \end{pmatrix}$$

Because the set$\{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n\}$ is orthonormal, you have

$$\langle \mathbf{p}_i | \mathbf{p}_j \rangle = \delta_{ij}$$

So, the matrix composed of dot products has the form

$$\mathbf{P}^T\mathbf{P} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix} = \mathbf{I}$$

This implies that $\mathbf{P}^T = \mathbf{P}^{-1}$ and you can conclude that P is orthogonal.

Conversely, if **P** is orthogonal, you can reverse the steps above to verify that the column vectors of **P** form an orthonormal set.

■

Theorem 4.20: Let **A** be $n \times n$ matrix. Then **A** is orthogonally diagonalizable and has real eigenvalues if and only if **A** is symmetric.

Proof:

The proof of the theorem in one direction is fairly straightforward. That is, if you assume **A** is orthogonally diagonalizable, then there exists an orthogonal matrix **P** such that $\mathbf{D} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$ is diagonal. Moreover, because $\mathbf{P}^T = \mathbf{P}^{-1}$, you have $\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1} = \mathbf{P}\mathbf{D}\mathbf{P}^T$ which implies that

$$\begin{aligned} \mathbf{A}^T &= (\mathbf{P}\mathbf{D}\mathbf{P}^T)^T \\ &= (\mathbf{P}^T)^T\mathbf{D}^T\mathbf{P}^T \\ &= \mathbf{P}\mathbf{D}\mathbf{P}^T \\ &= \mathbf{A} \end{aligned}$$

So, **A** is symmetric. We leave the remaining of the proof as exercise.

■

Orthogonal Diagonalization of a Symmetric Matrix

Let $\mathbf{A}$ be an $n \times n$ symmetric matrix.

1. Find all eigenvalues of $\mathbf{A}$ and determine the multiplicity of each.

2. For each eigenvalue of multiplicity 1, choose a unit eigenvector. (Choose any eigenvector and then normalize it.)

3. For each eigenvalue of multiplicity $k \geq 2$ find a set of k linearly independent eigenvectors.

4. The composite of steps 2 and 3 produces an orthonormal set of eigenvectors. Use these eigenvectors to form the columns of $\mathbf{P}$. The matrix $\mathbf{P}^{-1}\mathbf{AP} = \mathbf{P}^T\mathbf{AP} = \mathbf{D}$ will be diagonal. (The main diagonal entries of $\mathbf{D}$ are the eigenvalues of $\mathbf{A}$.)

Example 4.22

Find an orthogonal matrix $\mathbf{P}$ that orthogonally diagonalizes

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

Solution

1. The characteristic polynomial of $\mathbf{A}$ is

$$|\lambda\mathbf{I} - \mathbf{A}| = \begin{vmatrix} \lambda + 2 & -2 \\ -2 & \lambda - 1 \end{vmatrix} = (\lambda + 3)(\lambda - 2).$$

So the eigenvalues are $\lambda_1 = -3$ and $\lambda_2 = 2$.

2. For each eigenvalue, find an eigenvector. The eigenvectors $(-2,1)$ and $(1,2)$ form an orthogonal basis for $\mathbb{R}^2$. Each of these eigenvectors is normalized to produce an orthonormal basis.

$$\mathbf{p}_1 = \frac{(-2,1)}{\sqrt{5}}, \mathbf{p}_2 = \frac{(1,2)}{\sqrt{5}}$$

3. Because each eigenvalue has a multiplicity of 1, go directly to step 4.

4. Using $\mathbf{p}_1$ and $\mathbf{p}_2$ as column vectors, construct the matrix $\mathbf{P}$

$$\mathbf{P} = \begin{pmatrix} \frac{-2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \end{pmatrix}$$

Verify that is correct by computing $\mathbf{P}^{-1}\mathbf{AP} = \mathbf{P}^T\mathbf{AP}$

$$\mathbf{P}^T\mathbf{AP} = \begin{pmatrix} \frac{-2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \end{pmatrix} \begin{pmatrix} -2 & 2 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} \frac{-2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \end{pmatrix} = \begin{pmatrix} -3 & 0 \\ 0 & 2 \end{pmatrix}$$

4.8 p-norm in finite dimensions

The length of a vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ in the n-dimensional real vector space $\mathbb{R}^n$ is usually given by the Euclidean norm:

$$\|\mathbf{x}\| = (x_1^2 + x_2^2 + \cdots + x_n^2)^{\frac{1}{2}} \tag{4.107}$$

It follows directly from the definition that $\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$.

The formula for the Euclidean distance between two points $P_1 = (x_1, y_1, z_1)$ and $P_2 = (x_2, y_2, z_2)$ in 3-dimensional space is

$$d(P_1, P_2) = ((x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2)^{\frac{1}{2}} \tag{4.108}$$

The formula above, however, is not always the way we measure distance between points laying in a 3-dimensional space. For example, we can think of the Earth as being a subset of three-dimensional space, and the surface of the Earth as being the surface of a sphere. when measuring the distance between points on the Earth's surface, say from Salt Lake City to Rome. We do not draw a line through the two points and measure the distance along those points. This distance would correspond to the distance traveled if a tunnel was dug in a straight line through the Earth, starting at Salt Lake and ending at Rome. This is not very practical; one usually does not travel between cities by tunneling from one to the other. Instead, we measure the distance between two points P_1 and P_2 on the Earth by measuring the short path starting at P_1 and ending at P_2 that stays on the surface of the Earth. In many situations, the Euclidean distance is insufficient for capturing the actual distances in a given space. An analogy to this is suggested by taxi drivers in a grid street plan who should measure distance not in terms of the length of the straight line to their destination, but in terms of the rectilinear distance, which takes into account that streets are either orthogonal or parallel to each other (see figure 4.2). The class of p-norms generalizes these two examples and has an abundance of applications in many parts of mathematics, physics, and computer science.

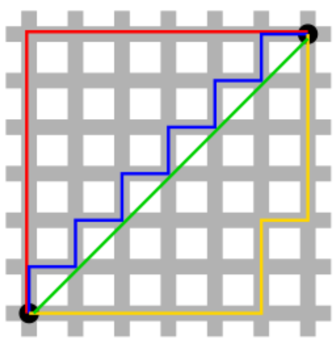


Figure 4.2

There are many useful measures of length (many different norms).

Definition: For a real number $p \geq 1$, the p-norm or ℓ^p-norm of $\mathbf{x}$ is defined by

$$\|\mathbf{x}\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{\frac{1}{p}} \tag{4.109}$$

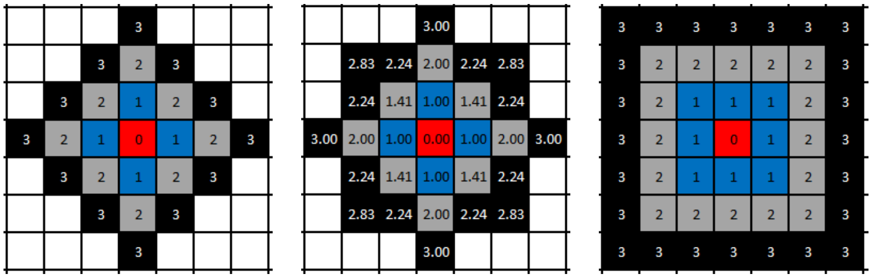
Some norms

ℓ^1-norm, 1-norm or the Manhattan norm: $\|\mathbf{x}\|_1 = |x_1| + |x_2| + \cdots + |x_n|$

ℓ^2-norm, 2-norm or the Euclidean norm: $\|\mathbf{x}\|_2 = \sqrt{|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2}$

ℓ^∞-norm, ∞-norm or the Chebyshev norm: $\|\mathbf{x}\|_\infty = \max\{|x_1|, |x_2|, \ldots |x_n|\}$

See figures (4.3).



