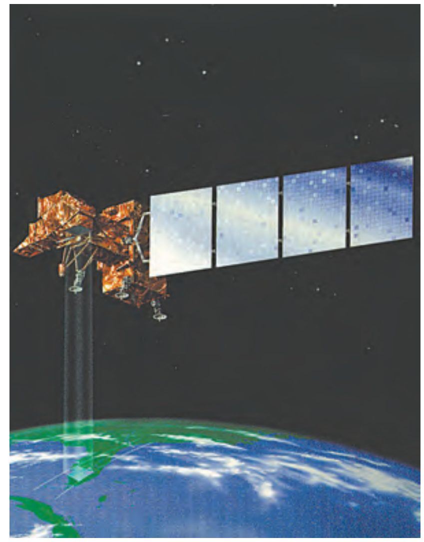
7 Symmetric Matrices and Quadratic Forms



INTRODUCTORY EXAMPLE

Multichannel Image Processing

Around the world in little more than 80 *minutes*, the two Landsat satellites streak silently across the sky in near polar orbits, recording images of terrain and coastline, in swaths 185 kilometers wide. Every 16 days, each satellite passes over almost every square kilometer of the earth's surface, so any location can be monitored every 8 days.

The Landsat images are useful for many purposes. Developers and urban planners use them to study the rate and direction of urban growth, industrial development, and other changes in land usage. Rural countries can analyze soil moisture, classify the vegetation in remote regions, and locate inland lakes and streams. Governments can detect and assess damage from natural disasters, such as forest fires, lava flows, floods, and hurricanes. Environmental agencies can identify pollution from smokestacks and measure water temperatures in lakes and rivers near power plants.

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.

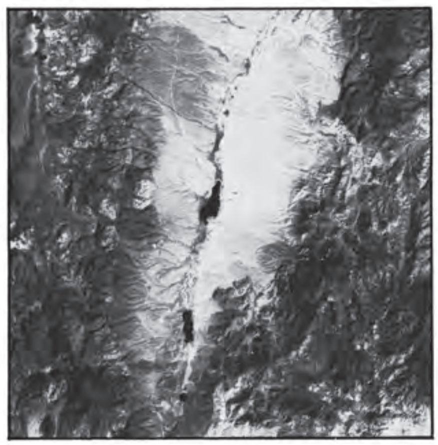
Principal component analysis is an effective way to suppress redundant information and provide in only one or two composite images most of the information from the initial data. Roughly speaking, the goal is to find a special linear combination of the images, that is, a list of weights that at each pixel 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. Additional *component* images can also be constructed, by criteria that will be explained in Section 7.5.

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.

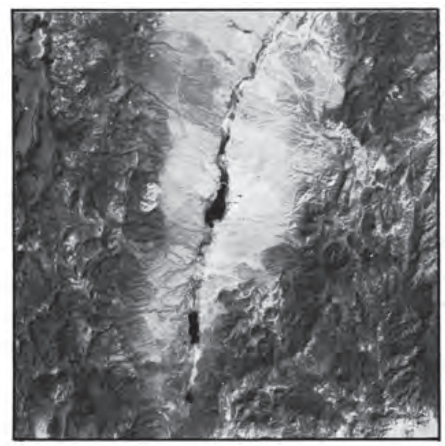
Earth Satellite Corporation of Rockville, Maryland, which kindly supplied the photos shown here, is experimenting with images from 224 separate spectral bands. Principal component analysis, essential for such massive data sets, typically reduces the data to about 15 usable principal components.

WEB

(a) Spectral band 1: Visible blue.



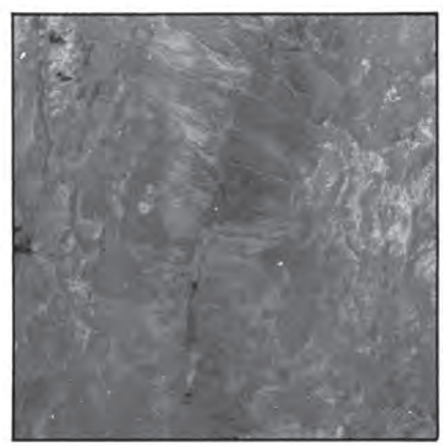
(b) Spectral band 4: Near infrared.



(c) Spectral band 7: Mid-infrared.

(d) Principal component 1: 93.5%.

(e) Principal component 2: 5.3%.



(f) Principal component 3: 1.2%.

Symmetric matrices arise more often in applications, in one way or another, than any other major class of matrices. The theory is rich and beautiful, depending in an essential way on both diagonalization from Chapter 5 and orthogonality from Chapter 6. The diagonalization of a symmetric matrix, described in Section 7.1, is the foundation for the discussion in Sections 7.2 and 7.3 concerning quadratic forms. Section 7.3, in turn, is needed for the final two sections on the singular value decomposition and on the image processing described in the introductory example. Throughout the chapter, all vectors and matrices have real entries.

7.1 DIAGONALIZATION OF SYMMETRIC MATRICES

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:

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

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

■

To begin the study of symmetric matrices, it is helpful to review the diagonalization process of Section 5.3.

EXAMPLE 2 If possible, diagonalize the matrix $A = \begin{bmatrix} 6 & -2 & -1 \\ -2 & 6 & -1 \\ -1 & -1 & 5 \end{bmatrix}$.

SOLUTION The characteristic equation of A is

$$0 = -\lambda^3 + 17\lambda^2 - 90\lambda + 144 = -(\lambda - 8)(\lambda - 6)(\lambda - 3)$$

Standard calculations produce a basis for each eigenspace:

$$\lambda = 8: \ \mathbf{v}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}; \qquad \lambda = 6: \ \mathbf{v}_2 = \begin{bmatrix} -1 \\ -1 \\ 2 \end{bmatrix}; \qquad \lambda = 3: \ \mathbf{v}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

These three vectors form a basis for $\mathbb{R}^3$. In fact, it is easy to check that $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is an *orthogonal* basis for $\mathbb{R}^3$. Experience from Chapter 6 suggests that an *orthonormal* basis might be useful for calculations, so here are the normalized (unit) eigenvectors.

$$\mathbf{u}_1 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} -1/\sqrt{6} \\ -1/\sqrt{6} \\ 2/\sqrt{6} \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$$

Let

$$P = \begin{bmatrix} -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{bmatrix}, \quad D = \begin{bmatrix} 8 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

Then $A = PDP^{-1}$, as usual. But this time, since P is square and has orthonormal columns, P is an *orthogonal* matrix, and P^{-1} is simply P^T. (See Section 6.2.) ■

Theorem 1 explains why the eigenvectors in Example 2 are orthogonal—they correspond to distinct eigenvalues.

THEOREM 1

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

PROOF Let $\mathbf{v}_1$ and $\mathbf{v}_2$ be eigenvectors that correspond to distinct eigenvalues, say, λ_1 and λ_2. To show that $\mathbf{v}_1 \cdot \mathbf{v}_2 = 0$, compute

$$\begin{aligned} \lambda_1 \mathbf{v}_1 \cdot \mathbf{v}_2 &= (\lambda_1 \mathbf{v}_1)^T \mathbf{v}_2 = (A\mathbf{v}_1)^T \mathbf{v}_2 && \text{Since } \mathbf{v}_1 \text{ is an eigenvector} \\ &= (\mathbf{v}_1^T A^T)\mathbf{v}_2 = \mathbf{v}_1^T (A\mathbf{v}_2) && \text{Since } A^T = A \\ &= \mathbf{v}_1^T (\lambda_2 \mathbf{v}_2) && \text{Since } \mathbf{v}_2 \text{ is an eigenvector} \\ &= \lambda_2 \mathbf{v}_1^T \mathbf{v}_2 = \lambda_2 \mathbf{v}_1 \cdot \mathbf{v}_2 \end{aligned}$$

Hence $(\lambda_1 - \lambda_2)\mathbf{v}_1 \cdot \mathbf{v}_2 = 0$. But $\lambda_1 - \lambda_2 \neq 0$, so $\mathbf{v}_1 \cdot \mathbf{v}_2 = 0$. ■

The special type of diagonalization in Example 2 is crucial for the theory of symmetric matrices. An $n \times n$ matrix A is said to be **orthogonally diagonalizable** if there are an orthogonal matrix P (with $P^{-1} = P^T$) and a diagonal matrix D such that

$$A = PDP^T = PDP^{-1} \tag{1}$$

Such a diagonalization requires n linearly independent and orthonormal eigenvectors. When is this possible? If A is orthogonally diagonalizable as in (1), then

$$A^T = (PDP^T)^T = P^{TT} D^T P^T = PDP^T = A$$

Thus A is symmetric! Theorem 2 below shows that, conversely, every symmetric matrix is orthogonally diagonalizable. The proof is much harder and is omitted; the main idea for a proof will be given after Theorem 3.

THEOREM 2

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

This theorem is rather amazing, because the work in Chapter 5 would suggest that it is usually impossible to tell when a matrix is diagonalizable. But this is not the case for symmetric matrices.

The next example treats a matrix whose eigenvalues are not all distinct.

EXAMPLE 3 Orthogonally diagonalize the matrix $A = \begin{bmatrix} 3 & -2 & 4 \\ -2 & 6 & 2 \\ 4 & 2 & 3 \end{bmatrix}$, whose characteristic equation is

$$0 = -\lambda^3 + 12\lambda^2 - 21\lambda - 98 = -(\lambda - 7)^2(\lambda + 2)$$

SOLUTION The usual calculations produce bases for the eigenspaces:

$$\lambda = 7: \mathbf{v}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \mathbf{v}_2 = \begin{bmatrix} -1/2 \\ 1 \\ 0 \end{bmatrix}; \qquad \lambda = -2: \mathbf{v}_3 = \begin{bmatrix} -1 \\ -1/2 \\ 1 \end{bmatrix}$$

Although $\mathbf{v}_1$ and $\mathbf{v}_2$ are linearly independent, they are not orthogonal. Recall from Section 6.2 that the projection of $\mathbf{v}_2$ onto $\mathbf{v}_1$ is $\dfrac{\mathbf{v}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1$, and the component of $\mathbf{v}_2$ orthogonal to $\mathbf{v}_1$ is

$$\mathbf{z}_2 = \mathbf{v}_2 - \frac{\mathbf{v}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 = \begin{bmatrix} -1/2 \\ 1 \\ 0 \end{bmatrix} - \frac{-1/2}{2}\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -1/4 \\ 1 \\ 1/4 \end{bmatrix}$$

Then $\{\mathbf{v}_1, \mathbf{z}_2\}$ is an orthogonal set in the eigenspace for $\lambda = 7$. (Note that $\mathbf{z}_2$ is a linear combination of the eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$, so $\mathbf{z}_2$ is in the eigenspace. This construction of $\mathbf{z}_2$ is just the Gram–Schmidt process of Section 6.4.) Since the eigenspace is two-dimensional (with basis $\mathbf{v}_1, \mathbf{v}_2$), the orthogonal set $\{\mathbf{v}_1, \mathbf{z}_2\}$ is an *orthogonal basis* for the eigenspace, by the Basis Theorem. (See Section 2.9 or 4.5.)

Normalize $\mathbf{v}_1$ and $\mathbf{z}_2$ to obtain the following orthonormal basis for the eigenspace for $\lambda = 7$:

$$\mathbf{u}_1 = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} -1/\sqrt{18} \\ 4/\sqrt{18} \\ 1/\sqrt{18} \end{bmatrix}$$

An orthonormal basis for the eigenspace for $\lambda = -2$ is

$$\mathbf{u}_3 = \frac{1}{\|2\mathbf{v}_3\|}2\mathbf{v}_3 = \frac{1}{3}\begin{bmatrix} -2 \\ -1 \\ 2 \end{bmatrix} = \begin{bmatrix} -2/3 \\ -1/3 \\ 2/3 \end{bmatrix}$$

By Theorem 1, $\mathbf{u}_3$ is orthogonal to the other eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$. Hence $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ is an orthonormal set. Let

$$P = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3\,] = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{18} & -2/3 \\ 0 & 4/\sqrt{18} & -1/3 \\ 1/\sqrt{2} & 1/\sqrt{18} & 2/3 \end{bmatrix}, \quad D = \begin{bmatrix} 7 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Then P orthogonally diagonalizes A, and $A = PDP^{-1}$. ■

In Example 3, the eigenvalue 7 has multiplicity two and the eigenspace is two-dimensional. This fact is not accidental, as the next theorem shows.

The Spectral Theorem

The set of eigenvalues of a matrix A is sometimes called the *spectrum* of A, and the following description of the eigenvalues is called a *spectral theorem.*

THEOREM 3

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.

Part (a) follows from Exercise 24 in Section 5.5. Part (b) follows easily from part (d). (See Exercise 31.) Part (c) is Theorem 1. Because of (a), a proof of (d) can be given using Exercise 32 and the Schur factorization discussed in Supplementary Exercise 16 in Chapter 6. The details are omitted.

Spectral Decomposition

Suppose $A = PDP^{-1}$, where the columns of P are orthonormal eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_n$ of A and the corresponding eigenvalues $\lambda_1, \dots, \lambda_n$ are in the diagonal matrix D. Then, since $P^{-1} = P^T$,

$$A = PDP^T = \begin{bmatrix} \mathbf{u}_1 & \cdots & \mathbf{u}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_n^T \end{bmatrix}$$

$$= \begin{bmatrix} \lambda_1\mathbf{u}_1 & \cdots & \lambda_n\mathbf{u}_n \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_n^T \end{bmatrix}$$

Using the column–row expansion of a product (Theorem 10 in Section 2.4), we can write

$$A = \lambda_1\mathbf{u}_1\mathbf{u}_1^T + \lambda_2\mathbf{u}_2\mathbf{u}_2^T + \cdots + \lambda_n\mathbf{u}_n\mathbf{u}_n^T \tag{2}$$

This representation of A is called a **spectral decomposition** of A because it breaks up A into pieces determined by the spectrum (eigenvalues) of A. Each term in (2) is an $n \times n$ matrix of rank 1. For example, every column of $\lambda_1\mathbf{u}_1\mathbf{u}_1^T$ is a multiple of $\mathbf{u}_1$. Furthermore, each matrix $\mathbf{u}_j\mathbf{u}_j^T$ is a **projection matrix** in the sense that for each $\mathbf{x}$ in $\mathbb{R}^n$, the vector $(\mathbf{u}_j\mathbf{u}_j^T)\mathbf{x}$ is the orthogonal projection of $\mathbf{x}$ onto the subspace spanned by $\mathbf{u}_j$. (See Exercise 35.)

