Numerical Analysis

SEVENTH EDITION

Richard L. Burden

Youngstown State University

J. Douglas Faires

Youngstown State University

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2. The last two letters determine the type of matrix involved.
   a. RG: real, general
   b. RT: real triangular
   c. DS: real positive definite
   d. SF: real symmetric
   e. RB: real banded

For example, the routine LFTDS factors a real positive definite matrix.

The NAG Library has many subroutines for direct methods of solving linear systems similar to those in LAPACK and IMSL. For example, the subroutine F04AEF solves linear systems using Crout factorization. The subroutine F04ATF solves a single linear system using Crout factorization, as in F04AEF. The subroutine F04EAF solves a single linear system where the matrix is real and tridiagonal, and F04ASF solves a system when the matrix is real and positive definite. Inverse matrices can be computed by F07AJF after using F07ADF for an arbitrary real matrix and by F01ABF if the matrix is positive definite. A determinant can be computed using F03AAF. Factorizations can be obtained using F07ADF for the LU factorization of a real matrix and using F01LEF for a tridiagonal matrix. Linear systems can then be solved using F07AEF. Choleski's factorization of a positive definite matrix can be obtained using F07FDF, and a linear system can then be solved using F07FEF. The NAG library also includes the lower-level matrix-vector manipulations.

Further information on the numerical solution of linear systems and matrices can be found in Golub and Van Loan [GV], Forsythe and Moler [FM], and Stewart [Stew1]. The use of direct techniques for solving large sparse systems is discussed in detail in George and Liu [GL] and in Pissanetzky [Pi]. Coleman and Van Loan [CV] consider the use of BLAS, LINPACK, and MATLAB.

CHAPTER 7

Iterative Techniques in Matrix Algebra

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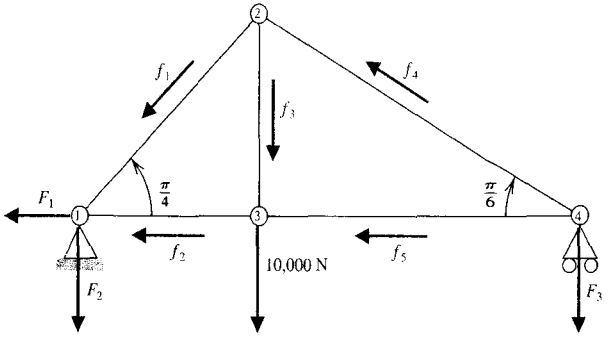
Trusses are lightweight structures capable of carrying heavy loads. In bridge design, the individual members of the truss are connected with rotatable pin joints that permit forces to be transferred from one member of the truss to another. The accompanying figure shows a truss that is held stationary at the lower left endpoint ①, is permitted to move horizontally at the lower right endpoint ④, and has pin joints at ①, ②, ③, and ④. A load of 10,000 newtons (N) is placed at the joint ③, and the forces on the members of the truss have magnitudes given by f_1, f_2, f_3, f_4, and f_5, as shown. The stationary support member has both a horizontal force F_1 and a vertical force F_2, but the movable support member has only the vertical force F_3.



If the truss is in static equilibrium, the forces at each joint must add to the zero vector, so the sum of the horizontal and vertical components of the forces at each joint must be 0. This produces the system of linear

[redacted]

equations shown in the accompanying table. An 8 × 8 matrix describing this system has 46 zero entries and only 18 nonzero entries. Matrices with a high percentage of zero entries are called *sparse* and are often solved using iterative, rather than direct, techniques. The iterative solution to this system is considered in Exercise 18 of Section 7.3.

Joint	Horizontal Component	Vertical Component
①	$-F_1 + \frac{\sqrt{2}}{2}f_1 + f_2 = 0$	$\frac{\sqrt{2}}{2}f_1 - F_2 = 0$
②	$-\frac{\sqrt{2}}{2}f_1 + \frac{\sqrt{3}}{2}f_4 = 0$	$-\frac{\sqrt{2}}{2}f_1 - f_3 + \frac{1}{2}f_4 = 0$
③	$-f_2 + f_5 = 0$	$f_3 - 10{,}000 = 0$
④	$-\frac{\sqrt{3}}{2}f_4 - f_5 = 0$	$\frac{1}{2}f_4 - F_3 = 0$

The methods presented in Chapter 6 used direct techniques to solve a system of $n \times n$ linear equations of the form $A\mathbf{x} = \mathbf{b}$. In this chapter, we present iterative methods to solve a system of this type.

7.1 Norms of Vectors and Matrices

In Chapter 2 we described iterative techniques for finding roots of equations of the form $f(x) = 0$. An initial approximation (or approximations) was found, and new approximations were then determined based on how well the previous approximations satisfied the equation. To discuss iterative methods for solving linear systems, we first need to be able to measure the distance between n-dimensional column vectors to determine whether a sequence of vectors converges to a solution of the system. In actuality, this measure is also needed when the solution is obtained by the direct methods presented in Chapter 6. Those methods required a large number of arithmetic operations, and using finite-digit arithmetic leads only to an approximation to an actual solution of the system.

Let $\mathbb{R}^n$ denote the set of all n-dimensional column vectors with real-number coefficients. To define a distance in $\mathbb{R}^n$ we use the notion of a norm.

Definition 7.1 A **vector norm** on $\mathbb{R}^n$ is a function, $\|\cdot\|$, from $\mathbb{R}^n$ into $\mathbb{R}$ with the following properties:

(i) $\|\mathbf{x}\| \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$,

(ii) $\|\mathbf{x}\| = 0$ if and only if $\mathbf{x} = \mathbf{0}$,

(iii) $\|\alpha\mathbf{x}\| = |\alpha|\|\mathbf{x}\|$ for all $\alpha \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^n$,

(iv) $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.

We will need only two specific norms on $\mathbb{R}^n$, although a third norm on $\mathbb{R}^n$ is prese in Exercise 2.

Since vectors in $\mathbb{R}^n$ are column vectors, it is convenient to use the transpose nota presented in Section 6.3 when a vector is represented in terms of its components. example, the vector

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

will be written $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$.

Definition 7.2 The l_2 and l_∞ norms for the vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ are defined by

$$\|\mathbf{x}\|_2 = \left\{\sum_{i=1}^{n} x_i^2\right\}^{1/2} \quad \text{and} \quad \|\mathbf{x}\|_\infty = \max_{1 \leq i \leq n} |x_i|.$$

The l_2 norm is called the **Euclidean norm** of the vector $\mathbf{x}$ since it represents the us notion of distance from the origin in case $\mathbf{x}$ is in $\mathbb{R}^1 \equiv \mathbb{R}$, $\mathbb{R}^2$, or $\mathbb{R}^3$. For example, the norm of the vector $\mathbf{x} = (x_1, x_2, x_3)^t$ gives the length of the straight line joining the poi $(0, 0, 0)$ and (x_1, x_2, x_3). Figure 7.1 shows the boundary of those vectors in $\mathbb{R}^2$ and $\mathbb{R}^3$ t have l_2 norm less than 1. Figure 7.2 is a similar illustration for the l_∞ norm.

Figure 7.1

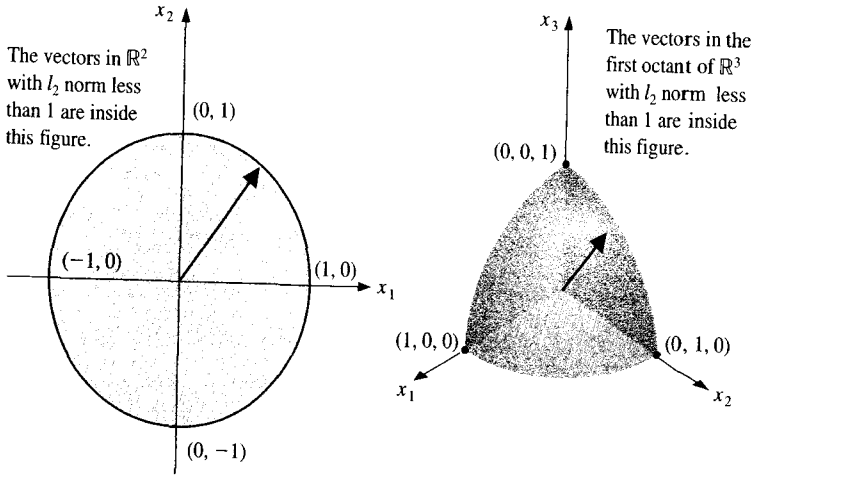
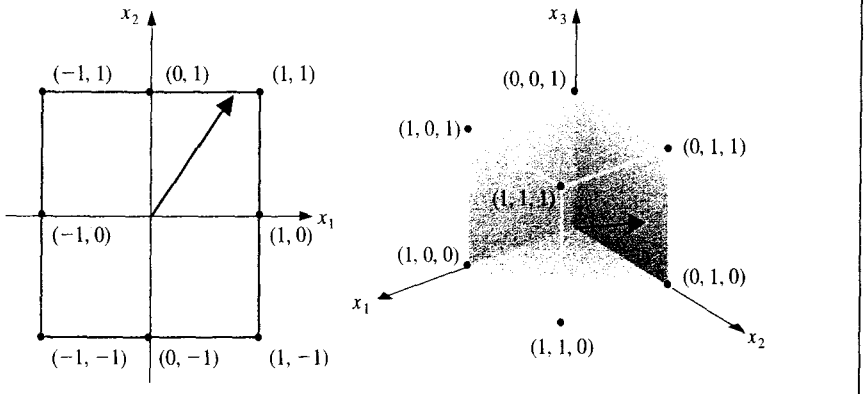


Figure 7.2



The vectors in $\mathbb{R}^2$ with l_∞ norm less than 1 are inside this figure.

The vectors in the first octant of $\mathbb{R}^3$ with l_∞ norm less than 1 are inside this figure.

EXAMPLE 1 The vector $\mathbf{x} = (-1, 1, -2)^t$ in $\mathbb{R}^3$ has norms

$$\|\mathbf{x}\|_2 = \sqrt{(-1)^2 + (1)^2 + (-2)^2} = \sqrt{6}$$

and

$$\|\mathbf{x}\|_\infty = \max\{|-1|, |1|, |-2|\} = 2. \quad \blacksquare$$

It is easy to show that the properties in Definition 7.1 hold for the l_∞ norm since they follow from similar results for absolute values. For example, if $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)^t$, then

$$\|\mathbf{x} + \mathbf{y}\|_\infty = \max_{1 \le i \le n} |x_i + y_i| \le \max_{1 \le i \le n} (|x_i| + |y_i|) \le \max_{1 \le i \le n} |x_i| + \max_{1 \le i \le n} |y_i| = \|\mathbf{x}\|_\infty + \|\mathbf{y}\|_\infty$$

To show that

$$\|\mathbf{x} + \mathbf{y}\|_2 \le \|\mathbf{x}\|_2 + \|\mathbf{y}\|_2, \quad \text{for each } \mathbf{x}, \mathbf{y} \in \mathbb{R}_n,$$

we need a famous inequality.

Theorem 7.3 **(Cauchy-Buniakowsky-Schwarz Inequality for Sums)**

For each $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)^t$ in $\mathbb{R}^n$,

$$\mathbf{x}^t\mathbf{y} = \sum_{i=1}^{n} x_i y_i \le \left\{\sum_{i=1}^{n} x_i^2\right\}^{1/2} \left\{\sum_{i=1}^{n} y_i^2\right\}^{1/2} = \|\mathbf{x}\| \cdot \|\mathbf{y}\|. \qquad (7.$$

Proof If $\mathbf{y} = \mathbf{0}$ or $\mathbf{x} = \mathbf{0}$, the result is immediate since both sides of the inequality are zero.

Suppose $\mathbf{y} \neq \mathbf{0}$ and $\mathbf{x} \neq \mathbf{0}$. For each $\lambda \in \mathbb{R}$,

$$0 \le \|\mathbf{x} - \lambda\mathbf{y}\|_2^2 = \sum_{i=1}^{n} (x_i - \lambda y_i)^2 = \sum_{i=1}^{n} x_i^2 - 2\lambda \sum_{i=1}^{n} x_i y_i + \lambda^2 \sum_{i=1}^{n} y_i^2,$$

and

$$2\lambda \sum_{i=1}^{n} x_i y_i \le \sum_{i=1}^{n} x_i^2 + \lambda^2 \sum_{i=1}^{n} y_i^2 = \|\mathbf{x}\|_2^2 + \lambda^2 \|\mathbf{y}\|_2^2.$$

Since $\|\mathbf{x}\|_2 > 0$ and $\|\mathbf{y}\|_2 > 0$, we can let $\lambda = \|\mathbf{x}\|_2 / \|\mathbf{y}\|_2$ to give

$$\left(2\frac{\|\mathbf{x}\|_2}{\|\mathbf{y}\|_2}\right)\left(\sum_{i=1}^{n} x_i y_i\right) \le \|\mathbf{x}\|_2^2 + \frac{\|\mathbf{x}\|_2^2}{\|\mathbf{y}\|_2^2}\|\mathbf{y}\|_2^2 = 2\|\mathbf{x}\|_2^2,$$

so

$$2\sum_{i=1}^{n} x_i y_i \le 2\|\mathbf{x}\|_2^2 \frac{\|\mathbf{y}\|_2}{\|\mathbf{x}\|_2} = 2\|\mathbf{x}\|_2 \|\mathbf{y}\|_2.$$

Thus,

$$\mathbf{x}^t\mathbf{y} = \sum_{i=1}^{n} x_i y_i \le \|\mathbf{x}\|_2 \|\mathbf{y}\|_2 = \left\{\sum_{i=1}^{n} x_i^2\right\}^{1/2} \left\{\sum_{i=1}^{n} y_i^2\right\}^{1/2}. \quad \blacksquare \blacksquare \blacksquare$$

With this result we see that for each $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$,

$$\|\mathbf{x} + \mathbf{y}\|_2^2 = \sum_{i=1}^{n} (x_i + y_i)^2 = \sum_{i=1}^{n} x_i^2 + 2\sum_{i=1}^{n} x_i y_i + \sum_{i=1}^{n} y_i^2 \le \|\mathbf{x}\|_2^2 + 2\|\mathbf{x}\|_2\|\mathbf{y}\|_2 + \|\mathbf{y}\|_2^2,$$

which gives the final norm property

$$\|\mathbf{x} + \mathbf{y}\|_2 \le \left(\|\mathbf{x}\|_2^2 + 2\|\mathbf{x}\|_2\|\mathbf{y}\|_2 + \|\mathbf{y}\|_2^2\right)^{1/2} = \|\mathbf{x}\|_2 + \|\mathbf{y}\|_2.$$

Since the norm of a vector gives a measure for the distance between an arbitrary vector and the zero vector, the **distance between two vectors** is defined as the norm of the difference of the vectors.

Definition 7.4 If $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)^t$ are vectors in $\mathbb{R}^n$, the l_2 and l_∞ distances between $\mathbf{x}$ and $\mathbf{y}$ are defined by

$$\|\mathbf{x} - \mathbf{y}\|_2 = \left\{\sum_{i=1}^{n} (x_i - y_i)^2\right\}^{1/2} \quad \text{and} \quad \|\mathbf{x} - \mathbf{y}\|_\infty = \max_{1 \le i \le n} |x_i - y_i|. \quad \blacksquare$$

EXAMPLE 2 The linear system

$$3.3330x_1 + 15920x_2 - 10.333x_3 = 15913,$$
$$2.2220x_1 + 16.710x_2 + 9.6120x_3 = 28.544,$$
$$1.5611x_1 + 5.1791x_2 + 1.6852x_3 = 8.4254$$

has solution $(x_1, x_2, x_3)^t = (1, 1, 1)^t$. If Gaussian elimination is performed in five-digit rounding arithmetic using maximal column pivoting (Algorithm 6.2), the solution obtained is

$$\tilde{\mathbf{x}} = (\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)^t = (1.2001, 0.99991, 0.92538)^t.$$

Measurements of $\mathbf{x} - \tilde{\mathbf{x}}$ are given by

$$\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty = \max\{|1 - 1.2001|, |1 - 0.99991|, |1 - 0.92538|\}$$
$$= \max\{0.2001, 0.00009, 0.07462\} = 0.2001$$

and

$$\|\mathbf{x} - \tilde{\mathbf{x}}\|_2 = \left[(1 - 1.2001)^2 + (1 - 0.99991)^2 + (1 - 0.92538)^2\right]^{1/2}$$
$$= [(0.2001)^2 + (0.00009)^2 + (0.07462)^2]^{1/2} = 0.21356.$$

Although the components $\tilde{x}_2$ and $\tilde{x}_3$ are good approximations to x_2 and x_3, the component $\tilde{x}_1$ is a poor approximation to x_1, and $|x_1 - \tilde{x}_1|$ dominates the norms. ■

The concept of distance in $\mathbb{R}^n$ is also used to define a limit of a sequence of vectors in this space.

Definition 7.5 A sequence $\{\mathbf{x}^{(k)}\}_{k=1}^\infty$ of vectors in $\mathbb{R}^n$ is said to **converge** to $\mathbf{x}$ with respect to the norm $\|\cdot\|$ if, given any $\varepsilon > 0$, there exists an integer $N(\varepsilon)$ such that

$$\|\mathbf{x}^{(k)} - \mathbf{x}\| < \varepsilon, \quad \text{for all } k \geq N(\varepsilon).$$

Theorem 7.6 The sequence of vectors $\{\mathbf{x}^{(k)}\}$ converges to $\mathbf{x}$ in $\mathbb{R}^n$ with respect to $\|\cdot\|_\infty$ if and only if $\lim_{k\to\infty} x_i^{(k)} = x_i$, for each $i = 1, 2, \ldots, n$.

Proof Suppose $\{\mathbf{x}^{(k)}\}$ converges to $\mathbf{x}$ with respect to $\|\cdot\|_\infty$. Given any $\varepsilon > 0$, there exists an integer $N(\varepsilon)$ such that for all $k \geq N(\varepsilon)$,

$$\max_{i=1,2,\ldots,n} |x_i^{(k)} - x_i| = \|\mathbf{x}^{(k)} - \mathbf{x}\|_\infty < \varepsilon.$$

This result implies that $|x_i^{(k)} - x_i| < \varepsilon$, for each $i = 1, 2, \ldots, n$, so $\lim_{k\to\infty} x_i^{(k)} = x_i$ for each i.

Conversely, suppose that $\lim_{k\to\infty} x_i^{(k)} = x_i$, for every $i = 1, 2, \ldots, n$. For a given $\varepsilon > 0$, let $N_i(\varepsilon)$ for each i represent an integer with the property that

$$|x_i^{(k)} - x_i| < \varepsilon,$$

whenever $k \geq N_i(\varepsilon)$.

Define $N(\varepsilon) = \max_{i=1,2,\ldots,n} N_i(\varepsilon)$. If $k \geq N(\varepsilon)$, then

$$\max_{i=1,2,\ldots,n} |x_i^{(k)} - x_i| = \|\mathbf{x}^{(k)} - \mathbf{x}\|_\infty < \varepsilon.$$

This implies that $\{\mathbf{x}^{(k)}\}$ converges to $\mathbf{x}$ with respect to $\|\cdot\|_\infty$. ■ ■ ■

EXAMPLE 3 Let $\mathbf{x}^{(k)} \in \mathbb{R}^4$ be defined by

$$\mathbf{x}^{(k)} = (x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, x_4^{(k)})^t = \left(1, 2 + \frac{1}{k}, \frac{3}{k^2}, e^{-k}\sin k\right)^t.$$

Since $\lim_{k\to\infty} 1 = 1$, $\lim_{k\to\infty}(2 + 1/k) = 2$, $\lim_{k\to\infty} 3/k^2 = 0$, and $\lim_{k\to\infty} e^{-k}\sin k = 0$, Theorem 7.6 implies that the sequence $\{\mathbf{x}^{(k)}\}$ converges to $(1, 2, 0, 0)^t$ with respect to $\|\cdot\|_\infty$. ■

To show directly that the sequence in Example 3 converges to $(1, 2, 0, 0)^t$ with respect to the l_2 norm is quite complicated. It is easier to prove the next result and apply it to this special case.

Theorem 7.7 For each $\mathbf{x} \in \mathbb{R}^n$,

$$\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_2 \leq \sqrt{n}\|\mathbf{x}\|_\infty.$$ ■

Proof Let x_j be a coordinate of $\mathbf{x}$ such that $\|\mathbf{x}\|_\infty = \max_{1\leq i\leq n} |x_i| = |x_j|$. Then

$$\|\mathbf{x}\|_\infty^2 = |x_j|^2 = x_j^2 \leq \sum_{i=1}^n x_i^2 = \|\mathbf{x}\|_2^2,$$

so

$$\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_2,$$

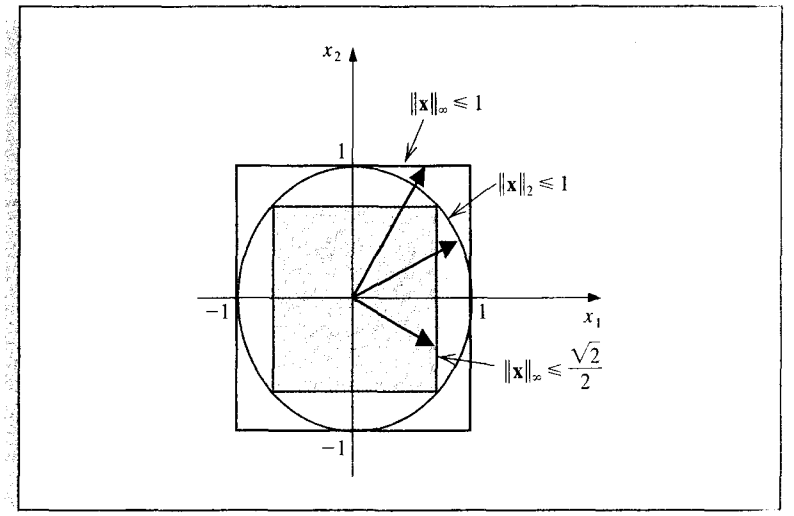
and

$$\|\mathbf{x}\|_2^2 = \sum_{i=1}^n x_i^2 \leq \sum_{i=1}^n x_j^2 = nx_j^2 = n\|\mathbf{x}\|_\infty^2,$$

so $\|\mathbf{x}\|_2 \leq \sqrt{n}\|\mathbf{x}\|_\infty$. ■ ■ ■

Figure 7.3 illustrates this result when $n = 2$.

Figure 7.3



EXAMPLE 4 In Example 3, we found that the sequence $\{\mathbf{x}^{(k)}\}$, defined by

$$\mathbf{x}^{(k)} = \left(1, 2 + \frac{1}{k}, \frac{3}{k^2}, e^{-k}\sin k\right)^t,$$

converges to $\mathbf{x} = (1, 2, 0, 0)^t$ with respect to $\|\cdot\|_\infty$. Given any $\varepsilon > 0$, there exists an integer $N(\varepsilon/2)$ with the property that

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_\infty < \frac{\varepsilon}{2},$$

whenever $k \geq N(\varepsilon/2)$. By Theorem 7.7, this implies that

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_2 < \sqrt{4}\|\mathbf{x}^{(k)} - \mathbf{x}\|_\infty < 2(\varepsilon/2) = \varepsilon,$$

when $k \geq N(\varepsilon/2)$. So $\{\mathbf{x}^{(k)}\}$ also converges to $\mathbf{x}$ with respect to $\|\cdot\|_2$. ■

It can be shown that all norms on $\mathbb{R}^n$ are equivalent with respect to convergence; that is, if $\|\cdot\|$ and $\|\cdot\|'$ are any two norms on $\mathbb{R}^n$ and $\{\mathbf{x}^{(k)}\}_{k=1}^\infty$ has the limit $\mathbf{x}$ with respect to $\|\cdot\|$, then $\{\mathbf{x}^{(k)}\}_{k=1}^\infty$ also has the limit $\mathbf{x}$ with respect to $\|\cdot\|'$. The proof of this fact for the general case can be found in [Or2, p. 8]. The case for the norms $\|\cdot\|_2$ and $\|\cdot\|_\infty$ follows from Theorem 7.7.

In the subsequent sections of this and later chapters, we will need methods for determining the distance between $n \times n$ matrices. This again requires the use of a norm.

