

By construction, the first k columns of Q are an orthonormal basis of $\text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$. From the proof of Theorem 12, $A = QR$ for some R . To find R , observe that $Q^T Q = I$, because the columns of Q are orthonormal. Hence

$$Q^T A = Q^T (QR) = IR = R$$

and

$$R = \begin{bmatrix} 1/2 & 1/2 & 1/2 & 1/2 \\ -3/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} \\ 0 & -2/\sqrt{6} & 1/\sqrt{6} & 1/\sqrt{6} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 3/2 & 1 \\ 0 & 3/\sqrt{12} & 2/\sqrt{12} \\ 0 & 0 & 2/\sqrt{6} \end{bmatrix} \quad \blacksquare$$

NUMERICAL NOTES

1. When the Gram–Schmidt process is run on a computer, roundoff error can build up as the vectors \mathbf{u}_k are calculated, one by one. For j and k large but unequal, the inner products $\mathbf{u}_j^T \mathbf{u}_k$ may not be sufficiently close to zero. This loss of orthogonality can be reduced substantially by rearranging the order of the calculations.¹ However, a different computer-based QR factorization is usually preferred to this modified Gram–Schmidt method because it yields a more accurate orthonormal basis, even though the factorization requires about twice as much arithmetic.
2. To produce a QR factorization of a matrix A , a computer program usually left-multiplies A by a sequence of orthogonal matrices until A is transformed into an upper triangular matrix. This construction is analogous to the left-multiplication by elementary matrices that produces an LU factorization of A .

PRACTICE PROBLEM

Let $W = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2\}$, where $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ and $\mathbf{x}_2 = \begin{bmatrix} 1/3 \\ 1/3 \\ -2/3 \end{bmatrix}$. Construct an orthonormal basis for W .

6.4 EXERCISES

In Exercises 1–6, the given set is a basis for a subspace W . Use the Gram–Schmidt process to produce an orthogonal basis for W .

1. $\begin{bmatrix} 3 \\ 0 \\ -1 \end{bmatrix}, \begin{bmatrix} 8 \\ 5 \\ -6 \end{bmatrix}$

2. $\begin{bmatrix} 0 \\ 4 \\ 2 \end{bmatrix}, \begin{bmatrix} 5 \\ 6 \\ -7 \end{bmatrix}$

3. $\begin{bmatrix} 2 \\ -5 \\ 1 \end{bmatrix}, \begin{bmatrix} 4 \\ -1 \\ 2 \end{bmatrix}$

5. $\begin{bmatrix} 1 \\ -4 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 7 \\ -7 \\ -4 \\ 1 \end{bmatrix}$

4. $\begin{bmatrix} 3 \\ -4 \\ 5 \end{bmatrix}, \begin{bmatrix} -3 \\ 14 \\ -7 \end{bmatrix}$

6. $\begin{bmatrix} 3 \\ -1 \\ 2 \\ -1 \end{bmatrix}, \begin{bmatrix} -5 \\ 9 \\ -9 \\ 3 \end{bmatrix}$

¹See *Fundamentals of Matrix Computations*, by David S. Watkins (New York: John Wiley & Sons, 1991), pp. 167–180.

7. Find an orthonormal basis of the subspace spanned by the vectors in Exercise 3.
8. Find an orthonormal basis of the subspace spanned by the vectors in Exercise 4.

Find an orthogonal basis for the column space of each matrix in Exercises 9–12.

$$\begin{array}{ll} 9. \begin{bmatrix} 3 & -5 & 1 \\ 1 & 1 & 1 \\ -1 & 5 & -2 \\ 3 & -7 & 8 \end{bmatrix} & 10. \begin{bmatrix} -1 & 6 & 6 \\ 3 & -8 & 3 \\ 1 & -2 & 6 \\ 1 & -4 & -3 \end{bmatrix} \\ 11. \begin{bmatrix} 1 & 2 & 5 \\ -1 & 1 & -4 \\ -1 & 4 & -3 \\ 1 & -4 & 7 \\ 1 & 2 & 1 \end{bmatrix} & 12. \begin{bmatrix} 1 & 3 & 5 \\ -1 & -3 & 1 \\ 0 & 2 & 3 \\ 1 & 5 & 2 \\ 1 & 5 & 8 \end{bmatrix} \end{array}$$

In Exercises 13 and 14, the columns of Q were obtained by applying the Gram–Schmidt process to the columns of A . Find an upper triangular matrix R such that $A = QR$. Check your work.

$$\begin{array}{ll} 13. A = \begin{bmatrix} 5 & 9 \\ 1 & 7 \\ -3 & -5 \\ 1 & 5 \end{bmatrix}, Q = \begin{bmatrix} 5/6 & -1/6 \\ 1/6 & 5/6 \\ -3/6 & 1/6 \\ 1/6 & 3/6 \end{bmatrix} \\ 14. A = \begin{bmatrix} -2 & 3 \\ 5 & 7 \\ 2 & -2 \\ 4 & 6 \end{bmatrix}, Q = \begin{bmatrix} -2/7 & 5/7 \\ 5/7 & 2/7 \\ 2/7 & -4/7 \\ 4/7 & 2/7 \end{bmatrix} \end{array}$$

15. Find a QR factorization of the matrix in Exercise 11.
16. Find a QR factorization of the matrix in Exercise 12.

In Exercises 17 and 18, all vectors and subspaces are in \mathbb{R}^n . Mark each statement True or False. Justify each answer.

