A **symmetric** matrix is a matrix A such that $A^T = A$. Such a matrix is necessarily square. Its main diagonal entries are arbitrary, but its other entries occur in pairs—on opposite sides of the main diagonal.

EXAMPLE 1 Of the following matrices, only the first three are symmetric:

$$\text{Symmetric:}\quad \begin{bmatrix} 1 & 0 \\ 0 & -3 \end{bmatrix}, \quad \begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & 8 \\ 0 & 8 & -7 \end{bmatrix}, \quad \begin{bmatrix} a & b & c \\ b & d & e \\ c & e & f \end{bmatrix}$$

$$\text{Nonsymmetric:}\quad \begin{bmatrix} 1 & -3 \\ 3 & 0 \end{bmatrix}, \quad \begin{bmatrix} 1 & -4 & 0 \\ -6 & 1 & -4 \\ 0 & -6 & 1 \end{bmatrix}, \quad \begin{bmatrix} 5 & 4 & 3 & 2 \\ 4 & 3 & 2 & 1 \\ 3 & 2 & 1 & 0 \end{bmatrix}$$

If A is symmetric, then any two eigenvectors from different eigenspaces are orthogonal.

An $n \times n$ matrix A is orthogonally diagonalizable if and only if A is a symmetric matrix.

The Spectral Theorem for Symmetric Matrices

An $n \times n$ symmetric matrix A has the following properties:

a. A has n real eigenvalues, counting multiplicities.

b. The dimension of the eigenspace for each eigenvalue λ equals the multiplicity of λ as a root of the characteristic equation.

c. The eigenspaces are mutually orthogonal, in the sense that eigenvectors corresponding to different eigenvalues are orthogonal.

d. A is orthogonally diagonalizable.

Until now, our attention in this text has focused on linear equations, except for the sums of squares encountered in Chapter 6 when computing $\mathbf{x}^T\mathbf{x}$. Such sums and more general expressions, called *quadratic forms*, occur frequently in applications of linear algebra to engineering (in design criteria and optimization) and signal processing (as output noise power). They also arise, for example, in physics (as potential and kinetic energy), differential geometry (as normal curvature of surfaces), economics (as utility functions), and statistics (in confidence ellipsoids). Some of the mathematical background for such applications flows easily from our work on symmetric matrices.

A **quadratic form** on $\mathbb{R}^n$ is a function Q defined on $\mathbb{R}^n$ whose value at a vector $\mathbf{x}$ in $\mathbb{R}^n$ can be computed by an expression of the form $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$, where A is an $n \times n$ symmetric matrix. The matrix A is called the **matrix of the quadratic form**.

The simplest example of a nonzero quadratic form is $Q(\mathbf{x}) = \mathbf{x}^T I\mathbf{x} = \|\mathbf{x}\|^2$. Examples 1 and 2 show the connection between any symmetric matrix A and the quadratic form $\mathbf{x}^T A\mathbf{x}$.

EXAMPLE 1 Let $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. Compute $\mathbf{x}^T A\mathbf{x}$ for the following matrices:

a. $A = \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix}$ b. $A = \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix}$

SOLUTION

a. $\mathbf{x}^T A\mathbf{x} = [\, x_1 \quad x_2 \,] \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = [\, x_1 \quad x_2 \,] \begin{bmatrix} 4x_1 \\ 3x_2 \end{bmatrix} = 4x_1^2 + 3x_2^2.$

b. There are two -2 entries in A. Watch how they enter the calculations. The $(1, 2)$-entry in A is in boldface type.

$$\begin{aligned}
\mathbf{x}^T A\mathbf{x} &= [\, x_1 \quad x_2 \,] \begin{bmatrix} 3 & \mathbf{-2} \\ -2 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = [\, x_1 \quad x_2 \,] \begin{bmatrix} 3x_1 - \mathbf{2}x_2 \\ -2x_1 + 7x_2 \end{bmatrix} \\
&= x_1(3x_1 - \mathbf{2}x_2) + x_2(-2x_1 + 7x_2) \\
&= 3x_1^2 - \mathbf{2}x_1x_2 - 2x_2x_1 + 7x_2^2 \\
&= 3x_1^2 - 4x_1x_2 + 7x_2^2
\end{aligned}$$

■

The presence of $-4x_1x_2$ in the quadratic form in Example 1(b) is due to the -2 entries off the diagonal in the matrix A. In contrast, the quadratic form associated with the diagonal matrix A in Example 1(a) has no x_1x_2 *cross-product* term.

EXAMPLE 2 For $\mathbf{x}$ in $\mathbb{R}^3$, let $Q(\mathbf{x}) = 5x_1^2 + 3x_2^2 + 2x_3^2 - x_1x_2 + 8x_2x_3$. Write this quadratic form as $\mathbf{x}^T A\mathbf{x}$.

SOLUTION The coefficients of x_1^2, x_2^2, x_3^2 go on the diagonal of A. To make A symmetric, the coefficient of x_ix_j for $i \neq j$ must be split evenly between the (i, j)- and (j, i)-entries in A. The coefficient of x_1x_3 is 0. It is readily checked that

$$Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x} = [\, x_1 \quad x_2 \quad x_3 \,] \begin{bmatrix} 5 & -1/2 & 0 \\ -1/2 & 3 & 4 \\ 0 & 4 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

■

EXAMPLE 3 Let $Q(\mathbf{x}) = x_1^2 - 8x_1x_2 - 5x_2^2$. Compute the value of $Q(\mathbf{x})$ for $\mathbf{x} = \begin{bmatrix} -3 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ -2 \end{bmatrix}$, and $\begin{bmatrix} 1 \\ -3 \end{bmatrix}$.

SOLUTION

$$\begin{aligned}
Q(-3, 1) &= (-3)^2 - 8(-3)(1) - 5(1)^2 = 28 \\
Q(2, -2) &= (2)^2 - 8(2)(-2) - 5(-2)^2 = 16 \\
Q(1, -3) &= (1)^2 - 8(1)(-3) - 5(-3)^2 = -20
\end{aligned}$$

■

In some cases, quadratic forms are easier to use when they have no cross-product terms—that is, when the matrix of the quadratic form is a diagonal matrix. Fortunately, the cross-product term can be eliminated by making a suitable change of variable.

Change of Variable in a Quadratic Form

If $\mathbf{x}$ represents a variable vector in $\mathbb{R}^n$, then a **change of variable** is an equation of the form

$$\mathbf{x} = P\mathbf{y}, \qquad \text{or equivalently,} \quad \mathbf{y} = P^{-1}\mathbf{x} \tag{1}$$

where P is an invertible matrix and $\mathbf{y}$ is a new variable vector in $\mathbb{R}^n$. Here $\mathbf{y}$ is the coordinate vector of $\mathbf{x}$ relative to the basis of $\mathbb{R}^n$ determined by the columns of P. (See Section 4.4.)

