(a) $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ **(b)** $\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$ **(c)** $\begin{bmatrix} 1 & 0 \\ 2 & -1 \\ 1 & 1 \end{bmatrix}$

(d) $\begin{bmatrix} 2 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & -2 & 1 \\ -1 & 1 & 2 \end{bmatrix}$ **(e)** $\begin{bmatrix} 0 & 2 & -1 \\ 1 & -1 & 3 \\ 2 & 1 & 0 \\ -1 & 4 & 1 \end{bmatrix}$

27. For each matrix **A** in Exercise 26, find a basis $\{\mathbf{v}_i\}$ for the Range(**A**) [= Col(**A**)] and a basis $\{\mathbf{w}_i\}$ for Null($\mathbf{A}^T$). Then verify that the $\mathbf{v}_i$ are orthogonal to the $\mathbf{w}_i$, as required by Theorem 7, part (ii).

28. For each of the following matrices **A**, express the 1's vector **1** as a unique sum, $\mathbf{1} = \mathbf{x}_1 + \mathbf{x}_2$ of a vector $\mathbf{x}_1$ in Row(**A**) and a vector $\mathbf{x}_2$ in Null(**A**).

(a) $\begin{bmatrix} 1 & -2 \\ -2 & 4 \end{bmatrix}$ **(b)** $\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$ **(c)** $\begin{bmatrix} 1 & 2 & 0 \\ 0 & 1 & 2 \end{bmatrix}$ **(d)** $\begin{bmatrix} 1 & 1 & 0 \\ 2 & 1 & 2 \\ 0 & 1 & 1 \end{bmatrix}$

29. Find a solution to $\mathbf{Ax} = \mathbf{1}$, for **A** the matrix in Exercise 28, part (c), in which **x** is in Row(**A**).

30. Use Theorem 8 to prove that if $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k$ are a linearly independent set of vectors in the row space of a matrix **A**, then $\mathbf{w}_i = \mathbf{A}\mathbf{v}_i$ are a linearly independent set of vectors in the range of **A**. Thus, if $\{\mathbf{v}_i\}$ are a basis for Row(**A**), then $\{\mathbf{A}\mathbf{v}_i\}$ are a basis for Col(**A**).

Section 5.4 Orthogonal Systems

In Section 5.3 we saw that the calculation of the pseudoinverse of a matrix **A** simplified greatly if the columns of **A** were orthogonal. In this section we examine sets of orthogonal vectors further. If a set of vectors, such as the columns of a matrix, are not orthogonal, we give a procedure to transform them into an equivalent set of orthogonal vectors. Finally, we generalize the idea of an orthogonal set of vectors to build vector spaces for continuous functions generated by an orthogonal set of functions. *The idea of projecting one vector onto another vector is used over and over again in this section.* Such projections provide simple solutions to systems of equations $\mathbf{Ax} = \mathbf{b}$ for which the columns of **A** are orthogonal.

The underlying computational property that makes it easy to work with orthogonal columns is, if **a**, **b** are orthogonal, their scalar product $\mathbf{a} \cdot \mathbf{b} = 0$. Scalar products are the building blocks for much of matrix algebra (e.g., each entry in the product of two matrices is a scalar product). Thus computations with orthogonal vectors create a lot of 0's and hence yield simple results.

The inverse $\mathbf{A}^{-1}$ of a matrix $\mathbf{A}$ with orthogonal columns $\mathbf{a}_i^C$ is easy to describe. It is essentially the same as the pseudoinverse: $\mathbf{A}^{-1}$ is formed by dividing each column $\mathbf{a}_i^C$ by $\mathbf{a}_i^C \cdot \mathbf{a}_i^C$, the sum of the squares of its entries, and forming the transpose of the resulting matrix. Thus, if $s_i = \mathbf{a}_i^C \cdot \mathbf{a}_i^C$, then

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{1}{s_1}\mathbf{a}_1^C \\ \frac{1}{s_2}\mathbf{a}_2^C \\ \vdots \\ \frac{1}{s_n}\mathbf{a}_n^C \end{bmatrix} \tag{1}$$

We verify (1) by noting that entry (i, j) in $\mathbf{A}^{-1}\mathbf{A}$ will be 0 if $i \neq j$ because $\mathbf{a}_i^C \cdot \mathbf{a}_j^C = 0$ (the columns are orthogonal). Entry (i, i) equals $(\mathbf{a}_i^C/s_i) \cdot \mathbf{a}_i^C = \mathbf{a}_i^C \cdot \mathbf{a}_i^C/(\mathbf{a}_i^C \cdot \mathbf{a}_i^C) = 1$.

Example 1. Inverse of Matrix with Orthogonal Columns

(i) Consider the matrix $\mathbf{A} = \begin{bmatrix} 3 & -4 \\ 4 & 3 \end{bmatrix}$, whose columns are othogonal. The sum of the squares of the entries in each column of $\mathbf{A}$ is $3^2 + 4^2 = 25$. If we divide each column by 25 and take the transpose, we obtain

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{3}{25} & \frac{4}{25} \\ -\frac{4}{25} & \frac{3}{25} \end{bmatrix}$$

The reader should check that this matrix is exactly what one would get by computing this 2-by-2 inverse using elimination.

(ii) Consider the orthogonal-column matrix

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

Its inverse, by (1), is

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{2}{6} & \frac{1}{6} & \frac{1}{6} \\ \frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{bmatrix}$$

Again the reader should check that $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$. ■

Let use use (1) to obtain a formula for the ith component x_i in the solution $\mathbf{x}$ to $\mathbf{Ax} = \mathbf{b}$. Given the inverse $\mathbf{A}^{-1}$, we can find $\mathbf{x}$ as $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$. The ith component in $\mathbf{A}^{-1}\mathbf{b}$ is the scalar product of ith row of $\mathbf{A}^{-1}$ with $\mathbf{b}$. By (1), the ith row of $\mathbf{A}^{-1}$ is $\mathbf{a}_i^C/(\mathbf{a}_i^C \cdot \mathbf{a}_i^C)$ and thus

$$x_i = \frac{\mathbf{a}_i^C \cdot \mathbf{b}}{\mathbf{a}_i^C \cdot \mathbf{a}_i^C} \tag{2}$$

Our old friend, the length of the projection of $\mathbf{b}$ onto column $\mathbf{a}_i^C$ (see Theorem 2 of Section 5.3).

A set of orthogonal vectors of unit length (whose norm is 1) are called **orthonormal**. The preceding formulas for x_i and $\mathbf{A}^{-1}$ become even nicer if the columns of $\mathbf{A}$ are orthonormal. In this case, $\mathbf{a}_i^C \cdot \mathbf{a}_i^C = 1$. Then the denominator in (2) is 1, so now the projection formula is $x_i = \mathbf{a}_i^C \cdot \mathbf{b}$. To obtain $\mathbf{A}^{-1}$, we divide each column of $\mathbf{A}$ by 1 and form the transpose: that is, $\mathbf{A}^{-1} = \mathbf{A}^T$. Summarizing this discussion, we have

Theorem 1

(i) If $\mathbf{A}$ is an n-by-n matrix whose columns are orthogonal, then $\mathbf{A}^{-1}$ is obtained by dividing the ith column of $\mathbf{A}$ by the sum of the squares of its entries and transposing the resulting matrix [see (1)]. The ith component x_i in the solution of $\mathbf{Ax} = \mathbf{b}$ is the length of the projection of $\mathbf{b}$ on $\mathbf{a}_i^C$: $x_i = \mathbf{a}_i^C \cdot \mathbf{b}/\mathbf{a}_i^C \cdot \mathbf{a}_i^C$.

(ii) If the columns of $\mathbf{A}$ are orthonormal, then the inverse $\mathbf{A}^{-1}$ is $\mathbf{A}^T$ and the length of the projection is just $x_i = \mathbf{a}_i^C \cdot \mathbf{b}$.

Suppose that we have a basis of n orthogonal vectors $\mathbf{q}_i$ for n-space. If $\mathbf{Q}$ has the $\mathbf{q}_i$ as its columns, the solution $\mathbf{x} = \mathbf{b}^*$ of $\mathbf{Qx} = \mathbf{b}$ will be a vector $\mathbf{b}^*$ of lengths of the projections of $\mathbf{b}$ onto each $\mathbf{q}_i$:

$$\mathbf{Qb}^* = b_1^*\mathbf{q}_1 + b_2^*\mathbf{q}_2 + \cdots + b_n^*\mathbf{q}_n = \mathbf{b} \tag{3}$$

Here the term $b_1^*\mathbf{q}_1$ is just the projection of $\mathbf{b}$ onto $\mathbf{q}_1$. So (3) simply says

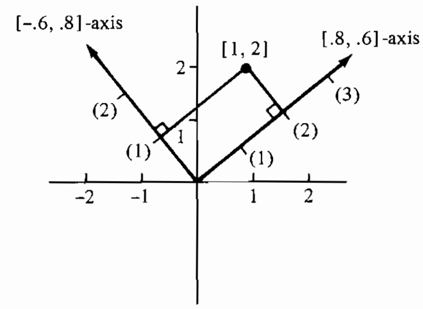
Corollary. Any n-vector $\mathbf{b}$ can be expressed as the sum of the projections of $\mathbf{b}$ onto a set of n orthogonal vectors $\mathbf{q}_i$.

