# Numerical Analysis Mathematics of Scientific Computing

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# 内容提要

- Solution of Equations by Iterative Methods
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4.6.1 Basic Concepts

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A general type of iterative process for solving the system Ax = b A certain matrix Q, called the **splitting matrix**,

$$Qx = (Q - A)x + b$$
 
$$Qx^{(k)} = (Q - A)x^{(k-1)} + b$$
 
$$x^{(k)} = (I - Q^{-1}A)x^{(k-1)} + Q^{-1}b$$

Our objective is to choose Q so that these two conditions are met:

- 1. The sequence  $[x^{(k)}]$  is easily computed.
- 2. The sequence  $[x^{(k)}]$  converges rapidly to a solution.

## THEOREM 1 (Theorem on Iterative Method Convergence)

If  $\parallel I-Q^{-1}A\parallel < 1$  for some subordinate matrix norm, then the sequence produced by the Equation  $Qx^{(k)}=(Q-A)x^{(k-1)}+b$  converges to the solution of Ax=b for any initial vector  $x^{(0)}$ .

#### Proof.

Since  $||I - Q^{-1}A|| < 1$ , A and Q are nonsingular.

$$x^{(k)} = (I - Q^{-1}A)x^{(k-1)} + Q^{-1}b$$

The actual solution x satisfies the equation  $x = (I - Q^{-1}A)x + Q^{-1}b$ 

$$x^{(k)} - x = (I - Q^{-1}A)(x^{(k-1)} - x)$$

$$||x^{(k)} - x|| \le ||(I - Q^{-1}A)|| ||(x^{(k-1)} - x)||$$

$$|| x^{(k)} - x || \le || (I - Q^{-1}A) ||^k || (x^{(0)} - x) ||$$

Since  $\parallel I - Q^{-1}A \parallel < 1$  We can conclude that  $\lim_{k \to \infty} \parallel x^{(k)} - x \parallel = 0$ 

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Q is chosen to be the identity matrix. The equation  $Qx^{(k)}=(Q-A)x^{(k-1)}+b$  in this case read as follows:

$$x^{(k)} = (I - A)x^{(k-1)} + b = x^{(k-1)} + r^{(k-1)}$$

where  $r^{(k-1)}$  is the residual vector,  $r^{(k-1)} = b - Ax^{(k-1)}$ . If ||I - A|| < 1 for some subordinate matrix norm, the Richardson iteration will produce a solution to Ax = b.

#### 4.6.2 Richardson Method

An algorithm of Richardson iteration is as follows: input n,  $(a_{ij})$ ,  $(b_i)$ ,  $(x_i)$ , Mfor k = 1 to M do for i = 1 to n do  $r_i \leftarrow b_i - \sum_{i=1}^n a_{ij} x_j$ end do for i = 1 to n do  $x_i \leftarrow x_i + r_i$ end do end do output k,  $(x_i)$ ,  $(r_i)$ 

```
function [k,x,r]=richardson(n,a,b,x,M)
   for k=1:M
       for i=1:n
3
            s=b(i)
4
            for j=1:n
5
                 s=s-a(i,j)*x(j)
            end
7
            r(i)=s
8
       end
9
       for i=1:n
10
            x(i)=x(i)+r(i)
11
       end
12
   end
13
```

4.6.3 Jacobi Method

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Q is the diagonal matrix whose diagonal entries are the same as those in the matrix  $A = (a_{ij})$ .  $Q^{-1}A$  is  $a_{ij}/a_{ii}$ , and hence

$$||I - Q^{-1}A||_{\infty} = \max_{1 \le i \le n} \sum_{\substack{j=1 \ i \ne i}}^{n} |a_{ij}/a_{ii}|$$

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## THEOREM 2 (Theorem on Convergence of Jacobi Method)

If A is diagonally dominant, then the sequence produced by the Jacobin iteration converges to the solution of Ax=b for any staring vector.

## Proof.

Diagonal dominance means that

$$|a_{ii}| > \sum_{\substack{j=1\\i \neq i}}^{n} |a_{ij}| \qquad (1 \le i \le n)$$

$$|| I - Q^{-1}A ||_{\infty} = \max_{1 \le i \le n} \sum_{\substack{j=1 \ i \ne i}}^{n} |a_{ij}/a_{ii}|$$