Manhattan Distance Euclidean Distance Chebyshev Distance

Figure 4.3. Manhattan, Euclidean, and Chebyshev Distance.

Theorem 4.21: $\|\mathbf{x}\|_\infty \le \|\mathbf{x}\|_2 \le \|\mathbf{x}\|_1$

Proof:

$$\begin{aligned}
\|\mathbf{x}\|_\infty &= \max\{|x_1|, |x_2|, \dots |x_n|\} \\
&= \max\left\{\sqrt{x_1^2}, \sqrt{x_2^2}, \dots, \sqrt{x_n^2}\right\} \\
&= \sqrt{x_k^2} \text{ for some } k \\
&\le \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} \\
&= \|\mathbf{x}\|_2 \\
&= \sqrt{|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2} \\
&\le \sqrt{(|x_1| + |x_2| + \cdots + |x_n|)^2} \\
&= \|\mathbf{x}\|_1
\end{aligned}$$

■

4.9 Lines, planes, hyperplanes and half-spaces in $\mathbb{R}^n$

The equation of a line means an equation in x and y whose solution set is a line in the (x, y) plane. The most popular form in algebra is the (slope-intercept form)

$$y = mx + c. \tag{4.110}$$

This in effect uses x as a parameter and writes y as a function of x: $y = f(x) = mx + c$. When $x = 0$, $y = c$ and the point $(0, c)$ is the intersection of the line with the y-axis. Thinking of a line as a geometrical object and not the graph of a function, it makes sense to treat x and y more evenhandedly. The general equation for a line (normal form) is

$$ax + by + d = 0, \tag{4.111}$$

with the stipulation that at least one of a or b is nonzero. This can easily be converted to slope-intercept form by solving for y:

$$y = \left(-\frac{a}{b}\right)x + \left(-\frac{d}{b}\right), \tag{4.112}$$

except for the special case $b = 0$, when the line is parallel to the y-axis.

If we set $x = t$, $-\infty < t < \infty$, then the solutions to (4.111) are

$$\mathbf{y} = (x, y) = \left(t, -\frac{a}{b}t - \frac{d}{b}\right) = t\left(1, -\frac{a}{b}\right) + \left(0, -\frac{d}{b}\right) = t\mathbf{v} + \mathbf{u}. \tag{4.113}$$

(4.113) is called the line L through $\mathbf{u}$ in the direction of $\mathbf{v}$. i.e., L is a line through $(0, -\frac{d}{b})$ in the direction of $(1, -\frac{a}{b})$. Equation (4.113) is called a vector equation for the line. Now let $\mathbf{n} = (a, b)$ and note that (4.111) is equivalent to

$$\langle \mathbf{n}, \mathbf{y} \rangle + d = 0. \tag{4.114}$$

Moreover, if $\mathbf{p} = (p_1, p_2)$ is a point on L, then

$$\langle \mathbf{n}, \mathbf{p} \rangle + d = 0, \tag{4.115}$$

which implies that $d = -\langle \mathbf{n}, \mathbf{p} \rangle$. Thus, we may write (4.115) as

$$\langle \mathbf{n}, \mathbf{y} \rangle - \langle \mathbf{n}, \mathbf{p} \rangle = 0 \tag{4.116}$$

and so we see that (4.116) is equivalent to the equation

$$\langle \mathbf{n}, (\mathbf{y} - \mathbf{p}) \rangle = 0. \tag{4.117}$$

Equation (4.117) is a normal equation for the line L and $\mathbf{n}$ is a normal vector for L. In words, (4.117) says that the line L consists of all points in $\mathbb{R}^2$ whose difference with $\mathbf{p}$ is orthogonal to $\mathbf{n}$. See figure 4.4.

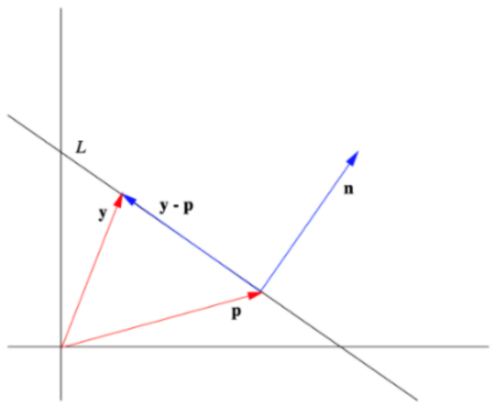


Figure 4.4. L is the set of points $\mathbf{y}$ for which $\mathbf{y}-\mathbf{p}$ is orthogonal to $\mathbf{n}$.

A plane in $\mathbb{R}^3$ has the equation

$$ax + by + cz + d = 0, \tag{4.118}$$

where at least one of the numbers a, b, c must be nonzero. If c is not zero, it is often useful to think of the plane as the graph of a function z of x and y. The equation can be rearranged like this:

$$z = -\left(\frac{a}{c}\right)x + \left(-\frac{b}{c}\right)y + \left(-\frac{d}{c}\right) \tag{4.119}$$

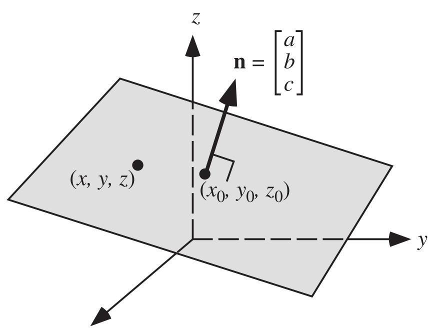


Figure 4.5. a plane with nonzero normal vector $\mathbf{n}$ through the point $\mathbf{x_0} = (x_0, y_0, z_0)$

The equation of a plane (figure 4.5) with nonzero normal vector $\mathbf{n} = (a, b, c)$ through the point $\mathbf{x_0} = (x_0, y_0, z_0)$ is

$$\langle \mathbf{n}, (\mathbf{x} - \mathbf{x_0}) \rangle = 0, \tag{4.120}$$

where $\mathbf{x} = (x, y, z)$. Plugging in gives the general equation of a plane,

$$ax + by + cz + d = 0, \tag{4.121}$$

where

$$d = -ax_0 - by_0 - cz_0. \tag{4.122}$$

A plane specified in this form therefore has x-, y-, and z-intercepts at

$$x=-\frac{d}{a}, y=-\frac{d}{b}, z=-\frac{d}{c}. \tag{4.123}$$

Now consider the case where P is the set of all points $\mathbf{y}=(x,y,z)$ in $\mathbb{R}^3$ that satisfy the equation

$$ax+by+cz+d=0, \tag{4.124}$$

where a, b, c, and d are scalars with at least one of a, b, and c not being 0. If for example, $a\neq 0$, then we may solve for x to obtain

$$x=-\frac{b}{a}y-\frac{c}{a}z-\frac{d}{a}. \tag{4.125}$$

If we set $y=t$, $-\infty<t<\infty$, and $z=s$, $-\infty<s<\infty$, the solutions to (4.125) are

$$\mathbf{y}=(x,y,z)=(-\frac{b}{a}t-\frac{c}{a}s-\frac{d}{a},t,s)=t(-\frac{b}{a},1,0)+s(-\frac{c}{a},0,1)+(-\frac{d}{a},0,0). \tag{4.126}$$

Thus, we see that P is a plane in $\mathbb{R}^3$. In analogy with the case of lines in $\mathbb{R}^2$, if we let $\mathbf{n}=(a,b,c)$ and let $\mathbf{p}=(p_1,p_2,p_3)$ be a point on P, then we have

$$\langle\mathbf{n},\mathbf{y}\rangle+d=ax+by+cz+d=0, \tag{4.127}$$

from which we see that $\langle\mathbf{n},\mathbf{p}\rangle=-d$, and so we may write (4.124) as

$$\langle\mathbf{n},(\mathbf{y}-\mathbf{p})\rangle=0. \tag{4.128}$$

We call (4.127) a normal equation for P and we call $\mathbf{n}$ a normal vector for P. In words, (4.128) says that the plane P consists of all points in $\mathbb{R}^3$ whose difference with $\mathbf{p}$ is orthogonal to $\mathbf{n}$. See Figure 4.6.