17. a. If $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is an orthogonal basis for W , then multiplying \mathbf{v}_3 by a scalar c gives a new orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2, c\mathbf{v}_3\}$.
- b. The Gram–Schmidt process produces from a linearly independent set $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ an orthogonal set $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ with the property that for each k , the vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ span the same subspace as that spanned by $\mathbf{x}_1, \dots, \mathbf{x}_k$.
- c. If $A = QR$, where Q has orthonormal columns, then $R = Q^T A$.
18. a. If $W = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ with $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ linearly independent, and if $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is an orthogonal set in W , then $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is a basis for W .
- b. If \mathbf{x} is not in a subspace W , then $\mathbf{x} - \text{proj}_W \mathbf{x}$ is not zero.
- c. In a QR factorization, say $A = QR$ (when A has linearly independent columns), the columns of Q form an orthonormal basis for the column space of A .

19. Suppose $A = QR$, where Q is $m \times n$ and R is $n \times n$. Show that if the columns of A are linearly independent, then R must be invertible. [Hint: Study the equation $R\mathbf{x} = \mathbf{0}$ and use the fact that $A = QR$.]

20. Suppose $A = QR$, where R is an invertible matrix. Show that A and Q have the same column space. [Hint: Given \mathbf{y} in $\text{Col } A$, show that $\mathbf{y} = Q\mathbf{x}$ for some \mathbf{x} . Also, given \mathbf{y} in $\text{Col } Q$, show that $\mathbf{y} = A\mathbf{x}$ for some \mathbf{x} .]

21. Given $A = QR$ as in Theorem 12, describe how to find an orthogonal $m \times m$ (square) matrix Q_1 and an invertible $n \times n$ upper triangular matrix R such that

$$A = Q_1 \begin{bmatrix} R \\ 0 \end{bmatrix}$$

The MATLAB `qr` command supplies this “full” QR factorization when $\text{rank } A = n$.

22. Let $\mathbf{u}_1, \dots, \mathbf{u}_p$ be an orthogonal basis for a subspace W of \mathbb{R}^n , and let $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be defined by $T(\mathbf{x}) = \text{proj}_W \mathbf{x}$. Show that T is a linear transformation.

23. Suppose $A = QR$ is a QR factorization of an $m \times n$ matrix A (with linearly independent columns). Partition A as $[A_1 \ A_2]$, where A_1 has p columns. Show how to obtain a QR factorization of A_1 , and explain why your factorization has the appropriate properties.

24. [M] Use the Gram–Schmidt process as in Example 2 to produce an orthogonal basis for the column space of

$$A = \begin{bmatrix} -10 & 13 & 7 & -11 \\ 2 & 1 & -5 & 3 \\ -6 & 3 & 13 & -3 \\ 16 & -16 & -2 & 5 \\ 2 & 1 & -5 & -7 \end{bmatrix}$$

25. [M] Use the method in this section to produce a QR factorization of the matrix in Exercise 24.

26. [M] For a matrix program, the Gram–Schmidt process works better with orthonormal vectors. Starting with $\mathbf{x}_1, \dots, \mathbf{x}_p$ as in Theorem 11, let $A = [\mathbf{x}_1 \ \dots \ \mathbf{x}_p]$. Suppose Q is an $n \times k$ matrix whose columns form an orthonormal basis for the subspace W_k spanned by the first k columns of A . Then for \mathbf{x} in \mathbb{R}^n , $QQ^T \mathbf{x}$ is the orthogonal projection of \mathbf{x} onto W_k (Theorem 10 in Section 6.3). If \mathbf{x}_{k+1} is the next column of A , then equation (2) in the proof of Theorem 11 becomes

$$\mathbf{v}_{k+1} = \mathbf{x}_{k+1} - Q(Q^T \mathbf{x}_{k+1})$$

(The parentheses above reduce the number of arithmetic operations.) Let $\mathbf{u}_{k+1} = \mathbf{v}_{k+1}/\|\mathbf{v}_{k+1}\|$. The new Q for the next step is $[Q \ \mathbf{u}_{k+1}]$. Use this procedure to compute the QR factorization of the matrix in Exercise 24. Write the keystrokes or commands you use.

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PRACTICE PROBLEMS

- Let $A = \begin{bmatrix} 1 & -3 & -3 \\ 1 & 5 & 1 \\ 1 & 7 & 2 \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} 5 \\ -3 \\ -5 \end{bmatrix}$. Find a least-squares solution of $A\mathbf{x} = \mathbf{b}$, and compute the associated least-squares error.
- What can you say about the least-squares solution of $A\mathbf{x} = \mathbf{b}$ when \mathbf{b} is orthogonal to the columns of A ?

6.5 EXERCISES

In Exercises 1–4, find a least-squares solution of $A\mathbf{x} = \mathbf{b}$ by (a) constructing the normal equations for $\hat{\mathbf{x}}$ and (b) solving for $\hat{\mathbf{x}}$.

