SOLUTION TO PRACTICE PROBLEM

Let $\mathbf{v}_1 = \mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ and $\mathbf{v}_2 = \mathbf{x}_2 - \dfrac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 = \mathbf{x}_2 - 0\mathbf{v}_1 = \mathbf{x}_2$. So $\{\mathbf{x}_1, \mathbf{x}_2\}$ is already orthogonal. All that is needed is to normalize the vectors. Let

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

Instead of normalizing $\mathbf{v}_2$ directly, normalize $\mathbf{v}_2' = 3\mathbf{v}_2$ instead:

$$\mathbf{u}_2 = \frac{1}{\|\mathbf{v}_2'\|}\mathbf{v}_2' = \frac{1}{\sqrt{1^2 + 1^2 + (-2)^2}}\begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{6} \\ 1/\sqrt{6} \\ -2/\sqrt{6} \end{bmatrix}$$

Then $\{\mathbf{u}_1, \mathbf{u}_2\}$ is an orthonormal basis for W.

6.5 LEAST-SQUARES PROBLEMS

The chapter's introductory example described a massive problem $A\mathbf{x} = \mathbf{b}$ that had no solution. Inconsistent systems arise often in applications, though usually not with such an enormous coefficient matrix. When a solution is demanded and none exists, the best one can do is to find an $\mathbf{x}$ that makes $A\mathbf{x}$ as close as possible to $\mathbf{b}$.

Think of $A\mathbf{x}$ as an *approximation* to $\mathbf{b}$. The smaller the distance between $\mathbf{b}$ and $A\mathbf{x}$, given by $\|\mathbf{b} - A\mathbf{x}\|$, the better the approximation. The **general least-squares problem** is to find an $\mathbf{x}$ that makes $\|\mathbf{b} - A\mathbf{x}\|$ as small as possible. The adjective "least-squares" arises from the fact that $\|\mathbf{b} - A\mathbf{x}\|$ is the square root of a sum of squares.

DEFINITION

If A is $m \times n$ and $\mathbf{b}$ is in $\mathbb{R}^m$, a **least-squares solution** of $A\mathbf{x} = \mathbf{b}$ is an $\hat{\mathbf{x}}$ in $\mathbb{R}^n$ such that

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \le \|\mathbf{b} - A\mathbf{x}\|$$

for all $\mathbf{x}$ in $\mathbb{R}^n$.

The most important aspect of the least-squares problem is that no matter what $\mathbf{x}$ we select, the vector $A\mathbf{x}$ will necessarily be in the column space, Col A. So we seek an $\mathbf{x}$ that makes $A\mathbf{x}$ the closest point in Col A to $\mathbf{b}$. See Fig. 1. (Of course, if $\mathbf{b}$ happens to be in Col A, then $\mathbf{b}$ *is* $A\mathbf{x}$ for some $\mathbf{x}$, and such an $\mathbf{x}$ is a "least-squares solution.")

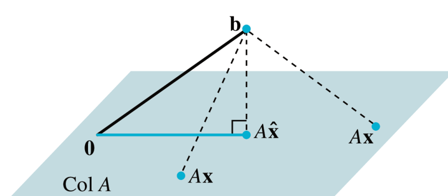

FIGURE 1 The vector $\mathbf{b}$ is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other $\mathbf{x}$.

Solution of the General Least-Squares Problem

Given A and $\mathbf{b}$ as above, apply the Best Approximation Theorem in Section 6.3 to the subspace Col A. Let

$$\hat{\mathbf{b}} = \text{proj}_{\text{Col } A}\, \mathbf{b}$$

Because $\hat{\mathbf{b}}$ is in the column space of A, the equation $A\mathbf{x} = \hat{\mathbf{b}}$ *is* consistent, and there is an $\hat{\mathbf{x}}$ in $\mathbb{R}^n$ such that

$$A\hat{\mathbf{x}} = \hat{\mathbf{b}} \tag{1}$$

Since $\hat{\mathbf{b}}$ is the closest point in Col A to $\mathbf{b}$, a vector $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$ if and only if $\hat{\mathbf{x}}$ satisfies (1). Such an $\hat{\mathbf{x}}$ in $\mathbb{R}^n$ is a list of weights that will build $\hat{\mathbf{b}}$ out of the columns of A. See Fig. 2. [There are many solutions of (1) if the equation has free variables.]