If the change of variable (1) is made in a quadratic form $\mathbf{x}^TA\mathbf{x}$, then

$$\mathbf{x}^TA\mathbf{x} = (P\mathbf{y})^TA(P\mathbf{y}) = \mathbf{y}^TP^TAP\mathbf{y} = \mathbf{y}^T(P^TAP)\mathbf{y} \tag{2}$$

and the new matrix of the quadratic form is P^TAP. Since A is symmetric, Theorem 2 guarantees that there is an *orthogonal* matrix P such that P^TAP is a diagonal matrix D, and the quadratic form in (2) becomes $\mathbf{y}^TD\mathbf{y}$. This is the strategy of the next example.

EXAMPLE 4 Make a change of variable that transforms the quadratic form in Example 3 into a quadratic form with no cross-product term.

SOLUTION The matrix of the quadratic form in Example 3 is

$$A = \begin{bmatrix} 1 & -4 \\ -4 & -5 \end{bmatrix}$$

The first step is to orthogonally diagonalize A. Its eigenvalues turn out to be $\lambda = 3$ and $\lambda = -7$. Associated unit eigenvectors are

$$\lambda = 3: \begin{bmatrix} 2/\sqrt{5} \\ -1/\sqrt{5} \end{bmatrix}; \qquad \lambda = -7: \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}$$

These vectors are automatically orthogonal (because they correspond to distinct eigenvalues) and so provide an orthonormal basis for $\mathbb{R}^2$. Let

$$P = \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix}, \qquad D = \begin{bmatrix} 3 & 0 \\ 0 & -7 \end{bmatrix}$$

Then $A = PDP^{-1}$ and $D = P^{-1}AP = P^TAP$, as pointed out earlier. A suitable change of variable is

$$\mathbf{x} = P\mathbf{y}, \qquad \text{where } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

Then

$$\begin{aligned} x_1^2 - 8x_1x_2 - 5x_2^2 &= \mathbf{x}^TA\mathbf{x} = (P\mathbf{y})^TA(P\mathbf{y}) \\ &= \mathbf{y}^TP^TAP\mathbf{y} = \mathbf{y}^TD\mathbf{y} \\ &= 3y_1^2 - 7y_2^2 \end{aligned}$$

■

To illustrate the meaning of the equality of quadratic forms in Example 4, we can compute $Q(\mathbf{x})$ for $\mathbf{x} = (2, -2)$ using the new quadratic form. First, since $\mathbf{x} = P\mathbf{y}$,

$$\mathbf{y} = P^{-1}\mathbf{x} = P^T\mathbf{x}$$

so

$$\mathbf{y} = \begin{bmatrix} 2/\sqrt{5} & -1/\sqrt{5} \\ 1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix}\begin{bmatrix} 2 \\ -2 \end{bmatrix} = \begin{bmatrix} 6/\sqrt{5} \\ -2/\sqrt{5} \end{bmatrix}$$

Hence

$$\begin{aligned} 3y_1^2 - 7y_2^2 &= 3(6/\sqrt{5})^2 - 7(-2/\sqrt{5})^2 = 3(36/5) - 7(4/5) \\ &= 80/5 = 16 \end{aligned}$$

This is the value of $Q(\mathbf{x})$ in Example 3 when $\mathbf{x} = (2, -2)$. See Fig. 1.

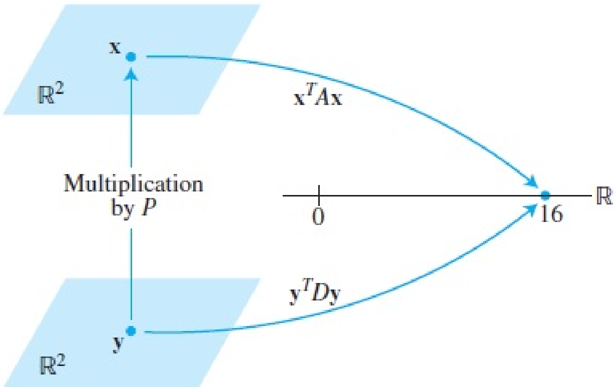


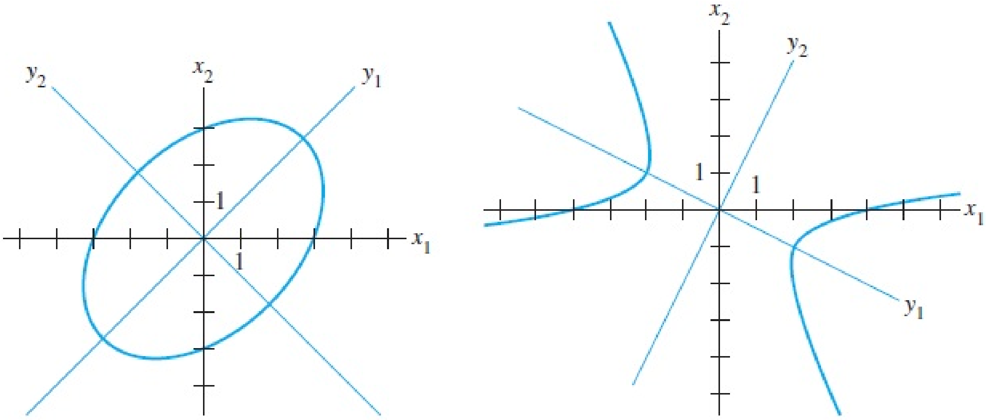
FIGURE 1 Change of variable in $\mathbf{x}^TA\mathbf{x}$.

EXAMPLE 5 The ellipse in Fig. 3(a) is the graph of the equation $5x_1^2 - 4x_1x_2 + 5x_2^2 = 48$. Find a change of variable that removes the cross-product term from the equation.

SOLUTION The matrix of the quadratic form is $A = \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$. The eigenvalues of A turn out to be 3 and 7, with corresponding unit eigenvectors

$$\mathbf{u}_1 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

Let $P = [\,\mathbf{u}_1 \quad \mathbf{u}_2\,] = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$. Then P orthogonally diagonalizes A, so the change of variable $\mathbf{x} = P\mathbf{y}$ produces the quadratic form $\mathbf{y}^T D\mathbf{y} = 3y_1^2 + 7y_2^2$. The new axes for this change of variable are shown in Fig. 3(a). ∎



(a) $5x_1^2 - 4x_1x_2 + 5x_2^2 = 48$

(b) $x_1^2 - 8x_1x_2 - 5x_2^2 = 16$

FIGURE 3 An ellipse and a hyperbola *not* in standard position.

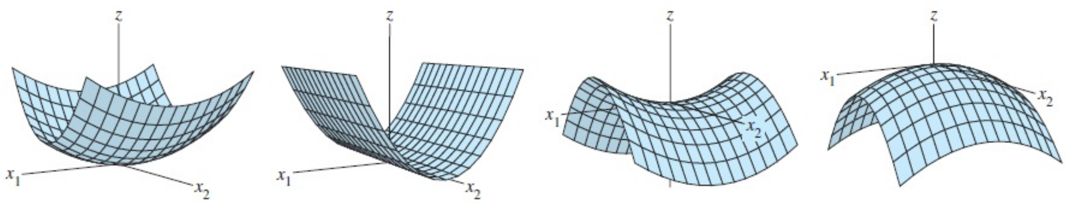
A quadratic form Q is:

a. **positive definite** if $Q(\mathbf{x}) > 0$ for all $\mathbf{x} \neq \mathbf{0}$,

b. **negative definite** if $Q(\mathbf{x}) < 0$ for all $\mathbf{x} \neq \mathbf{0}$,

c. **indefinite** if $Q(\mathbf{x})$ assumes both positive and negative values.