Definition 7.8 A **matrix norm** on the set of all $n \times n$ matrices is a real-valued function, $\|\cdot\|$, defined on this set, satisfying for all $n \times n$ matrices A and B and all real numbers α:

(i) $\|A\| \geq 0$;

(ii) $\|A\| = 0$, if and only if A is O, the matrix with all 0 entries;

(iii) $\|\alpha A\| = |\alpha|\|A\|$;

(iv) $\|A + B\| \leq \|A\| + \|B\|$;

(v) $\|AB\| \leq \|A\|\|B\|$. ■

The **distance between $n \times n$ matrices** A and B with respect to this matrix norm is $\|A - B\|$.

Although matrix norms can be obtained in various ways, the only norms we consider are those that are natural consequences of the vector norms l_2 and l_∞.

The following theorem is not difficult to show, and its proof is left as Exercise 13.

Theorem 7.9 If $\|\cdot\|$ is a vector norm on $\mathbb{R}^n$, then

$$\|A\| = \max_{\|\mathbf{x}\|=1} \|A\mathbf{x}\|$$

is a matrix norm. ■

This is called the **natural**, or *induced*, **matrix norm** associated with the vector norm. In this text, all matrix norms will be assumed to be natural matrix norms unless specified otherwise.

For any $\mathbf{z} \neq \mathbf{0}$, we have $\mathbf{x} = \mathbf{z}/\|\mathbf{z}\|$ as a unit vector. Hence,

$$\max_{\|\mathbf{x}\|=1} \|A\mathbf{x}\| = \max_{\mathbf{z}\neq\mathbf{0}} \left\|A\left(\frac{\mathbf{z}}{\|\mathbf{z}\|}\right)\right\| = \max_{\mathbf{z}\neq\mathbf{0}} \frac{\|A\mathbf{z}\|}{\|\mathbf{z}\|},$$

and we can alternatively write

$$\|A\| = \max_{\mathbf{z}\neq\mathbf{0}} \frac{\|A\mathbf{z}\|}{\|\mathbf{z}\|}. \tag{7.2}$$

The following corollary to Theorem 7.9 follows from this representation of $\|A\|$.

Corollary 7.10 For any vector $\mathbf{z} \neq \mathbf{0}$, matrix A, and any natural norm $\|\cdot\|$, we have

$$\|A\mathbf{z}\| \leq \|A\| \cdot \|\mathbf{z}\|.$$ ■

The measure given to a matrix under a natural norm describes how the matrix stretches unit vectors relative to that norm. The maximum stretch is the norm of the matrix. The matrix norms we will consider have the forms

$$\|A\|_\infty = \max_{\|\mathbf{x}\|_\infty=1} \|A\mathbf{x}\|_\infty, \quad \text{the } l_\infty \text{ norm,}$$

and

$$\|A\|_2 = \max_{\|\mathbf{x}\|_2=1} \|A\mathbf{x}\|_2, \quad \text{the } l_2 \text{ norm.}$$

Figure 7.4

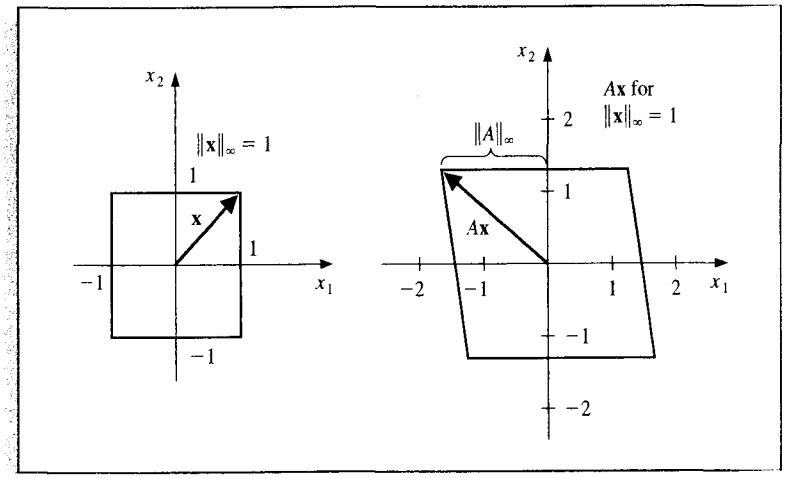
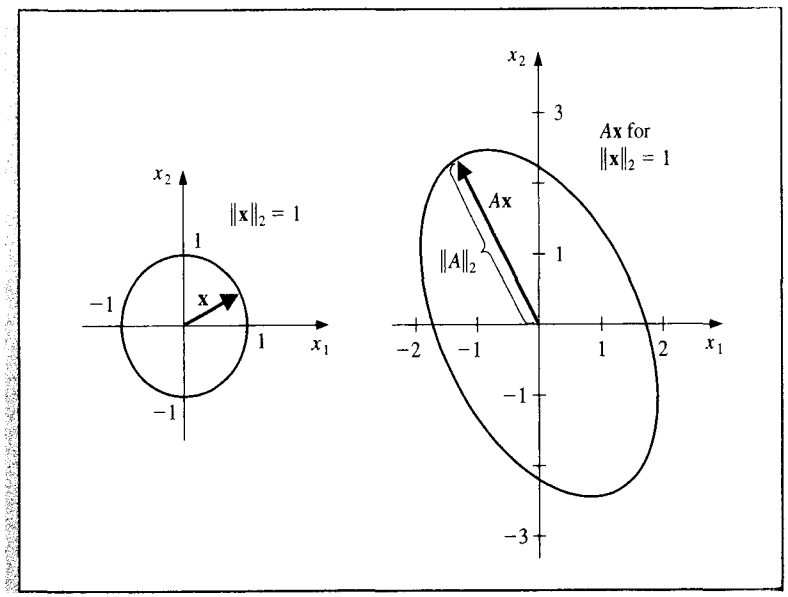


Figure 7.5



An illustration of these norms when $n = 2$ is shown in Figures 7.4 and 7.5. The l_∞ norm of a matrix can be easily computed from the entries of the matrix.

Theorem 7.11 If $A = (a_{ij})$ is an $n \times n$ matrix, then

$$\|A\|_\infty = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|.$$

Proof First we show that $\|A\|_\infty \le \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$. Let $\mathbf{x}$ be an n-dimensional vector with $1 = \|\mathbf{x}\|_\infty = \max_{1 \le i \le n} |x_i|$. Since $A\mathbf{x}$ is also an n-dimensional vector,

$$\|A\mathbf{x}\|_\infty = \max_{1 \le i \le n} |(A\mathbf{x})_i| = \max_{1 \le i \le n} \left| \sum_{j=1}^{n} a_{ij} x_j \right| \le \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}| \max_{1 \le j \le n} |x_j|.$$

But $\max_{1 \le j \le n} |x_j| = \|\mathbf{x}\|_\infty = 1$, so

$$\|A\mathbf{x}\|_\infty \le \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|.$$

Consequently,

$$\|A\|_\infty = \max_{\|\mathbf{x}\|_\infty = 1} \|A\mathbf{x}\|_\infty \le \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|. \tag{7.3}$$

Now we will show the opposite inequality, that $\|A\|_\infty \ge \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$. Let p be an integer with

$$\sum_{j=1}^{n} |a_{pj}| = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|,$$

and $\mathbf{x}$ be the vector with components

$$x_j = \begin{cases} 1, & \text{if } a_{pj} \ge 0, \\ -1, & \text{if } a_{pj} < 0. \end{cases}$$

Then $\|\mathbf{x}\|_\infty = 1$ and $a_{pj} x_j = |a_{pj}|$, for all $j = 1, 2, \ldots, n$, so

$$\|A\mathbf{x}\|_\infty = \max_{1 \le i \le n} \left| \sum_{j=1}^{n} a_{ij} x_j \right| \ge \left| \sum_{j=1}^{n} a_{pj} x_j \right| = \left| \sum_{j=1}^{n} |a_{pj}| \right| = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|.$$

This result implies that

$$\|A\|_\infty = \max_{\|\mathbf{x}\|_\infty = 1} \|A\mathbf{x}\|_\infty \ge \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|,$$

which, together with Inequality (7.3), gives

$$\|A\|_\infty = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|. \qquad \blacksquare \blacksquare \blacksquare$$

EXAMPLE 5 If

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

then

$$\sum_{j=1}^{3} |a_{1j}| = |1| + |2| + |-1| = 4,$$

$$\sum_{j=1}^{3} |a_{2j}| = |0| + |3| + |-1| = 4,$$

and

$$\sum_{j=1}^{3} |a_{3j}| = |5| + |-1| + |1| = 7;$$

so

$$\|A\|_\infty = \max\{4, 4, 7\} = 7. \quad \blacksquare$$

In the next section, we will discover an alternative method for finding the l_2 norm of a matrix.

EXERCISE SET 7.1

1. Find $\|\mathbf{x}\|_\infty$ and $\|\mathbf{x}\|_2$ for the following vectors.
   a. $\mathbf{x} = (3, -4, 0, \frac{3}{2})^t$
   b. $\mathbf{x} = (2, 1, -3, 4)^t$
   c. $\mathbf{x} = (\sin k, \cos k, 2^k)^t$ for a fixed positive integer k
   d. $\mathbf{x} = (4/(k+1), 2/k^2, k^2e^{-k})^t$ for a fixed positive integer k
2. a. Verify that the function $\|\cdot\|_1$, defined on $\mathbb{R}^n$ by

$$\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|,$$

   is a norm on $\mathbb{R}^n$.
   b. Find $\|\mathbf{x}\|_1$ for the vectors given in Exercise 1.
   c. Prove that for all $\mathbf{x} \in \mathbb{R}^n$, $\|\mathbf{x}\|_1 \geq \|\mathbf{x}\|_2$.
3. Prove that the following sequences are convergent, and find their limits.
   a. $\mathbf{x}^{(k)} = (1/k, e^{1-k}, -2/k^2)^t$
   b. $\mathbf{x}^{(k)} = \left(e^{-k}\cos k, k\sin(1/k), 3 + k^{-2}\right)^t$
   c. $\mathbf{x}^{(k)} = (ke^{-k^2}, (\cos k)/k, \sqrt{k^2+k} - k)^t$
   d. $\mathbf{x}^{(k)} = (e^{1/k}, (k^2+1)/(1-k^2), (1/k^2)(1+3+5+\cdots+(2k-1)))^t$
4. Find $\|\cdot\|_\infty$ for the following matrices.
   a. $\begin{bmatrix} 10 & 15 \\ 0 & 1 \end{bmatrix}$
   b. $\begin{bmatrix} 10 & 0 \\ 15 & 1 \end{bmatrix}$

   c. $\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$
   d. $\begin{bmatrix} 4 & -1 & 7 \\ -1 & 4 & 0 \\ -7 & 0 & 4 \end{bmatrix}$
5. The following linear systems $A\mathbf{x} = \mathbf{b}$ have $\mathbf{x}$ as the actual solution and $\tilde{\mathbf{x}}$ as an approximate solution. Compute $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty$ and $\|A\tilde{\mathbf{x}} - \mathbf{b}\|_\infty$.
   a. $\frac{1}{2}x_1 + \frac{1}{3}x_2 = \frac{1}{63}$,
      $\frac{1}{3}x_1 + \frac{1}{4}x_2 = \frac{1}{168}$,
      $\mathbf{x} = \left(\frac{1}{7}, -\frac{1}{6}\right)^t$,
      $\tilde{\mathbf{x}} = (0.142, -0.166)^t$.
   b. $x_1 + 2x_2 + 3x_3 = 1$,
      $2x_1 + 3x_2 + 4x_3 = -1$,
      $3x_1 + 4x_2 + 6x_3 = 2$,
      $\mathbf{x} = (0, -7, 5)^t$,
      $\tilde{\mathbf{x}} = (-0.33, -7.9, 5.8)^t$.
   c. $x_1 + 2x_2 + 3x_3 = 1$,
      $2x_1 + 3x_2 + 4x_3 = -1$,
      $3x_1 + 4x_2 + 6x_3 = 2$,
      $\mathbf{x} = (0, -7, 5)^t$,
      $\tilde{\mathbf{x}} = (-0.2, -7.5, 5.4)^t$.
   d. $0.04x_1 + 0.01x_2 - 0.01x_3 = 0.06$,
      $0.2x_1 + 0.5x_2 - 0.2x_3 = 0.3$,
      $x_1 + 2x_2 + 4x_3 = 11$,
      $\mathbf{x} = (1.827586, 0.6551724, 1.965517)^t$,
      $\tilde{\mathbf{x}} = (1.8, 0.64, 1.9)^t$.
6. The matrix norm $\|\cdot\|_1$, defined by $\|A\|_1 = \max_{\|\mathbf{x}\|_1 = 1} \|A\mathbf{x}\|_1$, can be computed using the formula

$$\|A\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^{n} |a_{ij}|,$$

   where the vector norm $\|\cdot\|_1$ is defined in Exercise 2. Find $\|\cdot\|_1$ for the matrices in Exercise 4.
7. Show by example that $\|\cdot\|_\oplus$, defined by $\|A\|_\oplus = \max_{1 \leq i,j \leq n} |a_{ij}|$, does not define a matrix norm.
8. Show that $\|\cdot\|_\otimes$, defined by

$$\|A\|_\otimes = \sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|,$$

   is a matrix norm. Find $\|\cdot\|_\otimes$ for the matrices in Exercise 4.
9. a. The Frobenius norm (which is not a natural norm) is defined for an $n \times n$ matrix A by

$$\|A\|_F = \left(\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^2 \right)^{1/2}.$$

   Show that $\|\cdot\|_F$ is a matrix norm.

b. Find $\|\cdot\|_F$ for the matrices in Exercise 4.

c. For any matrix A, show that $\|A\|_2 \leq \|A\|_F \leq n^{1/2}\|A\|_2$.

10. In Exercise 9 the Frobenius norm of a matrix was defined. Show that for any $n \times n$ matrix A and vector $\mathbf{x}$ in $\mathbb{R}^n$, $\|A\mathbf{x}\|_2 \leq \|A\|_F \|\mathbf{x}\|_2$.

11. Let S be a positive definite $n \times n$ matrix. For any $\mathbf{x}$ in $\mathbb{R}^n$ define $\|\mathbf{x}\| = (\mathbf{x}^t S\mathbf{x})^{1/2}$. Show that this defines a norm on $\mathbb{R}^n$. [*Hint:* Use Choleski factorization of S to show that $\mathbf{x}^t S\mathbf{y} = \mathbf{y}^t S\mathbf{x} \cdot (\mathbf{x}^t S\mathbf{x})^{1/2}(\mathbf{y}^t S\mathbf{y})^{1/2}$.]

12. Let S be a real and nonsingular matrix, and let $\|\cdot\|$ be any norm on $\mathbb{R}^n$. Define $\|\cdot\|'$ by $\|\mathbf{x}\|' = \|S\mathbf{x}\|$. Show that $\|\cdot\|'$ is also a norm on $\mathbb{R}^n$.

13. Prove that if $\|\cdot\|$ is a vector norm on $\mathbb{R}^n$, then $\|A\| = \max_{\|\mathbf{x}\|=1} \|A\mathbf{x}\|$ is a matrix norm.

14. The following excerpt from the *Mathematics Magazine* [Sz] gives an alternative way to prove the Cauchy-Buniakowsky-Schwarz Inequality.

a. Show that when $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{y} \neq \mathbf{0}$, we have

$$\frac{\sum_{i=1}^n x_i y_i}{\left(\sum_{i=1}^n x_i^2\right)^{1/2}\left(\sum_{i=1}^n y_i^2\right)^{1/2}} = 1 - \frac{1}{2}\sum_{i=1}^n \left(\frac{x_i}{\left(\sum_{j=1}^n x_j^2\right)^{1/2}} - \frac{y_i}{\left(\sum_{j=1}^n y_j^2\right)^{1/2}}\right)^2.$$

b. Use the result in part (a) to show that

$$\sum_{i=1}^n x_i y_i \leq \left(\sum_{i=1}^n x_i^2\right)^{1/2}\left(\sum_{i=1}^n y_i^2\right)^{1/2}.$$

7.2 Eigenvalues and Eigenvectors

An $n \times m$ matrix can be considered as a function that uses matrix multiplication to take m-dimensional vectors into n-dimensional vectors. A square matrix A takes the set of n-dimensional vectors into itself. In this case, certain nonzero vectors $\mathbf{x}$ are parallel to $A\mathbf{x}$, which means that a constant λ exists with $A\mathbf{x} = \lambda\mathbf{x}$. For these vectors, we have $(A - \lambda I)\mathbf{x} = \mathbf{0}$. There is a close connection between these numbers λ and the likelihood that an iterative method will converge. We will consider this connection in this section.

Definition 7.12 If A is a square matrix, the **characteristic polynomial** of A is defined by

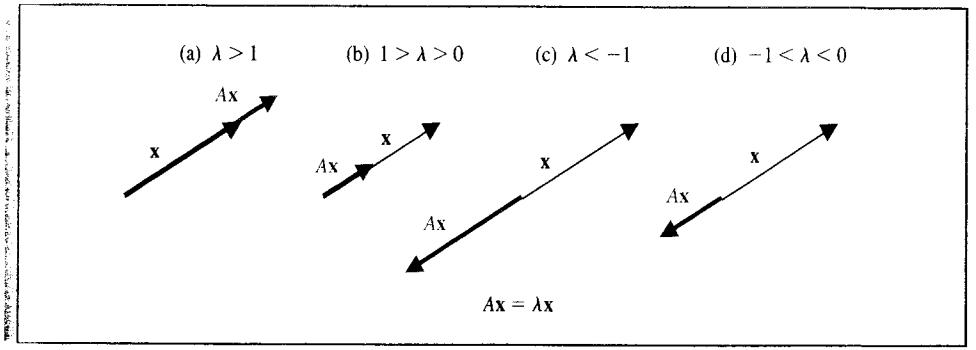
$$p(\lambda) = \det(A - \lambda I).$$ ■

It is not difficult to show (see Exercise 7) that p is an nth-degree polynomial and, consequently, has at most n distinct zeros, some of which may be complex. If λ is a zero of p, then, since $\det(A - \lambda I) = 0$, Theorem 6.16 in Section 6.4 implies that the linear system defined by $(A - \lambda I)\mathbf{x} = \mathbf{0}$ has a solution with $\mathbf{x} \neq \mathbf{0}$. We wish to study the zeros of p and the nonzero solutions corresponding to these systems.

Definition 7.13 If p is the characteristic polynomial of the matrix A, the zeros of p are **eigenvalues**, or characteristic values, of the matrix A. If λ is a eigenvalue of A and $\mathbf{x} \neq \mathbf{0}$ satisfies $(A - \lambda I)\mathbf{x} = \mathbf{0}$, then $\mathbf{x}$ is an **eigenvector**, or characteristic vector, of A corresponding to the eigenvalue λ. ■

If $\mathbf{x}$ is an eigenvector associated with the eigenvalue λ, then $A\mathbf{x} = \lambda\mathbf{x}$, so the matrix A takes the vector $\mathbf{x}$ into a scalar multiple of itself. If λ is real and $\lambda > 1$, then A has the effect of stretching $\mathbf{x}$ by a factor of λ, as illustrated in Figure 7.6(a). If $0 < \lambda < 1$, then A shrinks $\mathbf{x}$ by a factor of λ (see Figure 7.6(b)). When $\lambda < 0$, the effects are similar (see Figure 7.6(c) and (d)), although the direction of $A\mathbf{x}$ is reversed.

Figure 7.6



EXAMPLE 1 Let

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

To compute the eigenvalues of A, consider

$$p(\lambda) = \det(A - \lambda I) = \det\begin{bmatrix} 1-\lambda & 0 & 2 \\ 0 & 1-\lambda & -1 \\ -1 & 1 & 1-\lambda \end{bmatrix} = (1-\lambda)(\lambda^2 - 2\lambda + 4).$$

The eigenvalues of A are the solutions of $p(\lambda) = 0$, which are $\lambda_1 = 1$, $\lambda_2 = 1 + \sqrt{3}i$, and $\lambda_3 = 1 - \sqrt{3}i$.

An eigenvector $\mathbf{x}$ of A associated with λ_1 is a solution of the system $(A - \lambda_1 I)\mathbf{x} = \mathbf{0}$:

$$\begin{bmatrix} 0 & 0 & 2 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Thus,

$$2x_3 = 0, \quad -x_3 = 0, \quad \text{and} \quad -x_1 + x_2 = 0,$$

which implies that

$$x_3 = 0, \quad x_2 = x_1, \quad \text{and} \quad x_1 \text{ is arbitrary.}$$

The choice $x_1 = 1$ produces the eigenvector $(1, 1, 0)^t$ corresponding to the eigenvalue $\lambda_1 = 1$. For this choice, we have $\|(1, 1, 0)^t\|_\infty = 1$.

The choice $x_1 = \sqrt{2}/2$ produces an eigenvector corresponding to λ with

$$\left\| \left(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}, 0 \right)^t \right\|_2 = 1.$$

Since λ_2 and λ_3 are complex numbers, their corresponding eigenvectors are also complex. To find an eigenvector for λ_2, we solve the system

$$\begin{bmatrix} 1-(1+\sqrt{3}i) & 0 & 2 \\ 0 & 1-(1+\sqrt{3}i) & -1 \\ -1 & 1 & 1-(1+\sqrt{3}i) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

One solution to this system is the vector

$$\left(-\frac{2\sqrt{3}}{3}i, \frac{\sqrt{3}}{3}i, 1 \right)^t.$$

Similarly, the vector

$$\left(\frac{2\sqrt{3}}{3}i, -\frac{\sqrt{3}}{3}i, 1 \right)^t$$

is an eigenvector corresponding to the eigenvalue $\lambda_3 = 1 - \sqrt{3}i$. ■

Maple provides the function `Eigenvals` to compute eigenvalues and, optionally, eigenvectors of a matrix. For the example we enter the following:

```
>with(linalg);
>A:=matrix(3,3,[1,0,2,0,1,-1,-1,1,1]);
>evalf(Eigenvals(A));
```

$$[1.000000000 + 1.732050807I, \quad 1.000000000 - 1.732050807I, \quad 1.000000000]$$

This computes the eigenvalues

$$\lambda_2 = 1 + \sqrt{3}i, \quad \lambda_3 = 1 - \sqrt{3}i, \quad \lambda_1 = 1.$$

To compute both the eigenvalues and eigenvectors, use

```
>evalf(Eigenvals(A,B));
```

The eigenvalues are computed and displayed as before, and the eigenvectors are indicated in the columns of B. If the eigenvalues are all real, each column of B gives an eigenvector. However, for our example we display B using

```
>evalm(B);
```


$$B = \begin{bmatrix} 1.154700538 & .6324555321\ 10^{-10} & .7453559925 \\ -.5773502680 & .1264911064\ 10^{-9} & .7453559926 \\ -.2581988896\ 10^{-19} & 1.000000000 & -.72572776\ 10^{-11} \end{bmatrix}$$

The first two columns correspond to the real and imaginary parts of the eigenvectors corresponding to eigenvalues λ_2 and λ_3. Thus, an eigenvector for λ_2 is

$$\begin{bmatrix} 1.154700538 \\ -.5773502680 \\ -.2581988896\ 10^{-19} \end{bmatrix} + \begin{bmatrix} .6324555321\ 10^{-10} \\ .1264911064\ 10^{-9} \\ 1.000000000 \end{bmatrix} i \approx \begin{bmatrix} 1.154700538 \\ -.5773502680 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} i;$$

that is,

$$(1.154700538, -0.5773502680, i)^t = \left(\frac{2\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}, i \right)^t.$$

Since any multiple of an eigenvector is also an eigenvector, we have

$$(1, -0.5, 0.8660254i)$$

as an eigenvector. Multiplying each coordinate by $-(2\sqrt{3}/3)i$ gives the eigenvector in Example 1:

$$\left(-\frac{2\sqrt{3}}{3}i, \frac{\sqrt{3}}{3}i, 1 \right)^t.$$

Since λ_1 is real, the third column of B is an eigenvector corresponding to λ_1.

The notions of eigenvalues and eigenvectors are introduced here for a specific computational convenience, but these concepts arise frequently in the study of physical systems. In fact, they are of sufficient interest that Chapter 9 is devoted to their numerical approximation.

Definition 7.14 The **spectral radius** $\rho(A)$ of a matrix A is defined by

$$\rho(A) = \max |\lambda|, \quad \text{where } \lambda \text{ is an eigenvalue of } A.$$

(Recall that for complex $\lambda = \alpha + \beta i$, we have $|\lambda| = (\alpha^2 + \beta^2)^{1/2}$.) ■

For the matrix considered in Example 1,

$$\rho(A) = \max\{1, |1 + \sqrt{3}i|, |1 - \sqrt{3}i|\} = \max\{1, 2, 2\} = 2.$$

The spectral radius is closely related to the norm of a matrix, as shown in the following theorem.