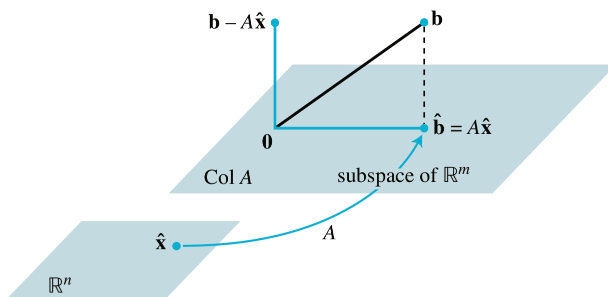

FIGURE 2 The least-squares solution $\hat{\mathbf{x}}$ is in $\mathbb{R}^n$.

Suppose $\hat{\mathbf{x}}$ satisfies $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$. By the Orthogonal Decomposition Theorem in Section 6.3, the projection $\hat{\mathbf{b}}$ has the property that $\mathbf{b} - \hat{\mathbf{b}}$ is orthogonal to Col A, so $\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to each column of A. If $\mathbf{a}_j$ is any column of A, then $\mathbf{a}_j \cdot (\mathbf{b} - A\hat{\mathbf{x}}) = 0$, and $\mathbf{a}_j^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0$. Since each $\mathbf{a}_j^T$ is a row of A^T,

$$A^T(\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0} \tag{2}$$

(This equation also follows from Theorem 3 in Section 6.1.) Thus

$$\begin{aligned} A^T\mathbf{b} - A^TA\hat{\mathbf{x}} &= \mathbf{0} \\ A^TA\hat{\mathbf{x}} &= A^T\mathbf{b} \end{aligned}$$

These calculations show that each least-squares solution of $A\mathbf{x} = \mathbf{b}$ satisfies the equation

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

The matrix equation (3) represents a system of equations called the **normal equations** for $A\mathbf{x} = \mathbf{b}$. A solution of (3) is often denoted by $\hat{\mathbf{x}}$.

THEOREM 13

The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$.

PROOF As shown above, the set of least-squares solutions is nonempty and each least-squares solution $\hat{\mathbf{x}}$ satisfies the normal equations. Conversely, suppose $\hat{\mathbf{x}}$ satisfies $A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$. Then $\hat{\mathbf{x}}$ satisfies (2) above, which shows that $\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to the rows of A^T and hence is orthogonal to the columns of A. Since the columns of A span Col A, the vector $\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to all of Col A. Hence the equation

$$\mathbf{b} = A\hat{\mathbf{x}} + (\mathbf{b} - A\hat{\mathbf{x}})$$

is a decomposition of $\mathbf{b}$ into the sum of a vector in Col A and a vector orthogonal to Col A. By the uniqueness of the orthogonal decomposition, $A\hat{\mathbf{x}}$ must be the orthogonal projection of $\mathbf{b}$ onto Col A. That is, $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$, and $\hat{\mathbf{x}}$ is a least-squares solution. ■

EXAMPLE 1 Find a least-squares solution of the inconsistent system $A\mathbf{x} = \mathbf{b}$ for

$$A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$$

SOLUTION To use normal equations (3), compute:

$$A^TA = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix}\begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}$$

$$A^T\mathbf{b} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix}\begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

Then the equation $A^TA\mathbf{x} = A^T\mathbf{b}$ becomes

$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

Row operations can be used to solve this system, but since A^TA is invertible and 2×2, it is probably faster to compute

$$(A^TA)^{-1} = \frac{1}{84}\begin{bmatrix} 5 & -1 \\ -1 & 17 \end{bmatrix}$$

and then to solve $A^TA\mathbf{x} = A^T\mathbf{b}$ as

$$\begin{aligned} \hat{\mathbf{x}} &= (A^TA)^{-1}A^T\mathbf{b} \\ &= \frac{1}{84}\begin{bmatrix} 5 & -1 \\ -1 & 17 \end{bmatrix}\begin{bmatrix} 19 \\ 11 \end{bmatrix} = \frac{1}{84}\begin{bmatrix} 84 \\ 168 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \end{aligned}$$ ■

In many calculations, A^TA is invertible, but this is not always the case. The next example involves a matrix of the sort that appears in what are called *analysis of variance* problems in statistics.