Also, Q is said to be **positive semidefinite** if $Q(\mathbf{x}) \geq 0$ for all $\mathbf{x}$, and to be **negative semidefinite** if $Q(\mathbf{x}) \leq 0$ for all $\mathbf{x}$. The quadratic forms in parts (a) and (b) of Fig. 4 are both positive semidefinite, but the form in (a) is better described as positive definite.



(a) $z = 3x_1^2 + 7x_2^2$ (b) $z = 3x_1^2$ (c) $z = 3x_1^2 - 7x_2^2$ (d) $z = -3x_1^2 - 7x_2^2$

FIGURE 4 Graphs of quadratic forms.

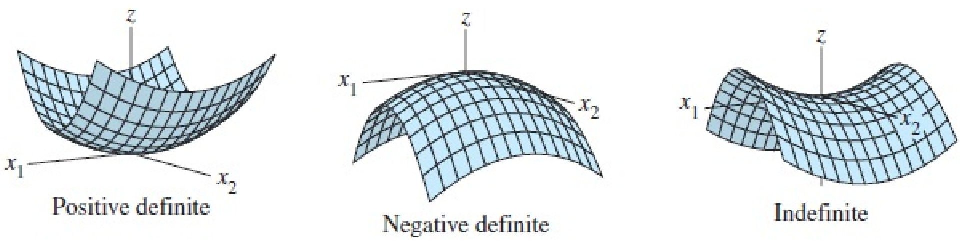
Quadratic Forms and Eigenvalues

Let A be an $n \times n$ symmetric matrix. Then a quadratic form $\mathbf{x}^T A\mathbf{x}$ is:

a. positive definite if and only if the eigenvalues of A are all positive,

b. negative definite if and only if the eigenvalues of A are all negative, or

c. indefinite if and only if A has both positive and negative eigenvalues.



EXAMPLE 6 Is $Q(\mathbf{x}) = 3x_1^2 + 2x_2^2 + x_3^2 + 4x_1x_2 + 4x_2x_3$ positive definite?

SOLUTION Because of all the plus signs, this form "looks" positive definite. But the matrix of the form is

$$A = \begin{bmatrix} 3 & 2 & 0 \\ 2 & 2 & 2 \\ 0 & 2 & 1 \end{bmatrix}$$

and the eigenvalues of A turn out to be 5, 2, and -1. So Q is an indefinite quadratic form, not positive definite. ■

The classification of a quadratic form is often carried over to the matrix of the form. Thus a **positive definite matrix** A is a *symmetric* matrix for which the quadratic form $\mathbf{x}^TA\mathbf{x}$ is positive definite. Other terms, such as **positive semidefinite matrix**, are defined analogously.

CONSTRAINED OPTIMIZATION

Engineers, economists, scientists, and mathematicians often need to find the maximum or minimum value of a quadratic form $Q(\mathbf{x})$ for $\mathbf{x}$ in some specified set. Typically, the problem can be arranged so that $\mathbf{x}$ varies over the set of unit vectors. This *constrained optimization problem* has an interesting and elegant solution. Example 6 below and the discussion in Section 7.5 will illustrate how such problems arise in practice.

The requirement that a vector $\mathbf{x}$ in $\mathbb{R}^n$ be a unit vector can be stated in several equivalent ways:

$$\|\mathbf{x}\| = 1, \qquad \|\mathbf{x}\|^2 = 1, \qquad \mathbf{x}^T\mathbf{x} = 1$$

and

$$x_1^2 + x_2^2 + \cdots + x_n^2 = 1 \tag{1}$$

The expanded version (1) of $\mathbf{x}^T\mathbf{x} = 1$ is commonly used in applications.

When a quadratic form Q has no cross-product terms, it is easy to find the maximum and minimum of $Q(\mathbf{x})$ for $\mathbf{x}^T\mathbf{x} = 1$.

EXAMPLE 1 Find the maximum and minimum values of $Q(\mathbf{x}) = 9x_1^2 + 4x_2^2 + 3x_3^2$ subject to the constraint $\mathbf{x}^T\mathbf{x} = 1$.

SOLUTION Since x_2^2 and x_3^2 are nonnegative, note that

$$4x_2^2 \le 9x_2^2 \qquad \text{and} \qquad 3x_3^2 \le 9x_3^2$$

and hence

$$\begin{aligned} Q(\mathbf{x}) &= 9x_1^2 + 4x_2^2 + 3x_3^2 \\ &\le 9x_1^2 + 9x_2^2 + 9x_3^2 \\ &= 9(x_1^2 + x_2^2 + x_3^2) \\ &= 9 \end{aligned}$$

whenever $x_1^2 + x_2^2 + x_3^2 = 1$. So the maximum value of $Q(\mathbf{x})$ cannot exceed 9 when $\mathbf{x}$ is a unit vector. Furthermore, $Q(\mathbf{x}) = 9$ when $\mathbf{x} = (1, 0, 0)$. Thus 9 is the maximum value of $Q(\mathbf{x})$ for $\mathbf{x}^T\mathbf{x} = 1$.

To find the minimum value of $Q(\mathbf{x})$, observe that

$$9x_1^2 \geq 3x_1^2, \qquad 4x_2^2 \geq 3x_2^2$$

and hence

$$Q(\mathbf{x}) \geq 3x_1^2 + 3x_2^2 + 3x_3^2 = 3(x_1^2 + x_2^2 + x_3^2) = 3$$

whenever $x_1^2 + x_2^2 + x_3^2 = 1$. Also, $Q(\mathbf{x}) = 3$ when $x_1 = 0$, $x_2 = 0$, and $x_3 = 1$. So 3 is the minimum value of $Q(\mathbf{x})$ when $\mathbf{x}^T\mathbf{x} = 1$. ■

EXAMPLE 2 Let $A = \begin{bmatrix} 3 & 0 \\ 0 & 7 \end{bmatrix}$, and let $Q(\mathbf{x}) = \mathbf{x}^TA\mathbf{x}$ for $\mathbf{x}$ in $\mathbb{R}^2$. Figure 1 displays the graph of Q. Figure 2 shows only the portion of the graph inside a cylinder; the intersection of the cylinder with the surface is the set of points (x_1, x_2, z) such that $z = Q(x_1, x_2)$ and $x_1^2 + x_2^2 = 1$. The "heights" of these points are the constrained values of $Q(\mathbf{x})$. Geometrically, the constrained optimization problem is to locate the highest and lowest points on the intersection curve.