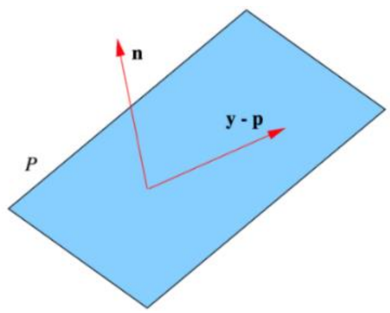


Figure 4.6. P is the set of points $\mathbf{y}$ for which $\mathbf{y}-\mathbf{p}$ is orthogonal to $\mathbf{n}$

Definition: Suppose $\mathbf{n}$ and $\mathbf{p}$ are vectors in $\mathbb{R}^n$ with $\mathbf{n}\neq\mathbf{0}$. The set of all vectors $\mathbf{y}$ in $\mathbb{R}^n$ which satisfy the equation

$$\langle\mathbf{n},(\mathbf{y}-\mathbf{p})\rangle=0, \tag{4.129}$$

or

$$\langle\mathbf{n},\mathbf{y}\rangle=b, \tag{4.130}$$

is called a hyperplane through the point $\mathbf{p}$. Where $b=\langle\mathbf{n},\mathbf{p}\rangle$. We call $\mathbf{n}$ a normal vector for the hyperplane and we call (4.129) a normal equation for the hyperplane.

In this terminology, a line in $\mathbb{R}^2$ is a hyperplane and a plane in $\mathbb{R}^3$ is a hyperplane.

Note that if we let $\mathbf{n}=(a_1,a_2,\dots,a_n)$, $\mathbf{p}=(p_1,p_2,\dots,p_n)$, and $\mathbf{y}=(y_1,y_2,\dots,y_n)$, then we may write (4.129) as

$$a_1(y_1-p_1)+a_2(y_2-p_2)+\cdots+a_n(y_n-p_n)=0, \tag{4.131}$$

or

$$a_1y_1+a_2y_2+\cdots+a_ny_n+d=0 \tag{4.132}$$

where $d=-\langle\mathbf{n},\mathbf{p}\rangle$.

The normal equation description of a hyperplane simplifies a number of geometric calculations. For example, given a hyperplane H through $\mathbf{p}$ with normal vector $\mathbf{n}$ and a point $\mathbf{q}$ in $\mathbb{R}^n$, the distance from $\mathbf{q}$ to H is simply the length of the projection of $\mathbf{q}-\mathbf{p}$ onto $\mathbf{n}$. Thus if $\mathbf{u}$ is the unit vector in direction of $\mathbf{n}$, then the distance from $\mathbf{q}$ to H is $|\langle(\mathbf{q}-\mathbf{p}),\mathbf{u}\rangle|$, (see figure 4.7). Moreover, if we let $d=-\langle\mathbf{p},\mathbf{n}\rangle$ as in (4.132), then we have

$$|\langle(\mathbf{q}-\mathbf{p}),\mathbf{u}\rangle| = |\langle\mathbf{q},\mathbf{u}\rangle-\langle\mathbf{p},\mathbf{u}\rangle| = \frac{\langle\mathbf{q},\mathbf{n}\rangle-\langle\mathbf{p},\mathbf{n}\rangle}{\|\mathbf{n}\|} = \frac{|\langle\mathbf{q},\mathbf{n}\rangle+d|}{\|\mathbf{n}\|}. \tag{4.133}$$

Note that, in particular, () may be used to find the distance from a point to a line in $\mathbb{R}^2$ and from a point to a plane in $\mathbb{R}^3$.

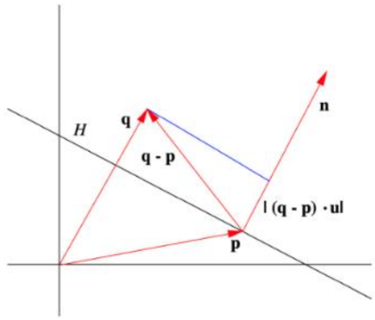


Figure 4.7. Distance from a point $\mathbf{q}$ to a hyperplane H.

Geometrically, an hyperplane $H=\{\mathbf{x}\colon\langle\mathbf{a},\mathbf{x}\rangle=b\}$, with $\|\mathbf{a}\|_2=1$, is a translation of the set of vectors orthogonal to $\mathbf{a}$. The direction of the translation is determined by $\mathbf{a}$, and the amount by b. Precisely, $|b|$ is the length of the closest point $\mathbf{x_0}$ on H from the origin, and the sign of b determines if H is away from the origin along the direction $\mathbf{a}$ or $-\mathbf{a}$. As we increase the magnitude of b, the hyperplane is shifting further away along $\pm\mathbf{a}$, depending on the sign of b. In the figure 4.8, the scalar b is positive, as $\mathbf{x_0}$ and $\mathbf{a}$ point to the same direction.

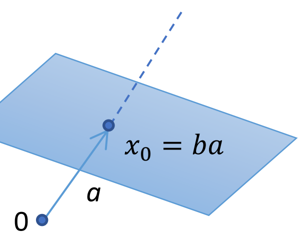


Figure 4.8. Geometry of hyperplanes

A half-space is a subset of $\mathbb{R}^n$ defined by a single inequality involving a scalar product.

Definition: A half-space in $\mathbb{R}^n$ is a set of the form

$$H=\{\mathbf{x}\colon\langle\mathbf{a},\mathbf{x}\rangle\geq b\}, \tag{4.134}$$

where $\mathbf{a}\in\mathbb{R}^n$, $\mathbf{a}\neq 0$, and $b\in\mathbb{R}$ are given.

Geometrically, figure 4.9, the half-space above is the set of points such that $\langle\mathbf{a},(\mathbf{x}-\mathbf{x_0})\rangle\geq 0$, that is, the angle between $\mathbf{x}-\mathbf{x_0}$ and $\mathbf{a}$ is acute (in $[-90,+90]$). Here $\mathbf{x_0}$ is the point closest to the origin on the hyperplane defined by the equality $\langle\mathbf{a}\cdot\mathbf{x}\rangle=b$. (When $\mathbf{a}$ is normalized, as in the picture, $\mathbf{x_0}=b\mathbf{a}$.)

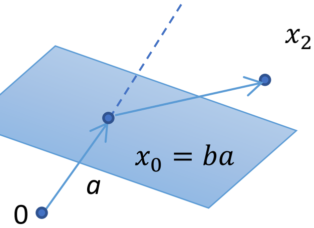


Figure 4.9. The half-space $\{\mathbf{x}\colon\langle\mathbf{a},\mathbf{x}\rangle\geq b\}$ is the set of points such that $\mathbf{x}-\mathbf{x_0}$ forms an acute angle with $\mathbf{a}$, where $\mathbf{x_0}$ is the projection of the origin on the boundary of the half-space.