EXAMPLE 2 Find a least-squares solution of $A\mathbf{x} = \mathbf{b}$ for

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

SOLUTION Compute

$$A^TA = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{bmatrix}$$

$$A^T\mathbf{b} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} -3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ -4 \\ 2 \\ 6 \end{bmatrix}$$

The augmented matrix for $A^TA\mathbf{x} = A^T\mathbf{b}$ is

$$\begin{bmatrix} 6 & 2 & 2 & 2 & 4 \\ 2 & 2 & 0 & 0 & -4 \\ 2 & 0 & 2 & 0 & 2 \\ 2 & 0 & 0 & 2 & 6 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & 1 & 3 \\ 0 & 1 & 0 & -1 & -5 \\ 0 & 0 & 1 & -1 & -2 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The general solution is $x_1 = 3 - x_4$, $x_2 = -5 + x_4$, $x_3 = -2 + x_4$, and x_4 is free. So the general least-squares solution of $A\mathbf{x} = \mathbf{b}$ has the form

$$\hat{\mathbf{x}} = \begin{bmatrix} 3 \\ -5 \\ -2 \\ 0 \end{bmatrix} + x_4 \begin{bmatrix} -1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

The next theorem gives useful criteria for determining when there is only one least-squares solution of $A\mathbf{x} = \mathbf{b}$. (Of course, the orthogonal projection $\hat{\mathbf{b}}$ is always unique.)

THEOREM 14

Let A be an $m \times n$ matrix. The following statements are logically equivalent:

a. The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for each $\mathbf{b}$ in $\mathbb{R}^m$.
b. The columns of A are linearly indpendent.
c. The matrix A^TA is invertible.

When these statements are true, the least-squares solution $\hat{\mathbf{x}}$ is given by

$$\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b} \tag{4}$$

The main elements of a proof of Theorem 14 are outlined in Exercises 19–21, which also review concepts from Chapter 4. Formula (4) for $\hat{\mathbf{x}}$ is useful mainly for theoretical purposes and for hand calculations when A^TA is a 2×2 invertible matrix.

When a least-squares solution $\hat{\mathbf{x}}$ is used to produce $A\hat{\mathbf{x}}$ as an approximation to $\mathbf{b}$, the distance from $\mathbf{b}$ to $A\hat{\mathbf{x}}$ is called the **least-squares error** of this approximation.

EXAMPLE 3 Given A and $\mathbf{b}$ as in Example 1, determine the least-squares error in the least-squares solution of $A\mathbf{x} = \mathbf{b}$.

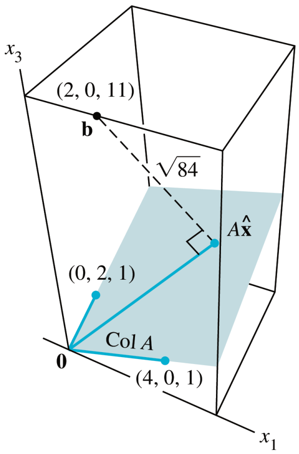

FIGURE 3

SOLUTION From Example 1,

$$\mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} \quad \text{and} \quad A\hat{\mathbf{x}} = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 4 \\ 3 \end{bmatrix}$$

Hence

$$\mathbf{b} - A\hat{\mathbf{x}} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} - \begin{bmatrix} 4 \\ 4 \\ 3 \end{bmatrix} = \begin{bmatrix} -2 \\ -4 \\ 8 \end{bmatrix}$$

and

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| = \sqrt{(-2)^2 + (-4)^2 + 8^2} = \sqrt{84}$$

The least-squares error is $\sqrt{84}$. For any $\mathbf{x}$ in $\mathbb{R}^2$, the distance between $\mathbf{b}$ and the vector $A\mathbf{x}$ is at least $\sqrt{84}$. See Fig. 3. Note that the least-squares solution $\hat{\mathbf{x}}$ itself does not appear in the figure. ■

Alternative Calculations of Least-Squares Solutions

The next example shows how to find a least-squares solution of $A\mathbf{x} = \mathbf{b}$ when the columns of A are orthogonal. Such matrices often appear in linear regression problems, discussed in the next section.