EXAMPLE 4 Construct a spectral decomposition of the matrix A that has the orthogonal diagonalization

$$A = \begin{bmatrix} 7 & 2 \\ 2 & 4 \end{bmatrix} = \begin{bmatrix} 2/\sqrt{5} & -1/\sqrt{5} \\ 1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} \begin{bmatrix} 8 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \\ -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix}$$

SOLUTION Denote the columns of P by $\mathbf{u}_1$ and $\mathbf{u}_2$. Then

$$A = 8\mathbf{u}_1\mathbf{u}_1^T + 3\mathbf{u}_2\mathbf{u}_2^T$$

To verify this decomposition of A, compute

$$\mathbf{u}_1\mathbf{u}_1^T = \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix} \begin{bmatrix} 2/\sqrt{5} & 1/\sqrt{5} \end{bmatrix} = \begin{bmatrix} 4/5 & 2/5 \\ 2/5 & 1/5 \end{bmatrix}$$

$$\mathbf{u}_2\mathbf{u}_2^T = \begin{bmatrix} -1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix} \begin{bmatrix} -1/\sqrt{5} & 2/\sqrt{5} \end{bmatrix} = \begin{bmatrix} 1/5 & -2/5 \\ -2/5 & 4/5 \end{bmatrix}$$

and

$$8\mathbf{u}_1\mathbf{u}_1^T + 3\mathbf{u}_2\mathbf{u}_2^T = \begin{bmatrix} 32/5 & 16/5 \\ 16/5 & 8/5 \end{bmatrix} + \begin{bmatrix} 3/5 & -6/5 \\ -6/5 & 12/5 \end{bmatrix} = \begin{bmatrix} 7 & 2 \\ 2 & 4 \end{bmatrix} = A \quad \blacksquare$$

NUMERICAL NOTE

When A is symmetric and not too large, modern high-performance computer algorithms calculate eigenvalues and eigenvectors with great precision. They apply a sequence of similarity transformations to A involving orthogonal matrices. The diagonal entries of the transformed matrices converge rapidly to the eigenvalues of A. (See the Numerical Notes in Section 5.2.) Using orthogonal matrices generally prevents numerical errors from accumulating during the process. When A is symmetric, the sequence of orthogonal matrices combines to form an orthogonal matrix whose columns are eigenvectors of A.

A nonsymmetric matrix cannot have a full set of orthogonal eigenvectors, but the algorithm still produces fairly accurate eigenvalues. After that, nonorthogonal techniques are needed to calculate eigenvectors.

PRACTICE PROBLEMS

1. Show that if A is a symmetric matrix, then A^2 is symmetric.
2. Show that if A is orthogonally diagonalizable, then so is A^2.

7.1 EXERCISES

Determine which of the matrices in Exercises 1–6 are symmetric.

1. $\begin{bmatrix} 3 & 5 \\ 5 & -7 \end{bmatrix}$

2. $\begin{bmatrix} -3 & 5 \\ -5 & 3 \end{bmatrix}$

3. $\begin{bmatrix} 2 & 2 \\ 4 & 4 \end{bmatrix}$

4. $\begin{bmatrix} 0 & 8 & 3 \\ 8 & 0 & -2 \\ 3 & -2 & 0 \end{bmatrix}$

5. $\begin{bmatrix} -6 & 2 & 0 \\ 0 & -6 & 2 \\ 0 & 0 & -6 \end{bmatrix}$

6. $\begin{bmatrix} 1 & 2 & 1 & 2 \\ 2 & 1 & 2 & 1 \\ 1 & 2 & 1 & 2 \end{bmatrix}$

Determine which of the matrices in Exercises 7–12 are orthogonal. If orthogonal, find the inverse.

7. $\begin{bmatrix} .6 & .8 \\ .8 & -.6 \end{bmatrix}$

8. $\begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$

9. $\begin{bmatrix} -5 & 2 \\ 2 & 5 \end{bmatrix}$

10. $\begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}$

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

12. $\begin{bmatrix} .5 & .5 & -.5 & -.5 \\ -.5 & .5 & -.5 & .5 \\ .5 & .5 & .5 & .5 \\ -.5 & .5 & .5 & -.5 \end{bmatrix}$

Orthogonally diagonalize the matrices in Exercises 13–22, giving an orthogonal matrix P and a diagonal matrix D. To save you time, the eigenvalues in Exercises 17–22 are: (17) 5, 2, −2; (18) 25, 3, −50; (19) 7, −2; (20) 13, 7, 1; (21) 9, 5, 1; (22) 2, 0.

13. $\begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$

14. $\begin{bmatrix} 1 & 5 \\ 5 & 1 \end{bmatrix}$

15. $\begin{bmatrix} 16 & -4 \\ -4 & 1 \end{bmatrix}$

16. $\begin{bmatrix} -7 & 24 \\ 24 & 7 \end{bmatrix}$

17. $\begin{bmatrix} 1 & 1 & 3 \\ 1 & 3 & 1 \\ 3 & 1 & 1 \end{bmatrix}$

18. $\begin{bmatrix} -2 & -36 & 0 \\ -36 & -23 & 0 \\ 0 & 0 & 3 \end{bmatrix}$

19. $\begin{bmatrix} 3 & -2 & 4 \\ -2 & 6 & 2 \\ 4 & 2 & 3 \end{bmatrix}$

20. $\begin{bmatrix} 7 & -4 & 4 \\ -4 & 5 & 0 \\ 4 & 0 & 9 \end{bmatrix}$

21. $\begin{bmatrix} 4 & 1 & 3 & 1 \\ 1 & 4 & 1 & 3 \\ 3 & 1 & 4 & 1 \\ 1 & 3 & 1 & 4 \end{bmatrix}$

22. $\begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$

23. Let $A = \begin{bmatrix} 3 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 3 \end{bmatrix}$ and $\mathbf{v} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$. Verify that 2 is an eigenvalue of A and $\mathbf{v}$ is an eigenvector. Then orthogonally diagonalize A.

24. Let $A = \begin{bmatrix} 5 & -4 & -2 \\ -4 & 5 & 2 \\ -2 & 2 & 2 \end{bmatrix}$, $\mathbf{v}_1 = \begin{bmatrix} -2 \\ 2 \\ 1 \end{bmatrix}$, and $\mathbf{v}_2 = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$. Verify that $\mathbf{v}_1$ and $\mathbf{v}_2$ are eigenvectors of A. Then orthogonally diagonalize A.

In Exercises 25 and 26, mark each statement True or False. Justify each answer.

25. a. An $n \times n$ matrix that is orthogonally diagonalizable must be symmetric.

b. If $A^T = A$ and if vectors $\mathbf{u}$ and $\mathbf{v}$ satisfy $A\mathbf{u} = 3\mathbf{u}$ and $A\mathbf{v} = 4\mathbf{v}$, then $\mathbf{u}\cdot\mathbf{v} = 0$.

c. An $n \times n$ symmetric matrix has n distinct real eigenvalues.

d. For a nonzero $\mathbf{v}$ in $\mathbb{R}^n$, the matrix $\mathbf{v}\mathbf{v}^T$ is called a projection matrix.

26. a. Every symmetric matrix is orthogonally diagonalizable.

b. If $B = PDP^T$, where $P^T = P^{-1}$ and D is a diagonal matrix, then B is a symmetric matrix.

c. An orthogonal matrix is orthogonally diagonalizable.

d. The dimension of an eigenspace of a symmetric matrix equals the multiplicity of the corresponding eigenvalue.

27. Suppose A is a symmetric $n \times n$ matrix and B is any $n \times m$ matrix. Show that B^TAB, B^TB, and BB^T are symmetric matrices.

28. Show that if A is an $n \times n$ symmetric matrix, then $(A\mathbf{x})\cdot\mathbf{y} = \mathbf{x}\cdot(A\mathbf{y})$ for all $\mathbf{x}, \mathbf{y}$ in $\mathbb{R}^n$.

29. Suppose A is invertible and orthogonally diagonalizable. Explain why A^{-1} is also orthogonally diagonalizable.

30. Suppose A and B are both orthogonally diagonalizable and $AB = BA$. Explain why AB is also orthogonally diagonalizable.

31. Let $A = PDP^{-1}$, where P is orthogonal and D is diagonal, and let λ be an eigenvalue of A of multiplicity k. Then λ appears k times on the diagonal of D. Explain why the dimension of the eigenspace for λ is k.

32. Suppose $A = PRP^{-1}$, where P is orthogonal and R is upper triangular. Show that if A is symmetric, then R is symmetric and hence is actually a diagonal matrix.

33. Construct a spectral decomposition of A from Example 2.

34. Construct a spectral decomposition of A from Example 3.

35. Let $\mathbf{u}$ be a unit vector in $\mathbb{R}^n$, and let $B = \mathbf{u}\mathbf{u}^T$.

a. Given any $\mathbf{x}$ in $\mathbb{R}^n$, compute $B\mathbf{x}$ and show that $B\mathbf{x}$ is the orthogonal projection of $\mathbf{x}$ onto $\mathbf{u}$, as described in Section 6.2.

b. Show that B is a symmetric matrix and $B^2 = B$.

c. Show that $\mathbf{u}$ is an eigenvector of B. What is the corresponding eigenvalue?

36. Let B be an $n \times n$ symmetric matrix such that $B^2 = B$. Any such matrix is called a **projection matrix** (or an **orthogonal projection matrix**). Given any $\mathbf{y}$ in $\mathbb{R}^n$, let $\hat{\mathbf{y}} = B\mathbf{y}$ and $\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$.

a. Show that $\mathbf{z}$ is orthogonal to $\hat{\mathbf{y}}$.

b. Let W be the column space of B. Show that $\mathbf{y}$ is the sum of a vector in W and a vector in $W^\perp$. Why does this prove that $B\mathbf{y}$ is the orthogonal projection of $\mathbf{y}$ onto the column space of B?

[M] Orthogonally diagonalize the matrices in Exercises 37–40. To practice the methods of this section, do not use an eigenvector routine from your matrix program. Instead, use the program to find the eigenvalues, and, for each eigenvalue λ, find an orthonormal basis for $\text{Nul}(A - \lambda I)$, as in Examples 2 and 3.

37. $\begin{bmatrix} 5 & 2 & 9 & -6 \\ 2 & 5 & -6 & 9 \\ 9 & -6 & 5 & 2 \\ -6 & 9 & 2 & 5 \end{bmatrix}$

38. $\begin{bmatrix} .38 & -.18 & -.06 & -.04 \\ -.18 & .59 & -.04 & .12 \\ -.06 & -.04 & .47 & -.12 \\ -.04 & .12 & -.12 & .41 \end{bmatrix}$

39. $\begin{bmatrix} .31 & .58 & .08 & .44 \\ .58 & -.56 & .44 & -.58 \\ .08 & .44 & .19 & -.08 \\ .44 & -.58 & -.08 & .31 \end{bmatrix}$

40. $\begin{bmatrix} 10 & 2 & 2 & -6 & 9 \\ 2 & 10 & 2 & -6 & 9 \\ 2 & 2 & 10 & -6 & 9 \\ -6 & -6 & -6 & 26 & 9 \\ 9 & 9 & 9 & 9 & -19 \end{bmatrix}$

SOLUTIONS TO PRACTICE PROBLEMS

1. $(A^2)^T = (AA)^T = A^TA^T$, by a property of transposes. By hypothesis, $A^T = A$. So $(A^2)^T = AA = A^2$, which shows that A^2 is symmetric.

2. If A is orthogonally diagonalizable, then A is symmetric, by Theorem 2. By Practice Problem 1, A^2 is symmetric and hence is orthogonally diagonalizable (Theorem 2).

7.2 QUADRATIC FORMS

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 $Q(\mathbf{x}) = \mathbf{x}^TA\mathbf{x}$, 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 $Q(\mathbf{x}) = \mathbf{x}^TI\mathbf{x} = \|\mathbf{x}\|^2$. Examples 1 and 2 show the connection between any symmetric matrix A and the quadratic form $\mathbf{x}^TA\mathbf{x}$.

EXAMPLE 1 Let $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. Compute $\mathbf{x}^TA\mathbf{x}$ 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. $\mathbf{x}^TA\mathbf{x} = [\, x_1 \quad x_2 \,]\begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = [\, x_1 \quad x_2 \,]\begin{bmatrix} 4x_1 \\ 3x_2 \end{bmatrix} = 4x_1^2 + 3x_2^2.$

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

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

■

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 $\mathbf{x}^TA\mathbf{x}$.

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

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

■

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

$$Q(-3, 1) = (-3)^2 - 8(-3)(1) - 5(1)^2 = 28$$
$$Q(2, -2) = (2)^2 - 8(2)(-2) - 5(-2)^2 = 16$$
$$Q(1, -3) = (1)^2 - 8(1)(-3) - 5(-3)^2 = -20$$

■

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

$$\begin{aligned} x_1^2 - 8x_1x_2 - 5x_2^2 &= \mathbf{x}^T A\mathbf{x} = (P\mathbf{y})^T A(P\mathbf{y}) \\ &= \mathbf{y}^T P^T A P\mathbf{y} = \mathbf{y}^T D\mathbf{y} \\ &= 3y_1^2 - 7y_2^2 \end{aligned}$$

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.

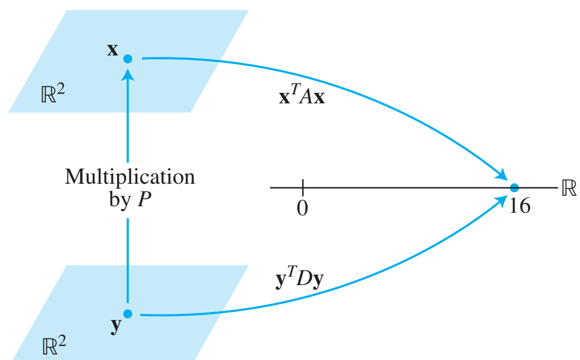


FIGURE 1 Change of variable in $\mathbf{x}^T A\mathbf{x}$.

Example 4 illustrates the following theorem. The proof of the theorem was essentially given before Example 4.

THEOREM 4

The Principal Axes Theorem

Let A be an $n \times n$ symmetric matrix. Then there is an orthogonal change of variable, $\mathbf{x} = P\mathbf{y}$, that transforms the quadratic form $\mathbf{x}^T A\mathbf{x}$ into a quadratic form $\mathbf{y}^T D\mathbf{y}$ with no cross-product term.

The columns of P in the theorem are called the **principal axes** of the quadratic form $\mathbf{x}^T A\mathbf{x}$. The vector $\mathbf{y}$ is the coordinate vector of $\mathbf{x}$ relative to the orthonormal basis of $\mathbb{R}^n$ given by these principal axes.