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

$$2. A = \begin{bmatrix} 2 & 1 \\ -2 & 0 \\ 2 & 3 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} -5 \\ 8 \\ 1 \end{bmatrix}$$

$$3. A = \begin{bmatrix} 1 & -2 \\ -1 & 2 \\ 0 & 3 \\ 2 & 5 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \\ 2 \end{bmatrix}$$

$$4. A = \begin{bmatrix} 1 & 3 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 5 \\ 1 \\ 0 \end{bmatrix}$$

In Exercises 5 and 6, describe all least-squares solutions of the equation $A\mathbf{x} = \mathbf{b}$.

$$5. A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 1 \\ 3 \\ 8 \\ 2 \end{bmatrix}$$

$$6. A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 7 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \end{bmatrix}$$

- Compute the least-squares error associated with the least-squares solution found in Exercise 3.
- Compute the least-squares error associated with the least-squares solution found in Exercise 4.

In Exercises 9–12, find (a) the orthogonal projection of \mathbf{b} onto $\text{Col } A$ and (b) a least-squares solution of $A\mathbf{x} = \mathbf{b}$.

$$9. A = \begin{bmatrix} 1 & 5 \\ 3 & 1 \\ -2 & 4 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 4 \\ -2 \\ -3 \end{bmatrix}$$

$$10. A = \begin{bmatrix} 1 & 2 \\ -1 & 4 \\ 1 & 2 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 3 \\ -1 \\ 5 \end{bmatrix}$$

$$11. A = \begin{bmatrix} 4 & 0 & 1 \\ 1 & -5 & 1 \\ 6 & 1 & 0 \\ 1 & -1 & -5 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 9 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$12. A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & -1 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 2 \\ 5 \\ 6 \\ 6 \end{bmatrix}$$

- Let $A = \begin{bmatrix} 3 & 4 \\ -2 & 1 \\ 3 & 4 \end{bmatrix}$, $\mathbf{b} = \begin{bmatrix} 11 \\ -9 \\ 5 \end{bmatrix}$, $\mathbf{u} = \begin{bmatrix} 5 \\ -1 \end{bmatrix}$, and $\mathbf{v} = \begin{bmatrix} 5 \\ -2 \end{bmatrix}$. Compute $A\mathbf{u}$ and $A\mathbf{v}$, and compare them with \mathbf{b} . Could \mathbf{u} possibly be a least-squares solution of $A\mathbf{x} = \mathbf{b}$? (Answer this without computing a least-squares solution.)

- Let $A = \begin{bmatrix} 2 & 1 \\ -3 & -4 \\ 3 & 2 \end{bmatrix}$, $\mathbf{b} = \begin{bmatrix} 5 \\ 4 \\ 4 \end{bmatrix}$, $\mathbf{u} = \begin{bmatrix} 4 \\ -5 \end{bmatrix}$, and $\mathbf{v} = \begin{bmatrix} 6 \\ -5 \end{bmatrix}$. Compute $A\mathbf{u}$ and $A\mathbf{v}$, and compare them with \mathbf{b} . Is it possible that at least one of \mathbf{u} or \mathbf{v} could be a least-squares solution of $A\mathbf{x} = \mathbf{b}$? (Answer this without computing a least-squares solution.)

In Exercises 15 and 16, use the factorization $A = QR$ to find the least-squares solution of $A\mathbf{x} = \mathbf{b}$.

$$15. A = \begin{bmatrix} 2 & 3 \\ 2 & 4 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 2/3 & -1/3 \\ 2/3 & 2/3 \\ 1/3 & -2/3 \end{bmatrix} \begin{bmatrix} 3 & 5 \\ 0 & 1 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 7 \\ 3 \\ 1 \end{bmatrix}$$

$$16. A = \begin{bmatrix} 1 & -1 \\ 1 & 4 \\ 1 & -1 \\ 1 & 4 \end{bmatrix} = \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \\ 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix} \begin{bmatrix} 2 & 3 \\ 0 & 5 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} -1 \\ 6 \\ 5 \\ 7 \end{bmatrix}$$

In Exercises 17 and 18, A is an $m \times n$ matrix and \mathbf{b} is in \mathbb{R}^m . Mark each statement True or False. Justify each answer.

- a. The general least-squares problem is to find an \mathbf{x} that makes $A\mathbf{x}$ as close as possible to \mathbf{b} .