EXAMPLE 4 Find a least-squares solution of $A\mathbf{x} = \mathbf{b}$ for

$$A = \begin{bmatrix} 1 & -6 \\ 1 & -2 \\ 1 & 1 \\ 1 & 7 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -1 \\ 2 \\ 1 \\ 6 \end{bmatrix}$$

SOLUTION Because the columns $\mathbf{a}_1$ and $\mathbf{a}_2$ of A are orthogonal, the orthogonal projection of $\mathbf{b}$ onto Col A is given by

$$\hat{\mathbf{b}} = \frac{\mathbf{b} \cdot \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_1}\mathbf{a}_1 + \frac{\mathbf{b} \cdot \mathbf{a}_2}{\mathbf{a}_2 \cdot \mathbf{a}_2}\mathbf{a}_2 = \frac{8}{4}\mathbf{a}_1 + \frac{45}{90}\mathbf{a}_2 \tag{5}$$

$$= \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \end{bmatrix} + \begin{bmatrix} -3 \\ -1 \\ 1/2 \\ 7/2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 5/2 \\ 11/2 \end{bmatrix}$$

Now that $\hat{\mathbf{b}}$ is known, we can solve $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$. But this is trivial, since we already know what weights to place on the columns of A to produce $\hat{\mathbf{b}}$. It is clear from (5) that

$$\hat{\mathbf{x}} = \begin{bmatrix} 8/4 \\ 45/90 \end{bmatrix} = \begin{bmatrix} 2 \\ 1/2 \end{bmatrix}$$ ■

In some cases, the normal equations for a least-squares problem can be *ill-conditioned*; that is, small errors in the calculations of the entries of A^TA can sometimes cause relatively large errors in the solution $\hat{\mathbf{x}}$. If the columns of A are linearly independent, the least-squares solution can often be computed more reliably through a QR factorization of A (described in Section 6.4).[1]

[1] The QR method is compared with the standard normal equation method in G. Golub and C. Van Loan, *Matrix Computations*, 3rd ed. (Baltimore: Johns Hopkins Press, 1996), pp. 230–231.

THEOREM 15

Given an $m \times n$ matrix A with linearly independent columns, let $A = QR$ be a QR factorization of A as in Theorem 12. Then, for each $\mathbf{b}$ in $\mathbb{R}^m$, the equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution, given by

$$\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b} \tag{6}$$

PROOF Let $\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$. Then

$$A\hat{\mathbf{x}} = QR\hat{\mathbf{x}} = QRR^{-1}Q^T\mathbf{b} = QQ^T\mathbf{b}$$

By Theorem 12, the columns of Q form an orthonormal basis for Col A. Hence, by Theorem 10, $QQ^T\mathbf{b}$ is the orthogonal projection $\hat{\mathbf{b}}$ of $\mathbf{b}$ onto Col A. Then $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$, which shows that $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$. The uniqueness of $\hat{\mathbf{x}}$ follows from Theorem 14. ■

NUMERICAL NOTE

Since R in Theorem 15 is upper triangular, $\hat{\mathbf{x}}$ should be calculated as the exact solution of the equation

$$R\mathbf{x} = Q^T\mathbf{b} \tag{7}$$

It is much faster to solve (7) by back-substitution or row operations than to compute R^{-1} and use (6).

EXAMPLE 5 Find the least-squares solution of $A\mathbf{x} = \mathbf{b}$ for

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

SOLUTION The QR factorization of A can be obtained as in Section 6.4.

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

Then

$$Q^T\mathbf{b} = \begin{bmatrix} 1/2 & 1/2 & 1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & 1/2 & -1/2 \end{bmatrix} \begin{bmatrix} 3 \\ 5 \\ 7 \\ -3 \end{bmatrix} = \begin{bmatrix} 6 \\ -6 \\ 4 \end{bmatrix}$$

The least-squares solution $\hat{\mathbf{x}}$ satisfies $R\mathbf{x} = Q^T\mathbf{b}$; that is,

$$\begin{bmatrix} 2 & 4 & 5 \\ 0 & 2 & 3 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ -6 \\ 4 \end{bmatrix}$$

This equation is solved easily and yields $\hat{\mathbf{x}} = \begin{bmatrix} 10 \\ -6 \\ 2 \end{bmatrix}$. ■

PRACTICE PROBLEMS

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

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

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

13. 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.)

14. 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.

17. 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 Col A.

c. A least-squares solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\hat{\mathbf{x}}$ such that $\|\mathbf{b} - A\mathbf{x}\| \leq \|\mathbf{b} - A\hat{\mathbf{x}}\|$ for all $\mathbf{x}$ in $\mathbb{R}^n$.

d. Any solution of $A^TA\mathbf{x} = A^T\mathbf{b}$ 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 Col A.

d. If $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$, then $\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b}$.

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 $A^TA\mathbf{x} = \mathbf{0}$. This will show that Nul A = Nul A^TA.

a. Show that if $A\mathbf{x} = \mathbf{0}$, then $A^TA\mathbf{x} = \mathbf{0}$.

b. Suppose $A^TA\mathbf{x} = \mathbf{0}$. Explain why $\mathbf{x}^TA^TA\mathbf{x} = \mathbf{0}$, and use this to show that $A\mathbf{x} = \mathbf{0}$.

