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 term *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.")

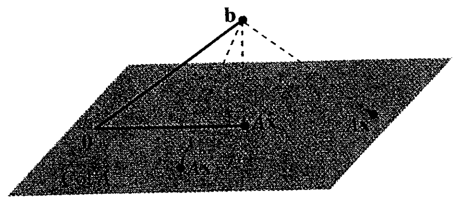


FIGURE 1 $\mathbf{b}$ is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other $\mathbf{x}$.

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.)

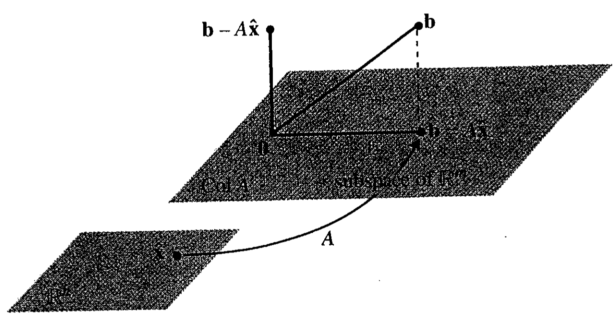


FIGURE 2 The least-squares solution $\hat{\mathbf{x}}$ is in $\mathbb{R}^n$.

Suppose that $\hat{\mathbf{x}}$ 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,

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

$$A^T\mathbf{b} - A^TA\hat{\mathbf{x}} = \mathbf{0}$$

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

[Equation (2) also follows from Theorem 3 in Section 6.1.] The matrix equation (3) represents a system of linear equations commonly referred to as the **normal equations for $\hat{\mathbf{x}}$**.

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 We have already shown that the set of least-squares solutions is nonempty and any such $\hat{\mathbf{x}}$ satisfies the normal equations. Conversely, suppose that $\hat{\mathbf{x}}$ 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

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

Solution To use (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 $A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$ 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 $(A^TA\hat{\mathbf{x}}) = A^T\mathbf{b}$ 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

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

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 $A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$ 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 a useful criterion for 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

The matrix A^TA is invertible if and only if the columns of A are linearly independent. In this case, the equation $A\mathbf{x} = \mathbf{b}$ has only one least-squares solution $\hat{\mathbf{x}}$, and it 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 $A\mathbf{x} = \mathbf{b}$.

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

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

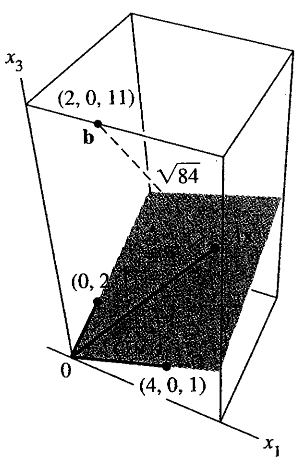


FIGURE 3

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

$$\begin{aligned} \hat{\mathbf{b}} &= \frac{\mathbf{b}\cdot\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_1}\mathbf{a}_1 + \frac{\mathbf{b}\cdot\mathbf{a}_2}{\mathbf{a}_2\cdot\mathbf{a}_2}\mathbf{a}_2 = \frac{8}{4}\mathbf{a}_1 + \frac{45}{90}\mathbf{a}_2 \\ &= \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \end{bmatrix} + \begin{bmatrix} -3 \\ -1 \\ 1/2 \\ 7/2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 5/2 \\ 11/2 \end{bmatrix} \end{aligned} \tag{5}$$

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]

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

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

[1]The QR method is compared with the standard normal equation method in G. Golub and C. Van Loan, *Matrix Computations*, 2nd ed. (Baltimore: Johns Hopkins Press, 1989), pp. 230–231.