4.10 Circle, spheres, hyperspheres and balls in $\mathbb{R}^n$

In two dimensions, the equation for a circle of radius r is

$$x^2 + y^2 = r^2 \tag{4.135}$$

In three dimensions, the equation for a 3-dimensional sphere (2-sphere) is

$$x^2 + y^2 + z^2 = r^2 \tag{4.136}$$

In hyperspace (space with more than three dimensions), the equation for an n-dimensional sphere ($(n-1)$-sphere) becomes

$$x_1^2 + x_2^2 + x_3^2 + \ldots + x_n^2 = r^2 \tag{4.137}$$

An n-sphere (a hypersphere) is the set of points in $(n+1)$-dimensional Euclidean space that are situated at a constant distance r from a fixed point, called the center. It is the generalization of an ordinary sphere in the ordinary three-dimensional space. The "radius" of a sphere is the constant distance of its points to the center. When the sphere has unit radius, it is usual to call it the unit n-sphere or (the n-sphere).

Definition: In terms of the standard norm, the n-sphere is defined as

$$S^n = \{\mathbf{x} \in \mathbb{R}^{n+1} : \|\mathbf{x}\|_2 = 1\} \tag{4.138}$$

and an n-sphere of radius r can be defined as

$$S^n = \{\mathbf{x} \in \mathbb{R}^{n+1} : \|\mathbf{x}\|_2 = r\} \tag{4.139}$$

The dimension of n-sphere is n, and must not be confused with the dimension $(n+1)$ of the Euclidean space in which it is naturally embedded. An n-sphere is the surface or boundary of an $(n+1)$-dimensional ball.

Definition: The set of points in $(n+1)$-space, $(x_1, x_2, \ldots, x_{n+1})$, that define an n-sphere, $S^n(r)$, is represented by the equation:

$$r^2 = \sum_{i=1}^{n+1} (x_i - c_i)^2 \tag{4.140}$$

where $c = (c_1, c_2, \ldots, c_{n+1})$ is a center point, and r is the radius.

In particular:

- the pair of points at the ends of a (one-dimensional) line segment is a 0-sphere,
- a circle, which is the one-dimensional circumference of a (two-dimensional) disk, is a 1-sphere,
- the two-dimensional surface of a three-dimensional ball is a 2-sphere, often simply called a sphere,

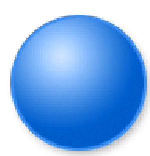


Figure 4.10. In Euclidean space, a ball is the volume bounded by a sphere

A ball is the solid figure bounded by a sphere; it is also called a solid sphere, figure 4.10. It may be a closed ball (including the boundary points that constitute the sphere) or an open ball (excluding them). These concepts are defined not only in three-dimensional Euclidean space but also for lower and higher dimensions spaces in general. A ball in n dimensions is called a hyperball or n-ball and is bounded by a hypersphere or $(n-1)$- sphere. Thus, for example,

- A 1-ball, a line segment, is the interior of a 0-sphere.
- A 2-ball, a disk, is the interior of a circle (1-sphere).
- A 3-ball, an ordinary ball, is the interior of a sphere (2-sphere).

Any normed vector space V with norm $\|\cdot\|$ is a metric space with the metric (distance function) $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|$. In such spaces, an arbitrary ball $B_r(\mathbf{y})$ of points $\mathbf{x}$ around a point $\mathbf{y}$ with a distance of less than r may be viewed as a scaled (by r) and translated (by $\mathbf{y}$) copy of a unit ball $B_1(0)$. Such "centered" balls with $\mathbf{y} = \mathbf{0}$ are denoted with $B(r)$.

In a Cartesian space $\mathbb{R}^n$ with the p-norm L_p, that is

$$\|\mathbf{x}\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{\frac{1}{p}} \tag{4.141}$$

Definition: an open ball around the origin with radius r is given by the set

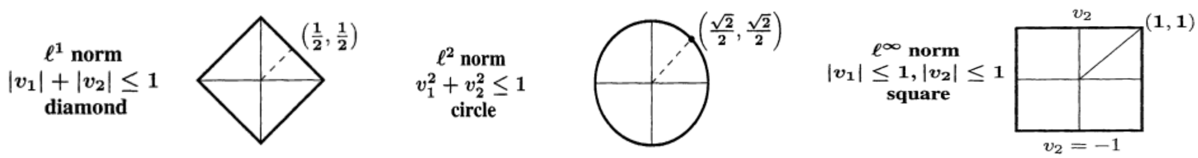
$$B(r) = \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{\frac{1}{p}} < r\} \tag{4.142}$$

A (Euclidean) ball (or just ball) in $\mathbb{R}^n$ has the form

$$B(\mathbf{x}_c, r) = \{\mathbf{x}: \|\mathbf{x} - \mathbf{x}_c\|_2 \leq r\} = \{\mathbf{x}: \langle(\mathbf{x} - \mathbf{x}_c), (\mathbf{x} - \mathbf{x}_c)\rangle \leq r^2\}. \tag{4.143}$$

For $n = 2$, in a 2-dimensional plane $\mathbb{R}^2$, "balls" according to the L_1-norm are bounded by squares with their diagonals parallel to the coordinate axes; those according to the L_∞ -norm have squares with their sides parallel to the coordinate axes as their boundaries. The L_2-norm generates the well known discs within circles, figure 4.11.

For $n = 3$, the L_1-balls are within octahedra with axes-aligned body diagonals, the L_∞-balls are within cubes with axes-aligned edges. Obviously, $p = 2$ generates the inner of usual spheres.



Manhattan Distance Euclidean Distance Chebyshev Distance

Figure 4.11

4.11 Ellipse, ellipsoid and hyperellipsoid in $\mathbb{R}^n$

Using a Cartesian coordinate system in which the origin is the center of the ellipse and the coordinate axes are axes of the ellipse, the implicit equation of the ellipse has the standard form

$$\frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} = 1 \tag{4.144}$$

where a, b are positive real numbers. The points $(a, 0)$ and $(0, b)$ lie on the curve. The line segments from the origin to these points are called the principal semi-axes of the ellipse, because a, b are half the length of the principal axes. They correspond to the semi-major axis and semi-minor axis of an ellipse. Hence,

$$\begin{aligned}
\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle &= (x_1 \quad x_2)\begin{pmatrix} \frac{1}{a^2} & 0 \\ 0 & \frac{1}{b^2} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\
&= (x_1 \quad x_2)\begin{pmatrix} \frac{1}{a^2}x_1 \\ \frac{1}{b^2}x_2 \end{pmatrix} \\
&= \frac{x_1^2}{a^2} + \frac{x_2^2}{b^2}
\end{aligned} \tag{4.145}$$

where $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, and $\mathbf{A} = \begin{pmatrix} \frac{1}{a^2} & 0 \\ 0 & \frac{1}{b^2} \end{pmatrix}$. The standard equation in $\mathbb{R}^n$ is

$$\frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \cdots + \frac{x_n^2}{a_n^2} = 1 \tag{4.146}$$

Definition: The ellipsoids is the set

$$\mathcal{E} = \{\mathbf{x} : \langle(\mathbf{x} - \mathbf{x}_c)|\mathbf{P}|(\mathbf{x} - \mathbf{x}_c)\rangle \leq 1\}, \tag{4.147}$$

$\mathbf{P}$ is symmetric and positive definite (i.e., $\mathbf{P} = \mathbf{P}^T$ and $\langle\mathbf{u}|\mathbf{P}|\mathbf{u}\rangle > 0$ whenever $\mathbf{u} \neq \mathbf{0}$). The vector $\mathbf{x}_c \in \mathbb{R}^n$ is the center of the ellipsoid.

The matrix $\mathbf{P}$ determines how far the ellipsoid extends in every direction from $\mathbf{x}_c$; the lengths of the semi-axes of $\mathcal{E}$ are given by $\sqrt{\lambda_i}$, where λ_i are the eigenvalues of $\mathbf{P}$. A ball is an ellipsoid with $\mathbf{P} = r^2\mathbf{I}$. Figure 4.11 shows an ellipsoid in $\mathbb{R}^2$.