Example 2. Conversion of Coordinates from One Basis to Another

Consider the orthonormal basis $\mathbf{q}_1 = [.8, .6]$, $\mathbf{q}_2 = [-.6, .8]$ for 2-space. To express the vector $\mathbf{b} = [1, 2]$ in terms of $\mathbf{q}_1$, $\mathbf{q}_2$ coordinates, we need to solve the system

$$b_1^* \begin{bmatrix} .8 \\ .6 \end{bmatrix} + b_2^* \begin{bmatrix} -.6 \\ .8 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

Figure 5.6



$$\begin{bmatrix} .8 & -.6 \\ .6 & .8 \end{bmatrix} \begin{bmatrix} b_1^* \\ b_2^* \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

or

$$b_1^* \begin{bmatrix} .8 \\ .6 \end{bmatrix} + b_2^* \begin{bmatrix} -.6 \\ .8 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$b_1^* = 2$, $b_2^* = 1$ are projections of $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ onto $\begin{bmatrix} .8 \\ .6 \end{bmatrix}$ and $\begin{bmatrix} -.6 \\ .8 \end{bmatrix}$.

or

$$\mathbf{Q}\mathbf{b}^* = \mathbf{b}, \qquad \text{where } \mathbf{Q} = [\mathbf{q}_1 \quad \mathbf{q}_2]$$

By Theorem 1,

$$\begin{aligned} b_1^* &= \mathbf{q}_1 \cdot \mathbf{b} = .8 \times 1 + .6 \times 2 = 2, \\ b_2^* &= \mathbf{q}_2 \cdot \mathbf{b} = -.6 \times 1 + .8 \times 2 = 1 \end{aligned}$$

where $b_1^*\mathbf{q}_1 = 2[.8, .6]$ is the projection of $\mathbf{b}$ on $\mathbf{q}_1$, and $b_2^*\mathbf{q}_2 = [-.6, .8]$ is the projection of $\mathbf{b}$ on $\mathbf{q}_2$. Thus $\mathbf{b} = [1, 2]$ is expressed as an $\mathbf{e}_1 - \mathbf{e}_2$ coordinate vector, while $\mathbf{b}^* = [2, 1]$ is the same vector expressed in $\mathbf{q}_1 - \mathbf{q}_2$ coordinates. A geometric picture of this conversion is given in Figure 5.6, where the vector [2, 1] is depicted as the sum of its projection onto $\mathbf{q}_1$ and onto $\mathbf{q}_2$. ■

Theorem 1 is a carbon copy of Theorem 5 of Section 5.3 about pseudoinverses when columns are orthogonal. As with the inverse, if $\mathbf{A}$'s columns are orthonormal, the pseudoinverse $\mathbf{A}^+$ of $\mathbf{A}$ will simply be $\mathbf{A}^T$. The following example gives a familiar illustration of this result and shows why orthogonal columns make inverses and pseudoinverse so similar.

Example 3. Pseudoinverse of Matrix with Orthonormal Columns

Let $\mathbf{I}_2$ be the first two columns of the 3-by-3 identity matrix.

$$\mathbf{I}_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Then

$$\mathbf{I}_2^+ = \mathbf{I}_2^T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

For any vector $\mathbf{b} = [b_1, b_2, b_3]$, the least-squares solution $\mathbf{x} = \mathbf{b}^*$ to $\mathbf{I}_2\mathbf{x} = \mathbf{b}$ is

$$\mathbf{b}^* = \mathbf{I}_2^+\mathbf{b} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

This result confirms our intuitive notion that $[b_1, b_2, 0]$ is the closest point in the x-y plane to the point $[b_1, b_2, b_3]$. ■

Optional

There is another interesting geometric fact about orthonormal columns (see the Exercises for the two-dimensional case).

Theorem 2. When $\mathbf{Q}$ has orthonormal columns, then solving $\mathbf{Qx} = \mathbf{b}$ for $\mathbf{b}^* = \mathbf{Q}^T\mathbf{b}$ is equivalent to performing the orthonormal change of basis $\mathbf{b} \rightarrow \mathbf{b}^* = \mathbf{Q}^T\mathbf{b}$. Such a basis change is simply a rotation of the coordinate axes, a reflection through a plane, or a combination of both. The entries in $\mathbf{Q}$ can be expressed in terms of the sines and cosines of the angles of this rotation.

For example, the rotation of axis in the plane by $\theta°$ is a linear transformation R of 2-space:

$$R: \quad \begin{aligned} x' &= x \cos \theta° + y \sin \theta° \\ y' &= -x \sin \theta° + y \cos \theta° \end{aligned} \qquad \text{or} \qquad \mathbf{u}' = \mathbf{Au}$$

where

$$\mathbf{A} = \begin{bmatrix} \cos \theta° & \sin \theta° \\ -\sin \theta° & \cos \theta° \end{bmatrix}$$

It is easy to check that $\mathbf{A}$ has orthonormal columns.

It follows that the distance between a pair of vectors and the angle that they form do not change with an orthonormal change of basis.

(**Note:** End of optional material.)

Orthogonal columns have another important advantage besides easy formulas. A highly nonorthogonal set of columns—that is, columns that are almost parallel—can result in unstable computations.

Example 4. Nonorthogonal Columns

Consider the following system of equations:

$$\begin{aligned} 1x_1 + .75x_2 &= 5 \\ 1x_1 + 1x_2 &= 7 \end{aligned} \tag{4}$$

Let us call the two column vectors in the coefficient matrix of (4): $\mathbf{u} = [1, 1]$ and $\mathbf{v} = [.75, 1]$. The cosine of their angle is, by Theorem 6 of Section 5.3,

$$\cos \theta(\mathbf{u}, \mathbf{v}) = \frac{\mathbf{u} \cdot \mathbf{v}}{|\mathbf{u}||\mathbf{v}|} = \frac{1.75}{\sqrt{2} \cdot 1.25} = .99 \tag{5}$$

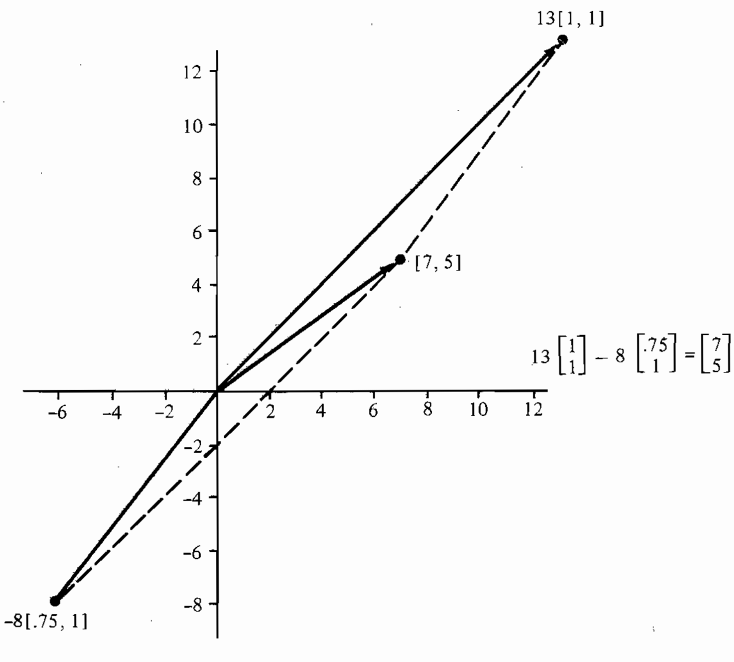
The angle with cosine of .99 is 8°. Thus **u** and **v** are almost parallel (almost the same vector). Representing *any* 2-vector **b** as a linear combination of two vectors that are almost the same is tricky, that is, unstable. For example, to solve (4) we must we find weights x_1, x_2 such that

$$x_1 \begin{bmatrix} 1 \\ 1 \end{bmatrix} + x_2 \begin{bmatrix} .75 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 7 \end{bmatrix} \tag{6}$$

The system (4) is the canoe-with-sail system from Section 1.1. We already know that calculations with **A**, the coefficient matrix in (4), are very unstable. In Section 3.5 we computed the condition number of **A** to be $c(\mathbf{A}) \simeq 16$. Recall that the condition number $c(\mathbf{A}) = \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\|$ measures how much a relative error in the entries of **A** (or in **b**) could affect the relative error in $\mathbf{x} = [x_1, x_2]$; in this case, a 5% error in **b** could cause an error 16 [$= c(\mathbf{A})$] times greater in **x**, a $16 \times 5\% = 80\%$ error.