Theorem 7.15 If A is an $n \times n$ matrix, then

(i) $\|A\|_2 = [\rho(A^t A)]^{1/2}$,

(ii) $\rho(A) \leq \|A\|$, for any natural norm $\|\cdot\|$. ■

Proof The proof of part (i) requires more information concerning eigenvalues than we presently have available. For the details involved in the proof, see [Or2, p. 21].

To prove part (ii), suppose λ is an eigenvalue of A with eigenvector $\mathbf{x}$ and $\|\mathbf{x}\| = 1$ (Exercise 6 ensures that such an eigenvector exists.) Since $A\mathbf{x} = \lambda\mathbf{x}$,

$$|\lambda| = |\lambda| \cdot \|\mathbf{x}\| = \|\lambda\mathbf{x}\| = \|A\mathbf{x}\| \leq \|A\|\|\mathbf{x}\| = \|A\|.$$

Thus,

$$\rho(A) = \max|\lambda| \leq \|A\|. \qquad \blacksquare \blacksquare \blacksquare$$

Part (i) of Theorem 7.15 implies that if A is symmetric, then $\|A\|_2 = \rho(A)$ (see Exercise 10).

An interesting and useful result, which is similar to part (ii) of Theorem 7.15, is that for any matrix A and any $\varepsilon > 0$, there exists a natural norm $\|\cdot\|$ with the property that $\rho(A) < \|A\| < \rho(A) + \varepsilon$. Consequently, $\rho(A)$ is the greatest lower bound for the natural norms on A. The proof of this result can be found in [Or2, p. 23].

EXAMPLE 2 If

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

then

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

To calculate $\rho(A^tA)$ we need the eigenvalues of A^tA. If

$$\begin{aligned} 0 &= \det(A^tA - \lambda I) \\ &= \det\begin{bmatrix} 3-\lambda & 2 & -1 \\ 2 & 6-\lambda & 4 \\ -1 & 4 & 5-\lambda \end{bmatrix} \\ &= -\lambda^3 + 14\lambda^2 - 42\lambda = -\lambda(\lambda^2 - 14\lambda + 42), \end{aligned}$$

then

$$\lambda = 0 \quad \text{or} \quad \lambda = 7 \pm \sqrt{7},$$

so

$$\|A\|_2 = \sqrt{\rho(A^tA)} = \sqrt{\max\{0, 7-\sqrt{7}, 7+\sqrt{7}\}} = \sqrt{7+\sqrt{7}} \approx 3.106. \quad \blacksquare$$

The operations in Example 2 can also be performed using Maple with


```
>with(linalg);
>A:=matrix(3,3,[1,1,0,1,2,1,-1,1,2]);
>B:=transpose(A);
>C:=multiply(A,B);
>evalf(Eigenvals(C));
```

$$[0.109767846510^{-8}, 4.354248690, 9.645751311]$$

Since $\|A\|_2 = \sqrt{\rho(A^tA)} = \sqrt{\rho(C)}$, we have

$$\|A\|_2 = \sqrt{9.645751311} = 3.105760987.$$

Maple also computes $\|A\|_2 = \sqrt{7+\sqrt{7}}$ directly with the command

```
>norm(A,2);
```

To determine the l_∞ norm of A, replace the last command with

```
>norm(A,infinity);
```

In studying iterative matrix techniques, it is of particular importance to know when powers of a matrix become small (that is, when all the entries approach zero). Matrices of this type are called *convergent*.

Definition 7.16 We call an $n \times n$ matrix A **convergent** if

$$\lim_{k\to\infty}(A^k)_{ij} = 0, \quad \text{for each } i = 1, 2, \ldots, n \text{ and } j = 1, 2, \ldots, n. \qquad \blacksquare$$

EXAMPLE 3 Let

$$A = \begin{bmatrix} \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{2} \end{bmatrix}.$$

Computing powers of A, we obtain:

$$A^2 = \begin{bmatrix} \frac{1}{4} & 0 \\ \frac{1}{4} & \frac{1}{4} \end{bmatrix}, \quad A^3 = \begin{bmatrix} \frac{1}{8} & 0 \\ \frac{3}{16} & \frac{1}{8} \end{bmatrix}, \quad A^4 = \begin{bmatrix} \frac{1}{16} & 0 \\ \frac{1}{8} & \frac{1}{16} \end{bmatrix},$$

and, in general,

$$A^k = \begin{bmatrix} (\frac{1}{2})^k & 0 \\ \frac{k}{2^{k+1}} & (\frac{1}{2})^k \end{bmatrix}.$$

Since

$$\lim_{k\to\infty}\left(\frac{1}{2}\right)^k = 0 \quad \text{and} \quad \lim_{k\to\infty}\frac{k}{2^{k+1}} = 0,$$

A is a convergent matrix. $\blacksquare$

Notice that the convergent matrix A in Example 3 has $\rho(A) = \frac{1}{2}$, since $\frac{1}{2}$ is the only eigenvalue of A. This illustrates the important connection that exists between the spectral radius of a matrix and the convergence of the matrix, as detailed in the following result.

Theorem 7.17 The following statements are equivalent.

(i) A is a convergent matrix.

(ii) $\lim_{n\to\infty} \|A^n\| = 0$, for some natural norm.

(iii) $\lim_{n\to\infty} \|A^n\| = 0$, for all natural norms.

(iv) $\rho(A) < 1$.

(v) $\lim_{n\to\infty} A^n\mathbf{x} = \mathbf{0}$, for every $\mathbf{x}$. ∎

The proof of this theorem can be found in [IK, p. 14].

EXERCISE SET 7.2

1. Compute the eigenvalues and associated eigenvectors of the following matrices.

   a. $\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$ b. $\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$

   c. $\begin{bmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix}$ d. $\begin{bmatrix} 1 & 1 \\ -2 & -2 \end{bmatrix}$

   e. $\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix}$ f. $\begin{bmatrix} -1 & 2 & 0 \\ 0 & 3 & 4 \\ 0 & 0 & 7 \end{bmatrix}$

   g. $\begin{bmatrix} 2 & 1 & 1 \\ 2 & 3 & 2 \\ 1 & 1 & 2 \end{bmatrix}$ h. $\begin{bmatrix} 3 & 2 & -1 \\ 1 & -2 & 3 \\ 2 & 0 & 4 \end{bmatrix}$

2. Find the spectral radius for each matrix in Exercise 1.
3. Which of the matrices in Exercise 1 are convergent?
4. Let $A_1 = \begin{bmatrix} 1 & 0 \\ \frac{1}{4} & \frac{1}{2} \end{bmatrix}$ and $A_2 = \begin{bmatrix} \frac{1}{2} & 0 \\ 16 & \frac{1}{2} \end{bmatrix}$. Show that A_1 is not convergent, but A_2 is convergent.
5. Find the $\|\cdot\|_2$ norm for the matrices in Exercise 1.
6. Show that if λ is a eigenvalue of a matrix A and $\|\cdot\|$ is a vector norm, then an eigenvector $\mathbf{x}$ associated with λ exists with $\|\mathbf{x}\| = 1$.
7. Show that the characteristic polynomial $p(\lambda) = \det(A - \lambda I)$ for the $n \times n$ matrix A is an nth-degree polynomial. [*Hint:* Expand $\det(A - \lambda I)$ along the first row, and use mathematical induction on n.]
8. a. Show that if A is an $n \times n$ matrix, then

$$\det A = \prod_{i=1}^{n} \lambda_i,$$

   where $\lambda_i, \ldots, \lambda_n$ are the eigenvalues of A. [*Hint:* Consider $p(0)$.]

   b. Show that A is singular if and only if $\lambda = 0$ is an eigenvalue of A.

9. Let λ be an eigenvalue of the $n \times n$ matrix A and $\mathbf{x} \neq \mathbf{0}$ be an associated eigenvector.
   a. Show that λ is also an eigenvalue of A^t.
   b. Show that for any integer $k \geq 1$, λ^k is an eigenvalue of A^k with eigenvector $\mathbf{x}$.
   c. Show that if A^{-1} exists, then $1/\lambda$ is an eigenvector of A^{-1} with eigenvector $\mathbf{x}$.
   d. Generalize parts (b) and (c) to $(A^{-1})^k$ for integers $k \geq 2$.
   e. Given the polynomial $q(x) = q_0 + q_1 x + \cdots + q_k x^k$, define $q(A)$ to be the matrix $q(A) = q_0 I + q_1 A + \cdots + q_k A^k$. Show that $q(\lambda)$ is an eigenvalue of $q(A)$ with eigenvector $\mathbf{x}$.
   f. Let $\alpha \neq \lambda$ be given. Show that if $A - \alpha I$ is a nonsingular, then $1/(\lambda - \alpha)$ is an eigenvalue of $(A - \alpha I)^{-1}$ with eigenvector $\mathbf{x}$.
10. Show that if A is symmetric, then $\|A\|_2 = \rho(A)$.
11. In Exercise 11 of Section 6.3, we assumed that the contribution a female beetle of a certain type made to the future years' beetle population could be expressed in terms of the matrix

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

    where the entry in the ith row and jth column represents the probabilistic contribution of a beetle of age j onto the next year's female population of age i.
    a. Does the matrix A have any real eigenvalues? If so, determine them and any associated eigenvectors.
    b. If a sample of this species was needed for laboratory test purposes that would have a constant proportion in each age group from year to year, what criteria could be imposed on the initial population to ensure that this requirement would be satisfied?
12. Find matrices A and B for which $\rho(A + B) > \rho(A) + \rho(B)$. (This shows that $\rho(A)$ cannot be a matrix norm.)
13. Show that if $\|\cdot\|$ is any natural norm, then $(1/\|A^{-1}\|) \leq |\lambda| \leq \|A\|$ for any eigenvalue λ of the nonsingular matrix A.

7.3 Iterative Techniques for Solving Linear Systems

In this section we describe the Jacobi and the Gauss-Seidel iterative methods, classic methods that date to the late eighteenth century. Iterative techniques are seldom used for solving linear systems of small dimension since the time required for sufficient accuracy exceeds that required for direct techniques such as Gaussian elimination. For large systems with a high percentage of 0 entries, however, these techniques are efficient in terms of both computer storage and computation. Systems of this type arise frequently in circuit analysis and in the numerical solution of boundary-value problems and partial-differential equations.

An iterative technique to solve the $n \times n$ linear system $A\mathbf{x} = \mathbf{b}$ starts with an initial approximation $\mathbf{x}^{(0)}$ to the solution $\mathbf{x}$ and generates a sequence of vectors $\{\mathbf{x}^{(k)}\}_{k=0}^{\infty}$ that converges to $\mathbf{x}$. Iterative techniques involve a process that converts the system $A\mathbf{x} = \mathbf{b}$ into an equivalent system of the form $\mathbf{x} = T\mathbf{x} + \mathbf{c}$ for some fixed matrix T and vector $\mathbf{c}$.

After the initial vector $\mathbf{x}^{(0)}$ is selected, the sequence of approximate solution vectors is generated by computing

$$\mathbf{x}^{(k)} = T\mathbf{x}^{(k-1)} + \mathbf{c},$$

for each $k = 1, 2, 3, \ldots$. This result should be reminiscent of the fixed-point iteration studied in Chapter 2.

EXAMPLE 1 The linear system $A\mathbf{x} = \mathbf{b}$ given by

$$\begin{aligned} E_1: &\quad 10x_1 - x_2 + 2x_3 = 6,\\ E_2: &\quad -x_1 + 11x_2 - x_3 + 3x_4 = 25,\\ E_3: &\quad 2x_1 - x_2 + 10x_3 - x_4 = -11,\\ E_4: &\quad 3x_2 - x_3 + 8x_4 = 15 \end{aligned}$$

has the unique solution $\mathbf{x} = (1, 2, -1, 1)^t$. To convert $A\mathbf{x} = \mathbf{b}$ to the form $\mathbf{x} = T\mathbf{x} + \mathbf{c}$, solve equation E_i for x_i, for each $i = 1, 2, 3, 4$, to obtain

$$\begin{aligned} x_1 &= \frac{1}{10}x_2 - \frac{1}{5}x_3 + \frac{3}{5},\\ x_2 &= \frac{1}{11}x_1 + \frac{1}{11}x_3 - \frac{3}{11}x_4 + \frac{25}{11},\\ x_3 &= -\frac{1}{5}x_1 + \frac{1}{10}x_2 + \frac{1}{10}x_4 - \frac{11}{10},\\ x_4 &= -\frac{3}{8}x_2 + \frac{1}{8}x_3 + \frac{15}{8}. \end{aligned}$$

Then $A\mathbf{x} = \mathbf{b}$ can be rewritten in the form $\mathbf{x} = T\mathbf{x} + \mathbf{c}$, with

$$T = \begin{bmatrix} 0 & \frac{1}{10} & -\frac{1}{5} & 0\\ \frac{1}{11} & 0 & \frac{1}{11} & -\frac{3}{11}\\ -\frac{1}{5} & \frac{1}{10} & 0 & \frac{1}{10}\\ 0 & -\frac{3}{8} & \frac{1}{8} & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{c} = \begin{bmatrix} \frac{3}{5}\\ \frac{25}{11}\\ -\frac{11}{10}\\ \frac{15}{8} \end{bmatrix}.$$

For an initial approximation, we let $\mathbf{x}^{(0)} = (0, 0, 0, 0)^t$. Then $\mathbf{x}^{(1)}$ is given by

$$\begin{aligned} x_1^{(1)} &= \frac{1}{10}x_2^{(0)} - \frac{1}{5}x_3^{(0)} + \frac{3}{5} = 0.6000,\\ x_2^{(1)} &= \frac{1}{11}x_1^{(0)} + \frac{1}{11}x_3^{(0)} - \frac{3}{11}x_4^{(0)} + \frac{25}{11} = 2.2727,\\ x_3^{(1)} &= -\frac{1}{5}x_1^{(0)} + \frac{1}{10}x_2^{(0)} + \frac{1}{10}x_4^{(0)} - \frac{11}{10} = -1.1000,\\ x_4^{(1)} &= -\frac{3}{8}x_2^{(0)} + \frac{1}{8}x_3^{(0)} + \frac{15}{8} = 1.8750. \end{aligned}$$

Additional iterates, $\mathbf{x}^{(k)} = (x_1^{(k)}, x_2^{(k)}, x_3^{(k)}, x_4^{(k)})^t$, are generated in a similar manner and are presented in Table 7.1.

Table 7.1

k	0	1	2	3	4	5	6	7	8	9	10
$x_1^{(k)}$	0.000	0.6000	1.0473	0.9326	1.0152	0.9890	1.0032	0.9981	1.0006	0.9997	1.0001
$x_2^{(k)}$	0.0000	2.2727	1.7159	2.053	1.9537	2.0114	1.9922	2.0023	1.9987	2.0004	1.9998
$x_3^{(k)}$	0.0000	−1.1000	−0.8052	−1.0493	−0.9681	−1.0103	−0.9945	−1.0020	−0.9990	−1.0004	−0.9998
$x_4^{(k)}$	0.0000	1.8750	0.8852	1.1309	0.9739	1.0214	0.9944	1.0036	0.9989	1.0006	0.9998

The decision to stop after ten iterations was based on the criterion

$$\frac{\|\mathbf{x}^{(10)} - \mathbf{x}^{(9)}\|_\infty}{\|\mathbf{x}^{(10)}\|_\infty} = \frac{8.0 \times 10^{-4}}{1.9998} < 10^{-3}.$$

In fact, $\|\mathbf{x}^{(10)} - \mathbf{x}\|_\infty = 0.0002$. ■

The method of Example 1 is called the **Jacobi iterative method**. It consists of solving the ith equation in $A\mathbf{x} = \mathbf{b}$ for x_i to obtain (provided $a_{ii} \neq 0$)

$$x_i = \sum_{\substack{j=1\\ j\neq i}}^{n} \left(-\frac{a_{ij}x_j}{a_{ii}}\right) + \frac{b_i}{a_{ii}}, \qquad \text{for } i = 1, 2, \ldots, n$$

and generating each $x_i^{(k)}$ from components of $\mathbf{x}^{(k-1)}$ for $k \geq 1$ by

$$x_i^{(k)} = \frac{\sum_{\substack{j=1\\ j\neq i}}^{n} \left(-a_{ij}x_j^{(k-1)}\right) + b_i}{a_{ii}}, \qquad \text{for } i = 1, 2, \ldots, n. \tag{7.4}$$

The method is written in the form $\mathbf{x}^{(k)} = T\mathbf{x}^{(k-1)} + \mathbf{c}$ by splitting A into its diagonal and off-diagonal parts. To see this, let D be the diagonal matrix whose diagonal entries are those of A, $-L$ be the strictly lower-triangular part of A, and $-U$ be the strictly upper-triangular part of A. With this notation,

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n}\\ a_{21} & a_{22} & \cdots & a_{2n}\\ \vdots & \vdots & & \vdots\\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

is split into

$$A = \begin{bmatrix} a_{11} & 0 & \cdots & 0\\ 0 & a_{22} & \ddots & \vdots\\ \vdots & \ddots & \ddots & 0\\ 0 & \cdots & 0 & a_{nn} \end{bmatrix} - \begin{bmatrix} 0 & \cdots & \cdots & 0\\ -a_{21} & \ddots & & \vdots\\ \vdots & \ddots & \ddots & \vdots\\ -a_{n1} & \cdots & -a_{n,n-1} & 0 \end{bmatrix} - \begin{bmatrix} 0 & -a_{12} & \cdots & -a_{1n}\\ \vdots & \ddots & \ddots & \vdots\\ \vdots & & \ddots & -a_{n-1,n}\\ 0 & \cdots & \cdots & 0 \end{bmatrix}$$

$$= D - L - U.$$

The equation $A\mathbf{x} = \mathbf{b}$, or $(D - L - U)\mathbf{x} = \mathbf{b}$, is then transformed into

$$D\mathbf{x} = (L + U)\mathbf{x} + \mathbf{b},$$

and, if D^{-1} exists, that is, if $a_{ii} \neq 0$ for each i, then

$$\mathbf{x} = D^{-1}(L + U)\mathbf{x} + D^{-1}\mathbf{b}.$$

This results in the matrix form of the Jacobi iterative technique:

$$\mathbf{x}^{(k)} = D^{-1}(L + U)\mathbf{x}^{(k-1)} + D^{-1}\mathbf{b}, \quad k = 1, 2, \ldots . \tag{7.5}$$

Introducing the notation $T_j = D^{-1}(L + U)$ and $\mathbf{c}_j = D^{-1}\mathbf{b}$, the Jacobi technique has the form

$$\mathbf{x}^{(k)} = T_j\mathbf{x}^{(k-1)} + \mathbf{c}_j. \tag{7.6}$$

In practice, Eq. (7.4) is used in computation and Eq. (7.6) for theoretical purposes.

Algorithm 7.1 implements the Jacobi iterative technique.

ALGORITHM 7.1

Jacobi Iterative

To solve $A\mathbf{x} = \mathbf{b}$ given an initial approximation $\mathbf{x}^{(0)}$:

INPUT the number of equations and unknowns n; the entries a_{ij}, $1 \leq i, j \leq n$ of the matrix A; the entries b_i, $1 \leq i \leq n$ of $\mathbf{b}$; the entries XO_i, $1 \leq i \leq n$ of $\mathbf{XO} = \mathbf{x}^{(0)}$; tolerance TOL; maximum number of iterations N.

OUTPUT the approximate solution $x_1, \ldots, x_n$ or a message that the number of iterations was exceeded.

Step 1 Set $k = 1$.

Step 2 While $(k \leq N)$ do Steps 3–6.

Step 3 For $i = 1, \ldots, n$

$$\text{set } x_i = \frac{-\sum_{\substack{j=1 \\ j \neq i}}^{n} (a_{ij}XO_j) + b_i}{a_{ii}}.$$

Step 4 If $\|\mathbf{x} - \mathbf{XO}\| < TOL$ then OUTPUT $(x_1, \ldots, x_n)$;
(*The procedure was successful.*)
STOP.

Step 5 Set $k = k + 1$.

Step 6 For $i = 1, \ldots, n$ set $XO_i = x_i$.

Step 7 OUTPUT ('Maximum number of iterations exceeded');
(*The procedure was successful.*)
STOP.

Step 3 of the algorithm requires that $a_{ii} \neq 0$, for each $i = 1, 2, \ldots, n$. If one of the a_{ii} entries is 0 and the system is nonsingular, a reordering of the equations can be performed so that no $a_{ii} = 0$. To speed convergence, the equations should be arranged so that a_{ii} is as large as possible. This subject is discussed in more detail later in this chapter.

Another possible stopping criterion in Step 4 is to iterate until

$$\frac{\|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\|}{\|\mathbf{x}^{(k)}\|}$$

is smaller than some prescribed tolerance. For this purpose, any convenient norm can be used, the usual being the l_∞ norm.

A possible improvement in Algorithm 7.1 can be seen by reconsidering Eq. (7.4). The components of $\mathbf{x}^{(k-1)}$ are used to compute $x_i^{(k)}$. Since, for $i > 1$, $x_1^{(k)}, \ldots, x_{i-1}^{(k)}$ have already been computed and are probably better approximations to the actual solutions $x_1, \ldots, x_{i-1}$ than $x_1^{(k-1)}, \ldots, x_{i-1}^{(k-1)}$, it seems more reasonable to compute $x_i^{(k)}$ using these most recently calculated values. That is, we can use

$$x_i^{(k)} = \frac{-\sum_{j=1}^{i-1}(a_{ij}x_j^{(k)}) - \sum_{j=i+1}^{n}(a_{ij}x_j^{(k-1)}) + b_i}{a_{ii}}, \tag{7.7}$$

for each $i = 1, 2, \ldots, n$, instead of Eq. (7.4). This modification is called the **Gauss-Seidel iterative technique** and is illustrated in the following example.

EXAMPLE 2 The linear system given by

$$\begin{aligned} 10x_1 - x_2 + 2x_3 &= 6, \\ -x_1 + 11x_2 - x_3 + 3x_4 &= 25, \\ 2x_1 - x_2 + 10x_3 - x_4 &= -11, \\ 3x_2 - x_3 + 8x_4 &= 15 \end{aligned}$$

was solved in Example 1 by the Jacobi iterative method. Incorporating Eq. (7.7) into Algorithm 7.1 gives the equations to be used for each $k = 1, 2, \ldots,$

$$\begin{aligned} x_1^{(k)} &= \frac{1}{10}x_2^{(k-1)} - \frac{1}{5}x_3^{(k-1)} + \frac{3}{5}, \\ x_2^{(k)} &= \frac{1}{11}x_1^{(k)} + \frac{1}{11}x_3^{(k-1)} - \frac{3}{11}x_4^{(k-1)} + \frac{25}{11}, \\ x_3^{(k)} &= -\frac{1}{5}x_1^{(k)} + \frac{1}{10}x_2^{(k)} + \frac{1}{10}x_4^{(k-1)} - \frac{11}{10}, \\ x_4^{(k)} &= -\frac{3}{8}x_2^{(k)} + \frac{1}{8}x_3^{(k)} + \frac{15}{8}. \end{aligned}$$

Letting $\mathbf{x}^{(0)} = (0, 0, 0, 0)^t$, we generate the iterates in Table 7.2.