- b. A least-squares solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\hat{\mathbf{x}}$ that satisfies $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$, where $\hat{\mathbf{b}}$ is the orthogonal projection of \mathbf{b} onto $\text{Col } A$.
- c. A least-squares solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\hat{\mathbf{x}}$ such that $\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$ for all \mathbf{x} in \mathbb{R}^n .
- d. Any solution of $A^T A\mathbf{x} = A^T \mathbf{b}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$.
- e. If the columns of A are linearly independent, then the equation $A\mathbf{x} = \mathbf{b}$ has exactly one least-squares solution.
18. a. If \mathbf{b} is in the column space of A , then every solution of $A\mathbf{x} = \mathbf{b}$ is a least-squares solution.
- b. The least-squares solution of $A\mathbf{x} = \mathbf{b}$ is the point in the column space of A closest to \mathbf{b} .
- c. A least-squares solution of $A\mathbf{x} = \mathbf{b}$ is a list of weights that, when applied to the columns of A , produces the orthogonal projection of \mathbf{b} onto $\text{Col } A$.
- d. If $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$, then $\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b}$.
- e. The normal equations always provide a reliable method for computing least-squares solutions.
- f. If A has a QR factorization, say $A = QR$, then the best way to find the least-squares solution of $A\mathbf{x} = \mathbf{b}$ is to compute $\hat{\mathbf{x}} = R^{-1} Q^T \mathbf{b}$.
19. Let A be an $m \times n$ matrix. Use the steps below to show that a vector \mathbf{x} in \mathbb{R}^n satisfies $A\mathbf{x} = \mathbf{0}$ if and only if $A^T A\mathbf{x} = \mathbf{0}$. This will show that $\text{Nul } A = \text{Nul } A^T A$.
- a. Show that if $A\mathbf{x} = \mathbf{0}$, then $A^T A\mathbf{x} = \mathbf{0}$.
- b. Suppose $A^T A\mathbf{x} = \mathbf{0}$. Explain why $\mathbf{x}^T A^T A\mathbf{x} = 0$, and use this to show that $A\mathbf{x} = \mathbf{0}$.
20. Let A be an $m \times n$ matrix such that $A^T A$ is invertible. Show that the columns of A are linearly independent. [Careful: You may not assume that A is invertible; it may not even be square.]
21. Let A be an $m \times n$ matrix whose columns are linearly independent. [Careful: A need not be square.]
- a. Use Exercise 19 to show that $A^T A$ is an invertible matrix.
- b. Explain why A must have at least as many rows as columns.
- c. Determine the rank of A .
22. Use Exercise 19 to show that $\text{rank } A^T A = \text{rank } A$. [Hint: How many columns does $A^T A$ have? How is this connected with the rank of $A^T A$?]
23. Suppose A is $m \times n$ with linearly independent columns and \mathbf{b} is in \mathbb{R}^m . Use the normal equations to produce a formula for $\hat{\mathbf{b}}$, the projection of \mathbf{b} onto $\text{Col } A$. [Hint: Find $\hat{\mathbf{x}}$ first. The formula does not require an orthogonal basis for $\text{Col } A$.]

24. Find a formula for the least-squares solution of $A\mathbf{x} = \mathbf{b}$ when the columns of A are orthonormal.

25. Describe all least-squares solutions of the system

$$x + y = 2$$

$$x + y = 4$$

26. [M] Example 3 in Section 4.8 displayed a low-pass linear filter that changed a signal $\{y_k\}$ into $\{y_{k+1}\}$ and changed a higher-frequency signal $\{w_k\}$ into the zero signal, where $y_k = \cos(\pi k/4)$ and $w_k = \cos(3\pi k/4)$. The following calculations will design a filter with approximately those properties. The filter equation is

$$a_0 y_{k+2} + a_1 y_{k+1} + a_2 y_k = z_k \quad \text{for all } k \quad (8)$$

Because the signals are periodic, with period 8, it suffices to study equation (8) for $k = 0, \dots, 7$. The action on the two signals described above translates into two sets of eight equations, shown below:

$$\begin{array}{c} y_{k+2} \quad y_{k+1} \quad y_k \\ k=0 \\ k=1 \\ \vdots \\ k=7 \end{array} \begin{bmatrix} 0 & .7 & 1 \\ -.7 & 0 & .7 \\ -1 & -.7 & 0 \\ -.7 & -1 & -.7 \\ 0 & -.7 & -1 \\ .7 & 0 & -.7 \\ 1 & .7 & 0 \\ .7 & 1 & .7 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{array}{c} y_{k+1} \\ .7 \\ 0 \\ -.7 \\ -1 \\ -.7 \\ 0 \\ .7 \\ 1 \end{array}$$

$$\begin{array}{c} w_{k+2} \quad w_{k+1} \quad w_k \\ k=0 \\ k=1 \\ \vdots \\ k=7 \end{array} \begin{bmatrix} 0 & -.7 & 1 \\ .7 & 0 & -.7 \\ -1 & .7 & 0 \\ .7 & -1 & .7 \\ 0 & .7 & -1 \\ -.7 & 0 & .7 \\ 1 & -.7 & 0 \\ -.7 & 1 & -.7 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{array}$$

Write an equation $A\mathbf{x} = \mathbf{b}$, where A is a 16×3 matrix formed from the two coefficient matrices above and where \mathbf{b} in \mathbb{R}^{16} is formed from the two right sides of the equations. Find a_0 , a_1 , and a_2 given by the least-squares solution of $A\mathbf{x} = \mathbf{b}$. (The .7 in the data above was used as an approximation for $\sqrt{2}/2$, to illustrate how a typical computation in an applied problem might proceed. If .707 were used instead, the resulting filter coefficients would agree to at least seven decimal places with $\sqrt{2}/4$, $1/2$, and $\sqrt{2}/4$, the values produced by exact arithmetic calculations.)

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6.6 EXERCISES

In Exercises 1–4, find the equation $y = \beta_0 + \beta_1 x$ of the least-squares line that best fits the given data points.