The two highest points on the curve are 7 units above the x_1x_2-plane, occurring where $x_1 = 0$ and $x_2 = \pm 1$. These points correspond to the eigenvalue 7 of A and the eigenvectors $\mathbf{x} = (0, 1)$ and $-\mathbf{x} = (0, -1)$. Similarly, the two lowest points on the curve are 3 units above the x_1x_2-plane. They correspond to the eigenvalue 3 and the eigenvectors $(1, 0)$ and $(-1, 0)$. ■

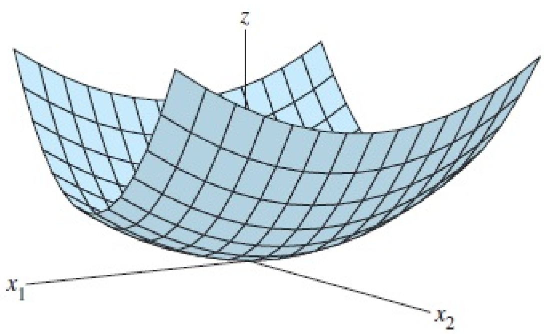


FIGURE 1 $z = 3x_1^2 + 7x_2^2$.

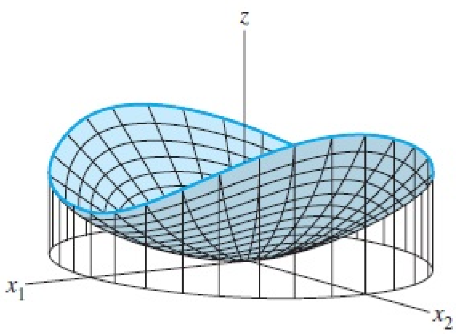


FIGURE 2 The intersection of $z = 3x_1^2 + 7x_2^2$ and the cylinder $x_1^2 + x_2^2 = 1$.

Every point on the intersection curve in Fig. 2 has a z-coordinate between 3 and 7, and for any number t between 3 and 7, there is a unit vector $\mathbf{x}$ such that $Q(\mathbf{x}) = t$. In other words, the set of all possible values of $\mathbf{x}^TA\mathbf{x}$, for $\|\mathbf{x}\| = 1$, is the closed interval $3 \leq t \leq 7$.

It can be shown that for any symmetric matrix A, the set of all possible values of $\mathbf{x}^T A\mathbf{x}$, for $\|\mathbf{x}\| = 1$, is a closed interval on the real axis. (See Exercise 13.) Denote the left and right endpoints of this interval by m and M, respectively. That is, let

$$m = \min\{\mathbf{x}^T A\mathbf{x} : \|\mathbf{x}\| = 1\}, \quad M = \max\{\mathbf{x}^T A\mathbf{x} : \|\mathbf{x}\| = 1\} \tag{2}$$

Exercise 12 asks you to prove that if λ is an eigenvalue of A, then $m \le \lambda \le M$. The next theorem says that m and M are themselves eigenvalues of A, just as in Example 2.[1]

> Let A be a symmetric matrix, and define m and M as in (2). Then M is the greatest eigenvalue λ_1 of A and m is the least eigenvalue of A. The value of $\mathbf{x}^T A\mathbf{x}$ is M when $\mathbf{x}$ is a unit eigenvector $\mathbf{u}_1$ corresponding to M. The value of $\mathbf{x}^T A\mathbf{x}$ is m when $\mathbf{x}$ is a unit eigenvector corresponding to m.

EXAMPLE 3 Let $A = \begin{bmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{bmatrix}$. Find the maximum value of the quadratic form $\mathbf{x}^T A\mathbf{x}$ subject to the constraint $\mathbf{x}^T\mathbf{x} = 1$, and find a unit vector at which this maximum value is attained.

SOLUTION By Theorem 6, the desired maximum value is the greatest eigenvalue of A. The characteristic equation turns out to be

$$0 = -\lambda^3 + 10\lambda^2 - 27\lambda + 18 = -(\lambda - 6)(\lambda - 3)(\lambda - 1)$$

The greatest eigenvalue is 6.

The constrained maximum of $\mathbf{x}^T A\mathbf{x}$ is attained when $\mathbf{x}$ is a unit eigenvector for $\lambda = 6$. Solve $(A - 6I)\mathbf{x} = \mathbf{0}$ and find an eigenvector $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$. Set $\mathbf{u}_1 = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$. ■

> Let A, λ_1, and $\mathbf{u}_1$ be as in Theorem 6. Then the maximum value of $\mathbf{x}^T A\mathbf{x}$ subject to the constraints
>
> $$\mathbf{x}^T\mathbf{x} = 1, \quad \mathbf{x}^T\mathbf{u}_1 = 0$$
>
> is the second greatest eigenvalue, λ_2, and this maximum is attained when $\mathbf{x}$ is an eigenvector $\mathbf{u}_2$ corresponding to λ_2.

EXAMPLE 4 Find the maximum value of $9x_1^2 + 4x_2^2 + 3x_3^2$ subject to the constraints $\mathbf{x}^T\mathbf{x} = 1$ and $\mathbf{x}^T\mathbf{u}_1 = 0$, where $\mathbf{u}_1 = (1, 0, 0)$. Note that $\mathbf{u}_1$ is a unit eigenvector corresponding to the greatest eigenvalue $\lambda = 9$ of the matrix of the quadratic form.

SOLUTION If the coordinates of $\mathbf{x}$ are x_1, x_2, x_3, then the constraint $\mathbf{x}^T\mathbf{u}_1 = 0$ means simply that $x_1 = 0$. For such a unit vector, $x_2^2 + x_3^2 = 1$, and

$$\begin{aligned} 9x_1^2 + 4x_2^2 + 3x_3^2 &= 4x_2^2 + 3x_3^2 \\ &\le 4x_2^2 + 4x_3^2 \\ &= 4(x_2^2 + x_3^2) \\ &= 4 \end{aligned}$$

Thus the constrained maximum of the quadratic form does not exceed 4. And this value is attained for $\mathbf{x} = (0, 1, 0)$, which is an eigenvector for the second greatest eigenvalue of the matrix of the quadratic form. ■

EXAMPLE 5 Let A be the matrix in Example 3 and let $\mathbf{u}_1$ be a unit eigenvector corresponding to the greatest eigenvalue of A. Find the maximum value of $\mathbf{x}^TA\mathbf{x}$ subject to the conditions

$$\mathbf{x}^T\mathbf{x} = 1, \quad \mathbf{x}^T\mathbf{u}_1 = 0 \tag{4}$$

SOLUTION From Example 3, the second greatest eigenvalue of A is $\lambda = 3$. Solve $(A - 3I)\mathbf{x} = \mathbf{0}$ to find an eigenvector, and normalize it to obtain

$$\mathbf{u}_2 = \begin{bmatrix} 1/\sqrt{6} \\ 1/\sqrt{6} \\ -2/\sqrt{6} \end{bmatrix}$$

The vector $\mathbf{u}_2$ is automatically orthogonal to $\mathbf{u}_1$ because the vectors correspond to different eigenvalues. Thus the maximum of $\mathbf{x}^TA\mathbf{x}$ subject to the constraints in (4) is 3, attained when $\mathbf{x} = \mathbf{u}_2$. ■

Let A be a symmetric $n \times n$ matrix with an orthogonal diagonalization $A = PDP^{-1}$, where the entries on the diagonal of D are arranged so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and where the columns of P are corresponding unit eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$. Then for $k = 2, \ldots, n$, the maximum value of $\mathbf{x}^TA\mathbf{x}$ subject to the constraints

$$\mathbf{x}^T\mathbf{x} = 1, \quad \mathbf{x}^T\mathbf{u}_1 = 0, \quad \ldots, \quad \mathbf{x}^T\mathbf{u}_{k-1} = 0$$

is the eigenvalue λ_k, and this maximum is attained at $\mathbf{x} = \mathbf{u}_k$.