Table 7.2

k	0	1	2	3	4	5
$x_1^{(k)}$	0.0000	0.6000	1.030	1.0065	1.0009	1.0001
$x_2^{(k)}$	0.0000	2.3272	2.037	2.0036	2.0003	2.0000
$x_3^{(k)}$	0.0000	−0.9873	−1.014	−1.0025	−1.0003	−1.0000
$x_4^{(k)}$	0.0000	0.8789	0.9844	0.9983	0.9999	1.0000

Since

$$\frac{\|\mathbf{x}^{(5)} - \mathbf{x}^{(4)}\|_\infty}{\|\mathbf{x}^{(5)}\|_\infty} = \frac{0.0008}{2.000} = 4 \times 10^{-4},$$

$\mathbf{x}^{(5)}$ is accepted as a reasonable approximation to the solution. Note that Jacobi's method in Example 1 required twice as many iterations for the same accuracy. ■

To write the Gauss-Seidel method in matrix form, multiply both sides of Eq. (7.7) by a_{ii} and collect all kth iterate terms, to give

$$a_{i1}x_1^{(k)} + a_{i2}x_2^{(k)} + \cdots + a_{ii}x_i^{(k)} = -a_{i,i+1}x_{i+1}^{(k-1)} - \cdots - a_{in}x_n^{(k-1)} + b_i,$$

for each $i = 1, 2, \ldots, n$. Writing all n equations gives

$$\begin{aligned}
a_{11}x_1^{(k)} &= -a_{12}x_2^{(k-1)} - a_{13}x_3^{(k-1)} - \cdots - a_{1n}x_n^{(k-1)} + b_1,\\
a_{21}x_1^{(k)} + a_{22}x_2^{(k)} &= -a_{23}x_3^{(k-1)} - \cdots - a_{2n}x_n^{(k-1)} + b_2,\\
&\vdots\\
a_{n1}x_1^{(k)} + a_{n2}x_2^{(k)} + \cdots + a_{nn}x_n^{(k)} &= b_n;
\end{aligned}$$

with the definitions of D, L, and U given previously, we have the Gauss-Seidel method represented by

$$(D - L)\mathbf{x}^{(k)} = U\mathbf{x}^{(k-1)} + \mathbf{b}$$

or

$$\mathbf{x}^{(k)} = (D - L)^{-1}U\mathbf{x}^{(k-1)} + (D - L)^{-1}\mathbf{b}, \quad \text{for each } k = 1, 2, \ldots. \tag{7.8}$$

Letting $T_g = (D - L)^{-1}U$ and $\mathbf{c}_g = (D - L)^{-1}\mathbf{b}$, the Gauss-Seidel technique has the form

$$\mathbf{x}^{(k)} = T_g\mathbf{x}^{(k-1)} + \mathbf{c}_g. \tag{7.9}$$

For the lower-triangular matrix $D - L$ to be nonsingular, it is necessary and sufficient that $a_{ii} \neq 0$, for each $i = 1, 2, \ldots, n$.

Algorithm 7.2 implements the Gauss-Seidel method.

ALGORITHM 7.2

Gauss-Seidel Iterative

To solve $A\mathbf{x} = \mathbf{b}$ given an initial approximation $\mathbf{x}^{(0)}$:

INPUT the number of equations and unknowns n; the entries a_{ij}, $1 \leq i, j \leq n$ of the matrix A; the entries b_i, $1 \leq i \leq n$ of $\mathbf{b}$; the entries XO_i, $1 \leq i \leq n$ of $\mathbf{XO} = \mathbf{x}^{(0)}$; tolerance TOL; maximum number of iterations N.

OUTPUT the approximate solution $x_1, \ldots, x_n$ or a message that the number of iterations was exceeded.

Step 1 Set $k = 1$.

Step 2 While $(k \leq N)$ do Steps 3–6.

Step 3 For $i = 1, \ldots, n$

$$\text{set } x_i = \frac{-\sum_{j=1}^{i-1} a_{ij}x_j - \sum_{j=i+1}^{n} a_{ij}XO_j + b_i}{a_{ii}}.$$

Step 4 If $\|\mathbf{x} - \mathbf{XO}\| < TOL$ then OUTPUT $(x_1, \ldots, x_n)$;
(The procedure was successful.)
STOP.

Step 5 Set $k = k + 1$.

Step 6 For $i = 1, \ldots, n$ set $XO_i = x_i$.

Step 7 OUTPUT ('Maximum number of iterations exceeded');
(The procedure was successful.)
STOP. ■

The comments following Algorithm 7.1 regarding reordering and stopping criteria also apply to the Gauss-Seidel Algorithm 7.2.

The results of Examples 1 and 2 appear to imply that the Gauss-Seidel method is superior to the Jacobi method. This is almost always true, but there are linear systems for which the Jacobi method converges and the Gauss-Seidel method does not (see Exercises 9 and 10).

To study the convergence of general iteration techniques, we consider the formula

$$\mathbf{x}^{(k)} = T\mathbf{x}^{(k-1)} + \mathbf{c}, \quad \text{for each } k = 1, 2, \ldots,$$

where $\mathbf{x}^{(0)}$ is arbitrary.

Lemma 7.18 If the spectral radius $\rho(T)$ satisfies $\rho(T) < 1$, then $(I - T)^{-1}$ exists, and

$$(I - T)^{-1} = I + T + T^2 + \cdots = \sum_{j=0}^{\infty} T^j. \quad ■$$

Proof Since $T\mathbf{x} = \lambda\mathbf{x}$ is true precisely when $(I - T)\mathbf{x} = (1 - \lambda)\mathbf{x}$, we have λ as an eigenvalue of T precisely when $1 - \lambda$ is an eigenvalue of $I - T$. But $|\lambda| \leq \rho(T) < 1$, so $\lambda = 1$ is not an eigenvalue of T, and 0 cannot be an eigenvalue of $I - T$. Hence, $(I - T)^{-1}$ exists.

Let $S_m = I + T + T^2 + \cdots + T^m$. Then

$$(I - T)S_m = (1 + T + T^2 + \cdots + T^m) - (T + T^2 + \cdots + T^{m+1}) = I - T^{m+1},$$

and, since T is convergent, the result at the end of Section 7.2 implies that

$$\lim_{m\to\infty} (I - T)S_m = \lim_{m\to\infty} (I - T^{m+1}) = I.$$

Thus, $(I - T)^{-1} = \lim_{m\to\infty} S_m = I + T + T^2 + \cdots = \sum_{j=0}^{\infty} T^j$. ■ ■ ■

Theorem 7.19 For any $\mathbf{x}^{(0)} \in \mathbb{R}^n$, the sequence $\{\mathbf{x}^{(k)}\}_{k=0}^{\infty}$ defined by

$$\mathbf{x}^{(k)} = T\mathbf{x}^{(k-1)} + \mathbf{c}, \quad \text{for each } k \geq 1, \tag{7.10}$$

converges to the unique solution of $\mathbf{x} = T\mathbf{x} + \mathbf{c}$ if and only if $\rho(T) < 1$. ■

Proof First assume that $\rho(T) < 1$. Then,

$$\begin{aligned}\mathbf{x}^{(k)} &= T\mathbf{x}^{(k-1)} + \mathbf{c} \\ &= T(T\mathbf{x}^{(k-2)} + \mathbf{c}) + \mathbf{c} \\ &= T^2\mathbf{x}^{(k-2)} + (T + I)\mathbf{c} \\ &\vdots \\ &= T^k\mathbf{x}^{(0)} + (T^{k-1} + \cdots + T + I)\mathbf{c}.\end{aligned}$$

Since $\rho(T) < 1$, the matrix T is convergent and

$$\lim_{k\to\infty} T^k\mathbf{x}^{(0)} = \mathbf{0}.$$

Lemma 7.18 implies that

$$\lim_{k\to\infty} \mathbf{x}^{(k)} = \lim_{k\to\infty} T^k\mathbf{x}^{(0)} + \left(\sum_{j=0}^{\infty} T^j\right)\mathbf{c} = \mathbf{0} + (I - T)^{-1}\mathbf{c} = (I - T)^{-1}\mathbf{c}.$$

Hence, the sequence $\{\mathbf{x}^{(k)}\}$ converges to the vector $\mathbf{x} \equiv (I - T)^{-1}\mathbf{c}$ and $\mathbf{x} = T\mathbf{x} + \mathbf{c}$.

To prove the converse, we show that for any $\mathbf{z} \in \mathbb{R}^n$, we have $\lim_{k\to\infty} T^k\mathbf{z} = \mathbf{0}$. By Theorem 7.17, this is equivalent to $\rho(T) < 1$.

Let $\mathbf{z}$ be an arbitrary vector, and $\mathbf{x}$ be the unique solution to $\mathbf{x} = T\mathbf{x} + \mathbf{c}$. Define $\mathbf{x}^{(0)} = \mathbf{x} - \mathbf{z}$, and, for $k \geq 1$, $\mathbf{x}^{(k)} = T\mathbf{x}^{(k-1)} + \mathbf{c}$. Then $\{\mathbf{x}^{(k)}\}$ converges to $\mathbf{x}$. Also,

$$\mathbf{x} - \mathbf{x}^{(k)} = (T\mathbf{x} + \mathbf{c}) - \left(T\mathbf{x}^{(k-1)} + \mathbf{c}\right) = T\left(\mathbf{x} - \mathbf{x}^{(k-1)}\right),$$

so

$$\mathbf{x} - \mathbf{x}^{(k)} = T\left(\mathbf{x} - \mathbf{x}^{(k-1)}\right) = T^2\left(\mathbf{x} - \mathbf{x}^{(k-2)}\right) = \cdots = T^k\left(\mathbf{x} - \mathbf{x}^{(0)}\right) = T^k\mathbf{z}.$$

Hence $\lim_{k\to\infty} T^k\mathbf{z} = \lim_{k\to\infty} T^k\left(\mathbf{x} - \mathbf{x}^{(0)}\right) = \lim_{k\to\infty}\left(\mathbf{x} - \mathbf{x}^{(k)}\right) = \mathbf{0}$.

Since $\mathbf{z} \in \mathbb{R}^n$ was arbitrary, this implies that T is a convergent matrix and that $\rho(T) < 1$. ■ ■ ■

The proof of the following corollary is similar to the proofs in Corollary 2.4. It is considered in Exercise 11.

Corollary 7.20 If $\|T\| < 1$ for any natural matrix norm and $\mathbf{c}$ is a given vector, then the sequence $\{\mathbf{x}^{(k)}\}_{k=0}^{\infty}$ defined by $\mathbf{x}^{(k)} = T\mathbf{x}^{(k-1)} + \mathbf{c}$ converges, for any $\mathbf{x}^{(0)} \in \mathbb{R}^n$, to a vector $\mathbf{x} \in \mathbb{R}^n$, and the following error bounds hold:

(i) $\|\mathbf{x} - \mathbf{x}^{(k)}\| \leq \|T\|^k\|\mathbf{x}^{(0)} - \mathbf{x}\|$;

(ii) $\|\mathbf{x} - \mathbf{x}^{(k)}\| \leq \frac{\|T\|^k}{1-\|T\|}\|\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\|$. ■

We have seen that the Jacobi and Gauss-Seidel iterative techniques can be written

$$\mathbf{x}^{(k)} = T_j\mathbf{x}^{(k-1)} + \mathbf{c}_j \quad \text{and} \quad \mathbf{x}^{(k)} = T_g\mathbf{x}^{(k-1)} + \mathbf{c}_g,$$

using the matrices

$$T_j = D^{-1}(L + U) \quad \text{and} \quad T_g = (D - L)^{-1}U.$$

If $\rho(T_j)$ or $\rho(T_g)$ is less than 1, then the corresponding sequence $\{\mathbf{x}^{(k)}\}_{k=0}^{\infty}$ will converge to the solution $\mathbf{x}$ of $A\mathbf{x} = \mathbf{b}$. For example, the Jacobi scheme has

$$\mathbf{x}^{(k)} = D^{-1}(L + U)\mathbf{x}^{(k-1)} + D^{-1}\mathbf{b},$$

and, if $\{\mathbf{x}^{(k)}\}_{k=0}^{\infty}$ converges to $\mathbf{x}$, then

$$\mathbf{x} = D^{-1}(L + U)\mathbf{x} + D^{-1}\mathbf{b}.$$

This implies that

$$D\mathbf{x} = (L + U)\mathbf{x} + \mathbf{b} \quad \text{and} \quad (D - L - U)\mathbf{x} = \mathbf{b}.$$

Since $D - L - U = A$, the solution $\mathbf{x}$ satisfies $A\mathbf{x} = \mathbf{b}$.

We can now give easily verified sufficiency conditions for convergence of the Jacobi and Gauss-Seidel methods. (To prove convergence for the Jacobi scheme, see Exercise 12, and for the Gauss-Seidel scheme, see [Or2, p. 120].)

Theorem 7.21 If A is strictly diagonally dominant, then for any choice of $\mathbf{x}^{(0)}$, both the Jacobi and Gauss-Seidel methods give sequences $\{\mathbf{x}^{(k)}\}_{k=0}^{\infty}$ that converge to the unique solution of $A\mathbf{x} = \mathbf{b}$. ■

The relationship of the rapidity of convergence to the spectral radius of the iteration matrix T can be seen from Corollary 7.20. Since the inequalities hold for any natural matrix norm, it follows from the statement after Theorem 7.15 that

$$\|\mathbf{x}^{(k)} - \mathbf{x}\| \approx \rho(T)^k\|\mathbf{x}^{(0)} - \mathbf{x}\|. \tag{7.11}$$

Thus, it is desirable to select the iterative technique with minimal $\rho(T) < 1$ for a particular system $A\mathbf{x} = \mathbf{b}$. No general results exist to tell which of the two techniques, Jacobi or Gauss-Seidel, will be most successful for an arbitrary linear system. In special cases, however, the answer is known, as is demonstrated in the following theorem. The proof of this result can be found in [Y, pp. 120–127].

Theorem 7.22 **(Stein-Rosenberg)**

If $a_{ij} \leq 0$, for each $i \neq j$ and $a_{ii} > 0$, for each $i = 1, 2, \ldots, n$, then one and only one of the following statements holds:

a. $0 \le \rho(T_g) < \rho(T_j) < 1$;

b. $1 < \rho(T_j) < \rho(T_g)$;

c. $\rho(T_j) = \rho(T_g) = 0$;

d. $\rho(T_j) = \rho(T_g) = 1$. ■

For the special case described in Theorem 7.22, we see from part (a) that when one method gives convergence, then both give convergence, and the Gauss-Seidel method converges faster than the Jacobi method. Part (b) indicates that when one method diverges then both diverge, and the divergence is more pronounced for the Gauss-Seidel method.

Since the rate of convergence of a procedure depends on the spectral radius of the matrix associated with the method, one way to select a procedure to accelerate convergence is to choose a method whose associated matrix has minimal spectral radius. Before describing a procedure for selecting such a method, we need to introduce a new means of measuring the amount by which an approximation to the solution to a linear system differs from the true solution to the system. The method makes use of the vector described in the following definition.

Definition 7.23 Suppose $\tilde{\mathbf{x}} \in \mathbb{R}^n$ is an approximation to the solution of the linear system defined by $A\mathbf{x} = \mathbf{b}$. The **residual vector** for $\tilde{\mathbf{x}}$ with respect to this system is $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}}$. ■

In procedures such as the Jacobi or Gauss-Seidel methods, a residual vector is associated with each calculation of an approximation component to the solution vector. The object is to generate a sequence of approximations that will cause the residual vectors to converge rapidly to zero. Suppose we let

$$\mathbf{r}_i^{(k)} = (r_{1i}^{(k)}, r_{2i}^{(k)}, \ldots, r_{ni}^{(k)})^t$$

denote the residual vector for the Gauss-Seidel method corresponding to the approximate solution vector $\mathbf{x}_i^{(k)}$ defined by

$$\mathbf{x}_i^{(k)} = (x_1^{(k)}, x_2^{(k)}, \ldots, x_{i-1}^{(k)}, x_i^{(k-1)}, \ldots, x_n^{(k-1)})^t.$$

The mth component of $\mathbf{r}_i^{(k)}$ is

$$r_{mi}^{(k)} = b_m - \sum_{j=1}^{i-1} a_{mj} x_j^{(k)} - \sum_{j=i}^{n} a_{mj} x_j^{(k-1)}, \tag{7.12}$$

or, equivalently,

$$r_{mi}^{(k)} = b_m - \sum_{j=1}^{i-1} a_{mj} x_j^{(k)} - \sum_{j=i+1}^{n} a_{mj} x_j^{(k-1)} - a_{mi} x_i^{(k-1)},$$

for each $m = 1, 2, \ldots, n$.

In particular, the ith component of $\mathbf{r}_i^{(k)}$ is

$$r_{ii}^{(k)} = b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} - a_{ii} x_i^{(k-1)},$$

so

$$a_{ii} x_i^{(k-1)} + r_{ii}^{(k)} = b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)}. \tag{7.13}$$

Recall, however, that in the Gauss-Seidel method, $x_i^{(k)}$ is chosen to be

$$x_i^{(k)} = \frac{1}{a_{ii}} \left[b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} \right], \tag{7.14}$$

so Eq. (7.13) can be rewritten as

$$a_{ii} x_i^{(k-1)} + r_{ii}^{(k)} = a_{ii} x_i^{(k)}.$$

Consequently, the Gauss-Seidel method can be characterized as choosing $x_i^{(k)}$ to satisfy

$$x_i^{(k)} = x_i^{(k-1)} + \frac{r_{ii}^{(k)}}{a_{ii}}. \tag{7.15}$$

We can derive another connection between the residual vectors and the Gauss-Seidel technique. Consider the residual vector $\mathbf{r}_{i+1}^{(k)}$, associated with the vector $\mathbf{x}_{i+1}^{(k)} = (x_1^{(k)}, \ldots, x_i^{(k)}, x_{i+1}^{(k-1)}, \ldots, x_n^{(k-1)})^t$. By (7.12), the ith component of $\mathbf{r}_{i+1}^{(k)}$ is

$$\begin{aligned} r_{i,i+1}^{(k)} &= b_i - \sum_{j=1}^{i} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} \\ &= b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} - a_{ii} x_i^{(k)}. \end{aligned}$$

Equation (7.14) implies that $r_{i,i+1}^{(k)} = 0$. In a sense, then, the Gauss-Seidel technique is also characterized choosing $x_{i+1}^{(k)}$ in such a way that the ith component of $\mathbf{r}_{i+1}^{(k)}$ is zero.

Choosing $x_{i+1}^{(k)}$ so that one coordinate of the residual vector is zero, however, is not the most efficient way to reduce the norm of the vector $\mathbf{r}_{i+1}^{(k)}$. If we modify the Gauss-Seidel procedure, as given by Eq. (7.15), to

$$x_i^{(k)} = x_i^{(k-1)} + \omega \frac{r_{ii}^{(k)}}{a_{ii}}, \tag{7.16}$$

for certain choices of positive ω, we can reduce the norm of the residual vector and obtain significantly faster convergence.

Methods involving Eq. (7.16) are called **relaxation methods**. For choices of ω with $0 < \omega < 1$, the procedures are called **under-relaxation methods** and can be used to obtain convergence of some systems that are not convergent by the Gauss-Seidel method. For choices of ω with $1 < \omega$, the procedures are called **over-relaxation methods**, which are used to accelerate the convergence for systems that are convergent by the Gauss-Seidel technique. These methods are abbreviated **SOR**, for **Successive Over-Relaxation**, and are particularly useful for solving the linear systems that occur in the numerical solution of certain partial-differential equations.

Before illustrating the advantages of the SOR method, we note that by using Eq. (7.13), Eq. (7.16) can be reformulated for calculation purposes to

$$x_i^{(k)} = (1-\omega)x_i^{(k-1)} + \frac{\omega}{a_{ii}}\left[b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(k-1)}\right].$$

To determine the matrix of the SOR method, we rewrite this as

$$a_{ii}x_i^{(k)} + \omega\sum_{j=1}^{i-1} a_{ij}x_j^{(k)} = (1-\omega)a_{ii}x_i^{(k-1)} - \omega\sum_{j=i+1}^{n} a_{ij}x_j^{(k-1)} + \omega b_i,$$

so that in vector form, we have

$$(D-\omega L)\mathbf{x}^{(k)} = [(1-\omega)D + \omega U]\mathbf{x}^{(k-1)} + \omega\mathbf{b}$$

or

$$\mathbf{x}^{(k)} = (D-\omega L)^{-1}[(1-\omega)D + \omega U]\mathbf{x}^{(k-1)} + \omega(D-\omega L)^{-1}\mathbf{b}. \tag{7.17}$$

If we let $T_\omega = (D-\omega L)^{-1}[(1-\omega)D+\omega U]$ and $\mathbf{c}_\omega = \omega(D-\omega L)^{-1}\mathbf{b}$, the SOR technique has the form

$$\mathbf{x}^{(k)} = T_\omega\mathbf{x}^{(k-1)} + \mathbf{c}_\omega. \tag{7.18}$$

EXAMPLE 3 The linear system $A\mathbf{x} = \mathbf{b}$ given by

$$\begin{aligned} 4x_1 + 3x_2 &= 24,\\ 3x_1 + 4x_2 - x_3 &= 30,\\ -x_2 + 4x_3 &= -24, \end{aligned}$$

has the solution $(3, 4, -5)^t$. The Gauss-Seidel method and the SOR method with $\omega = 1.25$ will be used to solve this system, using $\mathbf{x}^{(0)} = (1, 1, 1)^t$ for both methods. For each $k = 1, 2, \ldots$, the equations for the Gauss-Seidel method are

$$\begin{aligned} x_1^{(k)} &= -0.75x_2^{(k-1)} + 6,\\ x_2^{(k)} &= -0.75x_1^{(k)} + 0.25x_3^{(k-1)} + 7.5,\\ x_3^{(k)} &= 0.25x_2^{(k)} - 6, \end{aligned}$$

and the equations for the SOR method with $\omega = 1.25$ are

$$\begin{aligned} x_1^{(k)} &= -0.25x_1^{(k-1)} - 0.9375x_2^{(k-1)} + 7.5,\\ x_2^{(k)} &= -0.9375x_1^{(k)} - 0.25x_2^{(k-1)} + 0.3125x_3^{(k-1)} + 9.375,\\ x_3^{(k)} &= 0.3125x_2^{(k)} - 0.25x_3^{(k-1)} - 7.5. \end{aligned}$$

The first seven iterates for each method are listed in Tables 7.3 and 7.4. For the iterates to be accurate to seven decimal places, the Gauss-Seidel method requires 34 iterations, as opposed to 14 iterations for the over-relaxation method with $\omega = 1.25$. ■

Table 7.3 Gauss-Seidel

k	0	1	2	3	4	5	6	7
$x_1^{(k)}$	1	5.250000	3.1406250	3.0878906	3.0549316	3.0343323	3.0214577	3.0134110
$x_2^{(k)}$	1	3.812500	3.8828125	3.9267578	3.9542236	3.9713898	3.9821186	3.9888241
$x_3^{(k)}$	1	−5.046875	−5.0292969	−5.0183105	−5.0114441	−5.0071526	−5.0044703	−5.0027940

Table 7.4 SOR with $\omega = 1.25$

k	0	1	2	3	4	5	6	7
$x_1^{(k)}$	1	6.312500	2.6223145	3.1333027	2.9570512	3.0037211	2.9963276	3.0000498
$x_2^{(k)}$	1	3.5195313	3.9585266	4.0102646	4.0074838	4.0029250	4.0009262	4.0002586
$x_3^{(k)}$	1	−6.6501465	−4.6004238	−5.0966863	−4.9734897	−5.0057135	−4.9982822	−5.0003486

The obvious question to ask is how the appropriate value of ω is chosen. Although no complete answer to this question is known for the general $n \times n$ linear system, the following results can be used in certain situations.

Theorem 7.24 **(Kahan)**

If $a_{ii} \neq 0$, for each $i = 1, 2, \ldots, n$, then $\rho(T_\omega) \geq |\omega - 1|$. This implies that the SOR method can converge only if $0 < \omega < 2$. ■

The proof of this theorem is considered in Exercise 13. The proof of the next two results can be found in [Or2, pp. 123–133]. These results will be used in Chapter 12.

Theorem 7.25 **(Ostrowski-Reich)**

If A is a positive definite matrix and $0 < \omega < 2$, then the SOR method converges for any choice of initial approximate vector $\mathbf{x}^{(0)}$. ■

Theorem 7.26 If A is positive definite and tridiagonal, then $\rho(T_g) = [\rho(T_j)]^2 < 1$, and the optimal choice of ω for the SOR method is

$$\omega = \frac{2}{1 + \sqrt{1 - [\rho(T_j)]^2}}.$$

With this choice of ω, we have $\rho(T_\omega) = \omega - 1$. ■

EXAMPLE 4 The matrix

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

given in Example 3, is positive definite and tridiagonal, so Theorem 7.26 applies. Since

$$T_j = D^{-1}(L+U) = \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \begin{bmatrix} 0 & -3 & 0 \\ -3 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -0.75 & 0 \\ -0.75 & 0 & 0.25 \\ 0 & 0.25 & 0 \end{bmatrix},$$

we have

$$T_j - \lambda I = \begin{bmatrix} -\lambda & -0.75 & 0 \\ -0.75 & -\lambda & 0.25 \\ 0 & 0.25 & -\lambda \end{bmatrix},$$

so

$$\det(T_j - \lambda I) = -\lambda(\lambda^2 - 0.625).$$

Thus,

$$\rho(T_j) = \sqrt{0.625}$$

and

$$\omega = \frac{2}{1+\sqrt{1-[\rho(T_j)]^2}} = \frac{2}{1+\sqrt{1-0.625}} \approx 1.24.$$

This explains the rapid convergence obtained in Example 1 when using $\omega = 1.25$. ■

We close this section with Algorithm 7.3 for the SOR method.