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 from the equation

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

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 $R\hat{\mathbf{x}} = Q^T\mathbf{b}$; 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 $A\mathbf{x} = \hat{\mathbf{b}}$, 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 $\|\mathbf{b} - A\mathbf{x}\| \le \|\mathbf{b} - A\hat{\mathbf{x}}\|$ for all $\mathbf{x}$ in $\mathbb{R}^n$.

d. Any solution of $A^TA\hat{\mathbf{x}} = A^T\mathbf{b}$ 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 that $A^TA\mathbf{x} = \mathbf{0}$. 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 that 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

$$x + y = 2$$
$$x + y = 4$$

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

$$a_0y_{k+2} + a_1y_{k+1} + a_2y_k = z_k \quad \text{for all } k \tag{8}$$

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:

$$\begin{matrix} k=0 \\ k=1 \\ \vdots \\ \\ \\ \\ \\ k=7 \end{matrix} \overset{\begin{matrix} y_{k+2} & y_{k+1} & y_k \end{matrix}}{\begin{bmatrix} 0 & .7 & 1 \\ -.7 & 0 & .7 \\ -1 & -.7 & 0 \\ -.7 & -1 & -.7 \\ 0 & -.7 & -1 \\ .7 & 0 & -.7 \\ 1 & .7 & 0 \\ .7 & 1 & .7 \end{bmatrix}} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \overset{y_{k+1}}{\begin{bmatrix} .7 \\ 0 \\ -.7 \\ -1 \\ -.7 \\ 0 \\ .7 \\ 1 \end{bmatrix}};$$

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

Write an equation $A\mathbf{x} = \mathbf{b}$, where A is a 16×3 matrix formed from the two coefficient matrices above and $\mathbf{b}$ in $\mathbb{R}^{16}$ is formed from the two right sides of the equations. Find a_0, a_1, 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.)

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

One 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 readers may encounter later in their careers, 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**, $\boldsymbol{\beta}$ the **parameter vector**, and $\mathbf{y}$ 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 $(x_1, y_1), \dots, (x_n, y_n)$ that when graphed seem to lie close to a line. We want to determine the parameters β_0 and β_1 that make the line as "close" to the points as possible.

Suppose β_0 and β_1 are fixed and consider the line $y = \beta_0 + \beta_1 x$ in Fig. 1. Corresponding to each data point (x_j, y_j) there is a point $(x_j, \beta_0 + \beta_1 x_j)$ on the line with the same x-coordinate. We call y_j the *observed* value of y and $\beta_0 + \beta_1 x_j$ the *predicted* y-value (determined by the line). The difference between an observed y-value and a predicted y-value is called a *residual.*

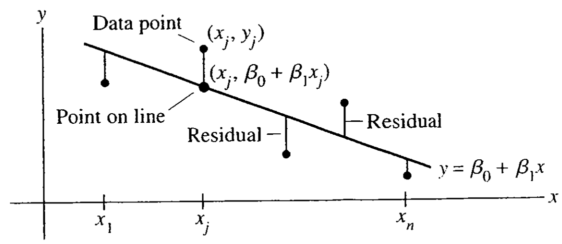


FIGURE 1 Fitting a line to experimental data.

There are several ways to measure how "close" the line is to the data. The usual choice (primarily because the mathematical calculations are simple) is to add the squares of the residuals. The **least-squares line** is the line $y = \beta_0 + \beta_1 x$ that minimizes the sum of the squares of the residuals. This line is also called a **line of regression of y on x**, because any errors in the data are assumed to be only in the y-coordinates. The coefficients β_0, β_1 of the line are called (linear) **regression coefficients.**[2]

---

[1]This notation is commonly used for least-squares lines instead of $y = mx + b$.
[2]If the measurement errors are in x instead of y, simply interchange the coordinates of the data (x_j, y_j) before plotting the points and computing the regression line. If both coordinates are subject to possible error, then you might choose the line that minimizes the sum of the squares of the *orthogonal* (perpendicular) distances from the points to the line. See the Practice Problems for Section 7.5.

