Numerical Analysis

10th ed

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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 $\mathbf{x}$, $\mathbf{y} \in \mathbb{R}$

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

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

Theorem (7.3: Cauchy-Bunyakovsky-Schwarz inequality)

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

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

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

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

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 the l_∞ norm if and only if $\lim_{k\to\infty} x_i^{(k)} = x_i$, for each $i = 1, 2, \ldots, n$.

Theorem (7.7)

For each $\mathbf{x} \in \mathbb{R}^n$, $\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_2 \leq \sqrt{n}\|\mathbf{x}\|_\infty$.

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)** $\|AB\| \leq \|A\|\|B\|$.

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.

Corollary (7.10)

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

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

Theorem (7.11)

If $A = (a_{ij})$ is an $n \times n$ matrix, then $\|A\|_\infty = \max_{1\leq i\leq n} \sum_{j=1}^{n} |a_{ij}|.$

Definition (7.12)

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

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

Definition (7.13)

If p is the characteristic polynomial of the matrix A, the zeros of p are called **eigenvalues**, or characteristic values, of the matrix A. If λ is an 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.

Definition (7.14)

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

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

(For complex $\lambda = \alpha + \beta i$, we define $|\lambda| = (\alpha^2 + \beta^2)^{1/2}$.)

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* $\|\cdot\|$.

Definition (7.16)

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

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

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 **Jacobi iterative method** is obtained by solving the *i*th equation in $A\mathbf{x} = \mathbf{b}$ for x_i to obtain (provided $a_{ii} \neq 0$)

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

For each $k \geq 1$, generate the components $x_i^{(k)}$ of $\mathbf{x}^{(k)}$ from the components of $\mathbf{x}^{(k-1)}$ by

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

Algorithm 7.1: JACOBI ITERATIVE TECHNIQUE

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.

Algorithm 7.1: JACOBI ITERATIVE TECHNIQUE

Step 1 Set $k = 1$.

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

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

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

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

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.

Possible improvement in Algorithm 7.1 can be seen by reconsidering the formula for $\mathbf{x}_i^{(k)}$ from the Jacobi iterative method. The components of $\mathbf{x}^{(k-1)}$ are used to compute all the components $x_i^{(k)}$ of $\mathbf{x}^{(k)}$. But, for $i > 1$, the components $x_1^{(k)}, \ldots, x_{i-1}^{(k)}$ of $\mathbf{x}^{(k)}$ have already been computed and are expected to be better approximations to the actual solutions $x_1, \ldots, x_{i-1}$ than are $x_1^{(k-1)}, \ldots, x_{i-1}^{(k-1)}$. It seems reasonable, then, to compute $x_i^{(k)}$ using these most recently calculated values. That is, to use

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

for each $i = 1, 2, \ldots, n$, instead of Eq. (7.5). This modification is called the **Gauss-Seidel iterative technique**

Algorithm 7.2: GAUSS-SEIDEL ITERATIVE TECHNIQUE

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.

Algorithm 7.2: GAUSS-SEIDEL ITERATIVE TECHNIQUE

Step 1 Set $k = 1$.

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

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

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

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

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.

Lemma (7.18)

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

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

Theorem (7.19)

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

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

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

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 $\mathbf{x} \in \mathbb{R}^n$, with $\mathbf{x} = T\mathbf{x} + \mathbf{c}$, and the following error bounds hold:

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

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

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 $A\mathbf{x} = \mathbf{b}$.

Theorem (7.22)

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:

(i) $0 \leq \rho(T_g) < \rho(T_j) < 1$;

(ii) $1 < \rho(T_j) < \rho(T_g)$;

(iii) $\rho(T_j) = \rho(T_g) = 0$;

(iv) $\rho(T_j) = \rho(T_g) = 1$.

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 $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}}$.

If we modify the Gauss-Seidel procedure, to

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

where

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

then for certain choices of positive ω the norm of the residual vector can be reduced and we obtain significantly faster convergence.

Methods involving the equation

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

are called **relaxation methods**.