A Geometric View of Principal Axes

Suppose $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$, where A is an invertible 2×2 symmetric matrix, and let c be a constant. It can be shown that the set of all $\mathbf{x}$ in $\mathbb{R}^2$ that satisfy

$$\mathbf{x}^T A\mathbf{x} = c \tag{3}$$

either corresponds to an ellipse (or circle), a hyperbola, two intersecting lines, or a single point, or contains no points at all. If A is a diagonal matrix, the graph is in *standard position*, such as in Fig. 2. If A is not a diagonal matrix, the graph of equation (3) is

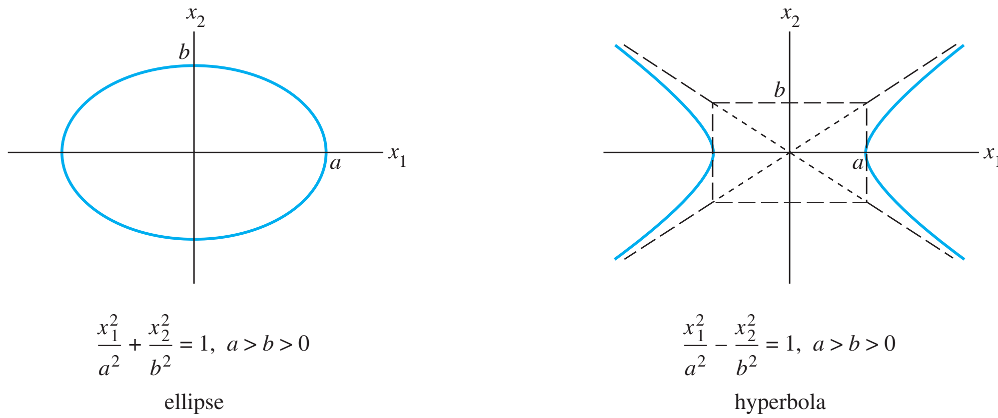


FIGURE 2 An ellipse and a hyperbola in standard position.

rotated out of standard position, as in Fig. 3. Finding the *principal axes* (determined by the eigenvectors of A) amounts to finding a new coordinate system with respect to which the graph is in standard position.

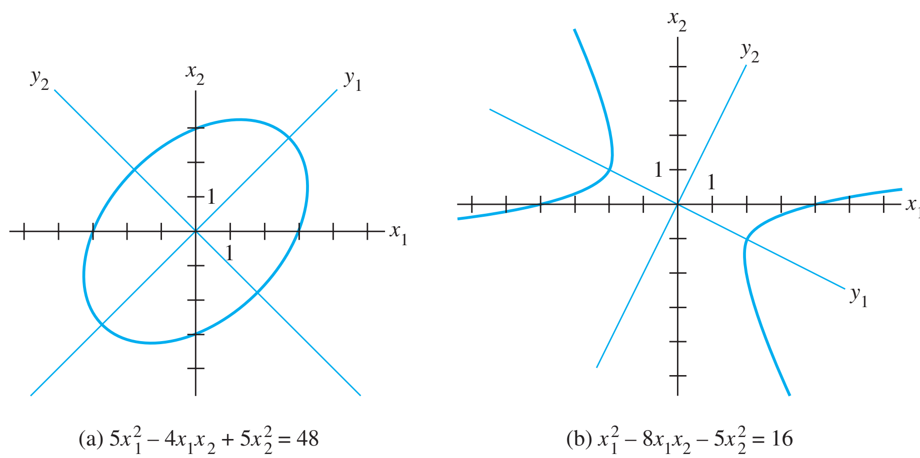


FIGURE 3 An ellipse and a hyperbola *not* in standard position.

The hyperbola in Fig. 3(b) is the graph of the equation $\mathbf{x}^TA\mathbf{x} = 16$, where A is the matrix in Example 4. The positive y_1-axis in Fig. 3(b) is in the direction of the first column of the matrix P in Example 4, and the positive y_2-axis is in the direction of the second column of P.

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.

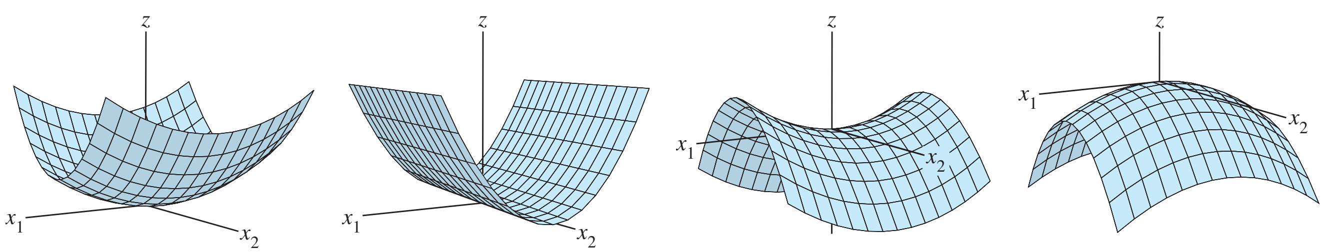
SOLUTION The matrix of the quadratic form is $A = \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$. The eigenvalues of A turn out to be 3 and 7, with corresponding unit eigenvectors

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

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). ■

Classifying Quadratic Forms

When A is an $n \times n$ matrix, the quadratic form $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$ is a real-valued function with domain $\mathbb{R}^n$. Figure 4 displays the graphs of four quadratic forms with domain $\mathbb{R}^2$. For each point $\mathbf{x} = (x_1, x_2)$ in the domain of a quadratic form Q, the graph displays the point (x_1, x_2, z) where $z = Q(\mathbf{x})$. Notice that except at $\mathbf{x} = \mathbf{0}$, the values of $Q(\mathbf{x})$ are all positive in Fig. 4(a) and all negative in Fig. 4(d). The horizontal cross-sections of the graphs are ellipses in Figs. 4(a) and 4(d) and hyperbolas in Fig. 4(c).



(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.

The simple 2×2 examples in Fig. 4 illustrate the following definitions.

DEFINITION

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.

Theorem 5 characterizes some quadratic forms in terms of eigenvalues.

THEOREM 5

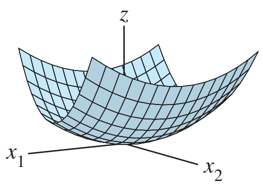
Quadratic Forms and Eigenvalues

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

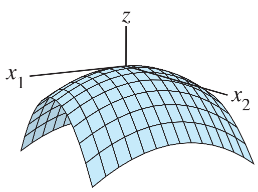
a. positive definite if and only if the eigenvalues of A are all positive,

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

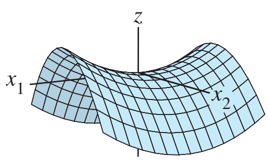
c. indefinite if and only if A has both positive and negative eigenvalues.



Positive definite



Negative definite



Indefinite

PROOF By the Principal Axes Theorem, there exists an orthogonal change of variable $\mathbf{x} = P\mathbf{y}$ such that

$$Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x} = \mathbf{y}^T D\mathbf{y} = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2 \tag{4}$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of A. Since P is invertible, there is a one-to-one correspondence between all nonzero $\mathbf{x}$ and all nonzero $\mathbf{y}$. Thus the values of $Q(\mathbf{x})$ for $\mathbf{x} \neq \mathbf{0}$ coincide with the values of the expression on the right side of (4), which is obviously controlled by the signs of the eigenvalues $\lambda_1, \ldots, \lambda_n$, in the three ways described in the theorem. ■

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 $\mathbf{x}^T A\mathbf{x}$ is positive definite. Other terms, such as **positive semidefinite matrix**, are defined analogously.

WEB

NUMERICAL NOTE

A fast way to determine whether a symmetric matrix A is positive definite is to attempt to factor A in the form $A = R^T R$, where R is upper triangular with positive diagonal entries. (A slightly modified algorithm for an LU factorization is one approach.) Such a *Cholesky factorization* is possible if and only if A is positive definite. See Supplementary Exercise 7 at the end of Chapter 7.

PRACTICE PROBLEM

Describe a positive semidefinite matrix A in terms of its eigenvalues.

WEB

7.2 EXERCISES

1. Compute the quadratic form $\mathbf{x}^T A\mathbf{x}$, when $A = \begin{bmatrix} 5 & 1/3 \\ 1/3 & 1 \end{bmatrix}$ and
   a. $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ b. $\mathbf{x} = \begin{bmatrix} 6 \\ 1 \end{bmatrix}$ c. $\mathbf{x} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$

2. Compute the quadratic form $\mathbf{x}^T A\mathbf{x}$, for $A = \begin{bmatrix} 4 & 3 & 0 \\ 3 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix}$ and
   a. $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ b. $\mathbf{x} = \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix}$ c. $\mathbf{x} = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$

3. Find the matrix of the quadratic form. Assume $\mathbf{x}$ is in $\mathbb{R}^2$.
   a. $10x_1^2 - 6x_1x_2 - 3x_2^2$ b. $5x_1^2 + 3x_1x_2$

4. Find the matrix of the quadratic form. Assume $\mathbf{x}$ is in $\mathbb{R}^2$.
   a. $20x_1^2 + 15x_1x_2 - 10x_2^2$ b. x_1x_2

5. Find the matrix of the quadratic form. Assume $\mathbf{x}$ is in $\mathbb{R}^3$.

a. $8x_1^2 + 7x_2^2 - 3x_3^2 - 6x_1x_2 + 4x_1x_3 - 2x_2x_3$

b. $4x_1x_2 + 6x_1x_3 - 8x_2x_3$

6. Find the matrix of the quadratic form. Assume $\mathbf{x}$ is in $\mathbb{R}^3$.

a. $5x_1^2 - x_2^2 + 7x_3^2 + 5x_1x_2 - 3x_1x_3$

b. $x_3^2 - 4x_1x_2 + 4x_2x_3$

7. Make a change of variable, $\mathbf{x} = P\mathbf{y}$, that transforms the quadratic form $x_1^2 + 10x_1x_2 + x_2^2$ into a quadratic form with no cross-product term. Give P and the new quadratic form.

8. Let A be the matrix of the quadratic form

$$9x_1^2 + 7x_2^2 + 11x_3^2 - 8x_1x_2 + 8x_1x_3$$

It can be shown that the eigenvalues of A are 3, 9, and 15. Find an orthogonal matrix P such that the change of variable $\mathbf{x} = P\mathbf{y}$ transforms $\mathbf{x}^T A\mathbf{x}$ into a quadratic form with no cross-product term. Give P and the new quadratic form.

Classify the quadratic forms in Exercises 9–18. Then make a change of variable, $\mathbf{x} = P\mathbf{y}$, that transforms the quadratic form into one with no cross-product term. Write the new quadratic form. Construct P using the methods of Section 7.1.

9. $3x_1^2 - 4x_1x_2 + 6x_2^2$

10. $9x_1^2 - 8x_1x_2 + 3x_2^2$

11. $2x_1^2 + 10x_1x_2 + 2x_2^2$

12. $-5x_1^2 + 4x_1x_2 - 2x_2^2$

13. $x_1^2 - 6x_1x_2 + 9x_2^2$

14. $8x_1^2 + 6x_1x_2$

15. **[M]** $-2x_1^2 - 6x_2^2 - 9x_3^2 - 9x_4^2 + 4x_1x_2 + 4x_1x_3 + 4x_1x_4 + 6x_3x_4$

16. **[M]** $4x_1^2 + 4x_2^2 + 4x_3^2 + 4x_4^2 + 3x_1x_2 + 3x_3x_4 - 4x_1x_4 + 4x_2x_3$

17. **[M]** $x_1^2 + x_2^2 + x_3^2 + x_4^2 + 9x_1x_2 - 12x_1x_4 + 12x_2x_3 + 9x_3x_4$

18. **[M]** $11x_1^2 - x_2^2 - 12x_1x_2 - 12x_1x_3 - 12x_1x_4 - 2x_3x_4$

19. What is the largest possible value of the quadratic form $5x_1^2 + 8x_2^2$ if $\mathbf{x} = (x_1, x_2)$ and $\mathbf{x}^T\mathbf{x} = 1$, that is, if $x_1^2 + x_2^2 = 1$? (Try some examples of $\mathbf{x}$.)

20. What is the largest value of the quadratic form $5x_1^2 - 3x_2^2$ if $\mathbf{x}^T\mathbf{x} = 1$?

In Exercises 21 and 22, matrices are $n \times n$ and vectors are in $\mathbb{R}^n$. Mark each statement True or False. Justify each answer.

21. a. The matrix of a quadratic form is a symmetric matrix.

b. A quadratic form has no cross-product terms if and only if the matrix of the quadratic form is a diagonal matrix.

c. The principal axes of a quadratic form $\mathbf{x}^T A\mathbf{x}$ are eigenvectors of A.

d. A positive definite quadratic form Q satisfies $Q(\mathbf{x}) > 0$ for all $\mathbf{x}$ in $\mathbb{R}^n$.

e. If the eigenvalues of a symmetric matrix A are all positive, then the quadratic form $\mathbf{x}^T A\mathbf{x}$ is positive definite.

f. A Cholesky factorization of a symmetric matrix A has the form $A = R^T R$, for an upper triangular matrix R with positive diagonal entries.

22. a. The expression $\|\mathbf{x}\|^2$ is a quadratic form.

b. If A is symmetric and P is an orthogonal matrix, then the change of variable $\mathbf{x} = P\mathbf{y}$ transforms $\mathbf{x}^T A\mathbf{x}$ into a quadratic form with no cross-product term.

c. If A is a 2×2 symmetric matrix, then the set of $\mathbf{x}$ such that $\mathbf{x}^T A\mathbf{x} = c$ (for a constant c) corresponds to either a circle, an ellipse, or a hyperbola.

d. An indefinite quadratic form is either positive semidefinite or negative semidefinite.

e. If A is symmetric and the quadratic form $\mathbf{x}^T A\mathbf{x}$ has only negative values for $\mathbf{x} \neq \mathbf{0}$, then the eigenvalues of A are all negative.

Exercises 23 and 24 show how to classify a quadratic form $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$, when $A = \begin{bmatrix} a & b \\ b & d \end{bmatrix}$ and $\det A \neq 0$, without finding the eigenvalues of A.

23. If λ_1 and λ_2 are the eigenvalues of A, then the characteristic polynomial of A can be written in two ways: $\det(A - \lambda I)$ and $(\lambda - \lambda_1)(\lambda - \lambda_2)$. Use this fact to show that $\lambda_1 + \lambda_2 = a + d$ (the diagonal entries of A) and $\lambda_1\lambda_2 = \det A$.

24. Verify the following statements.

a. Q is positive definite if $\det A > 0$ and $a > 0$.

b. Q is negative definite if $\det A > 0$ and $a < 0$.

c. Q is indefinite if $\det A < 0$.

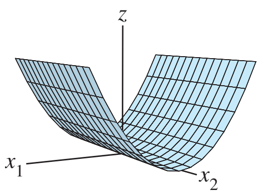
25. Show that if B is $m \times n$, then $B^T B$ is positive semidefinite; and if B is $n \times n$ and invertible, then $B^T B$ is positive definite.