If the data points were on the line, the parameters β_0 and β_1 would satisfy the equations

Predicted y-value		Observed y-value
$\beta_0 + \beta_1 x_1$	$=$	y_1
$\beta_0 + \beta_1 x_2$	$=$	y_2
$\vdots$		$\vdots$
$\beta_0 + \beta_1 x_n$	$=$	y_n

We can write this system as

$$X\boldsymbol{\beta} = \mathbf{y}, \quad \text{where } X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \tag{1}$$

Of course, if the data points don't lie on a line, then there are no parameters β_0, β_1 for which the predicted y-values in $X\boldsymbol{\beta}$ equal the observed y-values in $\mathbf{y}$, and $X\boldsymbol{\beta} = \mathbf{y}$ has no solution. This is a least-squares problem, $A\mathbf{x} = \mathbf{b}$, with different notation!

The square of the distance between the vectors $X\boldsymbol{\beta}$ and $\mathbf{y}$ is precisely the sum of the squares of the residuals. The $\boldsymbol{\beta}$ that minimizes this sum also minimizes the distance between $X\boldsymbol{\beta}$ and $\mathbf{y}$. *Computing the least-squares solution of $X\boldsymbol{\beta} = \mathbf{y}$ is equivalent to finding the $\boldsymbol{\beta}$ that determines the least-squares line in Fig. 1.*

EXAMPLE 1 Find the equation $y = \beta_0 + \beta_1 x$ of the least-squares line that best fits the data points (2, 1), (5, 2), (7, 3), (8, 3).

Solution Use the x-coordinates of the data to build the matrix X in (1) and the y-coordinates to build the vector $\mathbf{y}$:

$$X = \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}$$

For the least-squares solution of $X\boldsymbol{\beta} = \mathbf{y}$, obtain the normal equations (with the new notation):

$$X^T X \hat{\boldsymbol{\beta}} = X^T \mathbf{y}$$

That is, compute

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} = \begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix}$$

$$X^T\mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$$

The normal equations are

$$\begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$$

Hence

$$\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix}^{-1} \begin{bmatrix} 9 \\ 57 \end{bmatrix} = \frac{1}{84} \begin{bmatrix} 142 & -22 \\ -22 & 4 \end{bmatrix} \begin{bmatrix} 9 \\ 57 \end{bmatrix} = \frac{1}{84} \begin{bmatrix} 24 \\ 30 \end{bmatrix} = \begin{bmatrix} 2/7 \\ 5/14 \end{bmatrix}$$

Thus the least-squares line has the equation

$$y = \frac{2}{7} + \frac{5}{14}x$$

See Fig. 2.

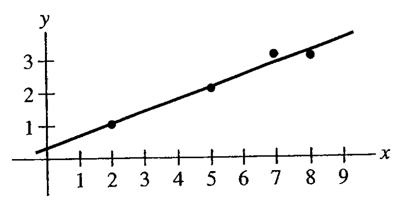


FIGURE 2 The least-squares line $y = \frac{2}{7} + \frac{5}{14}x$.

A common practice before computing a least-squares line is to compute the average $\bar{x}$ of the original x-values and form a new variable $x^* = x - \bar{x}$. The new x-data are said to be in **mean-deviation form**. In this case, the two columns of the design matrix will be orthogonal. Solution of the normal equations is simplified, just as in Example 4 of Section 6.5. See Exercises 17 and 18.

The General Linear Model

In some applications it is necessary to fit data points with something other than a straight line. In the examples that follow, the matrix equation is still $X\boldsymbol{\beta} = \mathbf{y}$, but the specific form of X changes from one problem to the next. Statisticians usually introduce a **residual vector** $\boldsymbol{\epsilon}$, defined by $\boldsymbol{\epsilon} = \mathbf{y} - X\boldsymbol{\beta}$, and write

$$\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

Any equation of this form is referred to as a **linear model**. Once X and $\mathbf{y}$ are determined, the goal is to minimize the length of $\boldsymbol{\epsilon}$, which amounts to finding a least-squares solution of $X\boldsymbol{\beta} = \mathbf{y}$. In each case, the least-squares solution $\hat{\boldsymbol{\beta}}$ is a solution of the normal equations

$$X^TX\hat{\boldsymbol{\beta}} = X^T\mathbf{y}$$

Least-Squares Fitting of Other Curves

When data points $(x_1, y_1), \ldots, (x_n, y_n)$ on a "scatter plot" do not lie close to any line, it may be appropriate to postulate some other functional relationship between x and y.