We solved (4) in Section 1.1 and obtained $x_1 = -1$, $x_2 = 7$. If we had solved for $\mathbf{b}' = [7, 5]$, we would have obtained the answer $x_1 = 13$, $x_2 = -8$ (see Figure 5.7 for a picture of this result). Or for $\mathbf{b}'' = [6, 6]$, $x_1 = 6$, $x_2 = 0$. ■

Figure 5.7



Reading the results of Example 4 in reverse, we see that when errors arise in solving an ill-conditioned system of equations $\mathbf{Ax} = \mathbf{b}$ (in which $\mathbf{A}$ has a large condition number), the problem should be that some column vector (or a linear combination of them) forms a small angle with another column vector—this means that the columns are almost linearly dependent. If the columns were close to mutually orthogonal, the system $\mathbf{Ax} = \mathbf{b}$ would be well-conditioned.

Principle. Let $\mathbf{A}$ be an n-by-n matrix with rank($\mathbf{A}$)= n so that the system of equations $\mathbf{Ax} = \mathbf{b}$ has a unique solution. The solution to $\mathbf{Ax} = \mathbf{b}$ will be more or less stable according to how close or far from orthogonal the column vectors of $\mathbf{A}$ are.

Suppose that the columns of the n-by-n matrix $\mathbf{A}$ are linearly independent but not orthogonal. We shall show how to find a new n-by-n matrix $\mathbf{A}^*$ of orthonormal columns (orthogonal and unit length) that are linear combinations of the columns of $\mathbf{A}$.

Our procedure can be applied to any basis $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_m$ of an m-dimensional space V and will yield a new basis of m orthonormal vectors $\mathbf{q}_i$ for V (unit-length vectors make calculations especially simple). The procedure is inductive in the sense that the first k $\mathbf{q}_i$ will be an orthonormal basis for the space V_k generated by the first k $\mathbf{a}_i$. The method is called **Gram–Schmidt orthogonalization**.

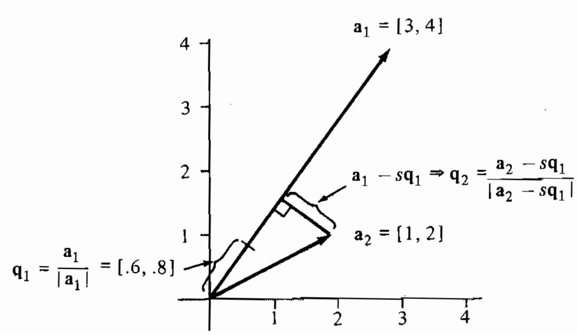
For $k = 1$, $\mathbf{q}_1$ should be a multiple of $\mathbf{a}_1$. To make $\mathbf{q}_1$ have norm 1, we set $\mathbf{q}_1 = \mathbf{a}_1/|\mathbf{a}_1|$. Next we must construct from $\mathbf{a}_2$ a second unit vector $\mathbf{q}_2$ orthogonal to $\mathbf{q}_1$. We divide $\mathbf{a}_2$ into two "parts": the part of $\mathbf{a}_2$ parallel to $\mathbf{q}_1$ and the part of $\mathbf{a}_2$ orthogonal (perpendicular) to $\mathbf{q}_1$ (see Figure 5.8). The component of $\mathbf{a}_2$ in $\mathbf{q}_1$'s direction is simply the projection of $\mathbf{a}_2$ onto $\mathbf{q}_1$. This projection is $s\mathbf{q}_1$, where the length s of the projection is

$$s = \frac{\mathbf{a}_2 \cdot \mathbf{q}_1}{\mathbf{q}_1 \cdot \mathbf{q}_1} = \mathbf{a}_2 \cdot \mathbf{q}_1 \tag{7}$$

since $\mathbf{q}_1 \cdot \mathbf{q}_1 = 1$. The rest of $\mathbf{a}_2$, the vector $\mathbf{a}_2 - s\mathbf{q}_1$, is orthogonal to the projection $s\mathbf{q}_1$, and hence orthogonal to $\mathbf{q}_1$. So $\mathbf{a}_2 - s\mathbf{q}_1$ is the orthogonal vector we want for $\mathbf{q}_2$. To have unit norm, we set $\mathbf{q}_2 = (\mathbf{a}_2 - s\mathbf{q}_1)/|\mathbf{a}_2 - s\mathbf{q}_1|$.

Let us show how the procedure works thus far.

Figure 5.8 Gram–Schmidt orthogonalization.



Example 5. Gram–Schmidt Orthogonalization in Two Dimensions

Suppose that $\mathbf{a}_1 = [3, 4]$ and $\mathbf{a}_2 = [2, 1]$ (see Figure 5.8). We set

$$\mathbf{q}_1 = \frac{\mathbf{a}_1}{|\mathbf{a}_1|} = \frac{[3, 4]}{5} = \left[\frac{3}{5}, \frac{4}{5}\right]$$

We project $\mathbf{a}_2$ onto $\mathbf{q}_1$ to get the part of $\mathbf{a}_2$ parallel to $\mathbf{q}_1$. From (7), the length of the projection is

$$s = \mathbf{a}_2 \cdot \mathbf{q}_1 = [2, 1] \cdot \left[\tfrac{3}{5}, \tfrac{4}{5}\right] = \tfrac{10}{5} = 2$$

and the projection is $s\mathbf{q}_1 = 2\left[\frac{3}{5}, \frac{4}{5}\right] = \left[\frac{6}{5}, \frac{8}{5}\right]$. Next we determine the other part of $\mathbf{a}_2$, the part orthogonal to $s\mathbf{q}_1$:

$$\mathbf{a}_2 - s\mathbf{q}_1 = [2, 1] - \left[\tfrac{6}{5}, \tfrac{8}{5}\right] = \left[\tfrac{4}{5}, -\tfrac{3}{5}\right]$$

Since $\left|\left[\frac{4}{5}, -\frac{3}{5}\right]\right| = 1$, then

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - s\mathbf{q}_1}{|\mathbf{a}_2 - s\mathbf{q}_1|} = \frac{\left[\frac{4}{5}, -\frac{3}{5}\right]}{1} = \left[\frac{4}{5}, -\frac{3}{5}\right]$$ ■

We extend the previous construction by finding the projections of $\mathbf{a}_3$ onto $\mathbf{q}_1$ and $\mathbf{q}_2$. Then the vector $\mathbf{a}_3 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2$, which is orthogonal to $\mathbf{q}_1$ and $\mathbf{q}_2$ should be $\mathbf{q}_3$; as before, we divide $\mathbf{a}_3 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2$ by its norm to make $\mathbf{q}_3$ unit length. We continue this process to find $\mathbf{q}_4$, $\mathbf{q}_5$, and so on.

Example 6. Gram–Schmidt Orthogonalization of 3-by-3 Matrix

Let us perform orthogonalization on the matrix $\mathbf{A}$ whose ith column we denote by $\mathbf{a}_i$.

$$\mathbf{A} = \begin{bmatrix} 0 & 3 & 2 \\ 3 & 5 & 5 \\ 4 & 0 & 5 \end{bmatrix} \tag{8}$$

First $\mathbf{q}_1 = \mathbf{a}_1/|\mathbf{a}_1| = [0, 3, 4]/5 = \left[0, \frac{3}{5}, \frac{4}{5}\right]$.

The length of the projection $\mathbf{a}_2$ onto $\mathbf{q}_1$ is

$$s = \mathbf{a}_2 \cdot \mathbf{q}_1 = 3 \cdot 0 + 5 \cdot \tfrac{3}{5} + 0 \cdot \tfrac{4}{5} = 3 \tag{9a}$$

So the projection of $\mathbf{a}_2$ onto $\mathbf{q}_1$ is

$$s\mathbf{q}_1 = 3\left[0, \tfrac{3}{5}, \tfrac{4}{5}\right] = \left[0, \tfrac{9}{5}, \tfrac{12}{5}\right]$$

Next we compute

$$\mathbf{a}_2 - s\mathbf{q}_1 = [3, 5, 0] - \left[0, \tfrac{9}{5}, \tfrac{12}{5}\right] = \left[3, \tfrac{16}{5}, -\tfrac{12}{5}\right]$$

where $|\mathbf{a}_2 - s\mathbf{q}_1| = \sqrt{9 + 256/25 + 144/25} = 5$. Then

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - s\mathbf{q}_1}{|\mathbf{a}_2 - s\mathbf{q}_1|} = \left[\frac{3}{5}, \frac{16}{25}, -\frac{12}{25}\right]$$

We compute the length of the projections of $\mathbf{a}_3$ onto $\mathbf{q}_1$ and $\mathbf{q}_2$:

$$\begin{aligned} s_1 &= \mathbf{a}_3 \cdot \mathbf{q}_1 = 2 \cdot 0 + \frac{5 \cdot 3}{5} + \frac{5 \cdot 4}{5} = 3 + 4 = 7 \\ s_2 &= \mathbf{a}_3 \cdot \mathbf{q}_2 = \frac{2 \cdot 3}{5} + \frac{5 \cdot 16}{25} + 5 \cdot \left(\frac{-12}{25}\right) \\ &= \frac{6}{5} + \frac{16}{5} - \frac{12}{5} = 2 \end{aligned} \tag{9b}$$