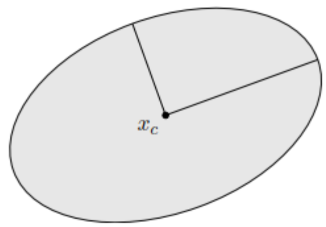


Figure 4.11

A hyper-ellipsoid, or ellipsoid of dimension $n-1$ in a Euclidean space of dimension n, is a quadric hypersurface defined by a polynomial of degree two that has a homogeneous part of degree two which is a positive definite quadratic form.

4.12 Quadratic form and definite matrix in $\mathbb{R}^n$

The reader should now be well aware of the important roles of matrices in the study of linear equations, which can be expressed in the form

$$a_1x_1 + a_2x_2 + \ldots + a_nx_n = b \tag{4.148}$$

The left side $a_1x_1 + a_2x_2 + \ldots + a_nx_n = \langle\mathbf{a}, \mathbf{x}\rangle$ of the equation is a (homogeneous) polynomial of degree 1 in n variables, called a linear form. In this section, we study a (homogeneous) polynomial of degree 2 in several variables, called a quadratic form, and show that matrices also play an important role in the study of a quadratic form.

A quadratic equation in two variables x and y is an equation of the form

$$ax^2 + 2bxy + cy^2 + dx + ey + f = 0, \tag{4.149}$$

in which the left side consists of a constant term f, a linear form $dx + ey$, and a quadratic form $ax^2 + 2bxy + cy^2$. Note that this quadratic form may be written in matrix notation as

$$ax^2 + 2bxy + cy^2 = \begin{pmatrix} x & y \end{pmatrix}\begin{pmatrix} a & b \\ b & c \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \langle\mathbf{x}|\mathbf{A}|\mathbf{x}\rangle \tag{4.150}$$

where

$$\mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix} \text{ and } \mathbf{A} = \begin{pmatrix} a & b \\ b & c \end{pmatrix} \tag{4.151}$$

Note also that the matrix $\mathbf{A}$ is taken to be a (real) symmetric matrix. Geometrically, the solution set of a quadratic equation in x and y usually represents a conic section, such as an ellipse, a parabola or a hyperbola in the xy-plane.

Definitions: An equation of the form

$$f(\mathbf{x}) = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_ix_j + \sum_{i=1}^{n} b_ix_i + c = 0 \tag{4.152}$$

where a_{ij}, b_i and c are real constants, is called a quadratic equation in n variables $x_1, x_2, \ldots, x_n$. In matrix form, it can be written as

$$f(\mathbf{x}) = \langle\mathbf{x}|\mathbf{A}|\mathbf{x}\rangle + \langle\mathbf{b}|\mathbf{x}\rangle + c = 0 \tag{4.153}$$

where $A = (a_{ij})$, $\mathbf{x} = (x_1 \ldots x_n)^T$ and $\mathbf{b} = (b_1 \ldots b_n)$ in $\mathbb{R}^n$.

(2) A linear form is a polynomial of degree 1 in n variables $x_1, x_2, \ldots, x_n$ of the form

$$\langle \mathbf{b}, \mathbf{x} \rangle = \sum_{i=1}^{n} b_i x_i \tag{4.154}$$

where $\mathbf{x} = (x_1 \dots x_n)^T$ and $\mathbf{b} = (b_1 \dots b_n)$ in $\mathbb{R}^n$.

(3) A quadratic form is a (homogeneous) polynomial of degree 2 in n variables $x_1, x_2, \dots, x_n$ of the form

$$q(\mathbf{x}) = \langle \mathbf{x}|\mathbf{A}|\mathbf{x} \rangle = (x_1 \dots x_n)\big(A_{ij}\big)\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij} x_i x_j \tag{4.155}$$

where $\mathbf{x} = (x_1 \dots x_n)^T \in \mathbb{R}^n$ and $\mathbf{A} = \big(A_{ij}\big)$ is a real n × n matrix.

Example 4.23

Consider the matrix $\mathbf{A} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$ and the vector $\mathbf{x}$.

Solution

q is given by

$$\begin{aligned} q = \langle \mathbf{x}|\mathbf{A}|\mathbf{x} \rangle &= (x_1 \quad x_2)\begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ &= (x_1 + 2x_2 \quad 2x_1 + x_2)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ &= x_1^2 + 2x_1x_2 + 2x_1x_2 + x_2^2 = x_1^2 + 4x_1x_2 + x_2^2 \end{aligned}$$

Example 4.24

Consider the 3 × 3 diagonal matrix $\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix}$ and a general 3 element vector $\mathbf{x}$.

Solution

The general quadratic form is given by

$$\begin{aligned} q = \langle \mathbf{x}|\mathbf{A}|\mathbf{x} \rangle &= (x_1 \quad x_2 \quad x_3)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ &= (x_1 \quad 2x_2 \quad 4x_3)\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ &= x_1^2 + 2x_2^2 + 4x_3^2 \end{aligned}$$

Example 4.25

Also consider the following matrix $\mathbf{A} = \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix}$.

Solution

The general quadratic form is given by

$$\begin{aligned} q = \langle \mathbf{x}|\mathbf{A}|\mathbf{x} \rangle &= (x_1 \quad x_2 \quad x_3)\begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ &= (-2x_1 + x_2 \quad x_1 - 2x_2 \quad -2x_3)\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ &= -2x_1^2 + x_1x_2 + x_1x_2 - 2x_2^2 - 2x_3^2 \\ &= -2x_1^2 + 2x_1x_2 - 2x_2^2 - 2x_3^2 \\ &= -2(x_1^2 - x_1x_2) - 2x_2^2 - 2x_3^2 \\ &= -2x_1^2 - 2(x_2^2 - x_1x_2) - 2x_3^2 \end{aligned}$$

Theorem 4.22: The matrix $\mathbf{A}$ in the definition of a quadratic form is any square matrix, but it can be restricted to be a symmetric matrix.

Proof:

In fact, any square matrix $\mathbf{A}$ is the sum of a symmetric part $\mathbf{B}$ ($\mathbf{B}^T = \mathbf{B}$) and a skew-symmetric part $\mathbf{C}$ ($\mathbf{C}^T = -\mathbf{C}$), say

$$\mathbf{A} = \mathbf{B} + \mathbf{C}, \qquad \mathbf{B} = \frac{1}{2}(\mathbf{A} + \mathbf{A}^T), \qquad \mathbf{C} = \frac{1}{2}(\mathbf{A} - \mathbf{A}^T)$$

where,

$$\mathbf{B}^T = \frac{1}{2}(\mathbf{A} + \mathbf{A}^T)^T = \frac{1}{2}(\mathbf{A}^T + (\mathbf{A}^T)^T) = \frac{1}{2}(\mathbf{A} + \mathbf{A}^T)$$

$$\mathbf{C}^T = \frac{1}{2}(\mathbf{A} - \mathbf{A}^T)^T = \frac{1}{2}(\mathbf{A}^T - (\mathbf{A}^T)^T) = \frac{1}{2}(\mathbf{A}^T - \mathbf{A}) = -\frac{1}{2}(\mathbf{A} - \mathbf{A}^T) = -\mathbf{C}$$

For the skew-symmetric matrix $\mathbf{C}$, we have

$$\langle \mathbf{x}|\mathbf{C}|\mathbf{x}\rangle = \langle \mathbf{x}|\mathbf{C}|\mathbf{x}\rangle^T = \langle \mathbf{x}|\mathbf{C}^T|\mathbf{x}\rangle = -\langle \mathbf{x}|\mathbf{C}|\mathbf{x}\rangle.$$

Since, $\langle \mathbf{x}|\mathbf{C}|\mathbf{x}\rangle$ is real number. Hence, $\langle \mathbf{x}|\mathbf{C}|\mathbf{x}\rangle = 0$. Therefore,

$$q(\mathbf{x}) = \langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \langle \mathbf{x}|(\mathbf{B}+\mathbf{C})|\mathbf{x}\rangle = \langle \mathbf{x}|\mathbf{B}|\mathbf{x}\rangle.$$

This means that, without loss of generality, one may assume that the matrix $\mathbf{A}$ in the definition of a quadratic form is a symmetric matrix.