The next three examples show how to fit data by curves that have the general form

$$y = \beta_0 f_0(x) + \beta_1 f_1(x) + \cdots + \beta_k f_k(x) \tag{2}$$

where the $f_0, \ldots, f_k$ are known functions and the $\beta_0, \ldots, \beta_k$ are parameters that must be determined. As we will see, equation (2) describes a linear model because it is linear in the unknown parameters.

For a particular value of x, (2) gives a predicted or "fitted" value of y. The difference between the observed value and the predicted value is the residual. The parameters $\beta_0, \ldots, \beta_k$ must be determined so as to minimize the sum of the squares of the residuals.

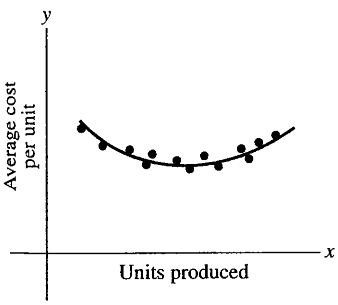


FIGURE 3 Average cost curve.

EXAMPLE 2 Suppose data points $(x_1, y_1), \ldots, (x_n, y_n)$ appear to lie along some sort of parabola instead of a straight line. For instance, if the x-coordinate denotes the production level for a company, and y denotes the average cost per unit of operating at a level of x units per day, then a typical average cost curve looks like a parabola that opens upward (Fig. 3). In ecology, a parabolic curve that opens downward is used to model the net primary production of nutrients in a plant, as a function of the surface area of the foliage (Fig. 4). Suppose we wish to approximate the data by an equation of the form

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 \tag{3}$$

Describe the linear model that produces a "least-squares fit" of the data by equation (3).

Solution Equation (3) describes the ideal relationship. Suppose that the actual values of the parameters are $\beta_0, \beta_1, \beta_2$. Then the coordinates of the first data point (x_1, y_1) satisfy an equation of the form

$$y_1 = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \epsilon_1$$

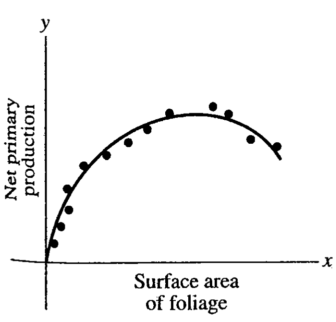


FIGURE 4 Production of nutrients.

where ϵ_1 is the residual error between the observed value y_1 and the predicted y-value $\beta_0 + \beta_1 x_1 + \beta_2 x_1^2$. Let us make a similar equation for each of the data points.

$$\begin{aligned}
y_1 &= \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \epsilon_1 \\
y_2 &= \beta_0 + \beta_1 x_2 + \beta_2 x_2^2 + \epsilon_2 \\
&\ \vdots \qquad\qquad \vdots \\
y_n &= \beta_0 + \beta_1 x_n + \beta_2 x_n^2 + \epsilon_n
\end{aligned}$$

It is a simple matter to write this system of equations in the form $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$. We find X by inspecting the first few rows of the system and looking for the pattern.

$$\underset{\mathbf{y}}{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}} = \underset{X}{\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix}} \underset{\boldsymbol{\beta}}{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}} + \underset{\boldsymbol{\epsilon}}{\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}}$$

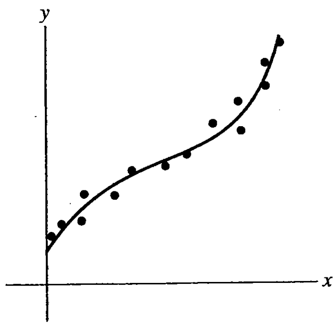


FIGURE 5 Data points along a cubic curve.

EXAMPLE 3 If data points tend to follow a pattern such as in Fig. 5, then an appropriate model might be an equation of the form

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$$

Such data, for instance, could come from a company's total costs, as a function of the level of production. Describe the linear model that gives a least-squares fit of this type to data $(x_1, y_1), \dots, (x_n, y_n)$.