Then

$$\begin{aligned} s_1\mathbf{q}_1 &= 7\left[0, \tfrac{3}{5}, \tfrac{4}{5}\right] = \left[0, \tfrac{21}{5}, \tfrac{28}{5}\right] \\ s_2\mathbf{q}_2 &= 2\left[\tfrac{3}{5}, \tfrac{16}{25}, -\tfrac{12}{25}\right] = \left[\tfrac{6}{5}, \tfrac{32}{25}, -\tfrac{24}{25}\right] \end{aligned}$$

and

$$\begin{aligned} \mathbf{a}_3 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2 &= [2, 5, 5] - \left[0, \tfrac{21}{5}, \tfrac{28}{5}\right] - \left[\tfrac{6}{5}, \tfrac{32}{25}, -\tfrac{24}{25}\right] \\ &= \left[\tfrac{4}{5}, -\tfrac{12}{25}, \tfrac{9}{25}\right] \end{aligned}$$

Since computation reveals that $|\mathbf{a}_3 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2| = 1$, then

$$\mathbf{q}_3 = (\mathbf{a}_3 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2) = \left[\tfrac{4}{5}, -\tfrac{12}{25}, \tfrac{9}{25}\right]$$

The matrix of these new orthogonal column vectors is

$$\mathbf{Q} = \begin{bmatrix} 0 & \frac{3}{5} & \frac{4}{5} \\ \frac{3}{5} & \frac{16}{25} & -\frac{12}{25} \\ \frac{4}{5} & -\frac{12}{25} & \frac{9}{25} \end{bmatrix} \tag{10}$$

■

In keeping with the principle above, the accuracy of this procedure depends on how close to and far from orthogonality the columns $\mathbf{a}_i$ are. If a linear combination of some $\mathbf{a}_i$ forms a small angle with another vector $\mathbf{a}_k$ (this means the matrix **A** has a large condition number), then the resulting $\mathbf{q}_i$ will have errors, making them not exactly orthogonal. However, more stable methods are available using advanced techniques, such as Householder transformations.

Suppose that the columns of **A** are not linearly independent. If, say, $\mathbf{a}_3$ is a linear combination of $\mathbf{a}_1$ and $\mathbf{a}_2$, then in the Gram–Schmidt procedure the error vector $\mathbf{a}_3 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2$ with respect to $\mathbf{q}_1$ and $\mathbf{q}_2$ will be $\mathbf{0}$. In this case we skip $\mathbf{a}_3$ and use $\mathbf{a}_4 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2$ to define $\mathbf{q}_3$. The number of vectors $\mathbf{q}_i$ formed will be the dimension of the column space of **A**, that is, rank(**A**).

The effect of the orthogonalization process can be represented by an upper triangular matrix **R** so that one obtains the matrix factorization

Theorem 3. Any m-by-n matrix **A** can be factored in the form

$$\mathbf{A} = \mathbf{QR} \tag{11}$$

where **Q** is the m-by-rank(**A**) matrix with orthonormal columns $\mathbf{q}_i$ obtained by Gram–Schmidt orthogonalization, and **R** is an upper triangular matrix of size rank(**A**)-by-n (described below).

For $i < j$, entry r_{ij} of **R** is $\mathbf{a}_j \cdot \mathbf{q}_i$, the projection of $\mathbf{a}_j$ onto $\mathbf{q}_i$. The diagonal entries in **R** are the sizes, before normalization, of the new columns: $r_{11} = |\mathbf{a}_1|$, $r_{22} = |\mathbf{a}_2 - s\mathbf{q}_1|$, $r_{33} = |\mathbf{a}_3 - s_1\mathbf{q}_1 - s_2\mathbf{q}_2|$, and so on.

Example 7. *QR* Decomposition

Give the **QR** decomposition for the matrix **A** in Example 6.

$$\mathbf{A} = \begin{bmatrix} 0 & 3 & 2 \\ 3 & 5 & 5 \\ 4 & 0 & 5 \end{bmatrix}$$

The orthonormal matrix **Q** is given in (10). We form **R** from the information about the sizes of new columns and the projections as described in the preceding paragraph. Here $r_{12} = s = 3$ in (9a), and $r_{13} = s_1 = 7$, $r_{23} = s_2 = 2$ in (9b). Then

$$\mathbf{QR} = \begin{bmatrix} 0 & \frac{3}{5} & \frac{4}{5} \\ \frac{3}{5} & \frac{16}{25} & -\frac{12}{25} \\ \frac{4}{5} & -\frac{12}{25} & \frac{9}{25} \end{bmatrix} \begin{bmatrix} 5 & 3 & 7 \\ 0 & 5 & 2 \\ 0 & 0 & 1 \end{bmatrix}$$

Let us compute the second column of **QR**—multiplying **Q** by $\mathbf{r}_2^C$, the second column of **R**—and show that the result is $\mathbf{a}_2$, the second column of **A**.

$$\begin{aligned} \mathbf{Qr}_2^C &= \begin{bmatrix} 0 & \frac{3}{5} & \frac{4}{5} \\ \frac{3}{5} & \frac{16}{25} & -\frac{12}{25} \\ \frac{4}{5} & -\frac{12}{25} & \frac{9}{25} \end{bmatrix} \begin{bmatrix} 3 \\ 5 \\ 0 \end{bmatrix} \\ &= 3 \begin{bmatrix} 0 \\ \frac{3}{5} \\ \frac{4}{5} \end{bmatrix} + 5 \begin{bmatrix} \frac{3}{5} \\ \frac{16}{25} \\ -\frac{12}{25} \end{bmatrix} + 0 \begin{bmatrix} \frac{4}{5} \\ -\frac{12}{25} \\ \frac{9}{25} \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \\ 0 \end{bmatrix} = \mathbf{a}_2 \end{aligned} \tag{12}$$

■

Columns of **Q** are obtained from linear combinations of the columns of **A**. Reversing this procedure yields the columns of **A** as linear combinations of the columns of **Q**. This reversal is what is accomplished by the matrix product **QR**. Consider the computation in (12). In terms of the columns $\mathbf{q}_i$ of **Q**, (12) is

$$3\mathbf{q}_1 + 5\mathbf{q}_2 + 0\mathbf{q}_3 = \mathbf{a}_2$$

or, in terms of **R**,

$$r_{12}\mathbf{q}_1 + r_{22}\mathbf{q}_2 = \mathbf{a}_2 \tag{13}$$

($\mathbf{a}_2$ equals its projection onto $\mathbf{q}_1$ plus its projection onto $\mathbf{q}_2$).

Next consider the formula for $\mathbf{q}_2$:

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - s\mathbf{q}_1}{|\mathbf{a}_2 - s\mathbf{q}_1|} = \frac{\mathbf{a}_2 - r_{12}\mathbf{q}_1}{r_{22}} \tag{14}$$

since $r_{22} = |\mathbf{a}_2 - s\mathbf{q}_1|$ and $r_{12} = s$. Solving for $\mathbf{a}_2$ in (14), we obtain (13)

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - r_{12}\mathbf{q}_1}{r_{22}} \quad \rightarrow \quad r_{12}\mathbf{q}_1 + r_{22}\mathbf{q}_2 = \mathbf{a}_2$$

The same analysis shows that the *j*th column in the product **QR** is just a reversal of the orthogonalization steps for finding $\mathbf{q}_j$.

The matrix **R** is upper triangular because column $\mathbf{a}_i$ is only involved in building columns $\mathbf{q}_i, \mathbf{q}_{i+1}, \ldots, \mathbf{q}_n$ of **Q**. *The* **QR** *decomposition is the column counterpart to the* **LU** *decomposition*, given in Section 3.2, in which the row combinations of Gaussian elimination are reversed to obtain the matrix **A** from its row-reduced matrix **U**.

The **QR** decomposition is used frequently in numerical procedures. We use it to find eigenvalues in the appendix to Section 5.5.

We will sketch one of its most frequent uses, finding the inverse or pseudoinverse of an ill-conditioned matrix. If **A** is an *n*-by-*n* matrix with linearly independent columns, the decomposition $\mathbf{A} = \mathbf{QR}$ yields

$$\mathbf{A}^{-1} = (\mathbf{QR})^{-1} = \mathbf{R}^{-1}\mathbf{Q}^{-1} = \mathbf{R}^{-1}\mathbf{Q}^T \tag{15}$$

The fact that $\mathbf{Q}^{-1} = \mathbf{Q}^T$ when **Q** has orthonormal columns was part of Theorem 1. Given the QR decomposition of A, (15) says that to get $\mathbf{A}^{-1}$, we only need to determine $\mathbf{R}^{-1}$. Since **R** is an upper triangular matrix, its inverse is obtained quickly by back substitution (see Exercise 12 of Section 3.5). When **A** is very ill-conditioned, one should compute $\mathbf{A}^{-1}$ via (15): first, determining the QR decomposition of A, using advanced (more stable) variations of the Gram–Schmidt procedure; then determining $\mathbf{R}^{-1}$; and thus obtaining $\mathbf{A}^{-1} = \mathbf{R}^{-1}\mathbf{Q}^T$.