■

Remark:

(1) A quadratic equation is said to be consistent if it has a solution, i.e., there is a vector $\mathbf{x} \in \mathbb{R}^n$ such that $f(\mathbf{x}) = 0$. Otherwise, it is said to be inconsistent. For instance, the equation $2x^2 + 3y^2 = -1$ is inconsistent. In the following discussion we will consider only consistent equations.

(2) From the definition of a quadratic form, one can see that, fixing a basis like the standard basis for $\mathbb{R}^n$, a quadratic form is associated with a unique symmetric matrix, which is called the matrix representation of the quadratic form q with respect to the basis chosen (the standard basis for $\mathbb{R}^n$). On the other hand, any (real) symmetric matrix $\mathbf{A}$ gives rise to a quadratic form $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle$. For example, for a symmetric matrix $\begin{pmatrix} 8 & 2 \\ 2 & -1 \end{pmatrix}$ the equation $(x_1 \quad x_2)\begin{pmatrix} 8 & 2 \\ 2 & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ defines a quadratic form $8x_1^2 + 4x_1x_2 - x_2^2$.

Diagonalization of a quadratic form

To study the solution of a quadratic equation $f(\mathbf{x}) = 0$, we first consider an equation $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = c$ without a linear form. This quadratic form may be rewritten as the sum of two parts:

$$q(\mathbf{x}) = \langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \sum_{i=1}^{n} A_{ii}x_i^2 + 2\sum_{i<j} A_{ij}x_ix_j \tag{4.156}$$

in which the first part $\sum_{i=1}^{n} A_{ii}x_i^2$ is called the (perfect) square terms and the second part $\sum_{i\neq j} A_{ij}x_ix_j$ is called the cross-product terms. Actually, what makes it hard to sketch the quadratic surface is the cross-product terms. However, the symmetric matrix $\mathbf{A}$ can be orthogonally diagonalized, i. e., there exists an orthogonal matrix $\mathbf{P}$ ($\mathbf{P}^T = \mathbf{P}^{-1}$) such that

$$\mathbf{P}^T\mathbf{A}\mathbf{P} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{D} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{pmatrix} \tag{4.157}$$

Here, the diagonal entries λ_i's are the eigenvalues of $\mathbf{A}$ and the column vectors of $\mathbf{P}$ are their associated eigenvectors of $\mathbf{A}$. Then we get, by setting $\mathbf{x} = \mathbf{P}\mathbf{y}$,

$$\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \langle \mathbf{y}|\mathbf{P}^T\mathbf{A}\mathbf{P}|\mathbf{y}\rangle = \langle \mathbf{y}|\mathbf{D}|\mathbf{y}\rangle = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2, \tag{4.158}$$

which is a quadratic form without the cross-product terms. Consequently, we have proven the following theorem.

Theorem 4.23: Let $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle$ be a quadratic form in $\mathbf{x} = (x_1 \ldots x_n)^T \in \mathbb{R}^n$ for a symmetric matrix $\mathbf{A}$. Then there is a change of coordinates of $\mathbf{x}$ into $\mathbf{y} = \mathbf{P}^T\mathbf{x} = (y_1 \ldots y_n)^T$ such that

$$\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \langle \mathbf{y}|\mathbf{D}|\mathbf{y}\rangle = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2, \tag{4.159}$$

where $\mathbf{P}$ is an orthogonal matrix and $\mathbf{P}^T\mathbf{A}\mathbf{P} = \mathbf{D}$.

Remark:

(1) Recall that in above theorem the columns of the matrix P are the orthonormal eigenvectors of $\mathbf{A}$ and $\mathbf{y}$ is just the coordinate expression of $\mathbf{x}$ with respect to the orthonormal eigenvectors of $\mathbf{A}$. In fact, $\mathbf{P} = [Id]_\beta^\alpha$, where β is a basis consisting of orthonormal eigenvectors of $\mathbf{A}$ and α is the standard basis.

(2) The solution set of a quadratic equation of the form $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = c$ is a hypersurface in $\mathbb{R}^n$, that is, a curved surface that can be parameterized in $n-1$ variables. These are called $n-1$ -dimensional quadratic surfaces, with axes in the directions of eigenvectors. In particular, if $n = 2$, the solution set of a quadratic equation is called a quadratic curve, or more commonly a conic section. When $n = 3$, the quadratic surfaces are ellipsoids or hyperboloids depending on the signs of the eigenvalues of $\mathbf{A}$. Of course, a paraboloid is also a quadratic surface, but it appears when a linear form is present in the quadratic equation. The determination of the quadratic hypersurface depends on the signs of the eigenvalues of $\mathbf{A}$.

Example 4.26

Determine the conic section $3x^2 + 2xy + 3y^2 - 8 = 0$.

Solution

This equation can be written in the form

$$\begin{pmatrix} x & y \end{pmatrix}\begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = 8$$

The matrix $\mathbf{A} = \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$ has eigenvalues $\lambda_1 = 2$ and $\lambda_2 = 4$ with associated unit eigenvectors

$$\mathbf{v}_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$
$$\mathbf{v}_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

respectively, which form an orthonormal basis β. If α denotes the standard basis, then the transition matrix

$$\begin{aligned} \mathbf{P} &= \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} \cos 45 & \sin 45 \\ -\sin 45 & \cos 45 \end{pmatrix} \end{aligned}$$

which is a rotation through 45° in clockwise direction such that $\mathbf{P}^T = \mathbf{P}^{-1}$. It gives a change of coordinates, $\mathbf{x} = \mathbf{P}\mathbf{y}$, *i. e.*,

$$\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} \acute{x} \\ \acute{y} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}\acute{x} + \frac{1}{\sqrt{2}}\acute{y} \\ -\frac{1}{\sqrt{2}}\acute{x} + \frac{1}{\sqrt{2}}\acute{y} \end{pmatrix}$$

Thus, we get

$$\begin{aligned} 3x^2 + 2xy + 3y^2 &= \langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle \\ &= \langle \mathbf{y}|\mathbf{P}^T\mathbf{A}\mathbf{P}|\mathbf{y}\rangle \\ &= \langle \mathbf{y}|\mathbf{D}|\mathbf{y}\rangle \\ &= \mathbf{y}^T\begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}\mathbf{y} = 2(\acute{x})^2 + 4(\acute{y})^2 = 8 \end{aligned}$$

or

$$\frac{(\acute{x})^2}{4} + \frac{(\acute{y})^2}{2} = 1$$

Its solution set is just an ellipse with axes $\mathbf{v}_1 = \mathbf{P}^T\boldsymbol{e}_1$ and $\mathbf{v}_2 = \mathbf{P}^T\boldsymbol{e}_2$.