Solution By an analysis similar to that in Example 2, we obtain

Observation vector, Design matrix, Parameter vector, Residual vector

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Multiple Regression

Suppose an experiment involves two independent variables—say, u and v—and one dependent variable, y. A simple equation to predict y from u and v has the form

$$y = \beta_0 + \beta_1 u + \beta_2 v \tag{4}$$

A more general prediction equation might have the form

$$y = \beta_0 + \beta_1 u + \beta_2 v + \beta_3 u^2 + \beta_4 uv + \beta_5 v^2 \tag{5}$$

This equation is used in geology, for instance, to model erosion surfaces, glacial cirques, soil pH, and other quantities. In such cases, the least-squares fit is called a *trend surface*.

Both (4) and (5) lead to a linear model because they are linear in the unknown parameters (even though u and v are multiplied). In general, a linear model will arise whenever y is to be predicted by an equation of the form

$$y = \beta_0 f_0(u, v) + \beta_1 f_1(u, v) + \cdots + \beta_k f_k(u, v)$$

with $f_0, \dots, f_k$ any sort of known functions and $\beta_0, \dots, \beta_k$ unknown weights.

EXAMPLE 4 In geography, local models of terrain are constructed from data $(u_1, v_1, y_1), \dots, (u_n, v_n, y_n)$, where u_j, v_j, and y_j are latitude, longitude, and altitude, respectively. Describe the linear model based on (4) that gives a least-squares fit to such data. The solution is called the least-squares plane. See Fig. 6.

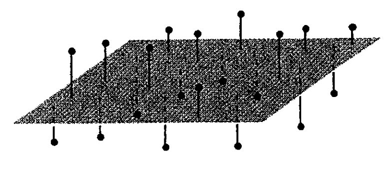


FIGURE 6 A least-squares plane.

Solution We expect the data to satisfy the following equations:

$$\begin{aligned} y_1 &= \beta_0 + \beta_1 u_1 + \beta_2 v_1 + \epsilon_1 \\ y_2 &= \beta_0 + \beta_1 u_2 + \beta_2 v_2 + \epsilon_2 \\ &\vdots \qquad\qquad \vdots \\ y_n &= \beta_0 + \beta_1 u_n + \beta_2 v_n + \epsilon_n \end{aligned}$$

This system has the matrix form $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where

Observation vector, Design matrix, Parameter vector, Residual vector

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & u_1 & v_1 \\ 1 & u_2 & v_2 \\ \vdots & \vdots & \vdots \\ 1 & u_n & v_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Example 4 shows that the linear model for multiple regression has the same abstract form as the model for the simple regression in the earlier examples. Linear algebra gives us the power to understand the general principle behind all the linear models. Once X is defined properly, the normal equations for $\boldsymbol{\beta}$ have the same matrix form, no matter how many variables are involved. Thus, for any linear model where X^TX is invertible, the least-squares $\hat{\boldsymbol{\beta}}$ is given by $(X^TX)^{-1}X^T\mathbf{y}$.

Further Reading

Krumbein, W. C., and F. A. Graybill, *An Introduction to Statistical Models in Geology* (New York: McGraw-Hill, 1965).

Unwin, David J., *An Introduction to Trend Surface Analysis*, Concepts and Techniques in Modern Geography, No. 5 (Norwich, England: Geo Books, 1975).

PRACTICE PROBLEM

When the monthly sales of a product are subject to seasonal fluctuations, a curve that approximates the sales data might have the form

$$y = \beta_0 + \beta_1 x + \beta_2 \sin(2\pi x/12)$$

where x is the time in months. The term $\beta_0 + \beta_1 x$ gives the basic sales trend, and the sine term reflects the seasonal changes in sales. Give the design matrix and the parameter vector for the linear model that leads to a least-squares fit of the equation above. Assume that the data are $(x_1, y_1), \ldots, (x_n, y_n)$.

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.