ALGORITHM 7.3

SOR

To solve $A\mathbf{x} = \mathbf{b}$ given the parameter ω and an initial approximation $\mathbf{x}^{(0)}$:

INPUT the number of equations and unknowns n; the entries a_{ij}, $1 \le i, j \le n$, of the matrix A; the entries b_i, $1 \le i \le n$, of $\mathbf{b}$; the entries XO_i, $1 \le i \le n$, of $\mathbf{XO} = \mathbf{x}^{(0)}$; the parameter ω; tolerance TOL; maximum number of iterations N.

OUTPUT the approximate solution $x_1, \ldots, x_n$ or a message that the number of iterations was exceeded.

Step 1 Set $k = 1$.

Step 2 While $(k \le N)$ do Steps 3–6.

Step 3 For $i = 1, \ldots, n$

$$\text{set } x_i = (1-\omega)XO_i + \frac{\omega(-\sum_{j=1}^{i-1} a_{ij}x_j - \sum_{j=i+1}^{n} a_{ij}XO_j + b_i)}{a_{ii}}.$$

Step 4 If $\|\mathbf{x} - \mathbf{XO}\| < TOL$ then OUTPUT $(x_1, \ldots, x_n)$;
(*The procedure was successful.*)
STOP.

Step 5 Set $k = k + 1$.

Step 6 For $i = 1, \ldots, n$ set $XO_i = x_i$.

Step 7 OUTPUT ('Maximum number of iterations exceeded');
(*The procedure was successful.*)
STOP. ■

EXERCISE SET 7.3

1. Find the first two iterations of the Jacobi method for the following linear systems, using $\mathbf{x}^{(0)} = \mathbf{0}$:

   a. $3x_1 - x_2 + x_3 = 1$,
   $3x_1 + 6x_2 + 2x_3 = 0$,
   $3x_1 + 3x_2 + 7x_3 = 4$.

   b. $10x_1 - x_2 = 9$,
   $-x_1 + 10x_2 - 2x_3 = 7$,
   $-2x_2 + 10x_3 = 6$.

   c. $10x_1 + 5x_2 = 6$,
   $5x_1 + 10x_2 - 4x_3 = 25$,
   $-4x_2 + 8x_3 - x_4 = -11$,
   $-x_3 + 5x_4 = -11$.

   d. $4x_1 + x_2 - x_3 + x_4 = -2$,
   $x_1 + 4x_2 - x_3 - x_4 = -1$,
   $-x_1 - x_2 + 5x_3 + x_4 = 0$,
   $x_1 - x_2 + x_3 + 3x_4 = 1$.

   e. $4x_1 + x_2 + x_3 + x_5 = 6$,
   $-x_1 - 3x_2 + x_3 + x_4 = 6$,
   $2x_1 + x_2 + 5x_3 - x_4 - x_5 = 6$,
   $-x_1 - x_2 - x_3 + 4x_4 = 6$,
   $2x_2 - x_3 + x_4 + 4x_5 = 6$.

   f. $4x_1 - x_2 - x_4 = 0$,
   $-x_1 + 4x_2 - x_3 - x_5 = 5$,
   $-x_2 + 4x_3 - x_6 = 0$,
   $-x_1 + 4x_4 - x_5 = 6$,
   $-x_2 - x_4 + 4x_5 - x_6 = -2$,
   $-x_3 - x_5 + 4x_6 = 6$.

2. Repeat Exercise 1 using the Gauss-Seidel method.
3. Use the Jacobi method to solve the linear systems in Exercise 1, with $TOL = 10^{-3}$ in the l_∞ norm.
4. Repeat Exercise 3 using the Gauss-Seidel Algorithm.
5. Find the first two iterations of the SOR method with $\omega = 1.1$ for the following linear systems, using $\mathbf{x}^{(0)} = \mathbf{0}$:

   a. $3x_1 - x_2 + x_3 = 1$,
   $3x_1 + 6x_2 + 2x_3 = 0$,
   $3x_1 + 3x_2 + 7x_3 = 4$.

   b. $10x_1 - x_2 = 9$,
   $-x_1 + 10x_2 - 2x_3 = 7$,
   $-2x_2 + 10x_3 = 6$.

c.
$$\begin{aligned} 10x_1 + 5x_2 &= 6,\\ 5x_1 + 10x_2 - 4x_3 &= 25,\\ -4x_2 + 8x_3 - x_4 &= -11,\\ -x_3 + 5x_4 &= -11. \end{aligned}$$

d.
$$\begin{aligned} 4x_1 + x_2 - x_3 + x_4 &= -2,\\ x_1 + 4x_2 - x_3 - x_4 &= -1,\\ -x_1 - x_2 + 5x_3 + x_4 &= 0,\\ x_1 - x_2 + x_3 + 3x_4 &= 1. \end{aligned}$$

e.
$$\begin{aligned} 4x_1 + x_2 + x_3 + x_5 &= 6,\\ -x_1 - 3x_2 + x_3 + x_4 &= 6,\\ 2x_1 + x_2 + 5x_3 - x_4 - x_5 &= 6,\\ -x_1 - x_2 - x_3 + 4x_4 &= 6,\\ 2x_2 - x_3 + x_4 + 4x_5 &= 6. \end{aligned}$$

f.
$$\begin{aligned} 4x_1 - x_2 - x_4 &= 0,\\ -x_1 + 4x_2 - x_3 - x_5 &= 5,\\ -x_2 + 4x_3 - x_6 &= 0,\\ -x_1 + 4x_4 - x_5 &= 6,\\ -x_2 - x_4 + 4x_5 - x_6 &= -2,\\ -x_3 - x_5 + 4x_6 &= 6. \end{aligned}$$

6. Repeat Exercise 1 using $\omega = 1.3$.
7. Use the SOR method with $\omega = 1.2$ to solve the linear systems in Exercise 5 with a tolerance $TOL = 10^{-3}$ in the l_∞ norm.
8. Determine which matrices in Exercise 5 are tridiagonal and positive definite. Repeat Exercise 7 for these matrices using the optimal choice of ω.
9. The linear system
$$\begin{aligned} 2x_1 - x_2 + x_3 &= -1,\\ 2x_1 + 2x_2 + 2x_3 &= 4,\\ -x_1 - x_2 + 2x_3 &= -5 \end{aligned}$$
has the solution $(1, 2, -1)^t$.
   a. Show that $\rho(T_j) = \frac{\sqrt{5}}{2} > 1$.
   b. Show that the Jacobi method with $\mathbf{x}^{(0)} = \mathbf{0}$ fails to give a good approximation after 25 iterations.
   c. Show that $\rho(T_g) = \frac{1}{2}$.
   d. Use the Gauss-Seidel method with $\mathbf{x}^{(0)} = \mathbf{0}$ to approximate the solution to the linear system to within 10^{-5} in the l_∞ norm.
10. The linear system
$$\begin{aligned} x_1 + 2x_2 - 2x_3 &= 7,\\ x_1 + x_2 + x_3 &= 2,\\ 2x_1 + 2x_2 + x_3 &= 5 \end{aligned}$$
has the solution $(1, 2, -1)^t$.
   a. Show that $\rho(T_j) = 0$.
   b. Use the Jacobi method with $\mathbf{x}^{(0)} = \mathbf{0}$ to approximate the solution to the linear system to within 10^{-5} in the l_∞ norm.
   c. Show that $\rho(T_g) = 2$.
   d. Show that the Gauss-Seidel method applied as in part (b) fails to give a good approximation in 25 iterations.

11. **a.** Prove that
$$\|\mathbf{x}^{(k)} - \mathbf{x}\| \le \|T\|^k \|\mathbf{x}^{(0)} - \mathbf{x}\| \quad \text{and} \quad \|\mathbf{x}^{(k)} - \mathbf{x}\| \le \frac{\|T\|^k}{1 - \|T\|} \|\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\|,$$
where T is an $n \times n$ matrix with $\|T\| < 1$ and
$$\mathbf{x}^{(k)} = T\mathbf{x}^{(k-1)} + \mathbf{c}, \quad k = 1, 2, \ldots,$$
with $\mathbf{x}^{(0)}$ arbitrary, $\mathbf{c} \in \mathbb{R}^n$, and $\mathbf{x} = T\mathbf{x} + \mathbf{c}$.
   b. Apply the bounds to Exercise 1, when possible, using the l_∞ norm.
12. Show that if A is strictly diagonally dominant, then $\|T_j\|_\infty < 1$.
13. Prove Theorem 7.24. [*Hint:* If $\lambda_1, \ldots, \lambda_n$ are eigenvalues of T_ω, then $\det T_\omega = \prod_{i=1}^n \lambda_i$. Since $\det D^{-1} = \det(D - \omega L)^{-1}$ and the determinant of a product of matrices is the product of the determinants of the factors, the result follows from Eq. (7.17).]
14. Suppose that an object can be at any one of $n + 1$ equally spaced points $x_0, x_1, \ldots, x_n$. When an object is at location x_i, it is equally likely to move to either x_{i-1} or x_{i+1} and cannot directly move to any other location. Consider the probabilities $\{P_i\}_{i=0}^n$ that an object starting at location x_i will reach the left endpoint x_0 before reaching the right endpoint x_n. Clearly, $P_0 = 1$ and $P_n = 0$. Since the object can move to x_i only from x_{i-1} or x_{i+1} and does so with probability $\frac{1}{2}$ for each of these locations,
$$P_i = \frac{1}{2}P_{i-1} + \frac{1}{2}P_{i+1}, \quad \text{for each } i = 1, 2, \ldots, n-1.$$
   a. Show that
$$\begin{bmatrix} 1 & -\frac{1}{2} & 0 & \cdots & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & \ddots & \vdots \\ 0 & -\frac{1}{2} & 1 & \ddots & 0 \\ \vdots & \ddots & \ddots & -\frac{1}{2} & -\frac{1}{2} \\ 0 & \cdots & 0 & -\frac{1}{2} & 1 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_{n-1} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$
   b. Solve this system using $n = 10$, 50, and 100.
   c. Change the probabilities to α and $1 - \alpha$ for movement to the left and right, respectively, and derive the linear system similar to the one in part (a).
   d. Repeat part (b) with $\alpha = \frac{1}{3}$.
15. Use all the applicable methods in this section to solve the linear system $A\mathbf{x} = \mathbf{b}$ to within 10^{-5} in the l_∞ norm, where the entries of A are
$$a_{i,j} = \begin{cases} 2i, & \text{when } j = i \text{ and } i = 1, 2, \ldots, 80,\\ 0.5i, & \text{when } \begin{cases} j = i + 2 \text{ and } i = 1, 2, \ldots, 78,\\ j = i - 2 \text{ and } i = 3, 4, \ldots, 80, \end{cases}\\ 0.25i, & \text{when } \begin{cases} j = i + 4 \text{ and } i = 1, 2, \ldots, 76,\\ j = i - 4 \text{ and } i = 5, 6, \ldots, 80, \end{cases}\\ 0, & \text{otherwise,} \end{cases}$$
and those of $\mathbf{b}$ are $b_i = \pi$, for each $i = 1, 2, \ldots, 80$.

16. Suppose that A is a positive definite.
    a. Show that we can write $A = D - L - L^t$, where D is diagonal with $d_{ii} > 0$ for each $1 \le i \le n$ and L is lower triangular. Further, show that $D - L$ is nonsingular.
    b. Let $T_g = (D - L)^{-1}L^t$ and $P = A - T_g^t A T_g$. Show that P is symmetric.
    c. Show that T_g can also be written as $T_g = I - (D - L)^{-1}A$.
    d. Let $Q = (D - L)^{-1}A$. Show that $T_g = I - Q$ and $P = Q^t[AQ^{-1} - A + (Q^t)^{-1}A]Q$.
    e. Show that $P = Q^t DQ$ and P is positive definite.
    f. Let λ be an eigenvalue of T_g with eigenvector $\mathbf{x} \neq \mathbf{0}$. Use part (b) to show that $\mathbf{x}^t P\mathbf{x} > 0$ implies that $|\lambda| < 1$.
    g. Show that T_g is convergent and prove that the Gauss-Seidel method converges.
17. Extend the method of proof in Exercise 16 to the SOR method with $0 < \omega < 2$.
18. The forces on the bridge truss described in the opening to this chapter satisfy the equations in the following table:

Joint	Horizontal Component	Vertical Component
①	$-F_1 + \frac{\sqrt{2}}{2}f_1 + f_2 = 0$	$\frac{\sqrt{2}}{2}f_1 - F_2 = 0$
②	$-\frac{\sqrt{2}}{2}f_1 + \frac{\sqrt{3}}{2}f_4 = 0$	$-\frac{\sqrt{2}}{2}f_1 - f_3 + \frac{1}{2}f_4 = 0$
③	$-f_2 + f_5 = 0$	$f_3 - 10{,}000 = 0$
④	$-\frac{\sqrt{3}}{2}f_4 - f_5 = 0$	$\frac{1}{2}f_4 - F_3 = 0$

This linear system can be placed in the matrix form

$$\begin{bmatrix} -1 & 0 & 0 & \frac{\sqrt{2}}{2} & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & -1 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & -1 \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 10{,}000 \\ 0 \\ 0 \end{bmatrix}.$$

    a. Explain why the system of equations was reordered.
    b. Approximate the solution of the resulting linear system to within 10^{-2} in the l_∞ norm using as initial approximation the vector all of whose entries are 1s and (i) the Gauss-Seidel method, (ii) the Jacobi method, and (iii) the SOR method with $\omega = 1.25$.

7.4 Error Bounds and Iterative Refinement

It seems intuitively reasonable that if $\tilde{\mathbf{x}}$ is an approximation to the solution $\mathbf{x}$ of $A\mathbf{x} = \mathbf{b}$ and the residual vector $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}}$ has the property that $\|\mathbf{r}\| = \|\mathbf{b} - A\tilde{\mathbf{x}}\|$ is small, then $\|\mathbf{x} - \tilde{\mathbf{x}}\|$ would be small as well. This is often the case, but certain systems, which occur frequently in practice, fail to have this property.

EXAMPLE 1 The linear system $A\mathbf{x} = \mathbf{b}$ given by

$$\begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 3.0001 \end{bmatrix}$$

has the unique solution $\mathbf{x} = (1, 1)^t$. The poor approximation $\tilde{\mathbf{x}} = (3, 0)^t$ has the residual vector

$$\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}} = \begin{bmatrix} 3 \\ 3.0001 \end{bmatrix} - \begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix} \begin{bmatrix} 3 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -0.0002 \end{bmatrix},$$

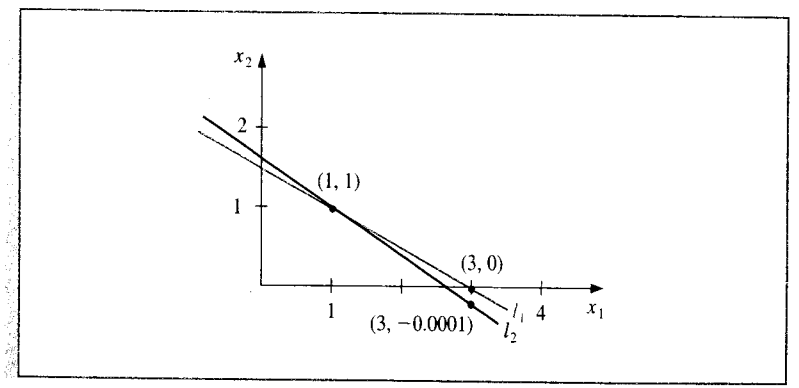
so $\|\mathbf{r}\|_\infty = 0.0002$. Although the norm of the residual vector is small, the approximation $\tilde{\mathbf{x}} = (3, 0)^t$ is obviously quite poor; in fact, $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty = 2$. ■

The difficulty in Example 1 is explained quite simply by noting that the solution to the system represents the intersection of the lines

$$l_1: \quad x_1 + 2x_2 = 3 \quad \text{and} \quad l_2: \quad 1.0001x_1 + 2x_2 = 3.0001.$$

The point $(3, 0)$ lies on l_1, and the lines are nearly parallel. This implies that $(3, 0)$ also lies close to l_2, even though it differs significantly from the solution of the system, given by the intersection point $(1, 1)$. (See Figure 7.7.)

Figure 7.7



Example 1 was clearly constructed to show the difficulties that can—and, in fact, do—arise. Had the lines not been nearly coincident, we would expect a small residual vector to imply an accurate approximation.

In the general situation, we cannot rely on the geometry of the system to give an indication of when problems might occur. We can, however, obtain this information by considering the norms of the matrix A and its inverse.

Theorem 7.27 Suppose that $\tilde{\mathbf{x}}$ is an approximation to the solution of $A\mathbf{x} = \mathbf{b}$, A is a nonsingular matrix, and $\mathbf{r}$ is the residual vector for $\tilde{\mathbf{x}}$. Then for any natural norm,

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| \le \|\mathbf{r}\| \cdot \|A^{-1}\|$$

and if $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{b} \neq \mathbf{0}$,

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \|A\| \cdot \|A^{-1}\| \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}. \tag{7.19}$$

■

Proof Since $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}} = A\mathbf{x} - A\tilde{\mathbf{x}}$ and A is nonsingular, $\mathbf{x} - \tilde{\mathbf{x}} = A^{-1}\mathbf{r}$. Theorem 7.11 in Section 7.1 implies that

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| = \|A^{-1}\mathbf{r}\| \leq \|A^{-1}\| \cdot \|\mathbf{r}\|.$$

Moreover, since $\mathbf{b} = A\mathbf{x}$, we have $\|\mathbf{b}\| \leq \|A\| \cdot \|\mathbf{x}\|$, so $1/\|\mathbf{x}\| \leq \|A\|/\|\mathbf{b}\|$ and

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \frac{\|A\| \cdot \|A^{-1}\|}{\|\mathbf{b}\|} \|\mathbf{r}\|. \qquad \blacksquare \blacksquare \blacksquare$$

The inequalities in Theorem 7.27 imply that $\|A^{-1}\|$ and $\|A\| \cdot \|A^{-1}\|$ provide an indication of the connection between the residual vector and the accuracy of the approximation. In general, the relative error $\|\mathbf{x} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\|$ is of most interest, and, by Inequality (7.19), this error is bounded by the product of $\|A\| \cdot \|A^{-1}\|$ with the relative residual for this approximation, $\|\mathbf{r}\|/\|\mathbf{b}\|$. Any convenient norm can be used for this approximation; the only requirement is that it be used consistently throughout.

Definition 7.28 The **condition number** of the nonsingular matrix A relative to a norm $\|\cdot\|$ is

$$K(A) = \|A\| \cdot \|A^{-1}\|. \qquad \blacksquare$$

With this notation, the inequalities in Theorem 7.27 become

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| \leq K(A) \frac{\|\mathbf{r}\|}{\|A\|}$$

and

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq K(A) \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}.$$

For any nonsingular matrix A and natural norm $\|\cdot\|$,

$$1 = \|I\| = \|A \cdot A^{-1}\| \leq \|A\| \cdot \|A^{-1}\| = K(A).$$

A matrix A is **well-conditioned** if $K(A)$ is close to 1, and is **ill-conditioned** when $K(A)$ is significantly greater than 1. Conditioning in this context refers to the relative security that a small residual vector implies a correspondingly accurate approximate solution.

EXAMPLE 2 The matrix for the system considered in Example 1 was

$$A = \begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix},$$

which has $\|A\|_\infty = 3.0001$. This norm would not be considered large. However,

$$A^{-1} = \begin{bmatrix} -10000 & 10000 \\ 5000.5 & -5000 \end{bmatrix}, \quad \text{so} \quad \|A^{-1}\|_\infty = 20000,$$

and for the infinity norm, $K(A) = (20000)(3.0001) = 60002$. The size of the condition number for this example should certainly keep us from making hasty accuracy decisions based on the residual of an approximation. ■

In Maple the condition number K_∞ can be computed as follows:

```
>with(linalg);
>A:=matrix(2,2,[1,2,1.0001,2]);
>cond(A);
```

60002.00000

Although the condition number of a matrix depends totally on the norms of the matrix and its inverse, in practice the calculation of the inverse is subject to roundoff error and is dependent on the accuracy with which the calculations are performed. If the operations involve arithmetic with t digits of accuracy, the approximate condition number for the matrix A is the norm of the matrix times the norm of the approximation to the inverse of A, which is obtained using t-digit arithmetic. In fact, this condition number also depends on the method used to calculate the inverse of A.

If we assume that the approximate solution to the linear system $A\mathbf{x} = \mathbf{b}$ is being determined using t-digit arithmetic and Gaussian elimination, it can be shown (see [FM, pp. 45–47]) that the residual vector $\mathbf{r}$ for the approximation $\tilde{\mathbf{x}}$ has

$$\|\mathbf{r}\| \approx 10^{-t} \|A\| \cdot \|\tilde{\mathbf{x}}\|. \tag{7.20}$$

From this approximation, an estimate for the effective condition number in t-digit arithmetic can be obtained without having to invert the matrix A. In actuality, this approximation assumes that all the arithmetic operations in the Gaussian elimination technique are performed using t-digit arithmetic but that the operations needed to determine the residual are done in double-precision (that is, $2t$-digit) arithmetic. This technique does not add significantly to the computational effort and eliminates much of the loss of accuracy involved with the subtraction of the nearly equal numbers that occur in the calculation of the residual.

The approximation for the t-digit condition number $K(A)$ comes from consideration of the linear system

$$A\mathbf{y} = \mathbf{r}.$$

The solution to this system can be readily approximated since the multipliers for the Gaussian elimination method have already been calculated. In fact $\tilde{\mathbf{y}}$, the approximate solution of $A\mathbf{y} = \mathbf{r}$, satisfies

$$\tilde{\mathbf{y}} \approx A^{-1}\mathbf{r} = A^{-1}(\mathbf{b} - A\tilde{\mathbf{x}}) = A^{-1}\mathbf{b} - A^{-1}A\tilde{\mathbf{x}} = \mathbf{x} - \tilde{\mathbf{x}}; \tag{7.21}$$

and

$$\mathbf{x} \approx \tilde{\mathbf{x}} + \tilde{\mathbf{y}}.$$

So $\tilde{\mathbf{y}}$ is an estimate of the error produced when $\tilde{\mathbf{x}}$ approximates the solution $\mathbf{x}$ to the original system. Equations (7.20) and (7.21) imply that

$$\|\tilde{\mathbf{y}}\| \approx \|\mathbf{x} - \tilde{\mathbf{x}}\| = \|A^{-1}\mathbf{r}\| \leq \|A^{-1}\| \cdot \|\mathbf{r}\| \approx \|A^{-1}\| \left(10^{-t}\|A\| \cdot \|\tilde{\mathbf{x}}\|\right) = 10^{-t}\|\tilde{\mathbf{x}}\|K(A)$$

This gives an approximation for the condition number involved with solving the system $A\mathbf{x} = \mathbf{b}$ using Gaussian elimination and the t-digit type of arithmetic just described:

$$K(A) \approx \frac{\|\tilde{\mathbf{y}}\|}{\|\tilde{\mathbf{x}}\|} 10^t. \tag{7.22}$$

EXAMPLE 3 The linear system given by

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 \\ 2.2220 & 16.710 & 9.6120 \\ 1.5611 & 5.1791 & 1.6852 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15913 \\ 28.544 \\ 8.4254 \end{bmatrix}$$

has the exact solution $\mathbf{x} = (1, 1, 1)^t$.