- (0, 1), (1, 1), (2, 2), (3, 2)
- (1, 0), (2, 1), (4, 2), (5, 3)
- (-1, 0), (0, 1), (1, 2), (2, 4)
- (2, 3), (3, 2), (5, 1), (6, 0)
- Let X be the design matrix used to find the least-squares line to fit data $(x_1, y_1), \dots, (x_n, y_n)$. Use a theorem in Section 6.5 to show that the normal equations have a unique solution if and only if the data include at least two data points with different x -coordinates.
- Let X be the design matrix in Example 2 corresponding to a least-squares fit of a parabola to data $(x_1, y_1), \dots, (x_n, y_n)$. Suppose x_1, x_2 , and x_3 are distinct. Explain why there is only one parabola that fits the data best, in a least-squares sense. (See Exercise 5.)
- A certain experiment produces the data (1, 1.8), (2, 2.7), (3, 3.4), (4, 3.8), (5, 3.9). Describe the model that produces a least-squares fit of these points by a function of the form

$$y = \beta_1 x + \beta_2 x^2$$

Such a function might arise, for example, as the revenue from the sale of x units of a product, when the amount offered for sale affects the price to be set for the product.

- Give the design matrix, the observation vector, and the unknown parameter vector.
 - [M] Find the associated least-squares curve for the data.
- A simple curve that often makes a good model for the variable costs of a company, as a function of the sales level x , has the form $y = \beta_1 x + \beta_2 x^2 + \beta_3 x^3$. There is no constant term because fixed costs are not included.
 - Give the design matrix and the parameter vector for the linear model that leads to a least-squares fit of the equation above, with data $(x_1, y_1), \dots, (x_n, y_n)$.
 - [M] Find the least-squares curve of the form above to fit the data (4, 1.58), (6, 2.08), (8, 2.5), (10, 2.8), (12, 3.1), (14, 3.4), (16, 3.8), and (18, 4.32), with values in thousands. If possible, produce a graph that shows the data points and the graph of the cubic approximation.
 - A certain experiment produces the data (1, 7.9), (2, 5.4), and (3, -9). Describe the model that produces a least-squares fit of these points by a function of the form

$$y = A \cos x + B \sin x$$

- Suppose radioactive substances A and B have decay constants of .02 and .07, respectively. If a mixture of these two substances at time $t = 0$ contains M_A grams of A and M_B grams of B, then a model for the total amount y of the mixture present at time t is

$$y = M_A e^{-.02t} + M_B e^{-.07t} \quad (6)$$

Suppose the initial amounts M_A and M_B are unknown, but a scientist is able to measure the total amounts present at several times and records the following points (t_i, y_i) : (10, 21.34), (11, 20.68), (12, 20.05), (14, 18.87), and (15, 18.30).

- Describe a linear model that can be used to estimate M_A and M_B .
- [M] Find the least-squares curve based on (6).



Halley's Comet last appeared in 1986 and will reappear in 2061.

- [M] According to Kepler's first law, a comet should have an elliptic, parabolic, or hyperbolic orbit (with gravitational attractions from the planets ignored). In suitable polar coordinates, the position (r, ϑ) of a comet satisfies an equation of the form

$$r = \beta + e(r \cdot \cos \vartheta)$$

where β is a constant and e is the *eccentricity* of the orbit, with $0 \leq e < 1$ for an ellipse, $e = 1$ for a parabola, and $e > 1$ for a hyperbola. Suppose observations of a newly discovered comet provide the data below. Determine the type of orbit, and predict where the comet will be when $\vartheta = 4.6$ (radians).³

ϑ	.88	1.10	1.42	1.77	2.14
r	3.00	2.30	1.65	1.25	1.01

- [M] A healthy child's systolic blood pressure p (in millimeters of mercury) and weight w (in pounds) are approximately related by the equation

$$\beta_0 + \beta_1 \ln w = p$$

Use the following experimental data to estimate the systolic blood pressure of a healthy child weighing 100 pounds.

³ The basic idea of least-squares fitting of data is due to K. F. Gauss (and, independently, to A. Legendre), whose initial rise to fame occurred in 1801 when he used the method to determine the path of the asteroid *Ceres*. Forty days after the asteroid was discovered, it disappeared behind the sun. Gauss predicted it would appear ten months later and gave its location. The accuracy of the prediction astonished the European scientific community.

w	44	61	81	113	131
$\ln w$	3.78	4.11	4.39	4.73	4.88
p	91	98	103	110	112

13. [M] To measure the takeoff performance of an airplane, the horizontal position of the plane was measured every second, from $t = 0$ to $t = 12$. The positions (in feet) were: 0, 8.8, 29.9, 62.0, 104.7, 159.1, 222.0, 294.5, 380.4, 471.1, 571.7, 686.8, and 809.2.

- Find the least-squares cubic curve $y = \beta_0 + \beta_1 t + \beta_2 t^2 + \beta_3 t^3$ for these data.
- Use the result of part (a) to estimate the velocity of the plane when $t = 4.5$ seconds.