For choices of ω with $0 < \omega < 1$, the procedures are called **under-relaxation methods**. We will be interested in choices of ω with $1 < \omega$, and these are called **over-relaxation methods**. They are used to accelerate the convergence for systems that are convergent by the Gauss-Seidel technique. The 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.

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 $0 < \omega < 2$.

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 $\rho(T_\omega) = \omega - 1$.

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}, $1 \leq i, j \leq n$, 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 $\mathbf{XO} = \mathbf{x}^{(0)}$; 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.

Algorithm 7.3: SOR

Step 1 Set $k = 1$.
Step 2 While ($k \leq N$) do Steps 3–6.
Step 3 For $i = 1, \ldots, n$ set

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

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.

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,*

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

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

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

Definition (7.28)

The **condition number** of the nonsingular matrix A relative to a norm $\|\cdot\|$ is $K(A) = \|A\| \cdot \|A^{-1}\|$.

Iterative refinement, or *Iterative improvement*, consists of performing iterations on the system whose right-hand side is the residual vector for successive approximations until satisfactory accuracy results.

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}, $1 \leq i, j \leq n$ of the matrix A; the entries b_i, $1 \leq i \leq n$ of $\mathbf{b}$; the maximum number of iterations N; tolerance TOL; number of digits of precision t.

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

Algorithm 7.4: ITERATIVE REFINEMENT

Step 0 Solve the system $A\mathbf{x} = \mathbf{b}$ for $x_1, \ldots, x_n$ by Gaussian elimination saving 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 ($k \leq N$) do Steps 3–9.

Step 3 For $i = 1, 2, \ldots, n$ (*Calculate* $\mathbf{r}$.) set $r_i = b_i - \sum_{j=1}^{n} a_{ij}x_j$.
(*Perform 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 ($COND$);
STOP. (*Procedure successful.*)

Step 8 Set $k = k + 1$.

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

Step 10 OUTPUT ('Max number iterations exceeded'); OUTPUT ($COND$);
STOP. (*Procedure unsuccessful.*)

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

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

Theorem (7.30)

Let $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^* \mathbf{y}$ *be the inner product notation.*
For any vectors $\mathbf{x}$, $\mathbf{y}$, *and* $\mathbf{z}$ *and any real number* α, *we have*

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

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

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

(d) $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$

(e) $\langle \mathbf{x}, \mathbf{x} \rangle = 0$ *if and only if* $\mathbf{x} = \mathbf{0}$

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* $\mathbf{x}^*$ *produces the minimal value of*

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

Theorem (7.32)

For any vectors $\mathbf{x}$, $\mathbf{y}$, *and* $\mathbf{z}$ *and any real number* α, *we have Let* $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ *be an A-orthogonal set of nonzero vectors* $(\langle \mathbf{v}^{(i)}, A\mathbf{v}^{(j)} \rangle = 0$, *if* $i \neq j$.) *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,* $A\mathbf{x}^{(n)} = \mathbf{b}$.

Theorem (7.33)

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

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

Preconditioning replaces a given system with one having the same solutions but with better convergence characteristics.

Algorithm 7.5: PRECONDITIONED CONJUGATE GRADIENT

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}, $1 \leq i, j \leq n$ of the matrix A; the entries b_j, $1 \leq j \leq n$ of the vector $\mathbf{b}$; the entries γ_{ij}, $1 \leq i, j \leq n$ of the preconditioning matrix C^{-1}, the entries x_i, $1 \leq i \leq n$ 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.

Chapter 7.6: Conjugate Gradient Method

Preconditioning replaces a given system with one having the same solutions but with better convergence characteristics.

Algorithm 7.5: PRECONDITIONED CONJUGATE GRADIENT

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'; $r_1, \ldots, r_n$);

STOP (*The procedure was successful.*)

Algorithm 7.5: PRECONDITIONED CONJUGATE GRADIENT

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

Algorithm 7.5: PRECONDITIONED CONJUGATE GRADIENT

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 exceeded.');
(*The procedure was unsuccessful.*)
STOP.