Using Gaussian elimination and five-digit rounding arithmetic leads successively to the augmented matrices

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 & \vdots & 15913 \\ 0 & -10596 & 16.501 & \vdots & 10580 \\ 0 & -7451.4 & 6.5250 & \vdots & -7444.9 \end{bmatrix}$$

and

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 & \vdots & 15913 \\ 0 & -10596 & 16.501 & \vdots & -10580 \\ 0 & 0 & -5.0790 & \vdots & -4.7000 \end{bmatrix}.$$

The approximate solution to this system is

$$\tilde{\mathbf{x}} = (1.2001, 0.99991, 0.92538)^t.$$

The residual vector corresponding to $\tilde{\mathbf{x}}$ is computed in double precision to be

$$\begin{aligned} \mathbf{r} &= \mathbf{b} - A\tilde{\mathbf{x}} \\ &= \begin{bmatrix} 15913 \\ 28.544 \\ 8.4254 \end{bmatrix} - \begin{bmatrix} 3.3330 & 15920 & -10.333 \\ 2.2220 & 16.710 & 9.6120 \\ 1.5611 & 5.1791 & 1.6852 \end{bmatrix} \begin{bmatrix} 1.2001 \\ 0.99991 \\ 0.92538 \end{bmatrix} \\ &= \begin{bmatrix} 15913 \\ 28.544 \\ 8.4254 \end{bmatrix} - \begin{bmatrix} 15913.00518 \\ 28.26987086 \\ 8.611560367 \end{bmatrix} = \begin{bmatrix} -0.00518 \\ 0.27412914 \\ -0.186160367 \end{bmatrix}, \end{aligned}$$

so

$$\|\mathbf{r}\|_\infty = 0.27413.$$

The estimate for the condition number given in the preceding discussion is obtained by first solving the system $A\mathbf{y} = \mathbf{r}$ for $\tilde{\mathbf{y}}$:

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 \\ 2.2220 & 16.710 & 9.6120 \\ 1.5611 & 5.1791 & 1.6852 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -0.00518 \\ 0.27413 \\ -0.18616 \end{bmatrix}.$$

This implies that $\tilde{\mathbf{y}} = (-0.20008, 8.9987 \times 10^{-5}, 0.074607)^t$. Using the estimate in Eq. (7.22) gives

$$K(A) \approx 10^5 \frac{\|\tilde{\mathbf{y}}\|_\infty}{\|\tilde{\mathbf{x}}\|_\infty} = \frac{10^5(0.20008)}{1.2001} = 16672. \tag{7.23}$$

To determine the *exact* condition number of A, we first must construct A^{-1}. Using five-digit rounding arithmetic for the calculations gives the approximation:

$$A^{-1} = \begin{bmatrix} -1.1701 \times 10^{-4} & -1.4983 \times 10^{-1} & 8.5416 \times 10^{-1} \\ 6.2782 \times 10^{-5} & 1.2124 \times 10^{-4} & -3.0662 \times 10^{-4} \\ -8.6631 \times 10^{-5} & 1.3846 \times 10^{-1} & -1.9689 \times 10^{-1} \end{bmatrix}.$$

Theorem 7.11 implies that $\|A^{-1}\|_\infty = 1.0041$ and $\|A\|_\infty = 15934$.

As a consequence, the ill-conditioned matrix A has

$$K(A) = (1.0041)(15934) = 15999.$$

The estimate in (7.23) is quite close to $K(A)$ and requires considerably less computational effort.

Since the actual solution $\mathbf{x} = (1, 1, 1)^t$ is known for this system, we can calculate both

$$\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty = 0.2001 \quad \text{and} \quad \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty}{\|\mathbf{x}\|_\infty} = \frac{0.2001}{1} = 0.2001.$$

The error bounds given in Theorem 7.27 for these values are

$$\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \leq K(A)\frac{\|\mathbf{r}\|_\infty}{\|A\|_\infty} = \frac{(15999)(0.27413)}{15934} = 0.27525$$

and

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty}{\|\mathbf{x}\|_\infty} \leq K(A)\frac{\|\mathbf{r}\|_\infty}{\|\mathbf{b}\|_\infty} = \frac{(15999)(0.27413)}{15913} = 0.27561. \quad \blacksquare$$

In Eq. (7.21), we used the estimate $\tilde{\mathbf{y}} \approx \mathbf{x} - \tilde{\mathbf{x}}$, where $\tilde{\mathbf{y}}$ is the approximate solution to the system $A\mathbf{y} = \mathbf{r}$. In general, $\tilde{\mathbf{x}} + \tilde{\mathbf{y}}$ is a more accurate approximation to the solution of the linear system $A\mathbf{x} = \mathbf{b}$ than the original approximation $\tilde{\mathbf{x}}$. The method using this assumption is called **iterative refinement**, or iterative improvement, and consists of performing iterations on the system whose right-hand side is the residual vector for successive approximations until satisfactory accuracy results.

If the process is applied using t-digit arithmetic and if $K_\infty(A) \approx 10^q$, then after k iterations of iterative refinement the solution has approximately the smaller of t and $k(t-q)$ correct digits. If the system is well-conditioned, one or two iterations will indicate that the solution is accurate. There is the possibility of significant improvement on ill-conditioned systems unless the matrix A is so ill-conditioned that $K_\infty(A) > 10^t$. In that situation, increased precision should be used for the calculations.

Algorithm 7.4 implements the Iterative Refinement technique.

ALGORITHM 7.4

Iterative Refinement

To approximate the solution to the linear system $A\mathbf{x} = \mathbf{b}$:

INPUT the number of equations and unknowns n; the entries a_{ij}, $1 \le i, j \le n$ of the matrix A; the entries b_i, $1 \le i \le n$ of $\mathbf{b}$; the maximum number of iterations N; tolerance TOL; number of digits of precision t.

OUTPUT the approximation $\mathbf{xx} = (xx_1, \ldots, xx_n)^t$ or a message that the number of iterations was exceeded, and an approximation $COND$ to $K_\infty(A)$.

Step 0 Solve the system $A\mathbf{x} = \mathbf{b}$ for $x_1, \ldots, x_n$ by Gaussian elimination saving the multipliers m_{ji}, $j = i+1, i+2, \ldots, n$, $i = 1, 2, \ldots, n-1$ and noting row interchanges.

Step 1 Set $k = 1$.

Step 2 While $(k \le N)$ do Steps 3–9.

Step 3 For $i = 1, 2, \ldots, n$ (*Calculate* $\mathbf{r}$.)

$$\text{set } r_i = b_i - \sum_{j=1}^{n} a_{ij} x_j.$$

(*Perform the computations in double-precision arithmetic.*)

Step 4 Solve the linear system $A\mathbf{y} = \mathbf{r}$ by using Gaussian elimination in the same order as in Step 0.

Step 5 For $i = 1, \ldots, n$ set $xx_i = x_i + y_i$.

Step 6 If $k = 1$ then set $COND = \dfrac{\|\mathbf{y}\|_\infty}{\|\mathbf{xx}\|_\infty} 10^t$.

Step 7 If $\|\mathbf{x} - \mathbf{xx}\|_\infty < TOL$ then OUTPUT ($\mathbf{xx}$);
OUTPUT ($COND$);
(*The procedure was successful.*)
STOP.

Step 8 Set $k = k + 1$.

Step 9 For $i = 1, \ldots, n$ set $x_i = xx_i$.

Step 10 OUTPUT ('Maximum number of iterations exceeded');
OUTPUT ($COND$);
(*The procedure was unsuccessful.*)
STOP. ■

If t-digit arithmetic is used, a recommended stopping procedure in Step 7 is to iterate until $|y_i^{(k)}| \le 10^{-t}$, for each $i = 1, 2, \ldots, n$.

EXAMPLE 4 In Example 3 we found the approximation to the problem we have been considering, using five-digit arithmetic and Gaussian elimination, to be

$$\tilde{\mathbf{x}}^{(1)} = (1.2001, 0.99991, 0.92538)^t$$

and the solution to $A\mathbf{y} = \mathbf{r}^{(1)}$ to be

$$\tilde{\mathbf{y}}^{(1)} = (-0.20008, 8.9987 \times 10^{-5}, 0.074607)^t.$$

By Step 5 in this algorithm,

$$\tilde{\mathbf{x}}^{(2)} = \tilde{\mathbf{x}}^{(1)} + \tilde{\mathbf{y}}^{(1)} = (1.0000, 1.0000, 0.99999)^t,$$

and the actual error in this approximation is

$$\|\mathbf{x} - \tilde{\mathbf{x}}^{(2)}\|_\infty = 1 \times 10^{-5}.$$

Using the suggested stopping technique for the algorithm, we compute $\mathbf{r}^{(2)} = \mathbf{b} - A\tilde{\mathbf{x}}^{(2)}$ and solve the system $A\mathbf{y}^{(2)} = \mathbf{r}^{(2)}$, which gives

$$\tilde{\mathbf{y}}^{(2)} = (1.5002 \times 10^{-9}, 2.0951 \times 10^{-10}, 1.0000 \times 10^{-5})^t.$$

Since $\|\tilde{\mathbf{y}}^{(2)}\|_\infty \le 10^{-5}$, we conclude that

$$\tilde{\mathbf{x}}^{(3)} = \tilde{\mathbf{x}}^{(2)} + \tilde{\mathbf{y}}^{(2)} = (1.0000, 1.0000, 1.0000)^t$$

is sufficiently accurate, which is certainly correct. ■

Throughout this section it has been assumed that in the linear system $A\mathbf{x} = \mathbf{b}$, A and $\mathbf{b}$ can be represented exactly. Realistically, the entries a_{ij} and b_j will be altered or perturbed by an amount δa_{ij} and δb_j, causing the linear system

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

to be solved in place of $A\mathbf{x} = \mathbf{b}$. Normally, if $\|\delta A\|$ and $\|\delta\mathbf{b}\|$ are small (on the order of 10^{-t}), the t-digit arithmetic should yield a solution $\tilde{\mathbf{x}}$ for which $\|\mathbf{x} - \tilde{\mathbf{x}}\|$ is correspondingly small. However, in the case of ill-conditioned systems, we have seen that even if A and $\mathbf{b}$ are represented exactly, rounding errors can cause $\|\mathbf{x} - \tilde{\mathbf{x}}\|$ to be large. The following theorem relates the perturbations of linear systems to the condition number of a matrix. The proof of this result can be found in [Or2, p. 33].

Theorem 7.29 Suppose A is nonsingular and

$$\|\delta A\| < \frac{1}{\|A^{-1}\|}.$$

The solution $\tilde{\mathbf{x}}$ to $(A + \delta A)\tilde{\mathbf{x}} = \mathbf{b} + \delta\mathbf{b}$ approximates the solution $\mathbf{x}$ of $A\mathbf{x} = \mathbf{b}$ with the error estimate

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \le \frac{K(A)\|A\|}{\|A\| - K(A)\|\delta A\|} \left(\frac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|} + \frac{\|\delta A\|}{\|A\|} \right). \tag{7.24}$$

■

The estimate in inequality (7.24) states that if the matrix A is well-conditioned (that is, $K(A)$ is not too large), then small changes in A and $\mathbf{b}$ produce correspondingly small changes in the solution $\mathbf{x}$. If, on the other hand, A is ill-conditioned, then small changes in A and $\mathbf{b}$ may produce large changes in $\mathbf{x}$.

The theorem is independent of the particular numerical procedure used to solve $A\mathbf{x} = \mathbf{b}$. It can be shown, by means of a backward error analysis (see [Wil1] or [Wil2]), that if Gaussian elimination with pivoting is used to solve $A\mathbf{x} = \mathbf{b}$ in t-digit arithmetic, the numerical solution $\tilde{\mathbf{x}}$ is the actual solution of a linear system:

$$(A + \delta A)\tilde{\mathbf{x}} = \mathbf{b}, \quad \text{where } \|\delta A\|_\infty \le f(n)10^{1-t} \max_{i,j,k} |a_{ij}^{(k)}|.$$

Wilkinson found in practice that $f(n) \approx n$ and, at worst, $f(n) \le 1.01(n^3 + 3n^2)$.

EXERCISE SET 7.4

1. Compute the condition numbers of the following matrices relative to $\|\cdot\|_\infty$.

a. $\begin{bmatrix} \frac{1}{2} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{4} \end{bmatrix}$

b. $\begin{bmatrix} 3.9 & 1.6 \\ 6.8 & 2.9 \end{bmatrix}$

c. $\begin{bmatrix} 1 & 2 \\ 1.00001 & 2 \end{bmatrix}$

d. $\begin{bmatrix} 1.003 & 58.09 \\ 5.550 & 321.8 \end{bmatrix}$

e. $\begin{bmatrix} 1 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & -1 \end{bmatrix}$

f. $\begin{bmatrix} 0.04 & 0.01 & -0.01 \\ 0.2 & 0.5 & -0.2 \\ 1 & 2 & 4 \end{bmatrix}$

2. The following linear systems $A\mathbf{x} = \mathbf{b}$ have $\mathbf{x}$ as the actual solution and $\tilde{\mathbf{x}}$ as an approximate solution. Using the results of Exercise 1, compute $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty$ and $K_\infty(A)\frac{\|\mathbf{b} - A\tilde{\mathbf{x}}\|_\infty}{\|A\|_\infty}$.

a. $\frac{1}{2}x_1 + \frac{1}{3}x_2 = \frac{1}{63}$,
$\frac{1}{3}x_1 + \frac{1}{4}x_2 = \frac{1}{168}$,
$\mathbf{x} = \left(\frac{1}{7}, -\frac{1}{6}\right)^t$,
$\tilde{\mathbf{x}} = (0.142, -0.166)^t$.

b. $3.9x_1 + 1.6x_2 = 5.5$,
$6.8x_1 + 2.9x_2 = 9.7$,
$\mathbf{x} = (1, 1)^t$,
$\tilde{\mathbf{x}} = (0.98, 1.1)^t$.

c. $x_1 + 2x_2 = 3$,
$1.0001x_1 + 2x_2 = 3.0001$,
$\mathbf{x} = (1, 1)^t$,
$\tilde{\mathbf{x}} = (0.96, 1.02)^t$.

d. $1.003x_1 + 58.09x_2 = 68.12$,
$5.550x_1 + 321.8x_2 = 377.3$,
$\mathbf{x} = (10, 1)^t$,
$\tilde{\mathbf{x}} = (-10, 1)^t$.

e. $x_1 - x_2 - x_3 = 2\pi$,
$x_2 - x_3 = 0$,
$-x_3 = \pi$.
$\mathbf{x} = (0, -\pi, -\pi)^t$,
$\tilde{\mathbf{x}} = (-0.1, -3.15, -3.14)^t$.

f. $0.04x_1 + 0.01x_2 - 0.01x_3 = 0.06$,
$0.2x_1 + 0.5x_2 - 0.2x_3 = 0.3$,
$x_1 + 2x_2 + 4x_3 = 11$,
$\mathbf{x} = (1.827586, 0.6551724, 1.965517)^t$,
$\tilde{\mathbf{x}} = (1.8, 0.64, 1.9)^t$.

3. The linear system

$$\begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 3.0001 \end{bmatrix}$$

has solution $(1, 1)^t$. Change A slightly to

$$\begin{bmatrix} 1 & 2 \\ 0.9999 & 2 \end{bmatrix},$$

and consider the linear system

$$\begin{bmatrix} 1 & 2 \\ 0.9999 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 3.0001 \end{bmatrix}.$$

Compute the new solution using five-digit rounding arithmetic, and compare the actual error to the estimate (7.24). Is A ill-conditioned?

4. The linear system $A\mathbf{x} = \mathbf{b}$ given by

$$\begin{bmatrix} 1 & 2 \\ 1.00001 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 3.00001 \end{bmatrix}$$

has solution $(1, 1)^t$. Use seven-digit rounding arithmetic to find the solution of the perturbed system

$$\begin{bmatrix} 1 & 2 \\ 1.000011 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3.00001 \\ 3.00003 \end{bmatrix},$$

and compare the actual error to the estimate (7.24). Is A ill-conditioned?

5. **a.** Use single precision on a computer to solve the following linear system using the Gaussian Elimination with Backward Substitution Algorithm 6.1.

$$\begin{aligned} \tfrac{1}{3}x_1 - \tfrac{1}{3}x_2 - \tfrac{1}{3}x_3 - \tfrac{1}{3}x_4 - \tfrac{1}{3}x_5 &= 1 \\ \tfrac{1}{3}x_2 - \tfrac{1}{3}x_3 - \tfrac{1}{3}x_4 - \tfrac{1}{3}x_5 &= 0 \\ \tfrac{1}{3}x_3 - \tfrac{1}{3}x_4 - \tfrac{1}{3}x_5 &= -1 \\ \tfrac{1}{3}x_4 - \tfrac{1}{3}x_5 &= 2 \\ \tfrac{1}{3}x_5 &= 7 \end{aligned}$$

b. Compute the condition number of the matrix for the system relative to $\|\cdot\|_\infty$.

c. Find the exact solution to the linear system.

6. The $n \times n$ *Hilbert matrix* $H^{(n)}$ defined by

$$H_{ij}^{(n)} = \frac{1}{i+j-1}, \quad 1 \le i, j \le n,$$

is an ill-conditioned matrix that arises in solving the normal equations for the coefficients of the least-squares polynomial (see Example 1 of Section 8.2).

a. Show that

$$[H^{(4)}]^{-1} = \begin{bmatrix} 16 & -120 & 240 & -140 \\ -120 & 1200 & -2700 & 1680 \\ 240 & -2700 & 6480 & -4200 \\ -140 & 1680 & -4200 & 2800 \end{bmatrix},$$

and compute $K_\infty(H^{(4)})$.

b. Show that

$$[H^{(5)}]^{-1} = \begin{bmatrix} 25 & -300 & 1050 & -1400 & 630 \\ -300 & 4800 & -18900 & 26880 & -12600 \\ 1050 & -18900 & 79380 & -117600 & 56700 \\ -1400 & 26880 & -117600 & 179200 & -88200 \\ 630 & -12600 & 56700 & -88200 & 44100 \end{bmatrix},$$

and compute $K_\infty(H^{(5)})$.

c. Solve the linear system

$$H^{(4)} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

using five-digit rounding arithmetic, and compare the actual error to that estimated by (7.24).

7. Show that if B is singular, then

$$\frac{1}{K(A)} \le \frac{\|A - B\|}{\|A\|}.$$

[*Hint:* There exists a vector with $\|\mathbf{x}\| = 1$, such that $B\mathbf{x} = \mathbf{0}$. Derive the estimate using $\|A\mathbf{x}\| \ge \|\mathbf{x}\| / \|A^{-1}\|$.]

8. Using Exercise 7, estimate the condition numbers for the following matrices:

a. $\begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix}$ **b.** $\begin{bmatrix} 3.9 & 1.6 \\ 6.8 & 2.9 \end{bmatrix}$

9. Use four-digit rounding arithmetic to compute the inverse H^{-1} of the 3×3 Hilbert matrix H, and then compute $\hat{H} = (H^{-1})^{-1}$. Determine $\|H - \hat{H}\|_\infty$.

7.5 The Conjugate Gradient Method

The conjugate gradient method of Hestenes and Stiefel [HS] was originally developed as a direct method designed to solve an $n \times n$ positive definite linear system. As a direct method it is generally inferior to Gaussian elimination with pivoting since both methods require n steps to determine a solution, and the steps of the conjugate gradient method are more computationally expensive than those in Gaussian elimination.

However, the conjugate gradient method is very useful when employed as an iterative approximation method for solving large sparse systems with nonzero entries occurring in predictable patterns. These problems frequently arise in the solution of boundary-value problems. When the matrix has been preconditioned to make the calculations more effective, good results are obtained in only about $\sqrt{n}$ steps. Employed in this way, the method is preferred over Gaussian elimination and the previously-discussed iterative methods.

Throughout this section we assume that the matrix A is positive definite. We will use the *inner product* notation

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^t \mathbf{y}, \tag{7.25}$$

where $\mathbf{x}$ and $\mathbf{y}$ are n-dimensional vectors. We will also need some additional standard results from linear algebra. A review of this material is found in Section 9.1.

The next result follows easily from the properties of transposes (see Exercise 12).

Theorem 7.30 For any vectors $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ and any real number α, we have

(i) $\langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{y}, \mathbf{x} \rangle$;

(ii) $\langle \alpha\mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x}, \alpha\mathbf{y} \rangle = \alpha \langle \mathbf{x}, \mathbf{y} \rangle$;

(iii) $\langle \mathbf{x} + \mathbf{z}, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{z}, \mathbf{y} \rangle$;

(iv) $\langle \mathbf{x}, \mathbf{x} \rangle \ge 0$;

(v) $\langle \mathbf{x}, \mathbf{x} \rangle = 0$ if and only if $\mathbf{x} = \mathbf{0}$. ■

When A is positive definite, $\langle \mathbf{x}, A\mathbf{x} \rangle = \mathbf{x}^t A\mathbf{x} > 0$ unless $\mathbf{x} = \mathbf{0}$. Also, since A is symmetric, we have $\mathbf{x}^t A\mathbf{y} = \mathbf{x}^t A^t \mathbf{y} = (A\mathbf{x})^t \mathbf{y}$, so in addition to the results in Theorem 7.30, we have for each $\mathbf{x}$ and $\mathbf{y}$,

$$\langle \mathbf{x}, A\mathbf{y} \rangle = \langle A\mathbf{x}, \mathbf{y} \rangle. \tag{7.26}$$

The following result is a basic tool in the development of the conjugate gradient method.

Theorem 7.31 The vector $\mathbf{x}^*$ is a solution to the positive definite linear system $A\mathbf{x} = \mathbf{b}$ if and only if $\mathbf{x}^*$ minimizes

$$g(\mathbf{x}) = \langle \mathbf{x}, A\mathbf{x} \rangle - 2\langle \mathbf{x}, \mathbf{b} \rangle. \quad ■$$

Proof Let $\mathbf{x}$ and $\mathbf{v} \neq \mathbf{0}$ be fixed vectors and t a real number variable. We have

$$\begin{aligned} g(\mathbf{x}+t\mathbf{v}) &= \langle \mathbf{x}+t\mathbf{v}, A\mathbf{x}+tA\mathbf{v}\rangle - 2\langle \mathbf{x}+t\mathbf{v}, \mathbf{b}\rangle \\ &= \langle \mathbf{x}, A\mathbf{x}\rangle + t\langle \mathbf{v}, A\mathbf{x}\rangle + t\langle \mathbf{x}, A\mathbf{v}\rangle + t^2\langle \mathbf{v}, A\mathbf{v}\rangle - 2\langle \mathbf{x}, \mathbf{b}\rangle - 2t\langle \mathbf{v}, \mathbf{b}\rangle \\ &= \langle \mathbf{x}, A\mathbf{x}\rangle - 2\langle \mathbf{x}, \mathbf{b}\rangle + 2t\langle \mathbf{v}, A\mathbf{x}\rangle - 2t\langle \mathbf{v}, \mathbf{b}\rangle + t^2\langle \mathbf{v}, A\mathbf{v}\rangle, \end{aligned}$$

so

$$g(\mathbf{x}+t\mathbf{v}) = g(\mathbf{x}) + 2t\langle \mathbf{v}, A\mathbf{x}-\mathbf{b}\rangle + t^2\langle \mathbf{v}, A\mathbf{v}\rangle. \tag{7.27}$$

Since $\mathbf{x}$ and $\mathbf{v}$ are fixed, we can define the quadratic function h in t by

$$h(t) = g(\mathbf{x}+t\mathbf{v}).$$

Then h assumes a minimal value when $h'(t) = 0$, because its t^2 coefficient, $\langle \mathbf{v}, A\mathbf{v}\rangle$, is positive. Since

$$h'(t) = 2\langle \mathbf{v}, A\mathbf{x}-\mathbf{b}\rangle + 2t\langle \mathbf{v}, A\mathbf{v}\rangle,$$

the minimum occurs when

$$\hat{t} = -\frac{\langle \mathbf{v}, A\mathbf{x}-\mathbf{b}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle} = \frac{\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle},$$

and, from Equation (7.27),

$$\begin{aligned} h(\hat{t}) &= g(\mathbf{x}) - 2\frac{\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle}\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}\rangle + \left(\frac{\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle}\right)^2 \langle \mathbf{v}, A\mathbf{v}\rangle \\ &= g(\mathbf{x}) - \frac{\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}\rangle^2}{\langle \mathbf{v}, A\mathbf{v}\rangle}. \end{aligned}$$

So, for any vector $\mathbf{v} \neq \mathbf{0}$, we have $g(\mathbf{x}+\hat{t}\mathbf{v}) < g(\mathbf{x})$ unless $\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}\rangle = 0$, in which case $g(\mathbf{x}) = g(\mathbf{x}+\hat{t}\mathbf{v})$. This is the basic result we need to prove Theorem 7.31.

Suppose $\mathbf{x}^*$ satisfies $A\mathbf{x}^* = \mathbf{b}$. Then $\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}^*\rangle = 0$ for any vector $\mathbf{v}$, and $g(\mathbf{x})$ cannot be made any smaller than $g(\mathbf{x}^*)$. Thus, $\mathbf{x}^*$ minimizes g.