EXAMPLE 6 During the next year, a county government is planning to repair x hundred miles of public roads and bridges and to improve y hundred acres of parks and recreation areas. The county must decide how to allocate its resources (funds, equipment, labor, etc.) between these two projects. If it is more cost-effective to work simultaneously on both projects rather than on only one, then x and y might satisfy a *constraint* such as

$$4x^2 + 9y^2 \leq 36$$

See Fig. 3. Each point (x, y) in the shaded *feasible set* represents a possible public works schedule for the year. The points on the constraint curve, $4x^2 + 9y^2 = 36$, use the maximum amounts of resources available.

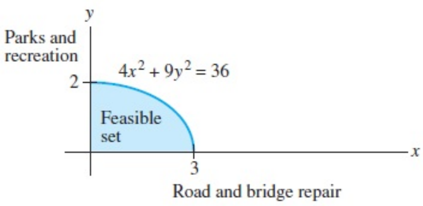


FIGURE 3 Public works schedules.

In choosing its public works schedule, the county wants to consider the opinions of the county residents. To measure the value, or *utility*, that the residents would assign to the various work schedules (x, y), economists sometimes use a function such as

$$q(x, y) = xy$$

The set of points (x, y) at which $q(x, y)$ is a constant is called an *indifference curve*. Three such curves are shown in Fig. 4. Points along an indifference curve correspond to alternatives that county residents as a group would find equally valuable.[2] Find the public works schedule that maximizes the utility function q.

SOLUTION The constraint equation $4x^2 + 9y^2 = 36$ does not describe a set of unit vectors, but a change of variable can fix that problem. Rewrite the constraint in the form

$$\left(\frac{x}{3}\right)^2 + \left(\frac{y}{2}\right)^2 = 1$$

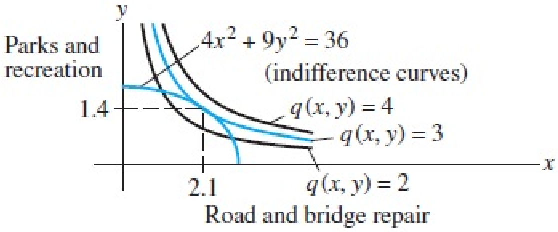


FIGURE 4 The optimum public works schedule is (2.1, 1.4).

and define

$$x_1 = \frac{x}{3}, \quad x_2 = \frac{y}{2}, \qquad \text{that is,} \quad x = 3x_1 \quad \text{and} \quad y = 2x_2$$

Then the constraint equation becomes

$$x_1^2 + x_2^2 = 1$$

and the utility function becomes $q(3x_1, 2x_2) = (3x_1)(2x_2) = 6x_1x_2$. Let $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. Then the problem is to maximize $Q(\mathbf{x}) = 6x_1x_2$ subject to $\mathbf{x}^T\mathbf{x} = 1$. Note that $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$, where

$$A = \begin{bmatrix} 0 & 3 \\ 3 & 0 \end{bmatrix}$$

The eigenvalues of A are ± 3, with eigenvectors $\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$ for $\lambda = 3$ and $\begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$ for $\lambda = -3$. Thus the maximum value of $Q(\mathbf{x}) = q(x_1, x_2)$ is 3, attained when $x_1 = 1/\sqrt{2}$ and $x_2 = 1/\sqrt{2}$.

In terms of the original variables, the optimum public works schedule is $x = 3x_1 = 3/\sqrt{2} \approx 2.1$ hundred miles of roads and bridges and $y = 2x_2 = \sqrt{2} \approx 1.4$ hundred acres of parks and recreational areas. The optimum public works schedule is the point where the constraint curve and the indifference curve $q(x, y) = 3$ just meet. Points (x, y) with a higher utility lie on indifference curves that do not touch the constraint curve. See Fig. 4. ■

The Singular Value Decomposition

Let A be an $m \times n$ matrix with rank r. Then there exists an $m \times n$ matrix Σ as in (3) for which the diagonal entries in D are the first r singular values of A, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$, and there exist an $m \times m$ orthogonal matrix U and an $n \times n$ orthogonal matrix V such that

$$A = U\Sigma V^T$$

EXAMPLE 4 Find a singular value decomposition of $A = \begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{bmatrix}$.

SOLUTION First, compute $A^T A = \begin{bmatrix} 9 & -9 \\ -9 & 9 \end{bmatrix}$. The eigenvalues of $A^T A$ are 18 and 0, with corresponding unit eigenvectors

$$\mathbf{v}_1 = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

These unit vectors form the columns of V:

$$V = [\,\mathbf{v}_1 \quad \mathbf{v}_2\,] = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

The singular values are $\sigma_1 = \sqrt{18} = 3\sqrt{2}$ and $\sigma_2 = 0$. Since there is only one nonzero singular value, the "matrix" D may be written as a single number. That is, $D = 3\sqrt{2}$. The matrix Σ is the same size as A, with D in its upper left corner:

$$\Sigma = \begin{bmatrix} D & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

To construct U, first construct $A\mathbf{v}_1$ and $A\mathbf{v}_2$:

$$A\mathbf{v}_1 = \begin{bmatrix} 2/\sqrt{2} \\ -4/\sqrt{2} \\ 4/\sqrt{2} \end{bmatrix}, \quad A\mathbf{v}_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

As a check on the calculations, verify that $\|A\mathbf{v}_1\| = \sigma_1 = 3\sqrt{2}$. Of course, $A\mathbf{v}_2 = \mathbf{0}$ because $\|A\mathbf{v}_2\| = \sigma_2 = 0$. The only column found for U so far is

$$\mathbf{u}_1 = \frac{1}{3\sqrt{2}} A\mathbf{v}_1 = \begin{bmatrix} 1/3 \\ -2/3 \\ 2/3 \end{bmatrix}$$

The other columns of U are found by extending the set $\{\mathbf{u}_1\}$ to an orthonormal basis for $\mathbb{R}^3$. In this case, we need two orthogonal unit vectors $\mathbf{u}_2$ and $\mathbf{u}_3$ that are orthogonal to $\mathbf{u}_1$. (See Fig. 3.) Each vector must satisfy $\mathbf{u}_1^T\mathbf{x} = 0$, which is equivalent to the equation $x_1 - 2x_2 + 2x_3 = 0$. A basis for the solution set of this equation is

$$\mathbf{w}_1 = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{w}_2 = \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix}$$