20. Let A be an $m \times n$ matrix such that A^TA 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^TA 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 rank A^TA = rank A. [*Hint:* How many columns does A^TA have? How is this connected with the rank of A^TA?]

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 Col A. [*Hint:* Find $\hat{\mathbf{x}}$ first. The formula does not require an orthogonal basis for 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

$$\begin{aligned} x + y &= 2 \\ x + y &= 4 \end{aligned}$$

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

$$a_0 y_{k+2} + a_1 y_{k+1} + a_2 y_k = z_k \qquad \text{for all } k \tag{8}$$

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

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

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

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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SOLUTIONS TO PRACTICE PROBLEMS

1. First, compute

$$A^TA = \begin{bmatrix} 1 & 1 & 1 \\ -3 & 5 & 7 \\ -3 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & -3 & -3 \\ 1 & 5 & 1 \\ 1 & 7 & 2 \end{bmatrix} = \begin{bmatrix} 3 & 9 & 0 \\ 9 & 83 & 28 \\ 0 & 28 & 14 \end{bmatrix}$$

$$A^T\mathbf{b} = \begin{bmatrix} 1 & 1 & 1 \\ -3 & 5 & 7 \\ -3 & 1 & 2 \end{bmatrix} \begin{bmatrix} 5 \\ -3 \\ -5 \end{bmatrix} = \begin{bmatrix} -3 \\ -65 \\ -28 \end{bmatrix}$$

Next, row reduce the augmented matrix for the normal equations, $A^TA\mathbf{x} = A^T\mathbf{b}$:

$$\begin{bmatrix} 3 & 9 & 0 & -3 \\ 9 & 83 & 28 & -65 \\ 0 & 28 & 14 & -28 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & 0 & -1 \\ 0 & 56 & 28 & -56 \\ 0 & 28 & 14 & -28 \end{bmatrix} \sim \cdots \sim \begin{bmatrix} 1 & 0 & -3/2 & 2 \\ 0 & 1 & 1/2 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The general least-squares solution is $x_1 = 2 + \frac{3}{2}x_3$, $x_2 = -1 - \frac{1}{2}x_3$, with x_3 free. For one specific solution, take $x_3 = 0$ (for example), and get

$$\hat{\mathbf{x}} = \begin{bmatrix} 2 \\ -1 \\ 0 \end{bmatrix}$$

To find the least-squares error, compute

$$\hat{\mathbf{b}} = A\hat{\mathbf{x}} = \begin{bmatrix} 1 & -3 & -3 \\ 1 & 5 & 1 \\ 1 & 7 & 2 \end{bmatrix} \begin{bmatrix} 2 \\ -1 \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ -3 \\ -5 \end{bmatrix}$$

It turns out that $\hat{\mathbf{b}} = \mathbf{b}$, so $\|\mathbf{b} - \hat{\mathbf{b}}\| = 0$. The least-squares error is zero because $\mathbf{b}$ happens to be in Col A.

2. If $\mathbf{b}$ is orthogonal to the columns of A, then the projection of $\mathbf{b}$ onto the column space of A is $\mathbf{0}$. In this case, a least-squares solution $\hat{\mathbf{x}}$ of $A\mathbf{x} = \mathbf{b}$ satisfies $A\hat{\mathbf{x}} = \mathbf{0}$.

6.6 APPLICATIONS TO LINEAR MODELS

A common task in science and engineering is to analyze and understand relationships among several quantities that vary. This section describes a variety of situations in which data are used to build or verify a formula that predicts the value of one variable as a function of other variables. In each case, the problem will amount to solving a least-squares problem.

For easy application of the discussion to real problems that you may encounter later in your career, we choose notation that is commonly used in the statistical analysis of scientific and engineering data. Instead of $A\mathbf{x} = \mathbf{b}$, we write $X\boldsymbol{\beta} = \mathbf{y}$ and refer to X as the **design matrix**, $\boldsymbol{\beta}$ as the **parameter vector**, and $\mathbf{y}$ as the **observation vector**.

Least-Squares Lines

The simplest relation between two variables x and y is the linear equation $y = \beta_0 + \beta_1 x$.[1] Experimental data often produce points $(x_1, y_1), \ldots, (x_n, y_n)$ that,

[1] This notation is commonly used for least-squares lines instead of $y = mx + b$.