Definition: Let $\mathbf{A} = (A_{ij}) \in M_{n\times n}(\mathbb{R})$ be a symmetric matrix and let $\mathbf{x} = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$. Then, $\mathbf{A}$ is said to be

(1) positive definite if $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \sum_{ij} A_{ij}x_ix_j > 0$ for all nonzero $\mathbf{x}$,
(2) positive semidefinite if $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \sum_{ij} A_{ij}x_ix_j \geq 0$ for all $\mathbf{x}$,
(3) negative definite if $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \sum_{ij} A_{ij}x_ix_j < 0$ for all nonzero $\mathbf{x}$,
(4) negative semidefinite if $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \sum_{ij} A_{ij}x_ix_j \leq 0$ for all $\mathbf{x}$,
(5) indefinite if $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle$ takes both positive and negative values.

Example 4.27

The real symmetric matrix

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

is positive definite, because the quadratic form satisfies

$$\begin{aligned}
\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle &= (x_1 \quad x_2 \quad x_3)\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\
&= (x_1 \quad x_2 \quad x_3)\begin{pmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 \end{pmatrix} \\
&= x_1(2x_1 - x_2) + x_2(-x_1 + 2x_2 - x_3) + x_3(-x_2 + 2x_3) \\
&= 2x_1^2 - 2x_1x_2 + 2x_2^2 - 2x_2x_3 + 2x_3^2 \\
&= x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 > 0
\end{aligned}$$

unless $x_1 = x_2 = x_3 = 0$.

Graphical analysis

When $\mathbf{x}$ has only two elements, we can graphically represent q in 3 dimensions. A positive definite quadratic form will always be positive except at the point where $\mathbf{x} = 0$. This gives a nice graphical representation where the plane at $\mathbf{x} = \mathbf{0}$ bounds the function from below. Figure 4.12 shows a positive definite quadratic form. Similarly, a negative definite quadratic form is bounded above by the plane $\mathbf{x} = \mathbf{0}$. Figure 4.13 shows a negative definite quadratic form. A positive semi-definite quadratic form is bounded below by the plane $\mathbf{x} = \mathbf{0}$ but will touch the plane at more than the single point $(0,0)$, it will touch the plane along a line. Figure 4.14 shows a positive semi-definite quadratic form. A negative semi-definite quadratic form is bounded above by the plane $\mathbf{x} = \mathbf{0}$ but will touch the plane at more than the single point $(0,0)$. It will touch the plane along a line. Figure 4.15 shows a negative-definite quadratic form. An indefinite quadratic form will not lie completely above or below the plane but will lie above for some values of $\mathbf{x}$ and below for other values of $\mathbf{x}$. Figure 4.16 shows an indefinite quadratic form.

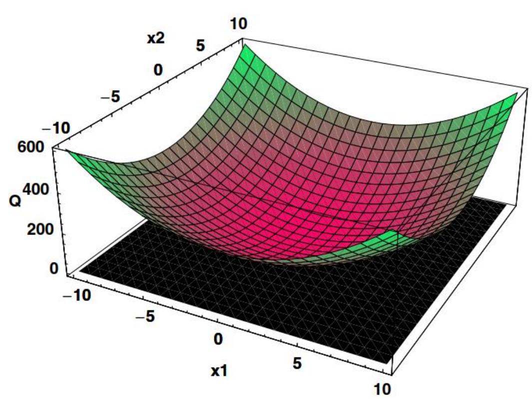


Figure 4.12. Positive Definite Quadratic Form $3x_1^2 + 3x_2^2$

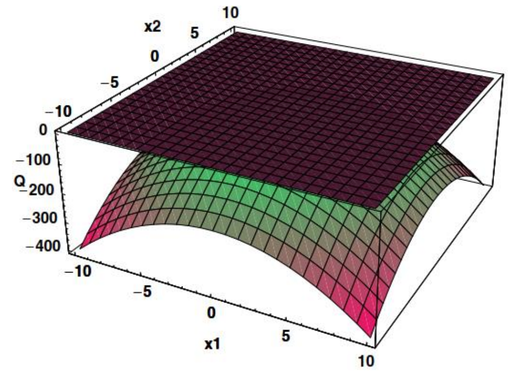


Figure 1.13. Negative Definite Quadratic Form $-2x_1^2 - 2x_2^2$

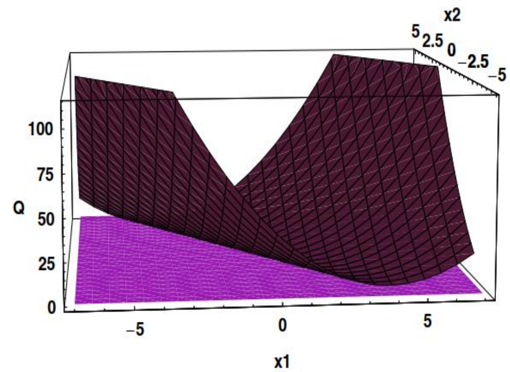


Figure 4.14. Positive Semi-Definite Quadratic Form $2x_1^2 + 4x_1x_2 + 2x_2^2$

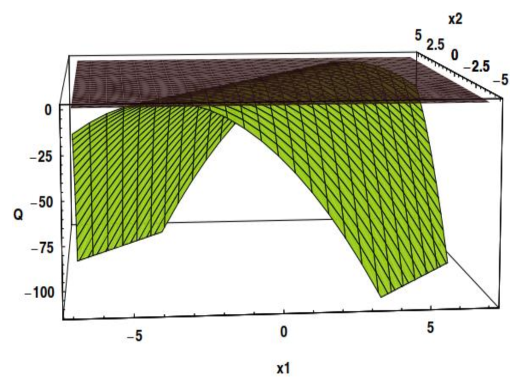


Figure 4.15. Negative Semi-Definite Quadratic Form $-2x_1^2 + 4x_1x_2 - 2x_2^2$

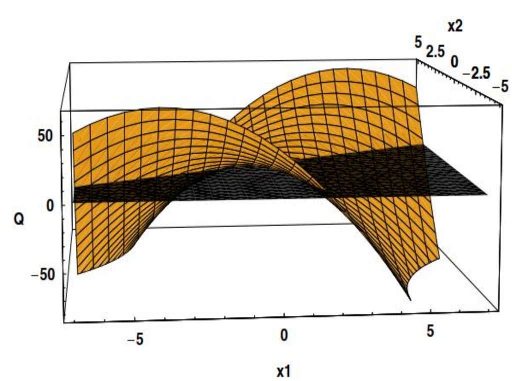


Figure 4.16. Indefinite Quadratic Form $-2x_1^2 + 4x_1x_2 + 2x_2^2$

To determine whether or not a matrix **A** is positive definite, one can diagonalize **A** so that

$$\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \sum_{i,j=1}^{n} A_{ij}x_i x_j = \langle \mathbf{y}|\mathbf{D}|\mathbf{y}\rangle = \sum_{i=1}^{n} \lambda_i y_i^2 \tag{4.160}$$

where $\mathbf{y} = \mathbf{P}^T\mathbf{x}$ for an orthogonal matrix **P** and the λ_i 's are eigenvalues of **A**. Therefore, $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle > 0$ for all nonzero $\mathbf{x} \in \mathbb{R}^n$ if and only if all the λ_i 's are positive. Consequently, we have the following characterization of positive definite matrices:

Theorem 4.24: A real symmetric $\mathrm{n} \times \mathrm{n}$ matrix **A** is positive definite if and only if all the eigenvalues of **A** are positive.