Equation (15) extends to pseudoinverses. That is, if **A** is an *m*-by-*n* matrix with linearly independent columns and $m > n$, then its pseudoinverse $\mathbf{A}^+$ can be computed as

$$\mathbf{A}^+ = \mathbf{R}^{-1}\mathbf{Q}^T \tag{16}$$

See the Exercises for instructions on how to verify (16) and examples of its use. *This formula for the pseudoinverse is the standard way pseudoinverses are computed in practice.* Even if one determines **Q** and **R** using the basic Gram–Schmidt procedure given above, the resulting $\mathbf{A}^+$ from (16) will be substantially more accurate than computing $\mathbf{A}^+$ using the standard formula $\mathbf{A}^+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$, because the matrix $\mathbf{A}^T\mathbf{A}$ tends to be ill-conditioned. For example, in the least-squares polynomial-fitting problem in Example 5 of Section 5.4, the condition number of the 3-by-3 matrix $\mathbf{X}^T\mathbf{X}$ was around 2000!

Principle. Because of conditioning problems, the pseudoinverse $\mathbf{A}^+$ of a matrix **A** should be computed by the formula $\mathbf{A}^+ = \mathbf{R}^{-1}\mathbf{Q}^T$, where **Q** and **R** are the matrices in the **QR** decomposition of **A**.

We now introduce a very different use of orthogonality. Our goal is to make a vector space for the set of all continuous functions. To make matters a little easier, let us focus on functions that can be expressed as a polynomial or infinite series in powers of x, such as $x^3 + 3x^2 - 4x + 1$ or e^x or $\sin x$.

Recall that the defining property of a vector space V is that if **u** and **v** are in V, then $r\mathbf{u} + s\mathbf{v}$ is also in V, for any scalars r, s. Clearly, linear combinations of polynomials (or infinite series) are again polynomials (or infinite series), so these functions form a vector space.

For a vector space of functions to be useful, we need a coordinate system, that is, a basis of independent functions $u_i(x)$ (functions that are not linearly dependent on each other) so that any function $f(x)$ can be expressed as a linear combination of these basis functions.

$$f(x) = f_1u_1(x) + f_2u_2(x) + \cdots \tag{17}$$

This basis will need to be infinite and the linear combinations of basis functions may also be infinite. The best basis would use orthogonal, or even better, orthonormal functions.

To make an orthogonal basis, we first need to extend the definition of a scalar, or inner, product $\mathbf{c} \cdot \mathbf{d}$ of vectors to an inner product of functions. The **inner product of two functions** $f(x)$ and $g(x)$ on the interval $[a, b]$ is defined as

$$f(x) \cdot g(x) = \int_a^b f(x)g(x)\,dx \tag{18}$$

This definition is a natural generalization of the standard inner product $\mathbf{c} \cdot \mathbf{d}$ in that both $\mathbf{c} \cdot \mathbf{d}$ and $f(x) \cdot g(x)$ form sums of term-by-term products of the respective entities, but in (18) we have a continuous sum, an integral.

With an inner product defined, most of the theory and formulas defined for vector spaces can be applied to our space of functions. The inner product tells us when two vectors **c**, **d** are orthogonal (if $\mathbf{c} \cdot \mathbf{d} = 0$), and allows us to compute coordinates c_i^* of **c** in an orthonormal basis $\mathbf{u}_i$: $c_i^* = \mathbf{c} \cdot \mathbf{u}_i$ (these coordinates are just the projections of **c** onto the $\mathbf{u}_i$). We can now do the same calculations for functions with (18).

The functional equivalent of the euclidean norm is defined by

$$|f(x)|^2 = f(x) \cdot f(x) = \int_a^b f(x)^2 \, dx \tag{19}$$

The counterpart of the sum norm $|\mathbf{c}|_s = \Sigma \, |c_i|$ for vectors is $|f(x)|_s = \int |f(x)| \, dx$.

An orthonormal basis for our functions on the interval $[a, b]$ will be a set of functions $\{u_i(x)\}$ which are orthogonal—by (18), $\int u_i(x)u_j(x) \, dx = 0$, for all $i \neq j$—and whose norms are 1—by (19), $\int u_i(x)^2 \, dx = 1$. Given such an orthonormal basis $\{u_i(x)\}$, the coordinates f_i of a function $f(x)$ in terms of the $u_i(x)$ are computed by the projection formula $f_i = f(x) \cdot u_i(x)$ used for n-dimensional orthonormal bases:

$$f(x) = [f(x) \cdot u_1(x)]u_1(x) + [f(x) \cdot u_2(x)]u_2(x) + \cdots \tag{20}$$

How do we find such an orthonormal basis? The first obvious choice is the set of powers of x: $1, x, x^2, x_3, \ldots$. These are linearly independent; that is, x^k cannot be expressed as a linear combination of smaller powers of x. Unfortunately, *there is no interval on which* 1, x, *and* x^2 *are mutually orthogonal.* On $[-1, 1]$, $1 \cdot x = \int x \, dx = 0$ and $x \cdot x^2 = \int x^3 \, dx = 0$, but $1 \cdot x^2 = \int x^2 \, dx = \frac{2}{3}$.

There are many sets of orthogonal functions that have been developed over the years. We shall mention two, Legendre polynomials and Fourier trigonometric functions.

The Gram–Schmidt orthogonalization procedure provides a way to build an orthonormal basis out of a basis of linearly independent vectors. The calculations in this procedure use inner products, and hence this procedure can be applied to the powers of x (which are linearly independent but, as we just said, far from orthogonal) to find an orthonormal set of polynomials.

When the interval is $[-1, 1]$, the polynomials obtained by orthogonalization are called **Legendre polynomials** $L_k(x)$. Actually, we shall not worry about making their norms equal to 1. As noted above, the functions $x^0 = 1$ and x are orthogonal on $[-1, 1]$. So $L_0(x) = 1$ and $L_1(x) = x$. Also, x^2 is orthogonal to x but not to 1 on $[-1, 1]$. We must subtract off the projection of x^2 onto 1:

$$L_2(x) = x^2 - \left(\frac{1 \cdot x^2}{1 \cdot 1}\right) 1 = x^2 - \frac{\int x^2 \, dx}{\int 1 \, dx} = x^2 - \frac{\frac{2}{3}}{2} = x^2 - \frac{1}{3} \tag{21}$$

A similar orthogonalization computation shows that $L_3(x) = x^3 - \frac{3}{5}x$.

Example 8. Approximating e^x by Legendre Polynomials

Let us use the first four Legendre polynomials $L_0(x) = 1$, $L_1(x) = x$, $L_2(x) = x^2 - \frac{1}{3}$, $L_3(x) = x^3 - 3x/5$ to approximate e^x on the interval $[-1, 1]$. We want the first four terms in (20):

$$\begin{aligned} e^x &\simeq w_0L_0 + w_1L_1(x) + w_2L_2(x) + w_3L_3(x) \\ &\simeq w_0 + w_1x + w_2\left(x^2 - \frac{1}{3}\right) + w_3\left(x^3 - \frac{3x}{5}\right) \end{aligned} \tag{22}$$

where $w_i = e^x \cdot L_i(x)/L_i(x) \cdot L_i(x) = \int e^x L_i(x)\,dx / \int L_i(x)^2\,dx$. For example,

$$w_2 = \frac{\int_{-1}^{1} e^x(x^2 - \frac{1}{3})\,dx}{\int_{-1}^{1} (x^2 - \frac{1}{3})^2\,dx}$$

With a little calculus, we compute the w_i to be (approximately)

$$w_0 = \frac{2.35}{2} = 1.18, \qquad w_1 = \frac{.736}{.667} = 1.10,$$

$$w_2 = \frac{.096}{.178} = .53, \qquad w_3 = \frac{.008}{.046} = .18$$

Then (22) becomes

$$e^x \simeq 1.18 + 1.10x + .53\left(x^2 - \frac{1}{3}\right) + .18\left(x^3 - \frac{3x}{5}\right) \tag{23}$$

If we collect like powers of x together on the right side, (23) simplifies to

$$e^x \simeq 1 + x + .53x^2 + .18x^3 \tag{24}$$

Comparing our approximation against the real values of e^x at the points $-1, -.5, 0, .5, 1$, we find

x	-1	$-.5$	0	.5	1
e^x	.37	.61	1	1.64	2.72
Legendre approximation	.37	.61	1	1.65	2.71