14. Let $\bar{x} = \frac{1}{n}(x_1 + \cdots + x_n)$ and $\bar{y} = \frac{1}{n}(y_1 + \cdots + y_n)$. Show that the least-squares line for the data $(x_1, y_1), \dots, (x_n, y_n)$ must pass through (\bar{x}, \bar{y}) . That is, show that \bar{x} and \bar{y} satisfy the linear equation $\bar{y} = \hat{\beta}_0 + \hat{\beta}_1 \bar{x}$. [Hint: Derive this equation from the vector equation $\mathbf{y} = X\hat{\boldsymbol{\beta}} + \boldsymbol{\epsilon}$. Denote the first column of X by $\mathbf{1}$. Use the fact that the residual vector $\boldsymbol{\epsilon}$ is orthogonal to the column space of X and hence is orthogonal to $\mathbf{1}$.]

Given data for a least-squares problem, $(x_1, y_1), \dots, (x_n, y_n)$, the following abbreviations are helpful:

$$\begin{aligned}\sum x &= \sum_{i=1}^n x_i, & \sum x^2 &= \sum_{i=1}^n x_i^2, \\ \sum y &= \sum_{i=1}^n y_i, & \sum xy &= \sum_{i=1}^n x_i y_i\end{aligned}$$

The normal equations for a least-squares line $y = \hat{\beta}_0 + \hat{\beta}_1 x$ may be written in the form

$$\begin{aligned}n\hat{\beta}_0 + \hat{\beta}_1 \sum x &= \sum y \\ \hat{\beta}_0 \sum x + \hat{\beta}_1 \sum x^2 &= \sum xy\end{aligned}\quad (7)$$

- Derive the normal equations (7) from the matrix form given in this section.
- Use a matrix inverse to solve the system of equations in (7) and thereby obtain formulas for $\hat{\beta}_0$ and $\hat{\beta}_1$ that appear in many statistics texts.

- Rewrite the data in Example 1 with new x -coordinates in mean deviation form. Let X be the associated design matrix. Why are the columns of X orthogonal?
 - Write the normal equations for the data in part (a), and solve them to find the least-squares line, $y = \beta_0 + \beta_1 x^*$, where $x^* = x - 5.5$.
- Suppose the x -coordinates of the data $(x_1, y_1), \dots, (x_n, y_n)$ are in mean deviation form, so that $\sum x_i = 0$. Show that if X is the design matrix for the least-squares line in this case, then $X^T X$ is a diagonal matrix.

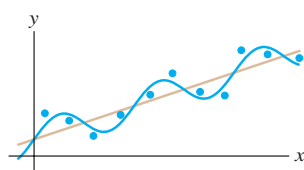
Exercises 19 and 20 involve a design matrix X with two or more columns and a least-squares solution $\hat{\boldsymbol{\beta}}$ of $\mathbf{y} = X\boldsymbol{\beta}$. Consider the following numbers.

- $\|X\hat{\boldsymbol{\beta}}\|^2$ —the sum of the squares of the “regression term.” Denote this number by $SS(R)$.
- $\|\mathbf{y} - X\hat{\boldsymbol{\beta}}\|^2$ —the sum of the squares for error term. Denote this number by $SS(E)$.
- $\|\mathbf{y}\|^2$ —the “total” sum of the squares of the y -values. Denote this number by $SS(T)$.

Every statistics text that discusses regression and the linear model $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$ introduces these numbers, though terminology and notation vary somewhat. To simplify matters, assume that the mean of the y -values is zero. In this case, $SS(T)$ is proportional to what is called the *variance* of the set of y -values.

- Justify the equation $SS(T) = SS(R) + SS(E)$. [Hint: Use a theorem, and explain why the hypotheses of the theorem are satisfied.] This equation is extremely important in statistics, both in regression theory and in the analysis of variance.
- Show that $\|X\hat{\boldsymbol{\beta}}\|^2 = \hat{\boldsymbol{\beta}}^T X^T \mathbf{y}$. [Hint: Rewrite the left side and use the fact that $\hat{\boldsymbol{\beta}}$ satisfies the normal equations.] This formula for $SS(R)$ is used in statistics. From this and from Exercise 19, obtain the standard formula for $SS(E)$:

$$SS(E) = \mathbf{y}^T \mathbf{y} - \hat{\boldsymbol{\beta}}^T X^T \mathbf{y}$$



Sales trend with seasonal fluctuations.

SOLUTION TO PRACTICE PROBLEM

Construct X and $\boldsymbol{\beta}$ so that the k th row of $X\boldsymbol{\beta}$ is the predicted y -value that corresponds to the data point (x_k, y_k) , namely,

$$\beta_0 + \beta_1 x_k + \beta_2 \sin(2\pi x_k/12)$$

It should be clear that

$$X = \begin{bmatrix} 1 & x_1 & \sin(2\pi x_1/12) \\ \vdots & \vdots & \vdots \\ 1 & x_n & \sin(2\pi x_n/12) \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

So p_2 is already orthogonal to q_1 , and we can take $q_2 = p_2$. For the projection of p_3 onto $W_2 = \text{Span}\{q_1, q_2\}$, compute

$$\begin{aligned}\langle p_3, q_1 \rangle &= \int_0^1 12t^2 \cdot 1 \, dt = 4t^3 \Big|_0^1 = 4 \\ \langle q_1, q_1 \rangle &= \int_0^1 1 \cdot 1 \, dt = t \Big|_0^1 = 1 \\ \langle p_3, q_2 \rangle &= \int_0^1 12t^2(2t-1) \, dt = \int_0^1 (24t^3 - 12t^2) \, dt = 2 \\ \langle q_2, q_2 \rangle &= \int_0^1 (2t-1)^2 \, dt = \frac{1}{6}(2t-1)^3 \Big|_0^1 = \frac{1}{3}\end{aligned}$$