On the other hand, suppose that $\mathbf{x}^*$ is a vector that minimizes g. Then for any vector $\mathbf{v}$, we have $g(\mathbf{x}^*+\hat{t}\mathbf{v}) \geq g(\mathbf{x}^*)$. Thus, $\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}^*\rangle = 0$. This implies that $\mathbf{b}-A\mathbf{x}^* = \mathbf{0}$ and, consequently, that $A\mathbf{x}^* = \mathbf{b}$. ▪ ▪ ▪

To begin the conjugate gradient method, we choose $\mathbf{x}$, an approximate solution to $A\mathbf{x}^* = \mathbf{b}$, and $\mathbf{v} \neq \mathbf{0}$, which gives a *search direction* in which to move away from $\mathbf{x}$ to improve the approximation. Let $\mathbf{r} = \mathbf{b}-A\mathbf{x}$ be the residual vector associated with $\mathbf{x}$ and

$$t = \frac{\langle \mathbf{v}, \mathbf{b}-A\mathbf{x}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle} = \frac{\langle \mathbf{v}, \mathbf{r}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle}.$$

If $\mathbf{r} \neq \mathbf{0}$ and if $\mathbf{v}$ and $\mathbf{r}$ are not orthogonal, then $\mathbf{x}+t\mathbf{v}$ gives a smaller value for g than $g(\mathbf{x})$ and is presumably closer to $\mathbf{x}^*$ than is $\mathbf{x}$. This suggests the following method.

Let $\mathbf{x}^{(0)}$ be an initial approximation to $\mathbf{x}^*$, and let $\mathbf{v}^{(1)} \neq \mathbf{0}$ be an initial search direction. For $k = 1, 2, 3, \ldots$, we compute

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{b}-A\mathbf{x}^{(k-1)}\rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)}\rangle},$$

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k\mathbf{v}^{(k)}$$

and choose a new search direction $\mathbf{v}^{(k+1)}$. The object is to make this selection so that the sequence of approximations $\{\mathbf{x}^{(k)}\}$ converges rapidly to $\mathbf{x}^*$.

To choose the search directions, we view g as a function of the components of $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$. Thus,

$$g(x_1, x_2, \ldots, x_n) = \langle \mathbf{x}, A\mathbf{x}\rangle - 2\langle \mathbf{x}, \mathbf{b}\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_ix_j - 2\sum_{i=1}^{n} x_ib_i.$$

Taking partial derivatives with respect to the component variables x_k gives

$$\frac{\partial g}{\partial x_k}(\mathbf{x}) = 2\sum_{i=1}^{n} a_{ki}x_i - 2b_k.$$

Therefore, the gradient of g is

$$\nabla g(\mathbf{x}) = \left(\frac{\partial g}{\partial x_1}(\mathbf{x}), \frac{\partial g}{\partial x_2}(\mathbf{x}), \ldots, \frac{\partial g}{\partial x_n}(\mathbf{x})\right)^t = 2(A\mathbf{x}-\mathbf{b}) = -2\mathbf{r},$$

where the vector $\mathbf{r}$ is the residual vector for $\mathbf{x}$.

From multivariable calculus, we know that the direction of greatest decrease in the value of $g(\mathbf{x})$ is the direction given by $-\nabla g(\mathbf{x})$; that is, in the direction of the residual $\mathbf{r}$. The method that chooses

$$\mathbf{v}^{(k+1)} = \mathbf{r}^{(k)} = \mathbf{b}-A\mathbf{x}^{(k)}$$

is called the *method of steepest descent*. Although we will see in Section 10.4 that this method has merit for nonlinear systems and optimization problems, it is not used for linear systems because of slow convergence.

An alternative approach uses a set of nonzero direction vectors $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ that satisfy

$$\langle \mathbf{v}^{(i)}, A\mathbf{v}^{(j)}\rangle = 0, \quad \text{if} \quad i \neq j.$$

This is called an **A-orthogonality condition**, and the set of vectors $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ is said to be **A-orthogonal**. It is not difficult to show that a set of A-orthogonal vectors associated with the positive definite matrix A is linearly independent. (See Exercise 13(a).) This set of search directions gives

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{b}-A\mathbf{x}^{(k-1)}\rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)}\rangle} = \frac{\langle \mathbf{v}^{(k)}, \mathbf{r}^{(k-1)}\rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)}\rangle}$$

and $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k\mathbf{v}^{(k)}$.

The following theorem shows that this choice of search directions gives convergence in at most n-steps, so as a direct method it produces the exact solution, assuming that the arithmetic is exact.

Theorem 7.32 Let $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ be an A-orthogonal set of nonzero vectors associated with the positive definite matrix A, and let $\mathbf{x}^{(0)}$ be arbitrary. Define

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} \quad \text{and} \quad \mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)},$$

for $k = 1, 2, \ldots, n$. Then, assuming exact arithmetic, $A\mathbf{x}^{(n)} = \mathbf{b}$. ■

Proof Since, for each $k = 1, 2, \ldots, n$,

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)},$$

we have

$$\begin{aligned} A\mathbf{x}^{(n)} &= A\mathbf{x}^{(n-1)} + t_n A\mathbf{v}^{(n)} \\ &= (A\mathbf{x}^{(n-2)} + t_{n-1} A\mathbf{v}^{(n-1)}) + t_n A\mathbf{v}^{(n)} \\ &\vdots \\ &= A\mathbf{x}^{(0)} + t_1 A\mathbf{v}^{(1)} + t_2 A\mathbf{v}^{(2)} + \cdots + t_n A\mathbf{v}^{(n)}, \end{aligned}$$

and subtracting $\mathbf{b}$ from this result yields

$$A\mathbf{x}^{(n)} - \mathbf{b} = A\mathbf{x}^{(0)} - \mathbf{b} + t_1 A\mathbf{v}^{(1)} + t_2 A\mathbf{v}^{(2)} + \cdots + t_n A\mathbf{v}^{(n)}.$$

We now take the inner product of both sides with the vector $\mathbf{v}^{(k)}$ and use the properties of inner products and the fact that A is symmetric to obtain

$$\begin{aligned} \langle A\mathbf{x}^{(n)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle &= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + t_1 \langle A\mathbf{v}^{(1)}, \mathbf{v}^{(k)} \rangle + \cdots + t_n \langle A\mathbf{v}^{(n)}, \mathbf{v}^{(k)} \rangle \\ &= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + t_1 \langle \mathbf{v}^{(1)}, A\mathbf{v}^{(k)} \rangle + \cdots + t_n \langle \mathbf{v}^{(n)}, A\mathbf{v}^{(k)} \rangle. \end{aligned}$$

The A-orthogonality property gives, for each k,

$$\langle A\mathbf{x}^{(n)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle = \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + t_k \langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle. \tag{7.28}$$

However,

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle},$$

so

$$\begin{aligned} & t_k \langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle \\ &= \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(k-1)} \rangle \\ &= \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} + A\mathbf{x}^{(0)} - A\mathbf{x}^{(1)} + \cdots - A\mathbf{x}^{(k-2)} + A\mathbf{x}^{(k-2)} - A\mathbf{x}^{(k-1)} \rangle \\ &= \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} \rangle + \langle \mathbf{v}^{(k)}, A\mathbf{x}^{(0)} - A\mathbf{x}^{(1)} \rangle + \cdots + \langle \mathbf{v}^{(k)}, A\mathbf{x}^{(k-2)} - A\mathbf{x}^{(k-1)} \rangle. \end{aligned}$$

But for any i,

$$\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + t_i \mathbf{v}^{(i)} \quad \text{and} \quad A\mathbf{x}^{(i)} = A\mathbf{x}^{(i-1)} + t_i A\mathbf{v}^{(i)},$$

so

$$A\mathbf{x}^{(i-1)} - A\mathbf{x}^{(i)} = -t_i A\mathbf{v}^{(i)}.$$

Thus,

$$t_k \langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle = \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} \rangle - t_1 \langle \mathbf{v}^{(k)}, A\mathbf{v}^{(1)} \rangle - \cdots - t_{k-1} \langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k-1)} \rangle.$$

Because of the A-orthogonality, $\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(i)} \rangle = 0$, for $i \neq k$, so

$$\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle t_k = \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} \rangle.$$

From Eq.(7.28),

$$\begin{aligned} \langle A\mathbf{x}^{(n)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle &= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} \rangle \\ &= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + \langle \mathbf{b} - A\mathbf{x}^{(0)}, \mathbf{v}^{(k)} \rangle \\ &= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle - \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle \\ &= 0. \end{aligned}$$

The vector $A\mathbf{x}^{(n)} - \mathbf{b}$ is orthogonal to the A-orthogonal set of vectors $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$. From this, it follows (see Exercise 13(b)) that $A\mathbf{x}^{(n)} - \mathbf{b} = \mathbf{0}$. ■ ■ ■

EXAMPLE 1 Consider the positive definite matrix

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

Let $\mathbf{v}^{(1)} = (1, 0, 0)^t$, $\mathbf{v}^{(2)} = (-3/4, 1, 0)^t$, and $\mathbf{v}^{(3)} = (-3/7, 4/7, 1)^t$. By direct calculation,

$$\langle \mathbf{v}^{(1)}, A\mathbf{v}^{(2)} \rangle = \mathbf{v}^{(1)t} A\mathbf{v}^{(2)} = (1, 0, 0) \begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -\frac{3}{4} \\ 1 \\ 0 \end{bmatrix} = 0,$$

$$\langle \mathbf{v}^{(1)}, A\mathbf{v}^{(3)} \rangle = (1, 0, 0) \begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -\frac{3}{7} \\ \frac{4}{7} \\ 1 \end{bmatrix} = 0,$$

and

$$\langle \mathbf{v}^{(2)}, A\mathbf{v}^{(3)} \rangle = \left(-\frac{3}{4}, 1, 0\right) \begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -\frac{3}{7} \\ \frac{4}{7} \\ 1 \end{bmatrix} = 0.$$

Thus, $\{\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}^{(3)}\}$ is an A-orthogonal set.

The linear system

$$\begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 24 \\ 30 \\ -24 \end{bmatrix},$$

has the exact solution $\mathbf{x}^* = (3, 4, -5)^t$. To approximate this solution, let $\mathbf{x}^{(0)} = (0, 0, 0)^t$. Since $\mathbf{b} = (24, 30, -24)^t$, we have

$$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = \mathbf{b} = (24, 30, -24)^t,$$

so

$$\langle \mathbf{v}^{(1)}, \mathbf{r}^{(0)} \rangle = \mathbf{v}^{(1)t}\mathbf{r}^{(0)} = 24, \quad \langle \mathbf{v}^{(1)}, A\mathbf{v}^{(1)} \rangle = 4, \quad \text{and} \quad t_0 = \frac{24}{4} = 6.$$

Thus,

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + t_0\mathbf{v}^{(1)} = (0, 0, 0)^t + 6(1, 0, 0)^t = (6, 0, 0)^t.$$

Continuing, we have

$$\mathbf{r}^{(1)} = \mathbf{b} - A\mathbf{x}^{(1)} = (0, 12, -24)^t; \quad t_1 = \frac{\langle \mathbf{v}^{(2)}, \mathbf{r}^{(1)} \rangle}{\langle \mathbf{v}^{(2)}, A\mathbf{v}^{(2)} \rangle} = \frac{12}{7/4} = \frac{48}{7};$$

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + t_1\mathbf{v}^{(2)} = (6, 0, 0)^t + \frac{48}{7}\left(-\frac{3}{4}, 1, 0\right)^t = \left(\frac{6}{7}, \frac{48}{7}, 0\right)^t;$$

$$\mathbf{r}^{(2)} = \mathbf{b} - A\mathbf{x}^{(2)} = \left(0, 0, -\frac{120}{7}\right); \quad t_2 = \frac{\langle \mathbf{v}^{(3)}, \mathbf{r}^{(2)} \rangle}{\langle \mathbf{v}^{(3)}, A\mathbf{v}^{(3)} \rangle} = \frac{-120/7}{24/7} = -5;$$

and

$$\mathbf{x}^{(3)} = \mathbf{x}^{(2)} + t_2\mathbf{v}^{(3)} = \left(\frac{6}{7}, \frac{48}{7}, 0\right)^t + (-5)\left(-\frac{3}{7}, \frac{4}{7}, 1\right)^t = (3, 4, -5)^t.$$

Since we applied the technique $n = 3$ times, this is the actual solution. ∎

Before discussing how to determine the A-orthogonal set, we will continue the development. The use of an A-orthogonal set $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ of direction vectors gives what is called a *conjugate direction* method. The following theorem shows the orthogonality of the residual vectors $\mathbf{r}^{(k)}$ and the direction vectors $\mathbf{v}^{(j)}$. A proof of this result using mathematical induction is considered in Exercise 14.

Theorem 7.33 The residual vectors $\mathbf{r}^{(k)}$, where $k = 1, 2, \ldots, n$, for a conjugate direction method, satisfy the equations

$$\langle \mathbf{r}^{(k)}, \mathbf{v}^{(j)} \rangle = 0, \quad \text{for each} \quad j = 1, 2, \ldots, k.$$ ∎

The conjugate gradient method of Hestenes and Stiefel chooses the search directions $\{\mathbf{v}^{(k)}\}$ during the iterative process so that the residual vectors $\{\mathbf{r}^{(k)}\}$ are mutually orthogonal. To construct the direction vectors $\{\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \ldots\}$ and the approximations $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots\}$, we start with an initial approximation $\mathbf{x}^{(0)}$ and use the steepest descent direction $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$ as the first search direction $\mathbf{v}^{(1)}$.

Assume that the conjugate directions $\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(k-1)}$ and the approximations $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(k-1)}$ have been computed with

$$\mathbf{x}^{(k-1)} = \mathbf{x}^{(k-2)} + t_{k-1}\mathbf{v}^{(k-1)},$$

where

$$\langle \mathbf{v}^{(i)}, A\mathbf{v}^{(j)} \rangle = 0 \quad \text{and} \quad \langle \mathbf{r}^{(i)}, \mathbf{r}^{(j)} \rangle = 0, \quad \text{for} \quad i \neq j.$$

If $\mathbf{x}^{(k-1)}$ is the solution to $A\mathbf{x} = \mathbf{b}$, we are done. Otherwise, $\mathbf{r}^{(k-1)} = \mathbf{b} - A\mathbf{x}^{(k-1)} \neq \mathbf{0}$ and Theorem 7.33 implies that $\langle \mathbf{r}^{(k-1)}, \mathbf{v}^{(i)} \rangle = 0$, for $i = 1, 2, \ldots, k-1$. We then use $\mathbf{r}^{(k-1)}$ to generate $\mathbf{v}^{(k)}$ by setting

$$\mathbf{v}^{(k)} = \mathbf{r}^{(k-1)} + s_{k-1}\mathbf{v}^{(k-1)}.$$

We want to choose s_{k-1} so that

$$\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k)} \rangle = 0.$$

Since

$$A\mathbf{v}^{(k)} = A\mathbf{r}^{(k-1)} + s_{k-1}A\mathbf{v}^{(k-1)}$$

and

$$\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k)} \rangle = \langle \mathbf{v}^{(k-1)}, A\mathbf{r}^{(k-1)} \rangle + s_{k-1}\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k-1)} \rangle,$$

we will have $\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k)} \rangle = 0$ when

$$s_{k-1} = -\frac{\langle \mathbf{v}^{(k-1)}, A\mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k-1)} \rangle}.$$

It can also be shown that with this choice of s_{k-1} we have $\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(i)} \rangle = 0$, for each $i = 1, 2, \ldots, k-2$ (see [Lu, p. 245]). Thus, $\{\mathbf{v}^{(1)}, \ldots \mathbf{v}^{(k)}\}$ is an A-orthogonal set.

Having chosen $\mathbf{v}^{(k)}$, we compute

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} = \frac{\langle \mathbf{r}^{(k-1)} + s_{k-1}\mathbf{v}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}$$

$$= \frac{\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} + s_{k-1}\frac{\langle \mathbf{v}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}.$$

By Theorem 7.33, $\langle \mathbf{v}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle = 0$, so

$$t_k = \frac{\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}. \tag{7.29}$$

Thus,

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)}.$$

To compute $\mathbf{r}^{(k)}$, we multiply by A and subtract $\mathbf{b}$ to obtain

$$A\mathbf{x}^{(k)} - \mathbf{b} = A\mathbf{x}^{(k-1)} - \mathbf{b} + t_k A\mathbf{v}^{(k)}$$

or

$$\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - t_k A\mathbf{v}^{(k)}.$$

Thus,

$$\langle \mathbf{r}^{(k)}, \mathbf{r}^{(k)} \rangle = \langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k)} \rangle - t_k \langle A\mathbf{v}^{(k)}, \mathbf{r}^{(k)} \rangle = -t_k \langle \mathbf{r}^{(k)}, A\mathbf{v}^{(k)} \rangle.$$

Further, from Eq. (7.29),

$$\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle = t_k \langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle,$$

so

$$s_k = -\frac{\langle \mathbf{v}^{(k)}, A\mathbf{r}^{(k)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} = -\frac{\langle \mathbf{r}^{(k)}, A\mathbf{v}^{(k)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}$$
$$= \frac{(1/t_k)\langle \mathbf{r}^{(k)}, \mathbf{r}^{(k)} \rangle}{(1/t_k)\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle} = \frac{\langle \mathbf{r}^{(k)}, \mathbf{r}^{(k)} \rangle}{\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}.$$

In summary, we have the formulas:

$$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}; \quad \mathbf{v}^{(1)} = \mathbf{r}^{(0)};$$

and, for $k = 1, 2, \ldots, n$,

$$t_k = \frac{\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle},$$
$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)},$$
$$\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - t_k A\mathbf{v}^{(k)},$$
$$s_k = \frac{\langle \mathbf{r}^{(k)}, \mathbf{r}^{(k)} \rangle}{\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle},$$
$$\mathbf{v}^{(k+1)} = \mathbf{r}^{(k)} + s_k \mathbf{v}^{(k)}. \tag{7.30}$$

Rather than presenting an algorithm for the conjugate gradient method using these formulas, we extend the method to include *preconditioning*.If the matrix A is ill-conditioned, the conjugate gradient method is highly susceptible to rounding errors. So, although the exact answer should be obtained in n steps, this is not usually the case. As a direct method the conjugate gradient method is not as good as Gaussian elimination with pivoting. The main use of the conjugate gradient method is as an iterative method applied to a better-

conditioned system. In this case an acceptable approximate solution is often obtained in about $\sqrt{n}$ steps.

To apply the method to a better-conditioned system, we want to select a nonsingular conditioning matrix C so that

$$\tilde{A} = C^{-1}A(C^{-1})^t$$

is better conditioned. To simplify the notation, we will use the matrix C^{-t} to refer to $(C^{-1})^t$.

Consider the linear system

$$\tilde{A}\tilde{\mathbf{x}} = \tilde{\mathbf{b}},$$

where $\tilde{\mathbf{x}} = C^t\mathbf{x}$ and $\tilde{\mathbf{b}} = C^{-1}\mathbf{b}$. Then

$$\tilde{A}\tilde{\mathbf{x}} = (C^{-1}AC^{-t})(C^t\mathbf{x}) = C^{-1}A\mathbf{x}.$$

Thus, we could solve $\tilde{A}\tilde{\mathbf{x}} = \tilde{\mathbf{b}}$ for $\tilde{\mathbf{x}}$ and then obtain $\mathbf{x}$ by multiplying by C^{-t}. However, instead of rewriting equations (7.30) using $\tilde{\mathbf{r}}^{(k)}$, $\tilde{\mathbf{v}}^{(k)}$, $\tilde{t}_k$, $\tilde{\mathbf{x}}^{(k)}$, and $\tilde{s}_k$, we incorporate the preconditioning implicitly.

Since

$$\tilde{\mathbf{x}}^{(k)} = C^t\mathbf{x}^{(k)},$$

we have

$$\tilde{\mathbf{r}}^{(k)} = \tilde{\mathbf{b}} - \tilde{A}\tilde{\mathbf{x}}^{(k)} = C^{-1}\mathbf{b} - (C^{-1}AC^{-t})C^t\mathbf{x}^{(k)} = C^{-1}(\mathbf{b} - A\mathbf{x}^{(k)}) = C^{-1}\mathbf{r}^{(k)}.$$

Let $\tilde{\mathbf{v}}^{(k)} = C^t\mathbf{v}^{(k)}$ and $\mathbf{w}^{(k)} = C^{-1}\mathbf{r}^{(k)}$. Then

$$\tilde{s}_k = \frac{\langle \tilde{\mathbf{r}}^{(k)}, \tilde{\mathbf{r}}^{(k)} \rangle}{\langle \tilde{\mathbf{r}}^{(k-1)}, \tilde{\mathbf{r}}^{(k-1)} \rangle} = \frac{\langle C^{-1}\mathbf{r}^{(k)}, C^{-1}\mathbf{r}^{(k)} \rangle}{\langle C^{-1}\mathbf{r}^{(k-1)}, C^{-1}\mathbf{r}^{(k-1)} \rangle},$$

so

$$\tilde{s}_k = \frac{\langle \mathbf{w}^{(k)}, \mathbf{w}^{(k)} \rangle}{\langle \mathbf{w}^{(k-1)}, \mathbf{w}^{(k-1)} \rangle}. \tag{7.31}$$

Thus,

$$\tilde{t}_k = \frac{\langle \tilde{\mathbf{r}}^{(k-1)}, \tilde{\mathbf{r}}^{(k-1)} \rangle}{\langle \tilde{\mathbf{v}}^{(k)}, \tilde{A}\tilde{\mathbf{v}}^{(k)} \rangle} = \frac{\langle C^{-1}\mathbf{r}^{(k-1)}, C^{-1}\mathbf{r}^{(k-1)} \rangle}{\langle C^t\mathbf{v}^{(k)}, C^{-1}AC^{-t}C^t\mathbf{v}^{(k)} \rangle} = \frac{\langle \mathbf{w}^{(k-1)}, \mathbf{w}^{(k-1)} \rangle}{\langle C^t\mathbf{v}^{(k)}, C^{-1}A\mathbf{v}^{(k)} \rangle}$$

and

$$\tilde{t}_k = \frac{\langle \mathbf{w}^{(k-1)}, \mathbf{w}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}. \tag{7.32}$$

Further,

$$\tilde{\mathbf{x}}^{(k)} = \tilde{\mathbf{x}}^{(k-1)} + \tilde{t}_k\tilde{\mathbf{v}}^{(k)}, \quad \text{so} \quad C^t\mathbf{x}^{(k)} = C^t\mathbf{x}^{(k-1)} + \tilde{t}_k C^t\mathbf{v}^{(k)}$$

and

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + \tilde{t}_k\mathbf{v}^{(k)}. \tag{7.33}$$

Continuing,

$$\tilde{\mathbf{r}}^{(k)} = \tilde{\mathbf{r}}^{(k-1)} - \tilde{t}_k \tilde{A}\tilde{\mathbf{v}}^{(k)},$$

so

$$C^{-1}\mathbf{r}^{(k)} = C^{-1}\mathbf{r}^{(k-1)} - \tilde{t}_k C^{-1}AC^{-t}\tilde{v}^{(k)}, \qquad \mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - \tilde{t}_k AC^{-t}C^t\mathbf{v}^{(k)},$$

and

$$\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - \tilde{t}_k A\mathbf{v}^{(k)}. \tag{7.34}$$

Finally,

$$\tilde{\mathbf{v}}^{(k+1)} = \tilde{\mathbf{r}}^{(k)} + \tilde{s}_k\tilde{\mathbf{v}}^{(k)} \quad \text{and} \quad C^t\mathbf{v}^{(k+1)} = C^{-1}\mathbf{r}^{(k)} + \tilde{s}_k C^t\mathbf{v}^{(k)},$$

so

$$\mathbf{v}^{(k+1)} = C^{-t}C^{-1}\mathbf{r}^{(k)} + \tilde{s}_k\mathbf{v}^{(k)} = C^{-t}\mathbf{w}^{(k)} + \tilde{s}_k\mathbf{v}^{(k)}. \tag{7.35}$$

The preconditioned conjugate gradient method is based on using equations (7.31)–(7.35) in the order (7.32), (7.33), (7.34), (7.31), (7.35). Algorithm 7.5 implements this procedure.