A pretty good fit. In particular, it is a better fit on $[-1, 1]$ than simply using the first terms of the power series for e^x, namely, $1 + x + x^2/2 + x^3/6$. The approximation gets more accurate as more Legendre polynomials are used. ■

Over the interval $[0, 2\pi]$ the trigonometric functions $(1/\sqrt{\pi}) \sin kx$ and $(1/\sqrt{\pi}) \cos kx$, for $k = 1, 2, \ldots$, plus the constant function $1/\sqrt{2\pi}$ are an orthonormal basis. To verify that they are orthogonal requires showing that

$$\frac{1}{\sqrt{\pi}} \sin jx \cdot \frac{1}{\sqrt{\pi}} \cos kx = \frac{1}{\pi} \int_0^{2\pi} \sin jx \cos kx \, dx = 0 \quad \text{for all } j, k$$

$$\frac{1}{\sqrt{\pi}} \sin jx \cdot \frac{1}{\sqrt{\pi}} \sin kx = \frac{1}{\pi} \int_0^{2\pi} \sin jx \sin kx \, dx = 0 \quad \text{for all } j \neq k$$

$$\frac{1}{\sqrt{\pi}} \cos jx \cdot \frac{1}{\sqrt{\pi}} \cos kx = \frac{1}{\pi} \int_0^{2\pi} \cos jx \cos kx \, dx = 0 \quad \text{for all } j \neq k$$

plus showing these trigonometric functions are orthogonal to a constant function. To verify that these trigonometric functions have unit length requires showing

$$\frac{1}{\sqrt{\pi}} \sin kx \cdot \frac{1}{\sqrt{\pi}} \sin kx = \frac{1}{\pi} \int_0^{2\pi} \sin^2 kx \, dx = 1 \qquad \text{for all } k$$

$$\frac{1}{\sqrt{\pi}} \cos kx \cdot \frac{1}{\sqrt{\pi}} \cos kx = \frac{1}{\pi} \int_0^{2\pi} \cos^2 kx \, dx = 1 \qquad \text{for all } k$$

When $u_{2k-1}(x) = (1/\sqrt{\pi}) \sin kx$ and $u_{2k}(x) = (1/\sqrt{\pi}) \cos kx$, $k = 1, 2, \ldots$ and $u_0(x) = 1/\sqrt{2\pi}$ in (20), this representation of $f(x)$ is called a **Fourier series**, and the coefficients $f(x) \cdot u_i(x)$ in (20) are called **Fourier coefficients**. Using Fourier series, we see that any piecewise continuous function can be expressed as a linear combination of sine and cosine waves. One important physical interpretation of this fact is that any complex electrical signal can be expressed as a sum of simple sinusoidal signals.

Example 9. Fourier Series Representation of a Jump Function

Let us determine the Fourier series representation of the discontinuous function: $f(x) = 1$ for $0 < x \leq \pi$ and $= 0$ for $\pi < x \leq 2\pi$. The Fourier coefficients $f(x) \cdot u_i(x)$ in (20) are

$$f(x) \cdot u_{2k-1}(x) = f(x) \cdot \frac{1}{\sqrt{\pi}} \sin kx = \frac{1}{\sqrt{\pi}} \int_0^{\pi} \sin kx \, dx$$

$$= \frac{1}{k\sqrt{\pi}} [-\cos kx]_0^{\pi} = \begin{cases} \dfrac{2}{k\sqrt{\pi}} & k \text{ odd} \\ 0 & k \text{ even} \end{cases}$$

$$f(x) \cdot u_{2k}(x) = f(x) \cdot \frac{1}{\sqrt{\pi}} \cos kx = \frac{1}{\sqrt{\pi}} \int_0^{\pi} \cos kx \, dx \qquad (25)$$

$$= \frac{1}{k\sqrt{\pi}} [\sin kx]_0^{\pi} = 0$$

Further, we calculate $f(x) \cdot 1/\sqrt{2\pi} = \sqrt{\pi/2}$, so the constant term of the Fourier series for this $f(x)$ is $(f(x) \cdot u_0(x))u_0(x) = \frac{1}{2}$.

By (25), only the odd sine terms occur. Letting an odd k be written as $2n - 1$, we obtain the Fourier series.

$$f(x) = \frac{1}{2} + \sum_{n=1}^{\infty} \frac{2}{(2n - 1)\sqrt{\pi}} \sin [(2n - 1)x] \qquad (26)$$

Figure 5.9 shows the approximation to $f(x)$ obtained when the first three sine terms in (26) are used (dashed line) and when the first eight sine terms are used. The fit is impressive. ■

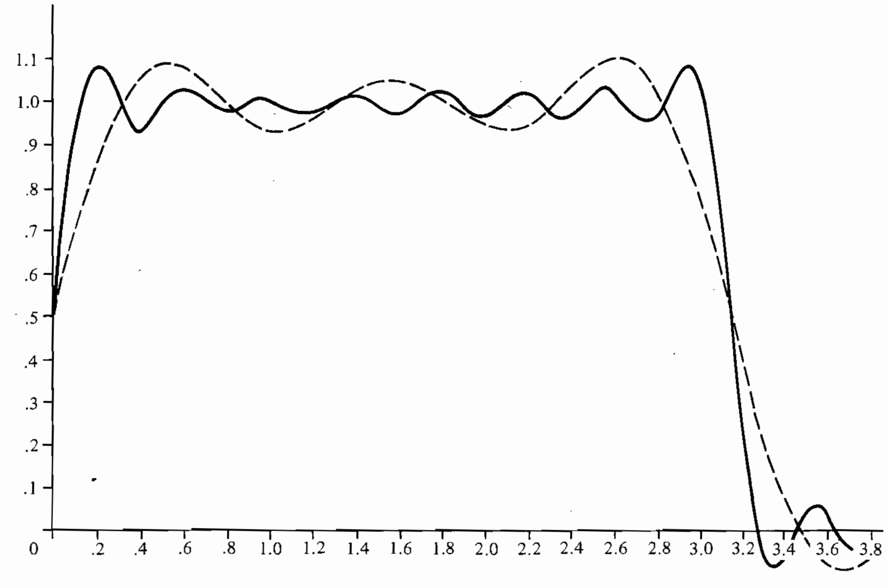


Figure 5.9 Dashed lines use first three trigonometric terms in Fourier series for $f(x)$. Solid lines use first eight terms.

Representing a function in terms of an orthonormal set of functions as in (20) has a virtually unlimited number of applications in the physical sciences and elsewhere. If one can solve a physical problem for the orthonormal basis functions, then one can typically obtain a solution for any function as a linear combination of the solutions for the basis functions. This is true for most differential equations associated with electrical circuits, vibrating bodies, and so on. Statisticians use Fourier series to analyze time-series patterns (see Example 3 of Section 1.5). The study of Fourier series is one of the major fields of mathematics.

We complete our discussion of vector spaces of functions by showing how badly conditioned the powers of x are as a basis for representing functions. Remember that the powers of x, x^i, $i = 0, 1, \ldots$, are linearly independent. The problem is that they are far from orthogonal.

Let us consider how we might approximate an arbitrary function $f(x)$ as a linear combination of, say, the powers of x up to x^5:

$$f(x) \simeq w_0 + w_1x + w_2x^2 + w_3x^3 + w_4x^4 + w_5x^5 \tag{27}$$

using the continuous version of least-squares theory. If $f(x)$ and the powers of x were vectors, not functions, then (27) would have the familiar matrix form $\mathbf{f} = \mathbf{A}\mathbf{w}$ and the approximate solution $\mathbf{w}$ would be given by $\mathbf{w} = \mathbf{A}^+\mathbf{f}$, where $\mathbf{A}^+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$.

Let us generalize $\mathbf{f} = \mathbf{A}\mathbf{w}$ to functions by letting the columns of a matrix be functions. We define the functional "matrix" $\mathbf{A}(x)$:

$$\mathbf{A}(x) = [1, x, x^2, x^3, x^4, x^5]$$

Now (27) becomes

$$f(x) = \mathbf{A}(x)\mathbf{w} \tag{28}$$

To find the approximate solution to (28), we need to compute the functional version of the pseudoinverse $\mathbf{A}(x)^+$: $\mathbf{A}(x)^+ = (\mathbf{A}(x)^T\mathbf{A}(x))^{-1}\mathbf{A}(x)^T$ and then find the vector $\mathbf{w}$ of coefficients in (27):

$$\mathbf{w} = \mathbf{A}(x)^+f(x) = (\mathbf{A}(x)^T\mathbf{A}(x))^{-1}(\mathbf{A}(x)^T\mathbf{f}(x) \tag{29}$$

The matrix $\mathbf{A}(x)^T$ has x^i as its ith "row", so the matrix product $\mathbf{A}(x)^T\mathbf{A}(x)$ involves computing the inner product of each 'row" of $\mathbf{A}(x)^T$ with each "column" of $\mathbf{A}(x)$:

$$\text{entry } (i, j) \text{ in } \mathbf{A}(x)^T\mathbf{A}(x) \text{ is } x^i \cdot x^j \ (= \textstyle\int x^ix^j\,dx)$$

Similarly, the matrix-"vector" product $\mathbf{A}(x)^Tf(x)$ is the vector of inner products $x^i \cdot f(x)$. The computations are simplest if we use the interval [0, 1]. Then entry (i, j) of $\mathbf{A}(x)^T\mathbf{A}(x)$ is

$$x^i \cdot x^j = \int_0^1 x^{i+j}\,dx = \left[\frac{x^{i+j+1}}{i+j+1}\right]_0^1 = \frac{1}{i+j+1} \tag{30}$$

For example, entry (1, 2) is $\int xx^2\,dx = \int x^3\,dx = \frac{1}{4}$. Note that we consider the constant function 1 ($= x^0$) to be the zeroth row of $\mathbf{A}(x)^T$.