26. Show that if an $n \times n$ matrix A is positive definite, then there exists a positive definite matrix B such that $A = B^T B$. [*Hint:* Write $A = PDP^T$, with $P^T = P^{-1}$. Produce a diagonal matrix C such that $D = C^T C$, and let $B = PCP^T$. Show that B works.]

27. Let A and B be symmetric $n \times n$ matrices whose eigenvalues are all positive. Show that the eigenvalues of $A + B$ are all positive. [*Hint:* Consider quadratic forms.]

28. Let A be an $n \times n$ invertible symmetric matrix. Show that if the quadratic form $\mathbf{x}^T A\mathbf{x}$ is positive definite, then so is the quadratic form $\mathbf{x}^T A^{-1}\mathbf{x}$. [*Hint:* Consider eigenvalues.]

SG Mastering: Diagonalization and Quadratic Forms 7–7



Positive semidefinite

SOLUTION TO PRACTICE PROBLEM

Make an orthogonal change of variable $\mathbf{x} = P\mathbf{y}$, and write

$$\mathbf{x}^T A\mathbf{x} = \mathbf{y}^T D\mathbf{y} = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2$$

as in equation (4). If an eigenvalue—say, λ_i—were negative, then $\mathbf{x}^T A\mathbf{x}$ would be negative for the $\mathbf{x}$ corresponding to $\mathbf{y} = \mathbf{e}_i$ (the ith column of I_n). So the eigenvalues of a positive semidefinite quadratic form must all be nonnegative. Conversely, if the eigenvalues are nonnegative, the expansion above shows that $\mathbf{x}^T A\mathbf{x}$ must be positive semidefinite.

7.3 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

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

and hence

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

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 $\mathbf{x}^T\mathbf{x} = 1$. ■

It is easy to see in Example 1 that the matrix of the quadratic form Q has eigenvalues 9, 4, and 3 and that the greatest and least eigenvalues equal, respectively, the (constrained) maximum and minimum of $Q(\mathbf{x})$. The same holds true for any quadratic form, as we shall see.

EXAMPLE 2 Let $A = \begin{bmatrix} 3 & 0 \\ 0 & 7 \end{bmatrix}$, and let $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$ 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 $(-1, 0)$. ■

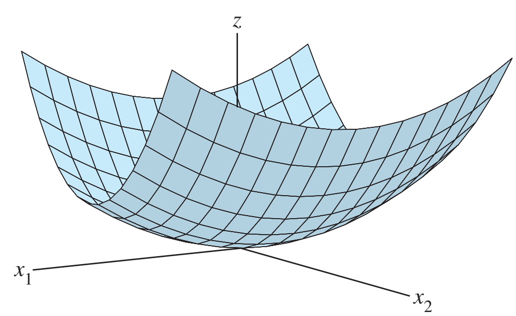


FIGURE 1 $z = 3x_1^2 + 7x_2^2$.

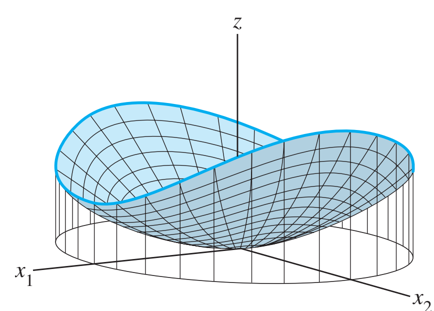


FIGURE 2 The intersection of $z = 3x_1^2 + 7x_2^2$ and the cylinder $x_1^2 + x_2^2 = 1$.

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 $\mathbf{x}^T A\mathbf{x}$, for $\|\mathbf{x}\| = 1$, is the closed interval $3 \le t \le 7$.

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]

THEOREM 6

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.

[1]The use of *minimum* and *maximum* in (2), and *least* and *greatest* in the theorem, refers to the natural ordering of the real numbers, not to magnitudes.

PROOF Orthogonally diagonalize A as PDP^{-1}. We know that

$$\mathbf{x}^T A\mathbf{x} = \mathbf{y}^T D\mathbf{y} \quad \text{when } \mathbf{x} = P\mathbf{y} \tag{3}$$

Also,

$$\|\mathbf{x}\| = \|P\mathbf{y}\| = \|\mathbf{y}\| \quad \text{for all } \mathbf{y}$$

because $P^T P = I$ and $\|P\mathbf{y}\|^2 = (P\mathbf{y})^T(P\mathbf{y}) = \mathbf{y}^T P^T P\mathbf{y} = \mathbf{y}^T\mathbf{y} = \|\mathbf{y}\|^2$. In particular, $\|\mathbf{y}\| = 1$ if and only if $\|\mathbf{x}\| = 1$. Thus $\mathbf{x}^T A\mathbf{x}$ and $\mathbf{y}^T D\mathbf{y}$ assume the same set of values as $\mathbf{x}$ and $\mathbf{y}$ range over the set of all unit vectors.

To simplify notation, suppose that A is a 3×3 matrix with eigenvalues $a \geq b \geq c$. Arrange the (eigenvector) columns of P so that $P = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3\,]$ and

$$D = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix}$$

Given any unit vector $\mathbf{y}$ in $\mathbb{R}^3$ with coordinates y_1, y_2, y_3, observe that

$$\begin{aligned} ay_1^2 &= ay_1^2 \\ by_2^2 &\leq ay_2^2 \\ cy_3^2 &\leq ay_3^2 \end{aligned}$$

and obtain these inequalities:

$$\begin{aligned} \mathbf{y}^T D\mathbf{y} &= ay_1^2 + by_2^2 + cy_3^2 \\ &\leq ay_1^2 + ay_2^2 + ay_3^2 \\ &= a(y_1^2 + y_2^2 + y_3^2) \\ &= a\|\mathbf{y}\|^2 = a \end{aligned}$$

Thus $M \leq a$, by definition of M. However, $\mathbf{y}^T D\mathbf{y} = a$ when $\mathbf{y} = \mathbf{e}_1 = (1, 0, 0)$, so in fact $M = a$. By (3), the $\mathbf{x}$ that corresponds to $\mathbf{y} = \mathbf{e}_1$ is the eigenvector $\mathbf{u}_1$ of A, because

$$\mathbf{x} = P\mathbf{e}_1 = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3\,]\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \mathbf{u}_1$$

Thus $M = a = \mathbf{e}_1^T D\mathbf{e}_1 = \mathbf{u}_1^T A\mathbf{u}_1$, which proves the statement about M. A similar argument shows that m is the least eigenvalue, c, and this value of $\mathbf{x}^T A\mathbf{x}$ is attained when $\mathbf{x} = P\mathbf{e}_3 = \mathbf{u}_3$. ■

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 $\mathbf{u}_1 = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$. ■

In Theorem 7 and in later applications, the values of $\mathbf{x}^T A\mathbf{x}$ are computed with additional constraints on the unit vector $\mathbf{x}$.

THEOREM 7

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.

Theorem 7 can be proved by an argument similar to the one above in which the theorem is reduced to the case where the matrix of the quadratic form is diagonal. The next example gives an idea of the proof for the case of a diagonal matrix.

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 $\mathbf{x}^T A\mathbf{x}$ 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 $\mathbf{x}^T A\mathbf{x}$ subject to the constraints in (4) is 3, attained when $\mathbf{x} = \mathbf{u}_2$. ■

The next theorem generalizes Theorem 7 and, together with Theorem 6, gives a useful characterization of *all* the eigenvalues of A. The proof is omitted.

THEOREM 8

> 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 $\mathbf{x} = \mathbf{u}_k$.

Theorem 8 will be helpful in Sections 7.4 and 7.5. The following application requires only Theorem 6.

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.

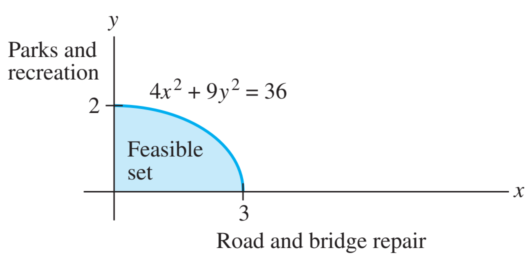


FIGURE 3 Public works schedules.

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

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

---

[2] Indifference curves are discussed in Michael D. Intriligator, Ronald G. Bodkin, and Cheng Hsiao, *Econometric Models, Techniques, and Applications* (Upper Saddle River, NJ: Prentice-Hall, 1996).

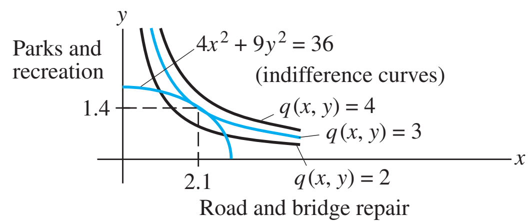


FIGURE 4 The optimum public works schedule is (2.1, 1.4).

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. ■

PRACTICE PROBLEMS

1. Let $Q(\mathbf{x}) = 3x_1^2 + 3x_2^2 + 2x_1x_2$. Find a change of variable that transforms Q into a quadratic form with no cross-product term, and give the new quadratic form.
2. With Q as in Problem 1, find the maximum value of $Q(\mathbf{x})$ subject to the constraint $\mathbf{x}^T\mathbf{x} = 1$, and find a unit vector at which the maximum is attained.

7.3 EXERCISES

In Exercises 1 and 2, find the change of variable $\mathbf{x} = P\mathbf{y}$ that transforms the quadratic form $\mathbf{x}^T A\mathbf{x}$ into $\mathbf{y}^T D\mathbf{y}$ as shown.

1. $5x_1^2 + 6x_2^2 + 7x_3^2 + 4x_1x_2 - 4x_2x_3 = 9y_1^2 + 6y_2^2 + 3y_3^2$
2. $3x_1^2 + 2x_2^2 + 2x_3^2 + 2x_1x_2 + 2x_1x_3 + 4x_2x_3 = 5y_1^2 + 2y_2^2$ [*Hint:* $\mathbf{x}$ and $\mathbf{y}$ must have the same number of coordinates, so the quadratic form shown here must have a coefficient of zero for y_3^2.]

In Exercises 3–6, find (a) the maximum value of $Q(\mathbf{x})$ subject to the constraint $\mathbf{x}^T\mathbf{x} = 1$, (b) a unit vector $\mathbf{u}$ where this maximum is attained, and (c) the maximum of $Q(\mathbf{x})$ subject to the constraints $\mathbf{x}^T\mathbf{x} = 1$ and $\mathbf{x}^T\mathbf{u} = 0$.

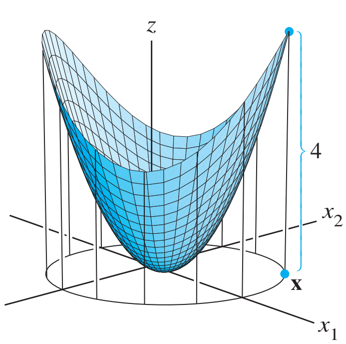
3. $Q(\mathbf{x}) = 5x_1^2 + 6x_2^2 + 7x_3^2 + 4x_1x_2 - 4x_2x_3$ (See Exercise 1.)

4. $Q(\mathbf{x}) = 3x_1^2 + 2x_2^2 + 2x_3^2 + 2x_1x_2 + 2x_1x_3 + 4x_2x_3$ (See Exercise 2.)
5. $Q(\mathbf{x}) = 5x_1^2 + 5x_2^2 - 4x_1x_2$
6. $Q(\mathbf{x}) = 7x_1^2 + 3x_2^2 + 3x_1x_2$
7. Let $Q(\mathbf{x}) = -2x_1^2 - x_2^2 + 4x_1x_2 + 4x_2x_3$. Find a unit vector $\mathbf{x}$ in $\mathbb{R}^3$ at which $Q(\mathbf{x})$ is maximized, subject to $\mathbf{x}^T\mathbf{x} = 1$. [*Hint:* The eigenvalues of the matrix of the quadratic form Q are 2, -1, and -4.]
8. Let $Q(\mathbf{x}) = 7x_1^2 + x_2^2 + 7x_3^2 - 8x_1x_2 - 4x_1x_3 - 8x_2x_3$. Find a unit vector $\mathbf{x}$ in $\mathbb{R}^3$ at which $Q(\mathbf{x})$ is maximized, subject to $\mathbf{x}^T\mathbf{x} = 1$. [*Hint:* The eigenvalues of the matrix of the quadratic form Q are 9 and -3.]
9. Find the maximum value of $Q(\mathbf{x}) = 7x_1^2 + 3x_2^2 - 2x_1x_2$, subject to the constraint $x_1^2 + x_2^2 = 1$. (Do not go on to find a vector where the maximum is attained.)
10. Find the maximum value of $Q(\mathbf{x}) = -3x_1^2 + 5x_2^2 - 2x_1x_2$, subject to the constraint $x_1^2 + x_2^2 = 1$. (Do not go on to find a vector where the maximum is attained.)
11. Suppose $\mathbf{x}$ is a unit eigenvector of a matrix A corresponding to an eigenvalue 3. What is the value of $\mathbf{x}^TA\mathbf{x}$?
12. Let λ be any eigenvalue of a symmetric matrix A. Justify the statement made in this section that $m \le \lambda \le M$, where m and M are defined as in (2). [*Hint:* Find an $\mathbf{x}$ such that $\lambda = \mathbf{x}^TA\mathbf{x}$.]
13. Let A be an $n \times n$ symmetric matrix, let M and m denote the maximum and minimum values of the quadratic form $\mathbf{x}^TA\mathbf{x}$, and denote corresponding unit eigenvectors by $\mathbf{u}_1$ and $\mathbf{u}_n$. The following calculations show that given any number t between M and m, there is a unit vector $\mathbf{x}$ such that $t = \mathbf{x}^TA\mathbf{x}$. Verify that $t = (1-\alpha)m + \alpha M$ for some number α between 0 and 1. Then let $\mathbf{x} = \sqrt{1-\alpha}\,\mathbf{u}_n + \sqrt{\alpha}\,\mathbf{u}_1$, and show that $\mathbf{x}^T\mathbf{x} = 1$ and $\mathbf{x}^TA\mathbf{x} = t$.

[M] In Exercises 14–17, follow the instructions given for Exercises 3–6.

14. $x_1x_2 + 3x_1x_3 + 30x_1x_4 + 30x_2x_3 + 3x_2x_4 + x_3x_4$
15. $3x_1x_2 + 5x_1x_3 + 7x_1x_4 + 7x_2x_3 + 5x_2x_4 + 3x_3x_4$
16. $4x_1^2 - 6x_1x_2 - 10x_1x_3 - 10x_1x_4 - 6x_2x_3 - 6x_2x_4 - 2x_3x_4$
17. $-6x_1^2 - 10x_2^2 - 13x_3^2 - 13x_4^2 - 4x_1x_2 - 4x_1x_3 - 4x_1x_4 + 6x_3x_4$

SOLUTIONS TO PRACTICE PROBLEMS



The maximum value of $Q(\mathbf{x})$ subject to $\mathbf{x}^T\mathbf{x} = 1$ is 4.