ALGORITHM 7.5

Preconditioned Conjugate Gradient Method

To solve $A\mathbf{x} = \mathbf{b}$ given the preconditioning matrix C^{-1} and the initial approximation $\mathbf{x}^{(0)}$:

INPUT the number of equations and unknowns n; the entries a_{ij}, $1 \le i, j \le n$ of the matrix A; the entries b_j, $1 \le j \le n$ of the vector $\mathbf{b}$; the entries γ_{ij}, $1 \le i, j \le n$ of the preconditioning matrix C^{-1}, the entries x_i, $1 \le i \le n$ of the initial approximation $\mathbf{x} = \mathbf{x}^{(0)}$; the maximum number of iterations N; tolerance TOL.

OUTPUT the approximate solution $x_1, \ldots x_n$ and the residual $r_1, \ldots r_n$ or a message that the number of iterations was exceeded.

Step 1 Set $\mathbf{r} = \mathbf{b} - A\mathbf{x}$; (*Compute* $\mathbf{r}^{(0)}$.)
$\mathbf{w} = C^{-1}\mathbf{r}$; (*Note:* $\mathbf{w} = \mathbf{w}^{(0)}$)
$\mathbf{v} = C^{-t}\mathbf{w}$; (*Note:* $\mathbf{v} = \mathbf{v}^{(1)}$)
$\alpha = \sum_{j=1}^{n} w_j^2$.

Step 2 Set $k = 1$.

Step 3 While $(k \le N)$ do Steps 4–7.

Step 4 If $\|\mathbf{v}\| < TOL$, then
OUTPUT ('Solution vector'; $x_1, \ldots, x_n$);
OUTPUT ('with residual'; $r_1, \ldots, r_n$);
(*The procedure was successful.*)
STOP

Step 5 Set $\mathbf{u} = A\mathbf{v}$; (*Note:* $\mathbf{u} = A\mathbf{v}^{(k)}$)
$t = \dfrac{\alpha}{\sum_{j=1}^{n} v_j u_j}$; (*Note:* $t = t_k$)

$\mathbf{x} = \mathbf{x} + t\mathbf{v}$; (*Note:* $\mathbf{x} = \mathbf{x}^{(k)}$)
$\mathbf{r} = \mathbf{r} - t\mathbf{u}$; (*Note:* $\mathbf{r} = \mathbf{r}^{(k)}$)
$\mathbf{w} = C^{-1}\mathbf{r}$; (*Note:* $\mathbf{w} = \mathbf{w}^{(k)}$)
$\beta = \sum_{j=1}^{n} w_j^2$. (*Note:* $\beta = \langle \mathbf{w}^{(k)}, \mathbf{w}^{(k)} \rangle$)

Step 6 If $|\beta| < TOL$ then
if $\|\mathbf{r}\| < TOL$ then
OUTPUT('Solution vector'; $x_1, \ldots, x_n$);
OUTPUT('with residual'; $r_1, \ldots, r_n$);
(*The procedure was successful.*)
STOP

Step 7 Set $s = \beta/\alpha$; $(s = s_k)$
$\mathbf{v} = C^{-t}\mathbf{w} + s\mathbf{v}$; (*Note:* $\mathbf{v} = \mathbf{v}^{(k+1)}$)
$\alpha = \beta$; (*Update* α.)
$k = k + 1$.

Step 8 If $(k > n)$ then
OUTPUT ('The maximum number of iterations was exceeded.');
(*The procedure was unsuccessful.*)
STOP. ■

The next example illustrates the calculations in an easy problem.

EXAMPLE 2 The linear system $A\mathbf{x} = \mathbf{b}$ given by

$$\begin{aligned} 4x_1 + 3x_2 &= 24, \\ 3x_1 + 4x_2 - x_3 &= 30, \\ -x_2 + 4x_3 &= -24 \end{aligned}$$

has solution $(3, 4, -5)^t$ and was considered in Example 3 of Section 7.3. In that example, both the Gauss-Seidel method and SOR method were used. We will use the conjugate gradient method with no preconditioning, so $C = C^{-1} = I$. Let $\mathbf{x}^{(0)} = (0, 0, 0)^t$. Then

$$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = \mathbf{b} = (24, 30, -24)^t;$$

$$\mathbf{w} = C^{-1}\mathbf{r}^{(0)} = (24, 30, -24)^t;$$

$$\mathbf{v}^{(1)} = C^{-t}\mathbf{w} = (24, 30, -24)^t;$$

$$\alpha = \langle \mathbf{w}, \mathbf{w} \rangle = 2052.$$

We start the first iteration with $k = 1$. Then

$$\mathbf{u} = A\mathbf{v}^{(1)} = (186.0, 216.0, -126.0)^t;$$

$$t_1 = \frac{\alpha}{\langle \mathbf{v}^{(1)}, \mathbf{u} \rangle} = 0.1469072165;$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + t_1\mathbf{v}^{(1)} = (3.525773196, 4.407216495, -3.525773196)^t;$$

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} - t_1\mathbf{u} = (-3.32474227, -1.73195876, -5.48969072)^t;$$

$$\mathbf{w} = C^{-1}\mathbf{r}^{(1)} = \mathbf{r}^{(1)};$$

$$\beta = \langle \mathbf{w}, \mathbf{w} \rangle = 44.19029651;$$

$$s_1 = \frac{\beta}{\alpha} = 0.02153523222;$$

$$\mathbf{v}^{(2)} = C^{-t}\mathbf{w} + s_1\mathbf{v}^{(1)} = (-2.807896697, -1.085901793, -6.006536293)^t.$$

Set

$$\alpha = \beta = 44.19029651.$$

We are now ready to begin the second iteration. We have

$$\mathbf{u} = A\mathbf{v}^{(2)} = (-14.48929217, -6.760760967, -22.94024338)^t;$$

$$t_2 = 0.2378157558;$$

$$\mathbf{x}^{(2)} = (2.858011121, 4.148971939, -4.954222164)^t;$$

$$\mathbf{r}^{(2)} = (0.121039698, -0.124143281, -0.034139402)^t;$$

$$\mathbf{w} = C^{-1}\mathbf{r}^{(2)} = \mathbf{r}^{(2)};$$

$$\beta = 0.03122766148;$$

$$s_2 = 0.0007066633163;$$

$$\mathbf{v}^{(3)} = (0.1190554504, -0.1249106480, -0.03838400086)^t.$$

Set

$$\alpha = \beta = 0.03122766148.$$

Finally, the third iteration gives

$$\mathbf{u} = A\mathbf{v}^{(3)} = (0.1014898976, -0.1040922099, -0.0286253554)^t;$$

$$t_3 = 1.192628008;$$

$$\mathbf{x}^{(3)} = (2.999999998, 4.000000002, -4.999999998)^t;$$

$$\mathbf{r}^{(3)} = (0.36 \times 10^{-8}, 0.39 \times 10^{-8}, -0.141 \times 10^{-8})^t.$$

Since $\mathbf{x}^{(3)}$ is nearly the exact solution, rounding error did not significantly effect the result. In Example 3 of Section 7.3, the Gauss-Seidel method required 34 iterations, and the SOR method, with $\omega = 1.25$, required 14 iterations for an accuracy of 10^{-7}. It should be noted, however, that in this example, we are really comparing a direct method to iterative methods. ■

The next example illustrates the effect of preconditioning on a poorly conditioned matrix. In this example and subsequently, we use $D^{-1/2}$ to represent the diagonal matrix whose entries are the reciprocals of the square roots of the diagonal entries of the coefficient matrix A.

EXAMPLE 3 The linear system $A\mathbf{x} = \mathbf{b}$ with

$$A = \begin{bmatrix} 0.2 & 0.1 & 1 & 1 & 0 \\ 0.1 & 4 & -1 & 1 & -1 \\ 1 & -1 & 60 & 0 & -2 \\ 1 & 1 & 0 & 8 & 4 \\ 0 & -1 & -2 & 4 & 700 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

has the solution

$$\mathbf{x}^* = (7.859713071, 0.4229264082, -0.07359223906, -0.5406430164, 0.01062616286)^t.$$

The matrix A is symmetric and positive definite but is ill-conditioned with condition number $K_\infty(A) = 13961.71$. We will use tolerance 0.01 and compare the results obtained from the Jacobi, Gauss-Seidel, and SOR (with $\omega = 1.25$) iterative methods and from the conjugate gradient method with $C^{-1} = I$. Then we precondition by choosing C^{-1} as $D^{-1/2}$, the diagonal matrix whose diagonal entries are the reciprocal of the positive square roots of the diagonal entries of the positive definite matrix A. The results are presented in Table 7.5. The preconditioned conjugate gradient method gives the most accurate approximation with the smallest number of iterations. ■

Table 7.5

Method	Number of Iterations	$\mathbf{x}^{(k)}$	$\|\mathbf{x}^* - \mathbf{x}^{(k)}\|_\infty$
Jacobi	49	(7.86277141, 0.42320802, −0.07348669, −0.53975964, 0.01062847)^t	0.00305834
Gauss-Seidel	15	(7.83525748, 0.42257868, −0.07319124, −0.53753055, 0.01060903)^t	0.02445559
SOR ($\omega = 1.25$)	7	(7.85152706, 0.42277371, −0.07348303, −0.53978369, 0.01062286)^t	0.00818607
Conjugate Gradient	5	(7.85341523, 0.42298677, −0.07347963, −0.53987920, 0.008628916)^t	0.00629785
Conjugate Gradient (Preconditioned)	4	(7.85968827, 0.42288329, −0.07359878, −0.54063200, 0.01064344)^t	0.00009312

The preconditioned conjugate gradient method is often used in the solution of large linear systems in which the matrix is sparse and positive definite. These systems must be solved to approximate solutions to boundary-value problems in ordinary-differential equations (Sections 11.3, 11.4, 11.5). The larger the system, the more impressive the conjugate gradient method becomes since it significantly reduces the number of iterations required. In these systems, the preconditioning matrix C is approximately equal to L in the Choleski factorization LL^t of A. Generally, small entries in A are ignored and Choleski's method is applied to obtain what is called an incomplete LL^t factorization of A. Thus, $C^{-t}C^{-1} \approx A^{-1}$ and a good approximation is obtained. More information about the conjugate gradient method can be found in Kelley [Kelley].

EXERCISE SET 7.5

1. The linear system

$$x_1 + \frac{1}{2}x_2 = \frac{5}{21},$$
$$\frac{1}{2}x_1 + \frac{1}{3}x_2 = \frac{11}{84}$$

has solution $(x_1, x_2)^t = (1/6, 1/7)^t$.

   a. Solve the linear system using Gaussian elimination with two-digit rounding arithmetic.
   b. Solve the linear system using the conjugate gradient method ($C = C^{-1} = I$) with two digit rounding arithmetic.
   c. Which method gives the better answer?
   d. Choose $C^{-1} = D^{-1/2}$. Does this choice improve the conjugate gradient method?

2. The linear system

$$0.1x_1 + 0.2x_2 = 0.3,$$
$$0.2x_1 + 113x_2 = 113.2$$

has solution $(x_1, x_2)^t = (1, 1)^t$. Repeat the directions for Exercise 1 on this linear system.

3. The linear system

$$x_1 + \frac{1}{2}x_2 + \frac{1}{3}x_3 = \frac{5}{6},$$
$$\frac{1}{2}x_1 + \frac{1}{3}x_2 + \frac{1}{4}x_3 = \frac{5}{12},$$
$$\frac{1}{3}x_1 + \frac{1}{4}x_2 + \frac{1}{5}x_3 = \frac{17}{60}$$

has solution $(1, -1, 1)^t$.

   a. Solve the linear system using Gaussian elimination with three-digit rounding arithmetic.
   b. Solve the linear system using the conjugate gradient method with three-digit rounding arithmetic.
   c. Does pivoting improve the answer in (a)?
   d. Repeat part (b) using $C^{-1} = D^{-1/2}$. Does this improve the answer in (b)?

4. Repeat Exercise 3 using single-precision arithmetic on a computer.

5. Perform only two steps of the conjugate gradient method with $C = C^{-1} = I$ on each of the following linear systems. Compare the results in parts (b), (c), (d), and (f) to those obtained in Exercises 1, 2, and 5 of Section 7.3.

   a. $3x_1 - x_2 + x_3 = 1,$
      $-x_1 + 6x_2 + 2x_3 = 0,$
      $x_1 + 2x_2 + 7x_3 = 4.$

   b. $10x_1 - x_2 = 9,$
      $-x_1 + 10x_2 - 2x_3 = 7,$
      $-2x_2 + 10x_3 = 6.$

   c. $10x_1 + 5x_2 = 6,$
      $5x_1 + 10x_2 - 4x_3 = 25,$
      $-4x_2 + 8x_3 - x_4 = -11,$
      $-x_3 + 5x_4 = -11.$

   d. $4x_1 + x_2 - x_3 + x_4 = -2,$
      $x_1 + 4x_2 - x_3 - x_4 = -1,$
      $-x_1 - x_2 + 5x_3 + x_4 = 0,$
      $x_1 - x_2 + x_3 + 3x_4 = 1.$

   e. $4x_1 + x_2 + x_3 + x_5 = 6,$
      $x_1 + 3x_2 + x_3 + x_4 = 6,$
      $x_1 + x_2 + 5x_3 - x_4 - x_5 = 6,$
      $x_2 - x_3 + 4x_4 = 6,$
      $x_1 - x_3 + 4x_5 = 6.$

   f. $4x_1 - x_2 - x_4 = 0,$
      $-x_1 + 4x_2 - x_3 - x_5 = 5,$
      $-x_2 + 4x_3 - x_6 = 0,$
      $-x_1 + 4x_4 - x_5 = 6,$
      $-x_2 - x_4 + 4x_5 - x_6 = -2,$
      $-x_3 - x_5 + 4x_6 = 6.$

6. Repeat Exercise 5 using $C^{-1} = D^{-1/2}$.

7. Repeat Exercise 5 with $TOL = 10^{-3}$ in the l_∞ norm. Compare the results in parts (b), (c), (d), and (f) to those obtained in Exercises 3, 4, and 7 of Section 7.3.

8. Repeat Exercise 7 using $C^{-1} = D^{-1/2}$.

9. Use (i) the Jacobi Method, (ii) the Gauss-Seidel method, (iii) the SOR method with $\omega = 1.3$, and (iv) the conjugate gradient method and preconditioning with $C^{-1} = D^{-1/2}$ to find solutions to the linear system $A\mathbf{x} = \mathbf{b}$ to within 10^{-5} in the l_∞ norm.

   a.
$$a_{i,j} = \begin{cases} 4, & \text{when } j = i \text{ and } i = 1, 2, \ldots, 16, \\ -1, & \text{when } \begin{cases} j = i+1 \text{ and } i = 1, 2, 3, 5, 6, 7, 9, 10, 11, 13, 14, 15, \\ j = i-1 \text{ and } i = 2, 3, 4, 6, 7, 8, 10, 11, 12, 14, 15, 16, \\ j = i+4 \text{ and } i = 1, 2, \ldots, 12, \\ j = i-4 \text{ and } i = 5, 6, \ldots, 16, \end{cases} \\ 0, & \text{otherwise} \end{cases}$$

   and

$$\mathbf{b} = (1.902207, 1.051143, 1.175689, 3.480083, 0.819600, -0.264419, -0.412789, 1.175689, 0.913337, -0.150209, -0.264419, 1.051143, 1.966694, 0.913337, 0.819600, 1.902207)^t$$

   b.
$$a_{i,j} = \begin{cases} 4, & \text{when } j = i \text{ and } i = 1, 2, \ldots, 25, \\ -1, & \text{when } \begin{cases} j = i+1 \text{ and } i = \begin{cases} 1, 2, 3, 4, 6, 7, 8, 9, 11, 12, 13, 14, \\ 16, 17, 18, 19, 21, 22, 23, 24, \end{cases} \\ j = i-1 \text{ and } i = \begin{cases} 2, 3, 4, 5, 7, 8, 9, 10, 12, 13, 14, 15, \\ 17, 18, 19, 20, 22, 23, 24, 25, \end{cases} \\ j = i+5 \text{ and } i = 1, 2, \ldots, 20, \\ j = i-5 \text{ and } i = 6, 7, \ldots, 25, \end{cases} \\ 0, & \text{otherwise} \end{cases}$$

and

$$\mathbf{b} = (1, 0, -1, 0, 2, 1, 0, -1, 0, 2, 1, 0, -1, 0, 2, 1, 0, -1, 0, 2, 1, 0, -1, 0, 2, 1, 0, -1, 0, 2)^t$$

c.

$$a_{i,j} = \begin{cases} 2i, & \text{when } j = i \text{ and } i = 1, 2, \ldots, 40, \\ -1, & \text{when } \begin{cases} j = i + 1 \text{ and } i = 1, 2, \ldots, 39, \\ j = i - 1 \text{ and } i = 2, 3, \ldots, 40, \end{cases} \\ 0, & \text{otherwise} \end{cases}$$

and $b_i = 1.5i - 6$, for each $i = 1, 2, \ldots, 40$

10. Solve the linear system in Exercise 12(a) and (b) of Section 7.3 using the conjugate gradient method with $C^{-1} = I$.

11. Let

$$A_1 = \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 4 \end{bmatrix}, \quad -I = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix},$$

$$\text{and} \quad 0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Form the 16×16 matrix A in partitioned form,

$$A = \begin{bmatrix} A_1 & -I & 0 & 0 \\ -I & A_1 & -I & 0 \\ 0 & -I & A_1 & -I \\ 0 & 0 & -I & A_1 \end{bmatrix}.$$

Let $\mathbf{b} = (1, 2, 3, 4, 5, 6, 7, 8, 9, 0, 1, 2, 3, 4, 5, 6)^t$.

a. Solve $A\mathbf{x} = \mathbf{b}$ using the conjugate gradient method with tolerance 0.05.

b. Solve $A\mathbf{x} = \mathbf{b}$ using the preconditioned conjugate gradient method with $C^{-1} = D^{1/2}$ and tolerance 0.05.

c. Is there any tolerance for which the methods of part (a) and part (b) require a different number of iterations?

12. Use the transpose properties given in Theorem 6.13 to prove Theorem 7.30.

13. **a.** Show that an A-orthogonal set of nonzero vectors associated with a positive definite matrix is linearly independent.

b. Show that if $\{\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \ldots, \mathbf{v}^{(n)}\}$ is a set of A-orthogonal nonzero vectors in $\mathbb{R}^n$ and $\mathbf{z}^t\mathbf{v}^{(i)} = \mathbf{0}$, for each $i = 1, 2, \ldots, n$, then $\mathbf{z} = \mathbf{0}$.

14. Prove Theorem 7.33 using mathematical induction as follows:

a. Show that $\langle \mathbf{r}^{(1)}, \mathbf{v}^{(1)} \rangle = 0$.

b. Assume that $\langle \mathbf{r}^{(k)}, \mathbf{v}^{(j)} \rangle = 0$, for each $k \leq l$ and $j = 1, 2, \ldots, k$, and show that this implies that $\langle \mathbf{r}^{(l+1)}, \mathbf{v}^{(j)} \rangle = 0$, for each $j = 1, 2, \ldots, l$.

c. Show that $\langle \mathbf{r}^{(l+1)}, \mathbf{v}^{(l+1)} \rangle = 0$.

7.6 Survey of Methods and Software

In this chapter we have studied iterative techniques to approximate the solution of linear systems. We began with the Jacobi method and the Gauss-Seidel method to introduce the iterative methods. Both methods require an arbitrary initial approximation $\mathbf{x}^{(0)}$ and generate a sequence of vectors $\mathbf{x}^{(i+1)}$ using an equation of the form

$$\mathbf{x}^{(i+1)} = T\mathbf{x}^{(i)} + \mathbf{c}.$$

It was noted that the method will converge if and only if the spectral radius of the iteration matrix $\rho(T) < 1$, and the smaller the spectral radius, the faster the convergence. Analysis of the residual vectors of the Gauss-Seidel technique led to the SOR iterative method, which involves a parameter ω to speed convergence.

These iterative methods and modifications are used extensively in the solution of linear systems which arise in the numerical solution of boundary value problems and partial differential equations (see Chapters 11 and 12). These systems are often very large, on the order of 10000 equations in 10000 unknowns, and are sparse with their nonzero entries in predictable positions. The iterative methods are also useful for other large sparse systems and are easily adapted for efficient use on parallel computers.

Almost all commercial and public domain packages that contain iterative methods for the solution of a linear system of equations require a preconditioner to be used with the method. Faster convergence of iterative solvers is often achieved by using a preconditioner. A preconditioner produces an equivalent system of equations that hopefully exhibits better convergence characteristics than the original system. The IMSL Library has the subroutine PCGRC, which is a preconditioned conjugate gradient method. The NAG Library has several subroutines, which are prefixed F11, for the iterative solution of linear systems. All of the subroutines are based on Krylov subspaces. Saad [Sa2] has a detailed description of Krylov subspace methods. The packages LINPACK and LAPACK contain only direct methods for the solution of linear systems; however, the packages do contain many subroutines that are used by the iterative solvers. The public domain packages IML++, ITPACK, SLAP, and Templates, contain iterative methods. MATLAB contains several iterative methods that are also based on Krylov subspaces. For example, the command x =PCG(A, b) executes the preconditioned conjugate gradient method to solve the linear system $Ax = b$. Some optional input parameters for PCG are, TOL a tolerance for convergence, MAXIT the maximum number of iterations, and M a preconditioner.

The concepts of condition number and poorly conditioned matrices were introduced in Section 7.4. Many of the subroutines for solving a linear system or for factoring a matrix into an LU factorization include checks for ill-conditioned matrices and also give an estimate of the condition number.

The subroutine SGETRF in LAPACK factors the real matrix A into an LU factorization and gives the row ordering for the permutation matrix P, where $PA = LU$. The subroutine SGECON gives the reciprocal of the condition number of A using the LU factorization computed by SGETRF. LAPACK also has subroutines to estimate the condition number for special matrices. For example, SPOTRF performs the Choleski factorization of a positive definite matrix A, and SPOCON estimates the reciprocal of the condition number using the Choleski factorization computed by SPOTRF.

The IMSL Library has subroutines that estimate the condition number. For example, the subroutine LFCRG computes an LU factorization $PA = LU$ of the matrix A and also gives an estimate of the condition number. The NAG Library has similar subroutines.

LAPACK, LINPACK, the IMSL Library, and the NAG Library have subroutines that improve on a solution to a linear system that is poorly conditioned. The subroutines test the condition number and then use iterative refinement to obtain the most accurate solution possible given the precision of the computer.

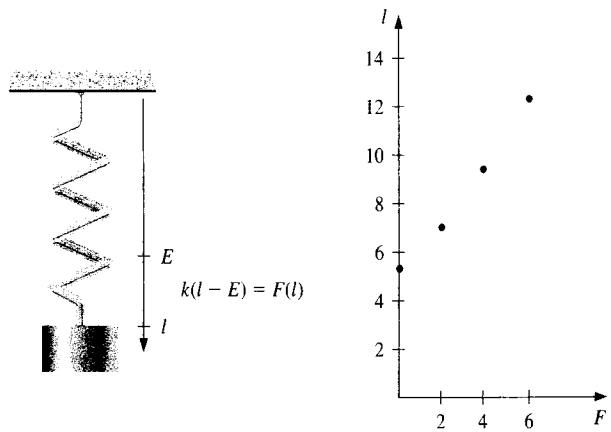
More information on the use of iterative methods for solving linear systems can be found in Varga [Var], Young [Y], Hageman and Young [HY], and in the recent book by Axelsson [Ax]. Iterative methods for large sparse systems are discussed in Barrett et al. [Barr], Hackbusch [Hac], Kelley [Kelley], and Saad [Sa2].

CHAPTER 8

Approximation Theory

. . .

Hooke's law states that when a force is applied to a spring constructed of uniform material, the length of the spring is a linear function of that force. We can write the linear function as $F(l) = k(l - E)$, where $F(l)$ represents the force required to stretch the spring l units, the constant E represents the length of the spring with no force applied, and the constant k is the spring constant.



Suppose we want to determine the spring constant for a spring that has initial length 5.3 in. We apply forces of 2, 4, and 6 lb to the spring and find that its length increases to 7.0, 9.4, and 12.3 in., respectively. A quick examination shows that the points (0, 5.3), (2, 7.0), (4, 9.4), and (6, 12.3) do not quite lie in a straight line. Although we could simply use one random pair of these data points to approximate the spring constant, it would seem more reasonable to find the line that *best* approximates