Then

$$\text{proj}_{W_2} p_3 = \frac{\langle p_3, q_1 \rangle}{\langle q_1, q_1 \rangle} q_1 + \frac{\langle p_3, q_2 \rangle}{\langle q_2, q_2 \rangle} q_2 = \frac{4}{1} q_1 + \frac{2}{1/3} q_2 = 4q_1 + 6q_2$$

and

$$q_3 = p_3 - \text{proj}_{W_2} p_3 = p_3 - 4q_1 - 6q_2$$

As a function, $q_3(t) = 12t^2 - 4 - 6(2t-1) = 12t^2 - 12t + 2$. The orthogonal basis for the subspace W is $\{q_1, q_2, q_3\}$. ■

PRACTICE PROBLEMS

Use the inner product axioms to verify the following statements.

1. $\langle \mathbf{v}, \mathbf{0} \rangle = \langle \mathbf{0}, \mathbf{v} \rangle = 0$.
2. $\langle \mathbf{u}, \mathbf{v} + \mathbf{w} \rangle = \langle \mathbf{u}, \mathbf{v} \rangle + \langle \mathbf{u}, \mathbf{w} \rangle$.

6.7 EXERCISES

1. Let \mathbb{R}^2 have the inner product of Example 1, and let $\mathbf{x} = (1, 1)$ and $\mathbf{y} = (5, -1)$.
 - a. Find $\|\mathbf{x}\|$, $\|\mathbf{y}\|$, and $|\langle \mathbf{x}, \mathbf{y} \rangle|^2$.
 - b. Describe all vectors (z_1, z_2) that are orthogonal to \mathbf{y} .
2. Let \mathbb{R}^2 have the inner product of Example 1. Show that the Cauchy–Schwarz inequality holds for $\mathbf{x} = (3, -2)$ and $\mathbf{y} = (-2, 1)$. [Suggestion: Study $|\langle \mathbf{x}, \mathbf{y} \rangle|^2$.]

Exercises 3–8 refer to \mathbb{P}_2 with the inner product given by evaluation at $-1, 0$, and 1 . (See Example 2.)

3. Compute $\langle p, q \rangle$, where $p(t) = 4 + t$, $q(t) = 5 - 4t^2$.
4. Compute $\langle p, q \rangle$, where $p(t) = 3t - t^2$, $q(t) = 3 + 2t^2$.
5. Compute $\|p\|$ and $\|q\|$, for p and q in Exercise 3.
6. Compute $\|p\|$ and $\|q\|$, for p and q in Exercise 4.
7. Compute the orthogonal projection of q onto the subspace spanned by p , for p and q in Exercise 3.
8. Compute the orthogonal projection of q onto the subspace spanned by p , for p and q in Exercise 4.
9. Let \mathbb{P}_3 have the inner product given by evaluation at $-3, -1, 1$, and 3 . Let $p_0(t) = 1$, $p_1(t) = t$, and $p_2(t) = t^2$.
 - a. Compute the orthogonal projection of p_2 onto the subspace spanned by p_0 and p_1 .
 - b. Find a polynomial q that is orthogonal to p_0 and p_1 , such that $\{p_0, p_1, q\}$ is an orthogonal basis for $\text{Span}\{p_0, p_1, p_2\}$. Scale the polynomial q so that its vector of values at $(-3, -1, 1, 3)$ is $(1, -1, -1, 1)$.
10. Let \mathbb{P}_3 have the inner product as in Exercise 9, with p_0, p_1 , and q the polynomials described there. Find the best approximation to $p(t) = t^3$ by polynomials in $\text{Span}\{p_0, p_1, q\}$.
11. Let p_0, p_1 , and p_2 be the orthogonal polynomials described in Example 5, where the inner product on \mathbb{P}_4 is given by evaluation at $-2, -1, 0, 1$, and 2 . Find the orthogonal projection of t^3 onto $\text{Span}\{p_0, p_1, p_2\}$.
12. Find a polynomial p_3 such that $\{p_0, p_1, p_2, p_3\}$ (see Exercise 11) is an orthogonal basis for the subspace \mathbb{P}_3 of \mathbb{P}_4 . Scale the polynomial p_3 so that its vector of values is $(-1, 2, 0, -2, 1)$.

13. Let A be any invertible $n \times n$ matrix. Show that for \mathbf{u}, \mathbf{v} in \mathbb{R}^n , the formula $\langle \mathbf{u}, \mathbf{v} \rangle = (A\mathbf{u}) \cdot (A\mathbf{v}) = (A\mathbf{u})^T (A\mathbf{v})$ defines an inner product on \mathbb{R}^n .
14. Let T be a one-to-one linear transformation from a vector space V into \mathbb{R}^n . Show that for \mathbf{u}, \mathbf{v} in V , the formula $\langle \mathbf{u}, \mathbf{v} \rangle = T(\mathbf{u}) \cdot T(\mathbf{v})$ defines an inner product on V .

Use the inner product axioms and other results of this section to verify the statements in Exercises 15–18.