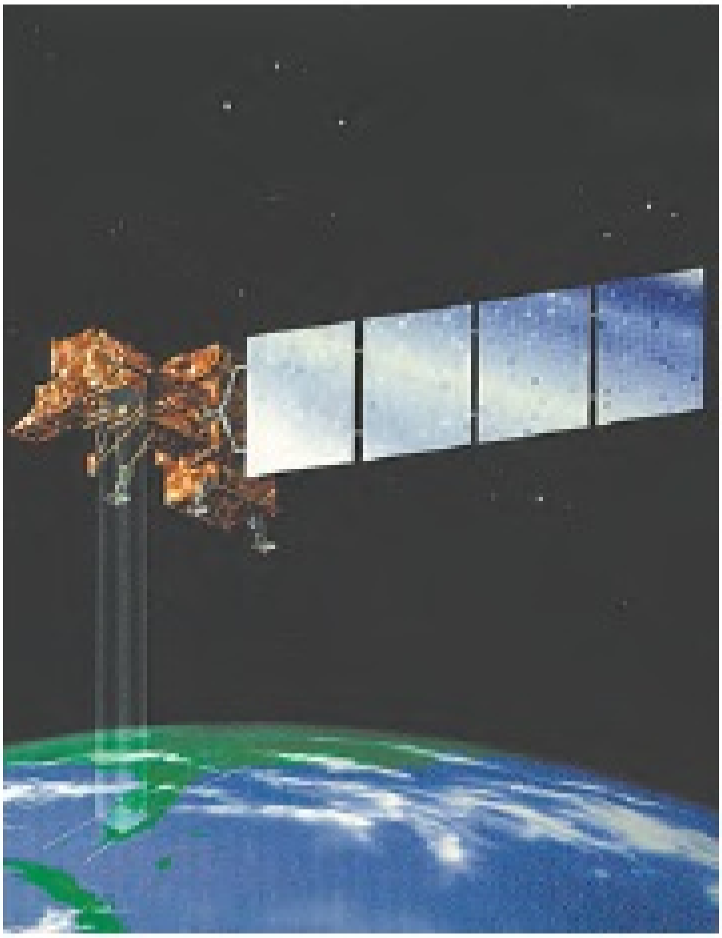
(Check that $\mathbf{w}_1$ and $\mathbf{w}_2$ are each orthogonal to $\mathbf{u}_1$.) Apply the Gram–Schmidt process (with normalizations) to $\{\mathbf{w}_1, \mathbf{w}_2\}$, and obtain

$$\mathbf{u}_2 = \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \\ 0 \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} -2/\sqrt{45} \\ 4/\sqrt{45} \\ 5/\sqrt{45} \end{bmatrix}$$

Finally, set $U = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3\,]$, take Σ and V^T from above, and write

$$A = \begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{bmatrix} = \begin{bmatrix} 1/3 & 2/\sqrt{5} & -2/\sqrt{45} \\ -2/3 & 1/\sqrt{5} & 4/\sqrt{45} \\ 2/3 & 0 & 5/\sqrt{45} \end{bmatrix} \begin{bmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

■



Sensors aboard the satellite acquire seven simultaneous images of any region on earth to be studied. The sensors record energy from separate wavelength bands—three in the visible light spectrum and four in infrared and thermal bands. Each image is digitized and stored as a rectangular array of numbers, each number indicating the signal intensity at a corresponding small point (or *pixel*) on the image. Each of the seven images is one channel of a *multichannel* or *multispectral image*.

The seven Landsat images of one fixed region typically contain much redundant information, since some features will appear in several images. Yet other features, because of their color or temperature, may reflect light that is recorded by only one or two sensors. One goal of multichannel image processing is to view the data in a way that extracts information better than studying each image separately.

Principal component analysis is an effective way to suppress redundant information and provide in only one or two composite images most of the information from the initial data. Roughly speaking, the goal is to find a special linear combination of the images, that is, a list of weights that at each pixel combine all seven corresponding image values into one new value. The weights are chosen in a way that makes the range of light intensities—the *scene variance*—in the composite image (called the *first principal component*) greater than that in any of the original images.

Principal component analysis is illustrated in the photos below, taken over Railroad Valley, Nevada. Images from three Landsat spectral bands are shown in (a)–(c). The total information in the three bands is rearranged in the three principal component images in (d)–(f). The first component (d) displays (or "explains") 93.5% of the scene variance present in the initial data. In this way, the three-channel initial data have been reduced to one-channel data, with a loss in some sense of only 6.5% of the scene variance.

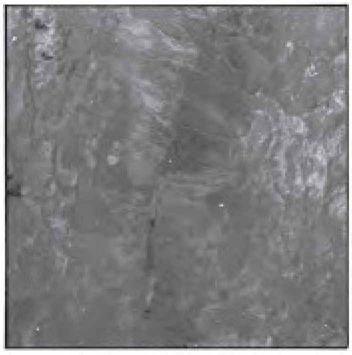
(a) Spectral band 1: Visible blue.

(b) Spectral band 4: Near infrared.

(c) Spectral band 7: Mid-infrared.

(d) Principal component 1: 93.5%.

(e) Principal component 2: 5.3%.



(f) Principal component 3: 1.2%.

Principal component analysis can be applied to any data that consist of lists of measurements made on a collection of objects or individuals. For instance, consider a chemical process that produces a plastic material. To monitor the process, 300 samples are taken of the material produced, and each sample is subjected to a battery of eight tests, such as melting point, density, ductility, tensile strength, and so on. The laboratory report for each sample is a vector in $\mathbb{R}^8$, and the set of such vectors forms an 8×300 matrix, called the **matrix of observations**.

EXAMPLE 1 An example of two-dimensional data is given by a set of weights and heights of N college students. Let $\mathbf{X}_j$ denote the **observation vector** in $\mathbb{R}^2$ that lists the weight and height of the jth student. If w denotes weight and h height, then the matrix of observations has the form

$$\begin{array}{cccc} \left[\begin{matrix} w_1 & w_2 & \cdots & w_N \\ h_1 & h_2 & \cdots & h_N \end{matrix}\right] \\ \uparrow \quad\ \uparrow \qquad\quad \uparrow \\ \mathbf{X}_1 \quad \mathbf{X}_2 \qquad\quad \mathbf{X}_N \end{array}$$

The set of observation vectors can be visualized as a two-dimensional *scatter plot*. See Fig. 1. ■

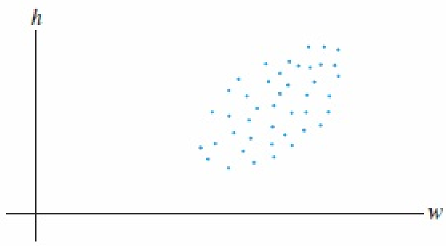


FIGURE 1 A scatter plot of observation vectors $\mathbf{X}_1, \ldots, \mathbf{X}_N$.