1. The matrix of the quadratic form is $A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$. It is easy to find the eigenvalues, 4 and 2, and corresponding unit eigenvectors, $\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$ and $\begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$. So the desired change of variable is $\mathbf{x} = P\mathbf{y}$, where $P = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$. (A common error here is to forget to normalize the eigenvectors.) The new quadratic form is $\mathbf{y}^TD\mathbf{y} = 4y_1^2 + 2y_2^2$.
2. The maximum of $Q(\mathbf{x})$ for $\mathbf{x}$ a unit vector is 4, and the maximum is attained at the unit eigenvector $\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$. [A common incorrect answer is $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$. This vector maximizes the quadratic form $\mathbf{y}^TD\mathbf{y}$ instead of $Q(\mathbf{x})$.]

7.4 THE SINGULAR VALUE DECOMPOSITION

The diagonalization theorems in Sections 5.3 and 7.1 play a part in many interesting applications. Unfortunately, as we know, not all matrices can be factored as $A = PDP^{-1}$ with D diagonal. However, a factorization $A = QDP^{-1}$ *is* possible for any $m \times n$ matrix A! A special factorization of this type, called the *singular value decomposition*, is one of the most useful matrix factorizations in applied linear algebra.

The singular value decomposition is based on the following property of the ordinary diagonalization that can be imitated for rectangular matrices: The absolute values of the eigenvalues of a symmetric matrix A measure the amounts that A stretches or shrinks certain vectors (the eigenvectors). If $A\mathbf{x} = \lambda\mathbf{x}$ and $\|\mathbf{x}\| = 1$, then

$$\|A\mathbf{x}\| = \|\lambda\mathbf{x}\| = |\lambda|\,\|\mathbf{x}\| = |\lambda| \tag{1}$$

If λ_1 is the eigenvalue with the greatest magnitude, then a corresponding unit eigenvector $\mathbf{v}_1$ identifies a direction in which the stretching effect of A is greatest. That is, the length of $A\mathbf{x}$ is maximized when $\mathbf{x} = \mathbf{v}_1$, and $\|A\mathbf{v}_1\| = |\lambda_1|$, by (1). This description of $\mathbf{v}_1$ and $|\lambda_1|$ has an analogue for rectangular matrices that will lead to the singular value decomposition.

EXAMPLE 1 If $A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}$, then the linear transformation $\mathbf{x} \mapsto A\mathbf{x}$ maps the unit sphere $\{\mathbf{x} : \|\mathbf{x}\| = 1\}$ in $\mathbb{R}^3$ onto an ellipse in $\mathbb{R}^2$, shown in Fig. 1. Find a unit vector $\mathbf{x}$ at which the length $\|A\mathbf{x}\|$ is maximized, and compute this maximum length.

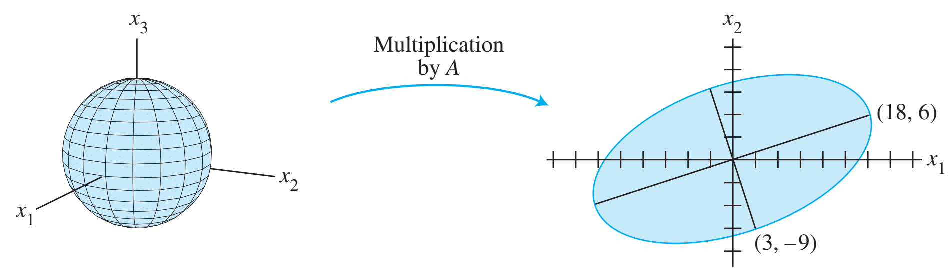


FIGURE 1 A transformation from $\mathbb{R}^3$ to $\mathbb{R}^2$.

SOLUTION The quantity $\|A\mathbf{x}\|^2$ is maximized at the same $\mathbf{x}$ that maximizes $\|A\mathbf{x}\|$, and $\|A\mathbf{x}\|^2$ is easier to study. Observe that

$$\|A\mathbf{x}\|^2 = (A\mathbf{x})^T(A\mathbf{x}) = \mathbf{x}^TA^TA\mathbf{x} = \mathbf{x}^T(A^TA)\mathbf{x}$$

Also, A^TA is a symmetric matrix, since $(A^TA)^T = A^TA^{TT} = A^TA$. So the problem now is to maximize the quadratic form $\mathbf{x}^T(A^TA)\mathbf{x}$ subject to the constraint $\|\mathbf{x}\| = 1$. By Theorem 6 in Section 7.3, the maximum value is the greatest eigenvalue λ_1 of A^TA. Also, the maximum value is attained at a unit eigenvector of A^TA corresponding to λ_1.

For the matrix A in this example,

$$A^TA = \begin{bmatrix} 4 & 8 \\ 11 & 7 \\ 14 & -2 \end{bmatrix}\begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix} = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix}$$

The eigenvalues of A^TA are $\lambda_1 = 360$, $\lambda_2 = 90$, and $\lambda_3 = 0$. Corresponding unit eigenvectors are, respectively,

$$\mathbf{v}_1 = \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} -2/3 \\ -1/3 \\ 2/3 \end{bmatrix}, \quad \mathbf{v}_3 = \begin{bmatrix} 2/3 \\ -2/3 \\ 1/3 \end{bmatrix}$$

The maximum value of $\|A\mathbf{x}\|^2$ is 360, attained when $\mathbf{x}$ is the unit vector $\mathbf{v}_1$. The vector $A\mathbf{v}_1$ is a point on the ellipse in Fig. 1 farthest from the origin, namely,

$$A\mathbf{v}_1 = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}\begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix} = \begin{bmatrix} 18 \\ 6 \end{bmatrix}$$

For $\|\mathbf{x}\| = 1$, the maximum value of $\|A\mathbf{x}\|$ is $\|A\mathbf{v}_1\| = \sqrt{360} = 6\sqrt{10}$. ∎

Example 1 suggests that the effect of A on the unit sphere in $\mathbb{R}^3$ is related to the quadratic form $\mathbf{x}^T(A^TA)\mathbf{x}$. In fact, the entire geometric behavior of the transformation $\mathbf{x} \mapsto A\mathbf{x}$ is captured by this quadratic form, as we shall see.

The Singular Values of an $m \times n$ Matrix

Let A be an $m \times n$ matrix. Then A^TA is symmetric and can be orthogonally diagonalized. Let $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ be an orthonormal basis for $\mathbb{R}^n$ consisting of eigenvectors of A^TA, and let $\lambda_1, \dots, \lambda_n$ be the associated eigenvalues of A^TA. Then, for $1 \le i \le n$,

$$\begin{aligned} \|A\mathbf{v}_i\|^2 &= (A\mathbf{v}_i)^T A\mathbf{v}_i = \mathbf{v}_i^T A^T A\mathbf{v}_i \\ &= \mathbf{v}_i^T(\lambda_i \mathbf{v}_i) && \text{Since } \mathbf{v}_i \text{ is an eigenvector of } A^TA \\ &= \lambda_i && \text{Since } \mathbf{v}_i \text{ is a unit vector} \end{aligned} \tag{2}$$

So the eigenvalues of A^TA are all nonnegative. By renumbering, if necessary, we may assume that the eigenvalues are arranged so that

$$\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n \ge 0$$

The **singular values** of A are the square roots of the eigenvalues of A^TA, denoted by $\sigma_1, \dots, \sigma_n$, and they are arranged in decreasing order. That is, $\sigma_i = \sqrt{\lambda_i}$ for $1 \le i \le n$. By equation (2), *the singular values of A are the lengths of the vectors* $A\mathbf{v}_1, \dots, A\mathbf{v}_n$.

EXAMPLE 2 Let A be the matrix in Example 1. Since the eigenvalues of A^TA are 360, 90, and 0, the singular values of A are

$$\sigma_1 = \sqrt{360} = 6\sqrt{10}, \quad \sigma_2 = \sqrt{90} = 3\sqrt{10}, \quad \sigma_3 = 0$$

From Example 1, the first singular value of A is the maximum of $\|A\mathbf{x}\|$ over all unit vectors, and the maximum is attained at the unit eigenvector $\mathbf{v}_1$. Theorem 7 in Section 7.3 shows that the second singular value of A is the maximum of $\|A\mathbf{x}\|$ over all unit vectors that are *orthogonal to* $\mathbf{v}_1$, and this maximum is attained at the second unit eigenvector, $\mathbf{v}_2$ (Exercise 22). For the $\mathbf{v}_2$ in Example 1,

$$A\mathbf{v}_2 = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix} \begin{bmatrix} -2/3 \\ -1/3 \\ 2/3 \end{bmatrix} = \begin{bmatrix} 3 \\ -9 \end{bmatrix}$$

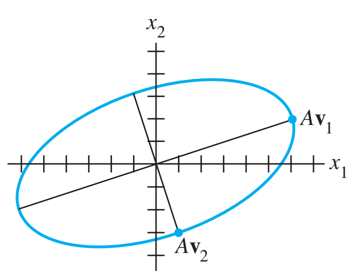


FIGURE 2

This point is on the minor axis of the ellipse in Fig. 1, just as $A\mathbf{v}_1$ is on the major axis. (See Fig. 2.) The first two singular values of A are the lengths of the major and minor semiaxes of the ellipse. ■

The fact that $A\mathbf{v}_1$ and $A\mathbf{v}_2$ are orthogonal in Fig. 2 is no accident, as the next theorem shows.

THEOREM 9 Suppose $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ is an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvectors of A^TA, arranged so that the corresponding eigenvalues of A^TA satisfy $\lambda_1 \ge \cdots \ge \lambda_n$, and suppose A has r nonzero singular values. Then $\{A\mathbf{v}_1, \dots, A\mathbf{v}_r\}$ is an orthogonal basis for Col A, and rank $A = r$.

PROOF Because $\mathbf{v}_i$ and $\lambda_j \mathbf{v}_j$ are orthogonal for $i \ne j$,

$$(A\mathbf{v}_i)^T(A\mathbf{v}_j) = \mathbf{v}_i^T A^T A\mathbf{v}_j = \mathbf{v}_i^T(\lambda_j \mathbf{v}_j) = 0$$

Thus $\{A\mathbf{v}_1, \dots, A\mathbf{v}_n\}$ is an orthogonal set. Furthermore, since the lengths of the vectors $A\mathbf{v}_1, \dots, A\mathbf{v}_n$ are the singular values of A, and since there are r nonzero singular values, $A\mathbf{v}_i \ne \mathbf{0}$ if and only if $1 \le i \le r$. So $A\mathbf{v}_1, \dots, A\mathbf{v}_r$ are linearly independent vectors, and they are in Col A. Finally, for any $\mathbf{y}$ in Col A—say, $\mathbf{y} = A\mathbf{x}$—we can write $\mathbf{x} = c_1\mathbf{v}_1 + \cdots + c_n\mathbf{v}_n$, and

$$\begin{aligned} \mathbf{y} = A\mathbf{x} &= c_1 A\mathbf{v}_1 + \cdots + c_r A\mathbf{v}_r + c_{r+1}A\mathbf{v}_{r+1} + \cdots + c_n A\mathbf{v}_n \\ &= c_1 A\mathbf{v}_1 + \cdots + c_r A\mathbf{v}_r + 0 + \cdots + 0 \end{aligned}$$

Thus $\mathbf{y}$ is in Span $\{A\mathbf{v}_1, \dots, A\mathbf{v}_r\}$, which shows that $\{A\mathbf{v}_1, \dots, A\mathbf{v}_r\}$ is an (orthogonal) basis for Col A. Hence rank $A = \dim \text{Col } A = r$. ■

NUMERICAL NOTE

In some cases, the rank of A may be very sensitive to small changes in the entries of A. The obvious method of counting the number of pivot columns in A does not work well if A is row reduced by a computer. Roundoff error often creates an echelon form with full rank.

In practice, the most reliable way to estimate the rank of a large matrix A is to count the number of nonzero singular values. In this case, extremely small nonzero singular values are assumed to be zero for all practical purposes, and the *effective rank* of the matrix is the number obtained by counting the remaining nonzero singular values.[1]

The Singular Value Decomposition

The decomposition of A involves an $m \times n$ "diagonal" matrix Σ of the form

$$\Sigma = \begin{array}{c} \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \begin{array}{l} \\ \leftarrow m-r \text{ rows} \end{array} \\ \qquad\quad \uparrow n-r \text{ columns} \end{array} \tag{3}$$

where D is an $r \times r$ diagonal matrix for some r not exceeding the smaller of m and n. (If r equals m or n or both, some or all of the zero matrices do not appear.)

THEOREM 10

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

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

Any factorization $A = U\Sigma V^T$, with U and V orthogonal, Σ as in (3), and positive diagonal entries in D, is called a **singular value decomposition** (or **SVD**) of A. The matrices U and V are not uniquely determined by A, but the diagonal entries of Σ are necessarily the singular values of A. See Exercise 19. The columns of U in such a decomposition are called **left singular vectors** of A, and the columns of V are called **right singular vectors** of A.

[1] In general, rank estimation is not a simple problem. For a discussion of the subtle issues involved, see Philip E. Gill, Walter Murray, and Margaret H. Wright, *Numerical Linear Algebra and Optimization*, vol. 1 (Redwood City, CA: Addison-Wesley, 1991), Sec. 5.8.

PROOF Let λ_i and $\mathbf{v}_i$ be as in Theorem 9, so that $\{A\mathbf{v}_1, \dots, A\mathbf{v}_r\}$ is an orthogonal basis for Col A. Normalize each $A\mathbf{v}_i$ to obtain an orthonormal basis $\{\mathbf{u}_1, \dots, \mathbf{u}_r\}$, where

$$\mathbf{u}_i = \frac{1}{\|A\mathbf{v}_i\|}A\mathbf{v}_i = \frac{1}{\sigma_i}A\mathbf{v}_i$$

and

$$A\mathbf{v}_i = \sigma_i \mathbf{u}_i \qquad (1 \le i \le r) \tag{4}$$

Now extend $\{\mathbf{u}_1, \dots, \mathbf{u}_r\}$ to an orthonormal basis $\{\mathbf{u}_1, \dots, \mathbf{u}_m\}$ of $\mathbb{R}^m$, and let

$$U = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_m\,] \quad \text{and} \quad V = [\,\mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_n\,]$$

By construction, U and V are orthogonal matrices. Also, from (4),

$$AV = [\,A\mathbf{v}_1 \quad \cdots \quad A\mathbf{v}_r \quad \mathbf{0} \quad \cdots \quad \mathbf{0}\,] = [\,\sigma_1\mathbf{u}_1 \quad \cdots \quad \sigma_r\mathbf{u}_r \quad \mathbf{0} \quad \cdots \quad \mathbf{0}\,]$$

Let D be the diagonal matrix with diagonal entries $\sigma_1, \dots, \sigma_r$, and let Σ be as in (3) above. Then

$$U\Sigma = [\,\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_m\,]\left[\begin{array}{cccc|c} \sigma_1 & & & 0 & \\ & \sigma_2 & & & 0 \\ & & \ddots & & \\ 0 & & & \sigma_r & \\ \hline & & 0 & & 0 \end{array}\right]$$

$$= [\,\sigma_1\mathbf{u}_1 \quad \cdots \quad \sigma_r\mathbf{u}_r \quad \mathbf{0} \quad \cdots \quad \mathbf{0}\,]$$
$$= AV$$

Since V is an orthogonal matrix, $U\Sigma V^T = AVV^T = A$. ■

The next two examples focus attention on the internal structure of a singular value decomposition. An efficient and numerically stable algorithm for this decomposition would use a different approach. See the Numerical Note at the end of the section.