So far, we have seen that it is important to determine whether or not a symmetric matrix **A** is positive definite. In most cases, the definition does not help much. But we have seen that theorem 4.24 gives us a practical characterization of positive definite matrices: **A** is positive definite if and only if all eigenvalues of **A** are positive. We will find some other practical criteria in terms of the determinant of the matrix. For this, we again look at the quadratic form in two variables, $q(x,y) = ax^2 + 2bxy + cy^2$, which may be rewritten in a complete square form as

$$q(x) = ax^2 + 2bxy + cy^2 = a\left(x + \frac{b}{a}y\right)^2 + (c - \frac{b^2}{a})y^2 \tag{4.161}$$

We see that q is positive definite, i.e., $q(x) = \langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle > 0$ for any nonzero vector $\mathbf{x} = (x,y) \in \mathbb{R}^2$, if and only if $a > 0$ and $ac > b^2$, or equivalently, the determinants of

$$(a) \text{ and } \begin{pmatrix} a & b \\ b & c \end{pmatrix} \tag{4.162}$$

are positive. The natural generalization of the above conditions will involve all n-submatrices of **A**, called the principal submatrices of **A**, which are defined as the upper left square submatrices

$$\mathbf{A}_1 = (a_{11}), \qquad \mathbf{A}_2 = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \qquad \mathbf{A}_3 = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \dots, \mathbf{A}_n = \mathbf{A} \tag{4.163}$$

or schematically represented in figure 4.17.

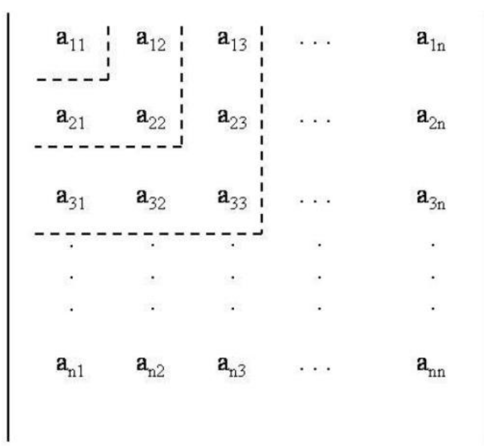


Figure 4.17. Naturally Ordered Principle Minors of a Matrix

With this construction, we have the following characterization of positive definite matrices.

Theorem 4.25: The following are equivalent for a real symmetric matrix **A**:
(1) A is positive definite, i. e., $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle > 0$ for all nonzero vector **x**;
(2) all the eigenvalues of **A** are positive;
(3) all the principal submatrices $\mathbf{A}_k$'s have positive determinants;
(4) all the pivots (without row interchanges) are positive;
(5) there exists a nonsingular matrix **W** such that $\mathbf{A} = \mathbf{W}^T\mathbf{W}$.

Proof:

(3) If $\mathbf{A}$ has positive eigenvalues λ_1, λ_2, ..., λ_n, then $\det \mathbf{A} = \lambda_1 \lambda_2 \ldots \lambda_n > 0$. To prove the same result for all the submatrices $\mathbf{A}_k$, we show that if $\mathbf{A}$ is positive definite, so is every $\mathbf{A}_k$. For each $k = 1, \ldots, n$, consider all the vectors whose last $n-k$ components are zero, say $\mathbf{x} = (x_1 \ldots x_k, 0, \ldots, 0)^T = (x_k, 0)^T$, where $\mathbf{x}_k$ is any vector in $\mathbb{R}^k$. Then

$$\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = (x_k, 0) \begin{pmatrix} A_k & * \\ & * \end{pmatrix} \begin{pmatrix} x_k \\ 0 \end{pmatrix} = \langle \mathbf{x}_k|\mathbf{A}_k|\mathbf{x}_k\rangle$$

Thus $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle > 0$ for all such nonzero $\mathbf{x}$ if and only if $\langle \mathbf{x}_k|\mathbf{A}_k|\mathbf{x}_k\rangle > 0$ for all nonzero $\mathbf{x}_k \in \mathbb{R}^k$ that is, $\mathbf{A}_k$'s are positive definite, all eigenvalues of $\mathbf{A}_k$ are positive, and its determinant is positive.

(4) Recall that the symmetric matrix $\mathbf{A}$ can be factorized uniquely into the form

$$\mathbf{A} = \mathbf{LDL}^T$$

where $\mathbf{L}$ is a lower triangular matrix with 1's on its diagonal and $\mathbf{D}$ is the diagonal matrix with the pivots d_k of $\mathbf{A}$ on the diagonal. But the k-th pivot d_k is exactly the ratio of $\det \mathbf{A}_k$ to $\det \mathbf{A}_{k-1}$:

$$\mathrm{d_k} = \frac{\det \mathbf{A}_\mathrm{k}}{\det \mathbf{A}_{\mathrm{k}-1}}$$

Hence, all d_k's are positive.

(5) Let $\mathbf{A} = \mathbf{LDL}^T$ as above with

$$\mathbf{D} = \begin{pmatrix} d_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & d_n \end{pmatrix}, d_i > 0$$

Define

$$\sqrt{\mathbf{D}} = \begin{pmatrix} \sqrt{d_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sqrt{d_n} \end{pmatrix}$$

Then, clearly $\det \sqrt{\mathbf{D}} > 0$, $\mathbf{D} = \sqrt{\mathbf{D}}\sqrt{\mathbf{D}}$ and $\left(\sqrt{\mathbf{D}}\right)^T = \sqrt{\mathbf{D}}$. Hence,

$$\mathbf{A} = \mathbf{LDL}^T = \left(\mathbf{L}\sqrt{\mathbf{D}}\right)\left(-\sqrt{\mathbf{D}}\mathbf{L}^T\right) = \left(\mathbf{L}\sqrt{\mathbf{D}}\right)\left(\mathbf{L}\sqrt{\mathbf{D}}\right)^T = \mathbf{W}^T\mathbf{W},$$

where $\mathbf{W} = \left(\mathbf{L}\sqrt{\mathbf{D}}\right)^T$, which is nonsingular since $\mathbf{L}$ and $\sqrt{\mathbf{D}}$ are.

If $\mathbf{A}$ is real symmetric and $\mathbf{A} = \mathbf{W}^T\mathbf{W}$, where $\mathbf{W}$ is nonsingular, then for $\mathbf{x} \neq 0$ we have

$$\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle = \langle \mathbf{x}|\mathbf{W}^T\mathbf{W}|\mathbf{x}\rangle = \langle \mathbf{Wx}|\mathbf{Wx}\rangle = ||\mathbf{Wx}||^2 > 0,$$

because $\mathbf{Wx} \neq 0$.

■

Example 4.28

As an example consider the matrix $G1$.

$$G1 = \begin{pmatrix} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

Solution

Element $a_{11} = 4 > 0$.

Now consider the first naturally occurring principal 2×2 submatrix $\begin{pmatrix} 4 & 2 \\ 2 & 9 \end{pmatrix} = 36 - 4 = 32 > 0$.

Now consider the determinant of the entire matrix $\begin{pmatrix} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{pmatrix} = 64 > 0$. This matrix is then positive definite.

We now consider semidefinite matrices. One can easily establish the following analogous theorem.

Theorem 4.26: The following are equivalent for a real symmetric matrix $\mathbf{A}$:
(1) A is positive semidefinite, i.e., $\langle \mathbf{x}|\mathbf{A}|\mathbf{x}\rangle \geq 0$ for all vectors $\mathbf{x}$;
(2) all the eigenvalues of $\mathbf{A}$ are non-negative.
(3) all the principal submatrices $\mathbf{A}_k$'s have nonnegative determinants.
(4) all the pivots (without row exchanges) are non-negative.
(5) there exists a matrix $\mathbf{W}$, possibly singular, such that $\mathbf{A} = \mathbf{W}^T\mathbf{W}$.

Example 4.29

As an example consider the matrix

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

Solution

Element $a_{11} = -2 < 0$. Now consider the first naturally occurring principal 2×2 submatrix

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

Now consider the determinant of the entire matrix

$$\begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix} = -6 < 0$$

This matrix is then negative definite.