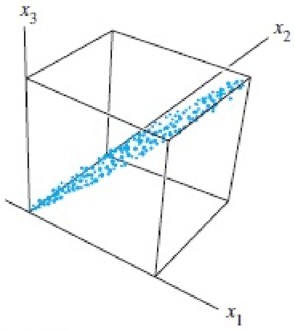


FIGURE 2
A scatter plot of spectral data for a satellite image.

EXAMPLE 2 The first three photographs of Railroad Valley, Nevada, shown in the chapter introduction, can be viewed as *one* image of the region, with *three spectral components*, because simultaneous measurements of the region were made at three separate wavelengths. Each photograph gives different information about the same physical region. For instance, the first pixel in the upper-left corner of each photograph corresponds to the same place on the ground (about 30 meters by 30 meters). To each pixel there corresponds an observation vector in $\mathbb{R}^3$ that lists the signal intensities for that pixel in the three spectral bands.

Typically, the image is 2000×2000 pixels, so there are 4 million pixels in the image. The data for the image form a matrix with 3 rows and 4 million columns (with columns arranged in any convenient order). In this case, the "multidimensional" character of the data refers to the three *spectral* dimensions rather than the two *spatial* dimensions that naturally belong to any photograph. The data can be visualized as a cluster of 4 million points in $\mathbb{R}^3$, perhaps as in Fig. 2. ■

Mean and Covariance

To prepare for principal component analysis, let $[\mathbf{X}_1 \ \cdots \ \mathbf{X}_N]$ be a $p \times N$ matrix of observations, such as described above. The **sample mean, M,** of the observation vectors $\mathbf{X}_1, \ldots, \mathbf{X}_N$ is given by

$$\mathbf{M} = \frac{1}{N}(\mathbf{X}_1 + \cdots + \mathbf{X}_N)$$

For the data in Fig. 1, the sample mean is the point in the "center" of the scatter plot. For $k = 1, \ldots, N$, let

$$\hat{\mathbf{X}}_k = \mathbf{X}_k - \mathbf{M}$$

The columns of the $p \times N$ matrix

$$B = [\hat{\mathbf{X}}_1 \ \ \hat{\mathbf{X}}_2 \ \ \cdots \ \ \hat{\mathbf{X}}_N]$$

have a zero sample mean, and B is said to be in **mean-deviation form**. When the sample mean is subtracted from the data in Fig. 1, the resulting scatter plot has the form in Fig. 3.

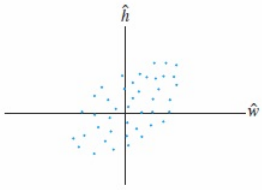


FIGURE 3
Weight–height data in mean-deviation form.

The **(sample) covariance matrix** is the $p \times p$ matrix S defined by

$$S = \frac{1}{N-1}BB^T$$

Since any matrix of the form BB^T is positive semidefinite, so is S. (See Exercise 25 in Section 7.2 with B and B^T interchanged.)

EXAMPLE 3 Three measurements are made on each of four individuals in a random sample from a population. The observation vectors are

$$\mathbf{X}_1 = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \quad \mathbf{X}_2 = \begin{bmatrix} 4 \\ 2 \\ 13 \end{bmatrix}, \quad \mathbf{X}_3 = \begin{bmatrix} 7 \\ 8 \\ 1 \end{bmatrix}, \quad \mathbf{X}_4 = \begin{bmatrix} 8 \\ 4 \\ 5 \end{bmatrix}$$

Compute the sample mean and the covariance matrix.

SOLUTION The sample mean is

$$\mathbf{M} = \frac{1}{4}\left(\begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} + \begin{bmatrix} 4 \\ 2 \\ 13 \end{bmatrix} + \begin{bmatrix} 7 \\ 8 \\ 1 \end{bmatrix} + \begin{bmatrix} 8 \\ 4 \\ 5 \end{bmatrix} \right) = \frac{1}{4}\begin{bmatrix} 20 \\ 16 \\ 20 \end{bmatrix} = \begin{bmatrix} 5 \\ 4 \\ 5 \end{bmatrix}$$

Subtract the sample mean from $\mathbf{X}_1, \dots, \mathbf{X}_4$ to obtain

$$\hat{\mathbf{X}}_1 = \begin{bmatrix} -4 \\ -2 \\ -4 \end{bmatrix}, \quad \hat{\mathbf{X}}_2 = \begin{bmatrix} -1 \\ -2 \\ 8 \end{bmatrix}, \quad \hat{\mathbf{X}}_3 = \begin{bmatrix} 2 \\ 4 \\ -4 \end{bmatrix}, \quad \hat{\mathbf{X}}_4 = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}$$

and

$$B = \begin{bmatrix} -4 & -1 & 2 & 3 \\ -2 & -2 & 4 & 0 \\ -4 & 8 & -4 & 0 \end{bmatrix}$$

The sample covariance matrix is

$$\begin{aligned} S &= \frac{1}{3}\begin{bmatrix} -4 & -1 & 2 & 3 \\ -2 & -2 & 4 & 0 \\ -4 & 8 & -4 & 0 \end{bmatrix} \begin{bmatrix} -4 & -2 & -4 \\ -1 & -2 & 8 \\ 2 & 4 & -4 \\ 3 & 0 & 0 \end{bmatrix} \\ &= \frac{1}{3}\begin{bmatrix} 30 & 18 & 0 \\ 18 & 24 & -24 \\ 0 & -24 & 96 \end{bmatrix} = \begin{bmatrix} 10 & 6 & 0 \\ 6 & 8 & -8 \\ 0 & -8 & 32 \end{bmatrix} \end{aligned}$$

To discuss the entries in $S = [s_{ij}]$, let $\mathbf{X}$ represent a vector that varies over the set of observation vectors and denote the coordinates of $\mathbf{X}$ by $x_1, \dots, x_p$. Then x_1, for example, is a scalar that varies over the set of first coordinates of $\mathbf{X}_1, \dots, \mathbf{X}_N$. For $j = 1, \dots, p$, the diagonal entry s_{jj} in S is called the **variance** of x_j.

The variance of x_j measures the spread of the values of x_j. (See Exercise 13.) In Example 3, the variance of x_1 is 10 and the variance of x_3 is 32. The fact that 32 is more than 10 indicates that the set of third entries in the response vectors contains a wider spread of values than the set of first entries.

The **total variance** of the data is the sum of the variances on the diagonal of S. In general, the sum of the diagonal entries of a square matrix S is called the **trace** of the matrix, written $\text{tr}(S)$. Thus

$$\{\text{total variance}\} = \text{tr}(S)$$

The entry s_{ij} in S for $i \neq j$ is called the **covariance** of x_i and x_j. Observe that in Example 3, the covariance between x_1 and x_3 is 0 because the $(1, 3)$-entry in S is 0. Statisticians say that x_1 and x_3 are **uncorrelated**. Analysis of the multivariate data in $\mathbf{X}_1, \dots, \mathbf{X}_N$ is greatly simplified when most or all of the variables $x_1, \dots, x_p$ are uncorrelated, that is, when the covariance matrix of $\mathbf{X}_1, \dots, \mathbf{X}_N$ is diagonal or nearly diagonal.