EXAMPLE 3 Use the results of Examples 1 and 2 to construct a singular value decomposition of $A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}$.

SOLUTION A construction can be divided into three steps.

SG Computing an SVD 7-10

Step 1. Find an orthogonal diagonalization of A^TA. That is, find the eigenvalues of A^TA and a corresponding orthonormal set of eigenvectors. If A had only two columns, the calculations could be done by hand. Larger matrices usually require a matrix program.[2] However, for the matrix A here, the eigendata for A^TA are provided in Example 1.

Step 2. Set up V and Σ. Arrange the eigenvalues of A^TA in decreasing order. In Example 1, the eigenvalues are already listed in decreasing order: 360, 90, and 0. The corresponding unit eigenvectors, $\mathbf{v}_1$, $\mathbf{v}_2$, and $\mathbf{v}_3$, are the right singular vectors of A. Using Example 1, construct

$$V = [\,\mathbf{v}_1 \quad \mathbf{v}_2 \quad \mathbf{v}_3\,] = \begin{bmatrix} 1/3 & -2/3 & 2/3 \\ 2/3 & -1/3 & -2/3 \\ 2/3 & 2/3 & 1/3 \end{bmatrix}$$

[2] See the *Study Guide* for software and graphing calculator commands. MATLAB, for instance, can produce both the eigenvalues and the eigenvectors with one command, `eig`.

The square roots of the eigenvalues are the singular values:

$$\sigma_1 = 6\sqrt{10}, \quad \sigma_2 = 3\sqrt{10}, \quad \sigma_3 = 0$$

The nonzero singular values are the diagonal entries of D. The matrix Σ is the same size as A, with D in its upper left corner and with 0's elsewhere.

$$D = \begin{bmatrix} 6\sqrt{10} & 0 \\ 0 & 3\sqrt{10} \end{bmatrix}, \qquad \Sigma = [\, D \quad 0 \,] = \begin{bmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{bmatrix}$$

Step 3. ***Construct U.*** When A has rank r, the first r columns of U are the normalized vectors obtained from $A\mathbf{v}_1, \dots, A\mathbf{v}_r$. In this example, A has two nonzero singular values, so rank $A = 2$. Recall from equation (2) and the paragraph before Example 2 that $\|A\mathbf{v}_1\| = \sigma_1$ and $\|A\mathbf{v}_2\| = \sigma_2$. Thus

$$\mathbf{u}_1 = \frac{1}{\sigma_1} A\mathbf{v}_1 = \frac{1}{6\sqrt{10}} \begin{bmatrix} 18 \\ 6 \end{bmatrix} = \begin{bmatrix} 3/\sqrt{10} \\ 1/\sqrt{10} \end{bmatrix}$$

$$\mathbf{u}_2 = \frac{1}{\sigma_2} A\mathbf{v}_2 = \frac{1}{3\sqrt{10}} \begin{bmatrix} 3 \\ -9 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{10} \\ -3/\sqrt{10} \end{bmatrix}$$

Note that $\{\mathbf{u}_1, \mathbf{u}_2\}$ is already a basis for $\mathbb{R}^2$. Thus no additional vectors are needed for U, and $U = [\, \mathbf{u}_1 \quad \mathbf{u}_2 \,]$. The singular value decomposition of A is

$$A = \underset{\substack{\uparrow \\ U}}{\begin{bmatrix} 3/\sqrt{10} & 1/\sqrt{10} \\ 1/\sqrt{10} & -3/\sqrt{10} \end{bmatrix}} \underset{\substack{\uparrow \\ \Sigma}}{\begin{bmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{bmatrix}} \underset{\substack{\uparrow \\ V^T}}{\begin{bmatrix} 1/3 & 2/3 & 2/3 \\ -2/3 & -1/3 & 2/3 \\ 2/3 & -2/3 & 1/3 \end{bmatrix}}$$

■

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

SOLUTION First, compute $A^TA = \begin{bmatrix} 9 & -9 \\ -9 & 9 \end{bmatrix}$. The eigenvalues of A^TA 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 $A\mathbf{v}_2$:

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

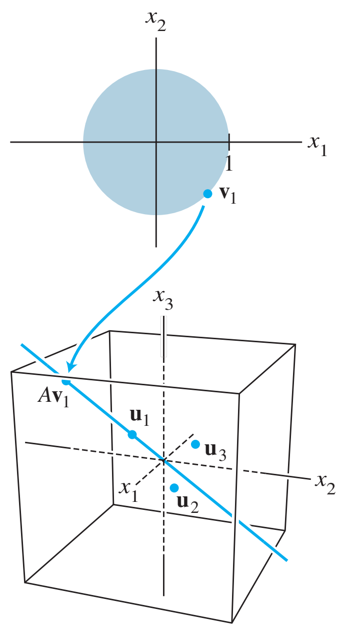


FIGURE 3

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

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

■

Applications of the Singular Value Decomposition

The SVD is often used to estimate the rank of a matrix, as noted above. Several other numerical applications are described briefly below, and an application to image processing is presented in Section 7.5.

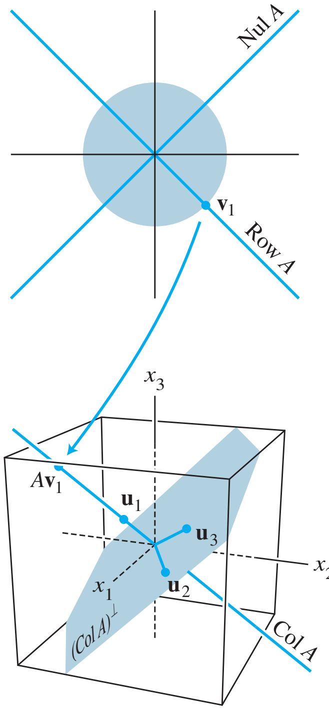
EXAMPLE 5 (The Condition Number) Most numerical calculations involving an equation $A\mathbf{x} = \mathbf{b}$ are as reliable as possible when the SVD of A is used. The two orthogonal matrices U and V do not affect lengths of vectors or angles between vectors (Theorem 7 in Section 6.2). Any possible instabilities in numerical calculations are identified in Σ. If the singular values of A are extremely large or small, roundoff errors are almost inevitable, but an error analysis is aided by knowing the entries in Σ and V.

If A is an invertible $n \times n$ matrix, then the ratio σ_1/σ_n of the largest and smallest singular values gives the **condition number** of A. Exercises 41–43 in Section 2.3 showed how the condition number affects the sensitivity of a solution of $A\mathbf{x} = \mathbf{b}$ to changes (or errors) in the entries of A. (Actually, a "condition number" of A can be computed in several ways, but the definition given here is widely used for studying $A\mathbf{x} = \mathbf{b}$.) ■

EXAMPLE 6 (Bases for Fundamental Subspaces) Given an SVD for an $m \times n$ matrix A, let $\mathbf{u}_1, \ldots, \mathbf{u}_m$ be the left singular vectors, $\mathbf{v}_1, \ldots, \mathbf{v}_n$ the right singular vectors, and $\sigma_1, \ldots, \sigma_n$ the singular values, and let r be the rank of A. By Theorem 9,

$$\{\mathbf{u}_1, \ldots, \mathbf{u}_r\} \tag{5}$$

is an orthonormal basis for Col A.



The fundamental subspaces in Example 4.

Recall from Theorem 3 in Section 6.1 that $(\text{Col } A)^\perp = \text{Nul } A^T$. Hence

$$\{\mathbf{u}_{r+1}, \dots, \mathbf{u}_m\} \tag{6}$$

is an orthonormal basis for Nul A^T.

Since $\|A\mathbf{v}_i\| = \sigma_i$ for $1 \le i \le n$, and σ_i is 0 if and only if $i > r$, the vectors $\mathbf{v}_{r+1}, \dots, \mathbf{v}_n$ span a subspace of Nul A of dimension $n - r$. By the Rank Theorem, dim Nul $A = n - \text{rank } A$. It follows that

$$\{\mathbf{v}_{r+1}, \dots, \mathbf{v}_n\} \tag{7}$$

is an orthonormal basis for Nul A, by the Basis Theorem (in Section 4.5).

From (5) and (6), the orthogonal complement of Nul A^T is Col A. Interchanging A and A^T, note that $(\text{Nul } A)^\perp = \text{Col } A^T = \text{Row } A$. Hence, from (7),

$$\{\mathbf{v}_1, \dots, \mathbf{v}_r\} \tag{8}$$

is an orthonormal basis for Row A.

Figure 4 summarizes (5)–(8), but shows the orthogonal basis $\{\sigma_1\mathbf{u}_1, \dots, \sigma_r\mathbf{u}_r\}$ for Col A instead of the normalized basis, to remind you that $A\mathbf{v}_i = \sigma_i\mathbf{u}_i$ for $1 \le i \le r$. Explicit orthonormal bases for the four fundamental subspaces determined by A are useful in some calculations, particularly in constrained optimization problems. ■

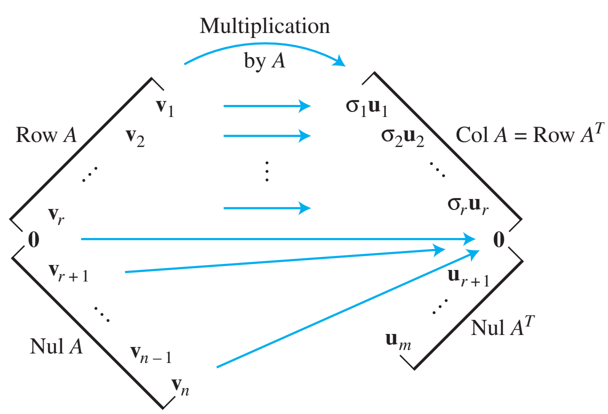


FIGURE 4 The four fundamental subspaces and the action of A.

The four fundamental subspaces and the concept of singular values provide the final statements of the Invertible Matrix Theorem. (Recall that statements about A^T have been omitted from the theorem, to avoid nearly doubling the number of statements.) The other statements were given in Sections 2.3, 2.9, 3.2, 4.6, and 5.2.

THEOREM

The Invertible Matrix Theorem (concluded)

Let A be an $n \times n$ matrix. Then the following statements are each equivalent to the statement that A is an invertible matrix.

u. $(\text{Col } A)^\perp = \{\mathbf{0}\}$.

v. $(\text{Nul } A)^\perp = \mathbb{R}^n$.

w. Row $A = \mathbb{R}^n$.

x. A has n nonzero singular values.

EXAMPLE 7 (Reduced SVD and the Pseudoinverse of A) When Σ contains rows or columns of zeros, a more compact decomposition of A is possible. Using the notation established above, let $r = \text{rank}\, A$, and partition U and V into submatrices whose first blocks contain r columns:

$$\begin{aligned} U &= [\, U_r \quad U_{m-r} \,], \quad \text{where } U_r = [\, \mathbf{u}_1 \quad \cdots \quad \mathbf{u}_r \,] \\ V &= [\, V_r \quad V_{n-r} \,], \quad \text{where } V_r = [\, \mathbf{v}_1 \quad \cdots \quad \mathbf{v}_r \,] \end{aligned}$$

Then U_r is $m \times r$ and V_r is $n \times r$. (To simplify notation, we consider U_{m-r} or V_{n-r} even though one of them may have no columns.) Then partitioned matrix multiplication shows that

$$A = [\, U_r \quad U_{m-r} \,] \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_r^T \\ V_{n-r}^T \end{bmatrix} = U_r D V_r^T \tag{9}$$

This factorization of A is called a **reduced singular value decomposition** of A. Since the diagonal entries in D are nonzero, D is invertible. The following matrix is called the **pseudoinverse** (also, the **Moore–Penrose inverse**) of A:

$$A^+ = V_r D^{-1} U_r^T \tag{10}$$

Supplementary Exercises 12–14 at the end of the chapter explore some of the properties of the reduced singular value decomposition and the pseudoinverse. ■

EXAMPLE 8 (Least-Squares Solution) Given the equation $A\mathbf{x} = \mathbf{b}$, use the pseudoinverse of A in (10) to define

$$\hat{\mathbf{x}} = A^+\mathbf{b} = V_r D^{-1} U_r^T \mathbf{b}$$

Then, from the SVD in (9),

$$\begin{aligned} A\hat{\mathbf{x}} &= (U_r D V_r^T)(V_r D^{-1} U_r^T \mathbf{b}) \\ &= U_r D D^{-1} U_r^T \mathbf{b} \qquad \text{Because } V_r^T V_r = I_r \\ &= U_r U_r^T \mathbf{b} \end{aligned}$$

It follows from (5) that $U_r U_r^T \mathbf{b}$ is the orthogonal projection $\hat{\mathbf{b}}$ of $\mathbf{b}$ onto Col A. (See Theorem 10 in Section 6.3.) Thus $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$. In fact, this $\hat{\mathbf{x}}$ has the smallest length among all least-squares solutions of $A\mathbf{x} = \mathbf{b}$. See Supplementary Exercise 14. ■

NUMERICAL NOTE

Examples 1–4 and the exercises illustrate the concept of singular values and suggest how to perform calculations by hand. In practice, the computation of A^TA should be avoided, since any errors in the entries of A are squared in the entries of A^TA. There exist fast iterative methods that produce the singular values and singular vectors of A accurately to many decimal places.

Further Reading

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PRACTICE PROBLEM

WEB

Given a singular value decomposition, $A = U\Sigma V^T$, find an SVD of A^T. How are the singular values of A and A^T related?

7.4 EXERCISES

Find the singular values of the matrices in Exercises 1–4.