15. $\langle \mathbf{u}, c\mathbf{v} \rangle = c\langle \mathbf{u}, \mathbf{v} \rangle$ for all scalars c .
16. If $\{\mathbf{u}, \mathbf{v}\}$ is an orthonormal set in V , then $\|\mathbf{u} - \mathbf{v}\| = \sqrt{2}$.
17. $\langle \mathbf{u}, \mathbf{v} \rangle = \frac{1}{4}\|\mathbf{u} + \mathbf{v}\|^2 - \frac{1}{4}\|\mathbf{u} - \mathbf{v}\|^2$.
18. $\|\mathbf{u} + \mathbf{v}\|^2 + \|\mathbf{u} - \mathbf{v}\|^2 = 2\|\mathbf{u}\|^2 + 2\|\mathbf{v}\|^2$.
19. Given $a \geq 0$ and $b \geq 0$, let $\mathbf{u} = \begin{bmatrix} \sqrt{a} \\ \sqrt{b} \end{bmatrix}$ and $\mathbf{v} = \begin{bmatrix} \sqrt{b} \\ \sqrt{a} \end{bmatrix}$. Use the Cauchy–Schwarz inequality to compare the geometric mean \sqrt{ab} with the arithmetic mean $(a + b)/2$.
20. Let $\mathbf{u} = \begin{bmatrix} a \\ b \end{bmatrix}$ and $\mathbf{v} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$. Use the Cauchy–Schwarz inequality to show that

$$\left(\frac{a+b}{2}\right)^2 \leq \frac{a^2 + b^2}{2}$$

Exercises 21–24 refer to $V = C[0, 1]$, with the inner product given by an integral, as in Example 7.

21. Compute $\langle f, g \rangle$, where $f(t) = 1 - 3t^2$ and $g(t) = t - t^3$.
22. Compute $\langle f, g \rangle$, where $f(t) = 5t - 3$ and $g(t) = t^3 - t^2$.
23. Compute $\|f\|$ for f in Exercise 21.
24. Compute $\|g\|$ for g in Exercise 22.
25. Let V be the space $C[-1, 1]$ with the inner product of Example 7. Find an orthogonal basis for the subspace spanned by the polynomials $1, t$, and t^2 . The polynomials in this basis are called *Legendre polynomials*.
26. Let V be the space $C[-2, 2]$ with the inner product of Example 7. Find an orthogonal basis for the subspace spanned by the polynomials $1, t$, and t^2 .
27. [M] Let \mathbb{P}_4 have the inner product as in Example 5, and let p_0, p_1, p_2 be the orthogonal polynomials from that example. Using your matrix program, apply the Gram–Schmidt process to the set $\{p_0, p_1, p_2, t^3, t^4\}$ to create an orthogonal basis for \mathbb{P}_4 .
28. [M] Let V be the space $C[0, 2\pi]$ with the inner product of Example 7. Use the Gram–Schmidt process to create an orthogonal basis for the subspace spanned by $\{1, \cos t, \cos^2 t, \cos^3 t\}$. Use a matrix program or computational program to compute the appropriate definite integrals.

SOLUTIONS TO PRACTICE PROBLEMS

1. By Axiom 1, $\langle \mathbf{v}, \mathbf{0} \rangle = \langle \mathbf{0}, \mathbf{v} \rangle$. Then $\langle \mathbf{0}, \mathbf{v} \rangle = \langle 0\mathbf{v}, \mathbf{v} \rangle = 0\langle \mathbf{v}, \mathbf{v} \rangle$, by Axiom 3, so $\langle \mathbf{0}, \mathbf{v} \rangle = 0$.
2. By Axioms 1, 2, and then 1 again, $\langle \mathbf{u}, \mathbf{v} + \mathbf{w} \rangle = \langle \mathbf{v} + \mathbf{w}, \mathbf{u} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle + \langle \mathbf{w}, \mathbf{u} \rangle = \langle \mathbf{u}, \mathbf{v} \rangle + \langle \mathbf{u}, \mathbf{w} \rangle$.

6.8 APPLICATIONS OF INNER PRODUCT SPACES

The examples in this section suggest how the inner product spaces defined in Section 6.7 arise in practical problems. The first example is connected with the massive least-squares problem of updating the North American Datum, described in the chapter's introductory example.

Weighted Least-Squares

Let \mathbf{y} be a vector of n observations, y_1, \dots, y_n , and suppose we wish to approximate \mathbf{y} by a vector $\hat{\mathbf{y}}$ that belongs to some specified subspace of \mathbb{R}^n . (In Section 6.5, $\hat{\mathbf{y}}$ was written as $A\mathbf{x}$ so that $\hat{\mathbf{y}}$ was in the column space of A .) Denote the entries in $\hat{\mathbf{y}}$ by $\hat{y}_1, \dots, \hat{y}_n$. Then the *sum of the squares for error*, or SS(E) , in approximating \mathbf{y} by $\hat{\mathbf{y}}$ is

$$\text{SS(E)} = (y_1 - \hat{y}_1)^2 + \cdots + (y_n - \hat{y}_n)^2 \quad (1)$$

This is simply $\|\mathbf{y} - \hat{\mathbf{y}}\|^2$, using the standard length in \mathbb{R}^n .