Principal Component Analysis

For simplicity, assume that the matrix $[\mathbf{X}_1 \ \cdots \ \mathbf{X}_N]$ is already in mean-deviation form. The goal of principal component analysis is to find an orthogonal $p \times p$ matrix $P = [\mathbf{u}_1 \ \cdots \ \mathbf{u}_p]$ that determines a change of variable, $\mathbf{X} = P\mathbf{Y}$, or

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_p \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{bmatrix}$$

with the property that the new variables $y_1, \dots, y_p$ are uncorrelated and are arranged in order of decreasing variance.

The orthogonal change of variable $\mathbf{X} = P\mathbf{Y}$ means that each observation vector $\mathbf{X}_k$ receives a "new name," $\mathbf{Y}_k$, such that $\mathbf{X}_k = P\mathbf{Y}_k$. Notice that $\mathbf{Y}_k$ is the coordinate vector of $\mathbf{X}_k$ with respect to the columns of P, and $\mathbf{Y}_k = P^{-1}\mathbf{X}_k = P^T\mathbf{X}_k$ for $k = 1, \dots, N$.

It is not difficult to verify that for any orthogonal P, the covariance matrix of $\mathbf{Y}_1, \dots, \mathbf{Y}_N$ is P^TSP (Exercise 11). So the desired orthogonal matrix P is one that makes P^TSP diagonal. Let D be a diagonal matrix with the eigenvalues $\lambda_1, \dots, \lambda_p$ of S on the diagonal, arranged so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq 0$, and let P be an orthogonal matrix whose columns are the corresponding unit eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_p$. Then $S = PDP^T$ and $P^TSP = D$.

The unit eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_p$ of the covariance matrix S are called the **principal components** of the data (in the matrix of observations). The **first principal component** is the eigenvector corresponding to the largest eigenvalue of S, the **second principal component** is the eigenvector corresponding to the second largest eigenvalue, and so on.

The first principal component $\mathbf{u}_1$ determines the new variable y_1 in the following way. Let $c_1, \dots, c_p$ be the entries in $\mathbf{u}_1$. Since $\mathbf{u}_1^T$ is the first row of P^T, the equation $\mathbf{Y} = P^T\mathbf{X}$ shows that

$$y_1 = \mathbf{u}_1^T\mathbf{X} = c_1x_1 + c_2x_2 + \cdots + c_px_p$$

Thus y_1 is a linear combination of the original variables $x_1, \dots, x_p$, using the entries in the eigenvector $\mathbf{u}_1$ as weights. In a similar fashion, $\mathbf{u}_2$ determines the variable y_2, and so on.

EXAMPLE 4 The initial data for the multispectral image of Railroad Valley (Example 2) consisted of 4 million vectors in $\mathbb{R}^3$. The associated covariance matrix is[1]

$$S = \begin{bmatrix} 2382.78 & 2611.84 & 2136.20 \\ 2611.84 & 3106.47 & 2553.90 \\ 2136.20 & 2553.90 & 2650.71 \end{bmatrix}$$

Find the principal components of the data, and list the new variable determined by the first principal component.

SOLUTION The eigenvalues of S and the associated principal components (the unit eigenvectors) are

$$\lambda_1 = 7614.23 \qquad \lambda_2 = 427.63 \qquad \lambda_3 = 98.10$$

$$\mathbf{u}_1 = \begin{bmatrix} .5417 \\ .6295 \\ .5570 \end{bmatrix} \quad \mathbf{u}_2 = \begin{bmatrix} -.4894 \\ -.3026 \\ .8179 \end{bmatrix} \quad \mathbf{u}_3 = \begin{bmatrix} .6834 \\ -.7157 \\ .1441 \end{bmatrix}$$

Using two decimal places for simplicity, the variable for the first principal component is

$$y_1 = .54x_1 + .63x_2 + .56x_3$$

This equation was used to create photograph (d) in the chapter introduction. The variables x_1, x_2, x_3 are the signal intensities in the three spectral bands. The values of x_1, converted to a gray scale between black and white, produced photograph (a). Similarly, the values of x_2 and x_3 produced photographs (b) and (c), respectively. At each pixel in photograph (d), the gray scale value is computed from y_1, a weighted linear combination of x_1, x_2, x_3. In this sense, photograph (d) "displays" the first principal component of the data. ■

In Example 4, the covariance matrix for the transformed data, using variables y_1, y_2, y_3, is

$$D = \begin{bmatrix} 7614.23 & 0 & 0 \\ 0 & 427.63 & 0 \\ 0 & 0 & 98.10 \end{bmatrix}$$

Although D is obviously simpler than the original covariance matrix S, the merit of constructing the new variables is not yet apparent. However, the variances of the variables y_1, y_2, y_3 appear on the diagonal of D, and obviously the first variance in D is much larger than the other two. As we shall see, this fact will permit us to view the data as essentially one-dimensional rather than three-dimensional.

Reducing the Dimension of Multivariate Data

Principal component analysis is potentially valuable for applications in which most of the variation, or dynamic range, in the data is due to variations in *only a few* of the new variables, $y_1, \dots, y_p$.

It can be shown that an orthogonal change of variables, $\mathbf{X} = P\mathbf{Y}$, does not change the total variance of the data. (Roughly speaking, this is true because left-multiplication by P does not change the lengths of vectors or the angles between them. See Exercise 12.) This means that if $S = PDP^T$, then

$$\begin{Bmatrix} \text{total variance} \\ \text{of } x_1, \dots, x_p \end{Bmatrix} = \begin{Bmatrix} \text{total variance} \\ \text{of } y_1, \dots, y_p \end{Bmatrix} = \operatorname{tr}(D) = \lambda_1 + \cdots + \lambda_p$$

The variance of y_j is λ_j, and the quotient $\lambda_j / \operatorname{tr}(S)$ measures the fraction of the total variance that is "explained" or "captured" by y_j.

EXAMPLE 5 Compute the various percentages of variance of the Railroad Valley multispectral data that are displayed in the principal component photographs, (d)–(f), shown in the chapter introduction.

SOLUTION The total variance of the data is

$$\operatorname{tr}(D) = 7614.23 + 427.63 + 98.10 = 8139.96$$

[Verify that this number also equals $\operatorname{tr}(S)$.] The percentages of the total variance explained by the principal components are

First component	Second component	Third component
$\dfrac{7614.23}{8139.96} = 93.5\%$	$\dfrac{427.63}{8139.96} = 5.3\%$	$\dfrac{98.10}{8139.96} = 1.2\%$

In a sense, 93.5% of the information collected by Landsat for the Railroad Valley region is displayed in photograph (d), with 5.3% in (e) and only 1.2% remaining for (f). ∎