1. $\begin{bmatrix} 1 & 0 \\ 0 & -3 \end{bmatrix}$ **2.** $\begin{bmatrix} -5 & 0 \\ 0 & 0 \end{bmatrix}$

3. $\begin{bmatrix} \sqrt{6} & 1 \\ 0 & \sqrt{6} \end{bmatrix}$ **4.** $\begin{bmatrix} \sqrt{3} & 2 \\ 0 & \sqrt{3} \end{bmatrix}$

Find an SVD of each matrix in Exercises 5–12. [*Hint:* In Exercise 11, one choice for U is $\begin{bmatrix} -1/3 & 2/3 & 2/3 \\ 2/3 & -1/3 & 2/3 \\ 2/3 & 2/3 & -1/3 \end{bmatrix}$. In Exercise 12, one column of U can be $\begin{bmatrix} 1/\sqrt{6} \\ -2/\sqrt{6} \\ 1/\sqrt{6} \end{bmatrix}$.]

5. $\begin{bmatrix} -3 & 0 \\ 0 & 0 \end{bmatrix}$ **6.** $\begin{bmatrix} -2 & 0 \\ 0 & -1 \end{bmatrix}$

7. $\begin{bmatrix} 2 & -1 \\ 2 & 2 \end{bmatrix}$ **8.** $\begin{bmatrix} 2 & 3 \\ 0 & 2 \end{bmatrix}$

9. $\begin{bmatrix} 7 & 1 \\ 0 & 0 \\ 5 & 5 \end{bmatrix}$ **10.** $\begin{bmatrix} 4 & -2 \\ 2 & -1 \\ 0 & 0 \end{bmatrix}$

11. $\begin{bmatrix} -3 & 1 \\ 6 & -2 \\ 6 & -2 \end{bmatrix}$ **12.** $\begin{bmatrix} 1 & 1 \\ 0 & 1 \\ -1 & 1 \end{bmatrix}$

13. Find the SVD of $A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}$ [*Hint:* Work with A^T.]

14. In Exercise 7, find a unit vector $\mathbf{x}$ at which $A\mathbf{x}$ has maximum length.

15. Suppose the factorization below is an SVD of a matrix A, with the entries in U and V rounded to two decimal places.

$$A = \begin{bmatrix} .40 & -.78 & .47 \\ .37 & -.33 & -.87 \\ -.84 & -.52 & -.16 \end{bmatrix} \begin{bmatrix} 7.10 & 0 & 0 \\ 0 & 3.10 & 0 \\ 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} .30 & -.51 & -.81 \\ .76 & .64 & -.12 \\ .58 & -.58 & .58 \end{bmatrix}$$

a. What is the rank of A?

b. Use this decomposition of A, with no calculations, to write a basis for Col A and a basis for Nul A. [*Hint:* First write the columns of V.]

16. Repeat Exercise 15 for the following SVD of a 3×4 matrix A:

$$A = \begin{bmatrix} -.86 & -.11 & -.50 \\ .31 & .68 & -.67 \\ .41 & -.73 & -.55 \end{bmatrix} \begin{bmatrix} 12.48 & 0 & 0 & 0 \\ 0 & 6.34 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} .66 & -.03 & -.35 & .66 \\ -.13 & -.90 & -.39 & -.13 \\ .65 & .08 & -.16 & -.73 \\ -.34 & .42 & -.84 & -.08 \end{bmatrix}$$

In Exercises 17–24, A is an $m \times n$ matrix with a singular value decomposition $A = U\Sigma V^T$, where U is an $m \times m$ orthogonal matrix, Σ is an $m \times n$ "diagonal" matrix with r positive entries and no negative entries, and V is an $n \times n$ orthogonal matrix. Justify each answer.

17. Suppose A is square and invertible. Find a singular value decomposition of A^{-1}.

18. Show that if A is square, then $|\det A|$ is the product of the singular values of A.

19. Show that the columns of V are eigenvectors of A^TA, the columns of U are eigenvectors of AA^T, and the diagonal entries of Σ are the singular values of A. [*Hint:* Use the SVD to compute A^TA and AA^T.]

20. Show that if A is an $n \times n$ positive definite matrix, then an orthogonal diagonalization $A = PDP^T$ is a singular value decomposition of A.

21. Show that if P is an orthogonal $m \times m$ matrix, then PA has the same singular values as A.

22. Justify the statement in Example 2 that the second singular value of a matrix A is the maximum of $\|A\mathbf{x}\|$ as $\mathbf{x}$ varies over all unit vectors orthogonal to $\mathbf{v}_1$, with $\mathbf{v}_1$ a right singular vector corresponding to the first singular value of A. [*Hint:* Use Theorem 7 in Section 7.3.]

23. Let $U = [\,\mathbf{u}_1 \ \ \cdots \ \ \mathbf{u}_m\,]$ and $V = [\,\mathbf{v}_1 \ \ \cdots \ \ \mathbf{v}_n\,]$, where the $\mathbf{u}_i$ and $\mathbf{v}_i$ are as in Theorem 10. Show that

$$A = \sigma_1\mathbf{u}_1\mathbf{v}_1^T + \sigma_2\mathbf{u}_2\mathbf{v}_2^T + \cdots + \sigma_r\mathbf{u}_r\mathbf{v}_r^T.$$

24. Using the notation of Exercise 23, show that $A^T\mathbf{u}_j = \sigma_j\mathbf{v}_j$ for $1 \le j \le r = \text{rank}\,A$.

25. Let $T : \mathbb{R}^n \to \mathbb{R}^m$ be a linear transformation. Describe how to find a basis $\mathcal{B}$ for $\mathbb{R}^n$ and a basis $\mathcal{C}$ for $\mathbb{R}^m$ such that the matrix for T relative to $\mathcal{B}$ and $\mathcal{C}$ is an $m \times n$ "diagonal" matrix.

[**M**] Compute an SVD of each matrix in Exercises 26 and 27. Report the final matrix entries accurate to two decimal places. Use the method of Examples 3 and 4.

26. $A = \begin{bmatrix} -18 & 13 & -4 & 4 \\ 2 & 19 & -4 & 12 \\ -14 & 11 & -12 & 8 \\ -2 & 21 & 4 & 8 \end{bmatrix}$

27. $A = \begin{bmatrix} 6 & -8 & -4 & 5 & -4 \\ 2 & 7 & -5 & -6 & 4 \\ 0 & -1 & -8 & 2 & 2 \\ -1 & -2 & 4 & 4 & -8 \end{bmatrix}$

28. [**M**] Compute the singular values of the 4×4 matrix in Exercise 9 in Section 2.3, and compute the condition number σ_1/σ_4.

29. [**M**] Compute the singular values of the 5×5 matrix in Exercise 10 in Section 2.3, and compute the condition number σ_1/σ_5.

SOLUTION TO PRACTICE PROBLEM

If $A = U\Sigma V^T$, where Σ is $m \times n$, then $A^T = (V^T)^T\Sigma^T U^T = V\Sigma^T U^T$. This is an SVD of A^T because V and U are orthogonal matrices and Σ^T is an $n \times m$ "diagonal" matrix. Since Σ and Σ^T have the same nonzero diagonal entries, A and A^T have the same nonzero singular values. [*Note:* If A is $2 \times n$, then AA^T is only 2×2 and its eigenvalues may be easier to compute (by hand) than the eigenvalues of A^TA.]

7.5 APPLICATIONS TO IMAGE PROCESSING AND STATISTICS

The satellite photographs in this chapter's introduction provide an example of multidimensional, or *multivariate*, data—information organized so that each datum in the data set is identified with a point (vector) in $\mathbb{R}^n$. The main goal of this section is to explain a technique, called *principal component analysis*, used to analyze such multivariate data. The calculations will illustrate the use of orthogonal diagonalization and the singular value decomposition.

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**.

Loosely speaking, we can say that the process control data are eight-dimensional. The next two examples describe data that can be visualized graphically.

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

$$\begin{bmatrix} w_1 & w_2 & \cdots & w_N \\ h_1 & h_2 & \cdots & h_N \end{bmatrix}$$
$$\begin{array}{cccc} \uparrow & \uparrow & & \uparrow \\ \mathbf{X}_1 & \mathbf{X}_2 & & \mathbf{X}_N \end{array}$$

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

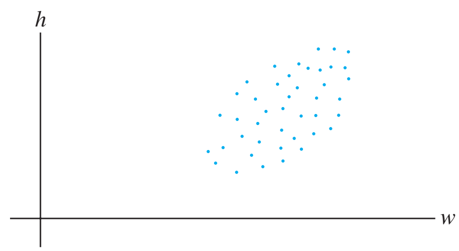

FIGURE 1 A scatter plot of observation vectors $\mathbf{X}_1, \dots, \mathbf{X}_N$.

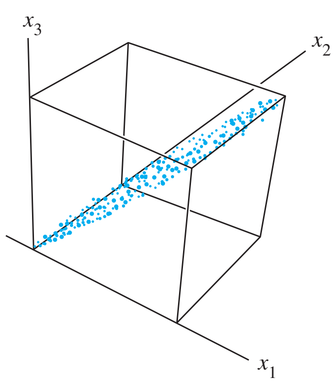

FIGURE 2
A scatter plot of spectral data for a satellite image.

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 $\mathbf{X}_1, \dots, \mathbf{X}_N$ 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 $k = 1, \dots, N$, 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.

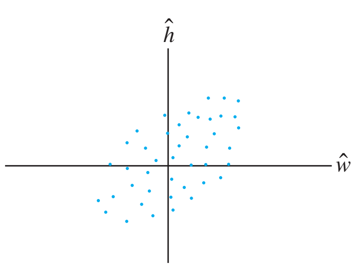

FIGURE 3
Weight–height data in mean-deviation form.

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 $\mathbf{X}_1, \ldots, \mathbf{X}_4$ 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 $x_1, \ldots, x_p$. Then x_1, for example, is a scalar that varies over the set of first coordinates of $\mathbf{X}_1, \ldots, \mathbf{X}_N$. For $j = 1, \ldots, p$, 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]

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

[1] Data for Example 4 and Exercises 5 and 6 were provided by Earth Satellite Corporation, Rockville, Maryland.

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

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

The variance of y_j is λ_j, and the quotient $\lambda_j / \text{tr}(S)$ 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

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

[Verify that this number also equals $\text{tr}(S)$.] 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). ■

The calculations in Example 5 show that the data have practically no variance in the third (new) coordinate. The values of y_3 are all close to zero. Geometrically, the data points lie nearly in the plane $y_3 = 0$, and their locations can be determined fairly accurately by knowing only the values of y_1 and y_2. In fact, y_2 also has relatively small variance, which means that the points lie approximately along a line, and the data are essentially one-dimensional. See Fig. 2, in which the data resemble a popsicle stick.

Characterizations of Principal Component Variables

If $y_1, \dots, y_p$ arise from a principal component analysis of a $p \times N$ matrix of observations, then the variance of y_1 is as large as possible in the following sense: If $\mathbf{u}$ is any unit vector and if $y = \mathbf{u}^T\mathbf{X}$, then the variance of the values of y as $\mathbf{X}$ varies over the original data $\mathbf{X}_1, \dots, \mathbf{X}_N$ turns out to be $\mathbf{u}^T S\mathbf{u}$. By Theorem 8 in Section 7.3, the maximum value of $\mathbf{u}^T S\mathbf{u}$, over all unit vectors $\mathbf{u}$, is the largest eigenvalue λ_1 of S, and this variance is attained when $\mathbf{u}$ is the corresponding eigenvector $\mathbf{u}_1$. In the same way, Theorem 8 shows that y_2 has maximum possible variance among all variables $y = \mathbf{u}^T\mathbf{X}$ that are *uncorrelated* with y_1. Likewise, y_3 has maximum possible variance among all variables uncorrelated with both y_1 and y_2, and so on.

NUMERICAL NOTE

The singular value decomposition is the main tool for performing principal component analysis in practical applications. If B is a $p \times N$ matrix of observations in mean-deviation form, and if $A = \left(1/\sqrt{N-1}\right)B^T$, then A^TA is the covariance matrix, S. The squares of the singular values of A are the p eigenvalues of S, and the right singular vectors of A are the principal components of the data.

As mentioned in Section 7.4, iterative calculation of the SVD of A is faster and more accurate than an eigenvalue decomposition of S. This is particularly true, for instance, in the hyperspectral image processing (with $p = 224$) mentioned in the chapter introduction. Principal component analysis is completed in seconds on specialized workstations.

Further Reading

Lillesand, Thomas M., and Ralph W. Kiefer, *Remote Sensing and Image Interpretation*, 4th ed. (New York: John Wiley, 2000).

PRACTICE PROBLEMS

The following table lists the weights and heights of five boys:

Boy	#1	#2	#3	#4	#5
Weight (lb)	120	125	125	135	145
Height (in.)	61	60	64	68	72

1. Find the covariance matrix for the data.
2. Make a principal component analysis of the data to find a single *size index* that explains most of the variation in the data.

7.5 EXERCISES

In Exercises 1 and 2, convert the matrix of observations to mean-deviation form, and construct the sample covariance matrix.

1. $\begin{bmatrix} 19 & 22 & 6 & 3 & 2 & 20 \\ 12 & 6 & 9 & 15 & 13 & 5 \end{bmatrix}$

2. $\begin{bmatrix} 1 & 5 & 2 & 6 & 7 & 3 \\ 3 & 11 & 6 & 8 & 15 & 11 \end{bmatrix}$

3. Find the principal components of the data for Exercise 1.

4. Find the principal components of the data for Exercise 2.

5. **[M]** A Landsat image with three spectral components was made of Homestead Air Force Base in Florida (after the base was hit by hurricane Andrew in 1992). The covariance matrix of the data is shown below. Find the first principal component of the data, and compute the percentage of the total variance that is contained in this component.

$$S = \begin{bmatrix} 164.12 & 32.73 & 81.04 \\ 32.73 & 539.44 & 249.13 \\ 81.04 & 249.13 & 189.11 \end{bmatrix}$$

6. **[M]** The covariance matrix below was obtained from a Landsat image of the Columbia River in Washington, using data from three spectral bands. Let x_1, x_2, x_3 denote the spectral components of each pixel in the image. Find a new variable of the form $y_1 = c_1x_1 + c_2x_2 + c_3x_3$ that has maximum possible variance, subject to the constraint that $c_1^2 + c_2^2 + c_3^2 = 1$. What percentage of the total variance in the data is explained by y_1?

$$S = \begin{bmatrix} 29.64 & 18.38 & 5.00 \\ 18.38 & 20.82 & 14.06 \\ 5.00 & 14.06 & 29.21 \end{bmatrix}$$

7. Let x_1, x_2 denote the variables for the two-dimensional data in Exercise 1. Find a new variable y_1 of the form $y_1 = c_1x_1 + c_2x_2$, with $c_1^2 + c_2^2 = 1$, such that y_1 has maximum possible variance over the given data. How much of the variance in the data is explained by y_1?