1. (0, 1), (1, 1), (2, 2), (3, 2)

2. (1, 0), (2, 1), (4, 2), (5, 3)

3. (−1, 0), (0, 1), (1, 2), (2, 4)

4. (2, 3), (3, 2), (5, 1), (6, 0)

5. Let X be the design matrix used to find the least-squares line to fit data $(x_1, y_1), \ldots, (x_n, y_n)$. 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.

6. Let X be the design matrix in Example 2 corresponding to a least-squares fit of a parabola to data $(x_1, y_1), \ldots, (x_n, y_n)$. Suppose that x_1, x_2, x_3 are distinct. Explain why there is only one parabola that fits the data best, in a least-squares sense. (See Exercise 5.)

7. A certain experiment produces data (1, 1.8), (2, 2.7), (3, 3.4), (4, 3.8), and (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.

a. Give the design matrix, the observation vector, and the unknown parameter vector.

b. **[M]** Find the associated least-squares curve for the data.

8. 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.

a. 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 $(x_1, y_1), \ldots, (x_n, y_n)$.

b. **[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), (18, 4.32), with values in thousands. If possible, produce a graph that shows the data points and the graph of the cubic approximation.

9. 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

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

10. 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

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

Suppose the initial amounts M_A, M_B are unknown, but a scientist is able to measure the total amount 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).

a. Describe a linear model that can be used to estimate M_A and M_B.

b. **[M]** Find the least-squares curve based on (6).

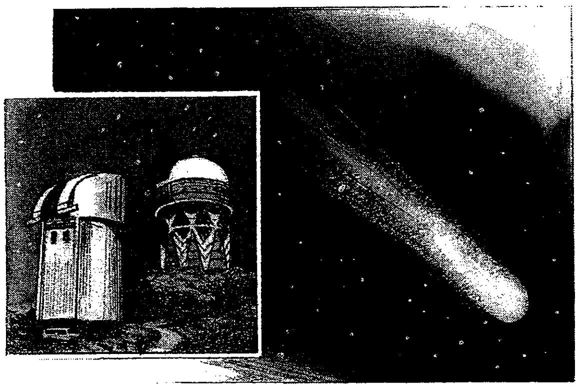
11. **[M]** According to Kepler's first law, a comet should have an elliptic, parabolic, or hyperbolic orbit (with gravitational attractions from the planets ignored). In suitable polar coordinates, the position (r, ϑ) of a comet satisfies an equation of the form

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

where β is a constant and e is the *eccentricity* of the orbit, with $0 \le e < 1$ for an ellipse, $e = 1$ for a parabola, and $e > 1$ for a hyperbola. Suppose that 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).[2]

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

[2] 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 he gave its location. The accuracy of the prediction astonished the European scientific community.



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

12. **[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.

w	44	61	81	113	131
$\ln w$	3.78	4.11	4.41	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, 809.2.

a. Find the least-squares cubic curve $y = \beta_0 + \beta_1 t + \beta_2 t^2 + \beta_3 t^3$ for these data.

b. Use the result of (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 $(x_1, y_1), \ldots, (x_n, y_n)$ 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 othogonal to $\mathbf{1}$.]

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

$\sum x = \sum_{i=1}^n x_i, \quad \sum x^2 = \sum_{i=1}^n x_i^2,$

$\sum y = \sum_{i=1}^n y_i, \quad \sum xy = \sum_{i=1}^n x_i y_i$

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

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

15. Derive the normal equations (7) from the matrix form given in this section.

16. 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.

17. a. 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?

b. 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 $x^* = x - 5.5$.

18. Suppose that the x-coordinates of the data $(x_1, y_1), \ldots, (x_n, y_n)$ 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^TX is a diagonal matrix.

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

(i) $\|X\hat{\boldsymbol{\beta}}\|^2$—the sum of the squares of the "regression term." Denote this number by SS(R).

(ii) $\|\mathbf{y} - X\hat{\boldsymbol{\beta}}\|^2$—the sum of the squares for error term. Denote this number by SS(E), the "least-squares error."

(iii) $\|\mathbf{y}\|^2$—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.

19. 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.

20. 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 18, obtain the standard formula for the least-squares error:

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