Computing all the inner products for $\mathbf{A}(x)^T\mathbf{A}(x)$ yields

$$\mathbf{A}(x)^T\mathbf{A}(x) = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} & \frac{1}{8} & \frac{1}{9} \\ \frac{1}{5} & \frac{1}{6} & \frac{1}{7} & \frac{1}{8} & \frac{1}{9} & \frac{1}{10} \\ \frac{1}{6} & \frac{1}{7} & \frac{1}{8} & \frac{1}{9} & \frac{1}{10} & \frac{1}{11} \end{bmatrix} \tag{31}$$

This matrix is very ill-conditioned since the columns are all similar to each other. When the fractions in (31) are expressed to six decimal places, such as $\frac{1}{3} = .333333$, the inverse given by the author's microcomputer was (with entries rounded to integer values)

Fractions expressed to six decimal places

$$(\mathbf{A}(x)^T\mathbf{A}(x))^{-1} =$$

$$\begin{bmatrix} 17 & -116 & -47 & 1{,}180 & -1{,}986 & 958 \\ -116 & 342 & 7{,}584 & -34{,}881 & 49{,}482 & -22{,}548 \\ -47 & 7{,}584 & -76{,}499 & 242{,}494 & -301{,}846 & 129{,}004 \\ 1{,}180 & -34{,}881 & 242{,}494 & 644{,}439 & 723{,}636 & -289{,}134 \\ -1{,}986 & 49{,}482 & -301{,}846 & 723{,}636 & -747{,}725 & 278{,}975 \\ 958 & -22{,}548 & 129{,}004 & -289{,}134 & 278{,}975 & -97{,}180 \end{bmatrix} \tag{32}$$

The (absolute) sum of the fifth column in (32) is about 2,000,000. The first column in (31) sums to about 2.5. So the condition number of $\mathbf{A}(x)^T\mathbf{A}(x)$, in the sum norm, is about $2{,}000{,}000 \times 2.5 = 5{,}000{,}000$. Now that is an ill-conditioned matrix!

We rounded fractions to six significant digits, but our condition number tells us that without a seventh significant digit, our numbers in (32) could be off by 500% error [a relative error of .000001 in $\mathbf{A}(x)^T\mathbf{A}(x)$ could yield answers off by a factor of 5 in pseudoinverse calculations]. Thus the numbers in (32) are worthless.

Suppose that we enter the matrix in (31) again, now expressing fractions to seven decimal places. The new inverse computation yields

Fractions expressed to seven decimal places

$$(\mathbf{A}(x)^T\mathbf{A}(x))^{-1} =$$

$$\begin{bmatrix} 51 & -1{,}051 & 6{,}160 & -1{,}475 & 15{,}419 & -5{,}845 \\ -1{,}051 & 26{,}385 & -165{,}765 & 410{,}749 & -438{,}029 & 168{,}208 \\ 6{,}160 & -165{,}765 & 1{,}079{,}198 & -2{,}731{,}939 & 2{,}955{,}103 & -1{,}146{,}281 \\ -1{,}475 & 410{,}749 & -2{,}731{,}939 & 7{,}017{,}359 & -7{,}671{,}190 & 2{,}999{,}546 \\ 15{,}419 & -438{,}029 & 2{,}955{,}103 & -7{,}671{,}190 & 8{,}454{,}598 & -3{,}327{,}362 \\ -5{,}845 & 168{,}208 & -1{,}146{,}281 & 2{,}999{,}546 & -3{,}327{,}362 & 1{,}316{,}523 \end{bmatrix} \tag{33}$$

We have a totally different matrix. Most of the entries in (33) are about 10 times larger than corresponding entries in (32). The sum of the fifth column in (33) is about 23,000,000. If we use (33), the condition number of $\mathbf{A}(x)^T\mathbf{A}(x)$ is around 56,000,000. Our entries in (33) were rounded to seven significant digits, but the condition number says eight significant digits were needed. Again our numbers are worthless. To compute the inverse accurately would require double-precision computation.

It is only fair to note that the ill-conditioned matrix (31) is famously bad. It is called a 6-by-6 *Hilbert matrix* [a Hilbert matrix has $1/(i + j + 1)$ in entry (i, j)].

Suppose that we used the numbers in (32) for $(\mathbf{A}(x)^T\mathbf{A}(x))^{-1}$ in computing the pseudoinverse. Let us proceed to calculate $\mathbf{A}(x)^+$ and then compute the coefficients in an approximation for a function by a fifth-degree polynomial. Let us choose $f(x) = e^x$. Then $(\mathbf{A}(x)^Te^x)$ is the vector of inner products $x^i \cdot e^i = \int x^ie^x\,dx$, $i = 0, 1, \ldots, 5$. Some calculus yields $\mathbf{A}(x)^Te^x = [2.718, 1, .718, .563, .465, .396]$ (expressed to three significant digits).

Now inserting our values for $(\mathbf{A}(x)^T\mathbf{A}(x))^{-1}$ and $\mathbf{A}^Te^x$ into (27), we obtain

$$\mathbf{w} = (\mathbf{A}(x)^T\mathbf{A}(x))^{-1}(\mathbf{A}(x)^Te^x) =$$

$$\begin{bmatrix} 17 & -116 & -47 & 1{,}180 & -1{,}986 & 958 \\ -116 & 342 & 7{,}584 & -34{,}881 & 49{,}482 & -22{,}548 \\ -47 & 7{,}584 & -76{,}499 & 242{,}494 & -301{,}846 & 129{,}004 \\ 1{,}180 & -34{,}881 & 242{,}494 & 644{,}439 & 723{,}636 & -289{,}134 \\ -1{,}986 & 49{,}482 & -301{,}846 & 723{,}636 & -747{,}725 & 278{,}975 \\ 958 & -22{,}548 & 129{,}004 & -289{,}134 & 278{,}975 & -97{,}180 \end{bmatrix} \cdot \begin{bmatrix} 2.718 \\ 1 \\ .718 \\ .563 \\ .465 \\ .396 \end{bmatrix}$$

$$= \begin{bmatrix} 17 \\ -87 \\ -219 \\ 1{,}611 \\ 2{,}449 \\ 1{,}135 \end{bmatrix} \tag{34}$$

Thus our fifth-degree polynomial approximation of e^x on the interval [0, 1] is

$$e^x \simeq 17 - 87x - 219x^2 + 1611x^3 + 2449x^4 + 1135x^5 \qquad (35)$$

Setting $x = 1$ in (35), we have $e^1 = 17 - 86 - 219 + 1611 + 2449 + 1135 = 4907$, pretty bad. Since our computed values in $(\mathbf{A}(x)^T\mathbf{A}(x))^{-1}$ are meaningless, such a bad approximation of e^x was to be expected.

Compare (35) with the Legendre polynomial approximation in Example 8.

Section 5.4 Exercises

Summary of Exercises

Exercises 1–11 involve inverses, pseudoinverses, and projections for matrices with orthogonal columns. Exercises 12–21 involve Gram–Schmidt orthogonalization and the **QR** decomposition. Exercises 22–30 present problems about functional inner products and functional approximation.

1. Compute the inverses of these matrices with orthogonal columns. Solve

$$\mathbf{Ax} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

where **A** is the matrix in part (b).

(a) $\begin{bmatrix} .6 & .8 \\ -.8 & .6 \end{bmatrix}$ **(b)** $\begin{bmatrix} 2 & 2 & 1 \\ -2 & 1 & 2 \\ 1 & -2 & 2 \end{bmatrix}$

2. Compute the inverses of these matrices with orthogonal columns.

(a) $\begin{bmatrix} -1 & 4 & -1 \\ 2 & 1 & -2 \\ 1 & 2 & 3 \end{bmatrix}$ **(b)** $\begin{bmatrix} 2 & -3 & 6 \\ -6 & 2 & 3 \\ 3 & 6 & 2 \end{bmatrix}$

(c) $\begin{bmatrix} .5 & -.5 & 1 \\ -.5 & .5 & 1 \\ 1 & .5 & 0 \end{bmatrix}$

Solve $\mathbf{Ax} = \mathbf{1}$, where **A** is the matrix in part (a).