8. Repeat Exercise 7 for the data in Exercise 2.

9. Suppose three tests are administered to a random sample of college students. Let $\mathbf{X}_1, \dots, \mathbf{X}_N$ be observation vectors in $\mathbb{R}^3$ that list the three scores of each student, and for $j = 1, 2, 3$, let x_j denote a student's score on the jth exam. Suppose the covariance matrix of the data is

$$S = \begin{bmatrix} 5 & 2 & 0 \\ 2 & 6 & 2 \\ 0 & 2 & 7 \end{bmatrix}$$

Let y be an "index" of student performance, with $y = c_1x_1 + c_2x_2 + c_3x_3$ and $c_1^2 + c_2^2 + c_3^2 = 1$. Choose c_1, c_2, c_3 so that the variance of y over the data set is as large as possible. [*Hint:* The eigenvalues of the sample covariance matrix are $\lambda = 3, 6$, and 9.]

10. **[M]** Repeat Exercise 9 with $S = \begin{bmatrix} 5 & 4 & 2 \\ 4 & 11 & 4 \\ 2 & 4 & 5 \end{bmatrix}$.

11. Given multivariate data $\mathbf{X}_1, \dots, \mathbf{X}_N$ (in $\mathbb{R}^p$) in mean-deviation form, let P be a $p \times p$ matrix, and define $\mathbf{Y}_k = P^T\mathbf{X}_k$ for $k = 1, \dots, N$.
    a. Show that $\mathbf{Y}_1, \dots, \mathbf{Y}_N$ are in mean-deviation form. [*Hint:* Let $\mathbf{w}$ be the vector in $\mathbb{R}^N$ with a 1 in each entry. Then $[\,\mathbf{X}_1 \ \cdots \ \mathbf{X}_N\,]\,\mathbf{w} = \mathbf{0}$ (the zero vector in $\mathbb{R}^p$).]
    b. Show that if the covariance matrix of $\mathbf{X}_1, \dots, \mathbf{X}_N$ is S, then the covariance matrix of $\mathbf{Y}_1, \dots, \mathbf{Y}_N$ is P^TSP.

12. Let $\mathbf{X}$ denote a vector that varies over the columns of a $p \times N$ matrix of observations, and let P be a $p \times p$ orthogonal matrix. Show that the change of variable $\mathbf{X} = P\mathbf{Y}$ does not change the total variance of the data. [*Hint:* By Exercise 11, it suffices to show that $\operatorname{tr}(P^TSP) = \operatorname{tr}(S)$. Use a property of the trace mentioned in Exercise 25 in Section 5.4.]

13. The sample covariance matrix is a generalization of a formula for the variance of a sample of N scalar measurements, say, $t_1, \dots, t_N$. If m is the average of $t_1, \dots, t_N$, then the *sample variance* is given by

$$\frac{1}{N-1}\sum_{k=1}^{n}(t_k - m)^2 \qquad (1)$$

Show how the sample covariance matrix, S, defined prior to Example 3, may be written in a form similar to (1). [*Hint:* Use partitioned matrix multiplication to write S as $1/(N-1)$ times the sum of N matrices of size $p \times p$. For $1 \le k \le N$, write $\mathbf{X}_k - \mathbf{M}$ in place of $\hat{\mathbf{X}}_k$.]

SOLUTIONS TO PRACTICE PROBLEMS

1. First arrange the data in mean-deviation form. The sample mean vector is easily seen to be $\mathbf{M} = \begin{bmatrix} 130 \\ 65 \end{bmatrix}$. Subtract $\mathbf{M}$ from the observation vectors (the columns in the table) and obtain

$$B = \begin{bmatrix} -10 & -5 & -5 & 5 & 15 \\ -4 & -5 & -1 & 3 & 7 \end{bmatrix}$$

Then the sample covariance matrix is

$$S = \frac{1}{5-1}\begin{bmatrix} -10 & -5 & -5 & 5 & 15 \\ -4 & -5 & -1 & 3 & 7 \end{bmatrix}\begin{bmatrix} -10 & -4 \\ -5 & -5 \\ -5 & -1 \\ 5 & 3 \\ 15 & 7 \end{bmatrix}$$

$$= \frac{1}{4}\begin{bmatrix} 400 & 190 \\ 190 & 100 \end{bmatrix} = \begin{bmatrix} 100.0 & 47.5 \\ 47.5 & 25.0 \end{bmatrix}$$

2. The eigenvalues of S are (to two decimal places)

$$\lambda_1 = 123.02 \quad \text{and} \quad \lambda_2 = 1.98$$

The unit eigenvector corresponding to λ_1 is $\mathbf{u} = \begin{bmatrix} .900 \\ .436 \end{bmatrix}$. (Since S is 2×2, the computations can be done by hand if a matrix program is not available.) For the *size index*, set

$$y = .900\hat{w} + .436\hat{h}$$

where $\hat{w}$ and $\hat{h}$ are weight and height, respectively, in mean-deviation form. The variance of this index over the data set is 123.02. Because the total variance is $\text{tr}(S) = 100 + 25 = 125$, the size index accounts for practically all (98.4%) of the variance of the data.

The original data for Practice Problem 1 and the line determined by the first principal component $\mathbf{u}$ are shown in Fig. 4. (In parametric vector form, the line is $\mathbf{x} = \mathbf{M} + t\mathbf{u}$.) It can be shown that the line is the best approximation to the data,

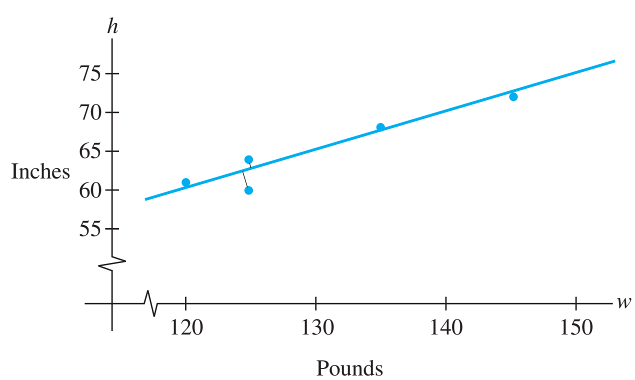

FIGURE 4 An orthogonal regression line determined by the first principal component of the data.

in the sense that the sum of the squares of the *orthogonal* distances to the line is minimized. In fact, principal component analysis is equivalent to what is termed *orthogonal regression*, but that is a story for another day. Perhaps we'll meet again.

CHAPTER 7 SUPPLEMENTARY EXERCISES

1. Mark each statement True or False. Justify each answer. In each part, A represents an $n \times n$ matrix.

a. If A is orthogonally diagonalizable, then A is symmetric.

b. If A is an orthogonal matrix, then A is symmetric.

c. If A is an orthogonal matrix, then $\|A\mathbf{x}\| = \|\mathbf{x}\|$ for all $\mathbf{x}$ in $\mathbb{R}^n$.

d. The principal axes of a quadratic form $\mathbf{x}^TA\mathbf{x}$ can be the columns of any matrix P that diagonalizes A.

e. If P is an $n \times n$ matrix with orthogonal columns, then $P^T = P^{-1}$.

f. If every coefficient in a quadratic form is positive, then the quadratic form is positive definite.

g. If $\mathbf{x}^TA\mathbf{x} > 0$ for some $\mathbf{x}$, then the quadratic form $\mathbf{x}^TA\mathbf{x}$ is positive definite.

h. By a suitable change of variable, any quadratic form can be changed into one with no cross-product term.

i. The largest value of a quadratic form $\mathbf{x}^TA\mathbf{x}$, for $\|\mathbf{x}\| = 1$, is the largest entry on the diagonal of A.

j. The maximum value of a positive definite quadratic form $\mathbf{x}^TA\mathbf{x}$ is the greatest eigenvalue of A.

k. A positive definite quadratic form can be changed into a negative definite form by a suitable change of variable $\mathbf{x} = P\mathbf{u}$, for some orthogonal matrix P.

l. An indefinite quadratic form is one whose eigenvalues are not definite.

m. If P is an $n \times n$ orthogonal matrix, then the change of variable $\mathbf{x} = P\mathbf{u}$ transforms $\mathbf{x}^TA\mathbf{x}$ into a quadratic form whose matrix is $P^{-1}AP$.

n. If U is $m \times n$ with orthogonal columns, then $UU^T\mathbf{x}$ is the orthogonal projection of $\mathbf{x}$ onto Col U.

o. If B is $m \times n$ and $\mathbf{x}$ is a unit vector in $\mathbb{R}^n$, then $\|B\mathbf{x}\| \le \sigma_1$, where σ_1 is the first singular value of B.

p. A singular value decomposition of an $m \times n$ matrix B can be written as $B = P\Sigma Q$, where P is an $m \times m$ orthogonal matrix, Q is an $n \times n$ orthogonal matrix, and Σ is an $m \times n$ "diagonal" matrix.

q. If A is $n \times n$, then A and A^TA have the same singular values.

2. Let $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ be an orthonormal basis for $\mathbb{R}^n$, and let $\lambda_1, \dots, \lambda_n$ be any real scalars. Define

$$A = \lambda_1\mathbf{u}_1\mathbf{u}_1^T + \cdots + \lambda_n\mathbf{u}_n\mathbf{u}_n^T$$

a. Show that A is symmetric.

b. Show that $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A.

3. Let A be an $n \times n$ symmetric matrix of rank r. Explain why the spectral decomposition of A represents A as the sum of r rank 1 matrices.

4. Let A be an $n \times n$ symmetric matrix.

a. Show that $(\text{Col } A)^\perp = \text{Nul } A$. [*Hint:* See Section 6.1.]

b. Show that each $\mathbf{y}$ in $\mathbb{R}^n$ can be written in the form $\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}$, with $\hat{\mathbf{y}}$ in Col A and $\mathbf{z}$ in Nul A.

5. Show that if $\mathbf{v}$ is an eigenvector of an $n \times n$ matrix A and $\mathbf{v}$ corresponds to a nonzero eigenvalue of A, then $\mathbf{v}$ is in Col A. [*Hint:* Use the definition of an eigenvector.]

6. Let A be an $n \times n$ symmetric matrix. Use Exercise 5 and an eigenvector basis for $\mathbb{R}^n$ to give a second proof of the decomposition in Exercise 4(b).

7. Prove that an $n \times n$ matrix A is positive definite if and only if A admits a *Cholesky factorization*, namely, $A = R^TR$ for some invertible upper triangular matrix R whose diagonal entries are all positive. [*Hint:* Use a QR factorization and Exercise 26 in Section 7.2.]

8. Use Exercise 7 to show that if A is positive definite, then A has an LU factorization, $A = LU$, where U has positive pivots on its diagonal. (The converse is true, too.)

If A is $m \times n$, then the matrix $G = A^TA$ is called the *Gram matrix of* A. In this case, the entries of G are the inner products of the columns of A. (See Exercises 9 and 10.)

9. Show that the Gram matrix of any matrix A is positive semidefinite, with the same rank as A. (See the Exercises in Section 6.5.)

10. Show that if an $n \times n$ matrix G is positive semidefinite and has rank r, then G is the Gram matrix of some $r \times n$ matrix A. This is called a *rank-revealing factorization* of G. [*Hint:* Consider the spectral decomposition of G, and first write G as BB^T for an $n \times r$ matrix B.]

11. Prove that any $n \times n$ matrix A admits a *polar decomposition* of the form $A = PQ$, where P is an $n \times n$ positive semidefinite matrix with the same rank as A and where Q is an $n \times n$ orthogonal matrix. [*Hint:* Use a singular value decomposition, $A = U\Sigma V^T$, and observe that $A = (U\Sigma U^T)(UV^T)$.] This decomposition is used, for instance, in mechanical engineering to model the deformation of a material. The matrix P describes the stretching or compression of the material (in the directions of the eigenvectors of P), and Q describes the rotation of the material in space.

Exercises 12–14 concern an $m \times n$ matrix A with a reduced singular value decomposition, $A = U_r D V_r^T$, and the pseudoinverse $A^+ = V_r D^{-1} U_r^T$.

12. Verify the properties of A^+:

a. For each $\mathbf{y}$ in $\mathbb{R}^m$, $AA^+\mathbf{y}$ is the orthogonal projection of $\mathbf{y}$ onto Col A.

b. For each $\mathbf{x}$ in $\mathbb{R}^n$, $A^+A\mathbf{x}$ is the orthogonal projection of $\mathbf{x}$ onto Row A.

c. $AA^+A = A$ and $A^+AA^+ = A^+$.

13. Suppose the equation $A\mathbf{x} = \mathbf{b}$ is consistent, and let $\mathbf{x}^+ = A^+\mathbf{b}$. By Exercise 23 in Section 6.3, there is exactly one vector $\mathbf{p}$ in Row A such that $A\mathbf{p} = \mathbf{b}$. The following steps prove that $\mathbf{x}^+ = \mathbf{p}$ and $\mathbf{x}^+$ is the *minimum length solution* of $A\mathbf{x} = \mathbf{b}$.

a. Show that $\mathbf{x}^+$ is in Row A. [*Hint:* Write $\mathbf{b}$ as $A\mathbf{x}$ for some $\mathbf{x}$, and use Exercise 12.]

b. Show that $\mathbf{x}^+$ is a solution of $A\mathbf{x} = \mathbf{b}$.

c. Show that if $\mathbf{u}$ is any solution of $A\mathbf{x} = \mathbf{b}$, then $\|\mathbf{x}^+\| \leq \|\mathbf{u}\|$, with equality only if $\mathbf{u} = \mathbf{x}^+$.

14. Given any $\mathbf{b}$ in $\mathbb{R}^m$, adapt Exercise 13 to show that $A^+\mathbf{b}$ is the *least-squares solution of minimum length*. [*Hint:* Consider the equation $A\mathbf{x} = \hat{\mathbf{b}}$, where $\hat{\mathbf{b}}$ is the orthogonal projection of $\mathbf{b}$ onto Col A.]

[**M**] In Exercises 15 and 16, construct the pseudoinverse of A. Begin by using a matrix program to produce the SVD of A, or, if that is not available, begin with an orthogonal diagonalization of A^TA. Use the pseudoinverse to solve $A\mathbf{x} = \mathbf{b}$, for $\mathbf{b} = (6, -1, -4, 6)$, and let $\hat{\mathbf{x}}$ be the solution. Make a calculation to verify that $\hat{\mathbf{x}}$ is in Row A. Find a nonzero vector $\mathbf{u}$ in Nul A, and verify that $\|\hat{\mathbf{x}}\| < \|\hat{\mathbf{x}} + \mathbf{u}\|$, which must be true by Exercise 13(c).

15. $A = \begin{bmatrix} -3 & -3 & -6 & 6 & 1 \\ -1 & -1 & -1 & 1 & -2 \\ 0 & 0 & -1 & 1 & -1 \\ 0 & 0 & -1 & 1 & -1 \end{bmatrix}$

16. $A = \begin{bmatrix} 4 & 0 & -1 & -2 & 0 \\ -5 & 0 & 3 & 5 & 0 \\ 2 & 0 & -1 & -2 & 0 \\ 6 & 0 & -3 & -6 & 0 \end{bmatrix}$

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