3. Show that if **A** is an n-by-n upper triangular matrix with orthonormal columns, **A** is the identity matrix **I**.

4. Compute the length k of the projection of **b** onto **a** and give the projection vector $k\mathbf{a}$.

(a) $\mathbf{a} = [0, 1, 0]$, $\mathbf{b} = [3, 2, 4]$
(b) $\mathbf{a} = [1, -1, 2]$, $\mathbf{b} = [2, 3, 1]$
(c) $\mathbf{a} = [\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$, $\mathbf{b} = [4, 1, 3]$
(d) $\mathbf{a} = [2, -1, 3]$, $\mathbf{b} = [-2, 5, 3]$

5. Express the vector [2, 1, 2] as a linear combination of the following orthogonal bases for three-dimensional space.
(a) $[1, -1, 2], [2, 2, 0], [-1, 1, 1]$
(b) $[\frac{2}{3}, \frac{1}{3}, -\frac{2}{3}], [\frac{1}{3}, \frac{2}{3}, \frac{2}{3}], [\frac{2}{3}, -\frac{2}{3}, \frac{1}{3}]$
(c) $[3, 1.5, 1], [1, -3, 1.5], [-1.5, 1, 3]$

6. Compute the pseudoinverse of

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

Find the least-squares solution to $\mathbf{Ax} = \mathbf{1}$.

7. Compute the pseudoinverse of

$$\mathbf{A} = \begin{bmatrix} 3 & 4 \\ 1 & -2 \\ 2 & -5 \end{bmatrix}$$

Find the least-squares solution to $\mathbf{Ax} = \mathbf{1}$.

8. Consider the regression model $\hat{z} = qx + ry + s$ for the following data, where the x-value is a scaled score (to have average value of 0) of high school grades, the y-value is a scaled score of SAT scores, and the z-value is a score of college grades.

x	-4	-2	0	2	4
y	2	-1	-2	-1	2
z	3	6	7	7	6

Determine q, r, and s. Note that the $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{1}$ vectors are mutually orthogonal.

9. Verify that Theorem 2 is true in two dimensions, namely, that a change from the standard $\{\mathbf{e}_1, \mathbf{e}_2\}$ basis to some other orthonormal basis $\{\mathbf{q}_1, \mathbf{q}_2\}$ corresponds to a rotation (around the origin) and possibly a reflection. Note that since $\mathbf{q}_1$, $\mathbf{q}_2$ have unit length, they are completely determined by knowing the (counterclockwise) angles θ_1, θ_2 they make with the positive $\mathbf{e}_1$ axis; also since $\mathbf{q}_1$, $\mathbf{q}_2$ are orthogonal, $|\theta_1 - \theta_2| = 90°$.

10. **(a)** Show that an orthonormal change of basis preserves lengths (in euclidean norm).
Hint: Verify that $(\mathbf{Qv}) \cdot (\mathbf{Qv}) = \mathbf{v} \cdot \mathbf{v}$ (where $\mathbf{Q}$ has orthonormal columns) by using the identity $(\mathbf{Ab}) \cdot (\mathbf{Cd}) = \mathbf{b}^T(\mathbf{A}^T\mathbf{C})\mathbf{d}$.
(b) Show that an orthonormal change of basis preserves angles.
Hint: Show that the cosine formula for the angle is unchanged by the method in part (a).

11. Compute the angle between the following pairs of nonorthogonal vectors. Which are close to orthogonal?
(a) [3, 2], [−3, 4] **(b)** [1, 2, 5], [2, 5, 3]
(c) [1, −3, 2], [−2, 4, −3]

12. Find the **QR** decomposition of the following matrices.

(a) $\begin{bmatrix} 3 & -1 \\ 4 & 1 \end{bmatrix}$ **(b)** $\begin{bmatrix} 2 & 1 \\ 1 & 1 \\ 2 & 3 \end{bmatrix}$ **(c)** $\begin{bmatrix} 1 & -1 & 2 \\ 2 & -1 & 1 \\ 2 & -2 & 2 \end{bmatrix}$ **(d)** $\begin{bmatrix} 2 & 3 & 1 \\ 1 & 1 & 1 \\ 2 & 1 & 2 \end{bmatrix}$

13. Use the Gram–Schmidt orthogonalization to find an orthonormal basis that generates the same vector space as the following bases:
(a) [1, 1], [2, −1] **(b)** [2, 1, 2], [4, 1, 1],
(c) [3, 1, 1], [1, 2, 1], [1, 1, 2]

14. **(a)** Compute the inverse of the matrix in Exercise 12, part (c) by first finding the **QR** decomposition of the matrix and then using (15) to get the inverse. (See Exercise 12 of Section 3.5 for instructions on computing $\mathbf{R}^{-1}$.) What is its condition number?
(b) Check your answer by computing the inverse by the regular elimination by pivoting method.

15. **(a)** Find the pseudoinverse $\mathbf{A}^+$ of the matrix $\mathbf{A}$ in Exercise 12, part (b) by using the **QR** decomposition of $\mathbf{A}$ and computing $\mathbf{A}^+$ as $\mathbf{A}^+ = \mathbf{R}^{-1}\mathbf{Q}^T$.
(b) Check your answer by finding the pseudoinverse from the formula $\mathbf{A}^+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$. Note that this is a very poorly conditioned matrix; compute the condition number of $(\mathbf{A}^T\mathbf{A})$.

16. Use (16) to find the pseudoinverse in solving the refinery problem in Example 3 of Section 5.3.

17. Use (16) to find the pseudoinverse in the following regression problems using the model $\hat{y} = qx + r$.
(a) (x, y) points: (0, 1), (2, 1), (4, 4)
(b) (x, y) points: (3, 2), (4, 5), (5, 5), (6, 5)
(c) (x, y) points: (−2, 1), (0, 1), (2, 4)

18. Use (16) to find the pseudoinverse in the least-squares polynomial-fitting problem in Example 5 of Section 5.3.

19. Verify (16): $\mathbf{A}^+ = \mathbf{R}^{-1}\mathbf{Q}^T$, by substituting $\mathbf{QR}$ for $\mathbf{A}$ (and $\mathbf{R}^T\mathbf{Q}^T$ for $\mathbf{A}^T$) in the pseudoinverse formula $\mathbf{A}^+ = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$ and simplifying (remember that $\mathbf{R}$ is invertible; we assume that the columns of $\mathbf{A}$ are linearly independent).

20. Show that if the columns of the m-by-n matrix $\mathbf{A}$ are linearly independent, the m-by-m matrix $\mathbf{R}$ of the $\mathbf{QR}$ decomposition must be invertible.

Hint: Show main diagonal entries of $\mathbf{R}$ are nonzero and then see Exercise 12 of Section 3.5 for instructions on computing inverse of $\mathbf{R}$.

21. Show that any set H of k orthonormal n-vectors can be extended to an orthonormal basis for n-dimensional space.

Hint: Form an n-by-$(k + n)$ matrix whose first k columns come from H and whose remaining n columns form the identity matrix; now apply the Gram–Schmidt orthogonalization to this matrix.

22. Over the interval $[0, 1]$, compute the following inner products: $x \cdot x$, $x \cdot x^3$, $x^3 \cdot x^3$.

23. Verify that the fourth Legendre polynomial is $x^3 - \frac{3}{5}x$.

24. Verify the values found for the weights w_1, w_2, w_3, and w_4 in Example 8.

Note: You must use integration by parts—or a table of integrals.

25. Approximate the following functions $f(x)$ as a linear combination of the first four Legendre polynomials over the interval $[-1, 1]$: $L_0(x) = 1$, $L_1(x) = x$, $L_2(x) = x^2 - \frac{1}{3}$, $L_3(x) = x^3 - 3x/5$.
(a) $f(x) = x^4$ **(b)** $f(x) = |x|$
(c) $f(x) = -1: x < 0, = 1: x \geq 0$

26. Approximate $x^3 + 2x - 1$ as a linear combination of the first four Legendre polynomials over the interval $[-1, 1]$: $L_0(x) = 1$, $L_1(x) = x$, $L_2(x) = x^2 - \frac{1}{2}$, $L_3(x) = x^3 - 3x/5$. Your "approximation" should equal $x^3 + 2x - 1$, since this polynomial is a linear combination of the functions 1, x, x^2, and x^3, from which the Legendre polynomials were derived by orthogonalization.

27. **(a)** Find the Legendre polynomial of degree 4.
(b) Find the Legendre polynomial of degree 5.

28. **(a)** Using the interval $[0, 1]$, instead of $[-1, 1]$, find three orthogonal polynomials of the form $K_0(x) = a$, $K_1(x) = bx + c$, and $K_2(x) = dx^2 + ex + f$.
(b) Find a least-squares approximation of x^4 on the interval $[0, 1]$ using your three polynomials in part (a).