We then conclude that  $||I - Q^{-1}A||_{\infty} < 1$ . By Theorem 1, the Jacobi iteration converges.

```
input n, (a_{ij}), (b_i), (x_i), M
for k=1 to M do
   for i = 1 to n do
   u_i \leftarrow (b_i - \sum_{j=1}^n a_{ij}x_j)/a(ii)
   end do
   for i = 1 to n do
   x_i \leftarrow u_i
   end do
   output k, (x_i)
end do
```

```
function [k, x]=jacobi(n,a,b,x,M)
   for k=1:M
3
       for i=1:n
            d=1/a(i,i)
            b(i)=d*b(i)
5
            for j=1:n
6
                 a(i,j)=d*a(i,j)
7
            end
8
       end
g
       for i=1:n
10
            u(i)=b(i)
11
            for j=1:n
12
             u(i)=u(i)-a(i,j)*x(j)
13
            end
14
             u(i)=u(i)+a(i,i)*x(i)
15
       end
16
       for i=1:n
17
            x(i)=u(i)
18
        end
19
```

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# **Basic Concepts**

- For arbitrary linear iterative processes.  $x^{(k)}=Gx^{(k-1)}+c$ , we set  $G=I-Q^{-1}A$  and  $c=Q^{-1}b$ .
- The characteristic equation of A:  $det(A \lambda I) = 0$
- The spectral radius of A:  $\rho(A) = \max\{|\lambda| : det(A \lambda I) = 0\}$
- If  $S^{-1}AS=B$ , the similar matrices matrices have the same eigenvalues.

## THEOREM 3 (Theorem on Similar Upper Trigngular Matrices)

Every square matrix is similar to an (possibly complex) upper triangular matrix whose off-diagonal elements are arbitrarily small.

### Proof.

Let A be an  $n \times n$  matrix. Schur's theoerm states that A is similar to an upper triangular matrix  $T=(t_{ij})$ , which may be complex. Let  $D=diag(\varepsilon,\varepsilon^2,...,\varepsilon^n)$ . The generic element of  $B=D^{-1}TD$  is  $t_{ij}\varepsilon^{j-i}$ . The elements above the diagonal can be made as small as we wish by decreasing  $\varepsilon$ .



## THEOREM 4 (Theorem on Spectral Radius)

The spectral radius function safisfies the equation

$$\rho(A) = \inf_{\|\cdot\|} \|A\|$$

in which the infimum is take over all subordinate matrix norms.

#### Proof.

First, we prove that  $\rho(A) \leq \inf_{\|.\|} \|A\|$ 

Let  $\lambda$  be any eigenvalue of A. Select a nonzero eigenvector x corresponding to  $\lambda$ .

$$|\lambda| \| x \| = \| \lambda x \| = \| Ax \| \le \| A \| \| x \|$$

$$|\lambda| \leq \parallel A \parallel$$
. We have  $\rho(A) \leq \inf_{\parallel \cdot \parallel} \parallel A \parallel$ 



## Proof.

Second, we prove that  $\inf_{\|\cdot\|} \|A\| \le \rho(A)$ 

For the reverse inequality, we use Theorem 3. We have

$$\parallel S^{-1}AS\parallel_{\infty}=\parallel D+T\parallel_{\infty}\leq \parallel D\parallel_{\infty}+\parallel T\parallel_{\infty}$$

Since D has the eigenvalues of A on its diagonal, it follows that

If the eigenvalues of 
$$\|D\|_{\infty} = \max_{1 \leq i \leq n} |\lambda| = \rho(A)$$

$$\|S^{-1}AS\|_{\infty} \leq \rho(A) + \varepsilon$$

$$\|A\|'_{\infty} = \|S^{-1}AS\|_{\infty}$$

$$\|nf_{\text{total}}\|A\| \leq \rho(A) + \varepsilon$$

$$\inf_{\|\cdot\|} \|A\| \le \rho(A) + \varepsilon$$

$$\inf_{\|\cdot\|} \|A\| \le \rho(A)$$

So 
$$\rho(A) = \inf_{\|\cdot\|} \|A\|$$

# THEOREM 5 (Theorem on Necessary and Sufficient Conditions for Iterative Method Convergence)

For the iteration formual  $x^{(k)} = Gx^{(k-1)} + c$  to produce a sequence converging to  $(I-G)^{-1}c$ , for any starting vector  $x^{(0)}$ , it is necessary and sufficient that the spectral radius of G be less than 1.

#### Proof.

First, Suppose that  $\rho(G) < 1$ . There is a subordinate matrix norm such that  $\parallel G \parallel < 1$ . We write

$$x^{(1)} = Gx^{(0)} + c$$

$$x^{(2)} = G^2 x^{(0)} + Gc + c$$

$$x^{(3)} = G^3 x^{(0)} + G^2 c + Gc + c$$

The general formula is 
$$x^{(k)} = G^k x^{(0)} + \sum_{j=0}^{k-1} G^j c$$

$$\parallel G^k x^{(0)} \parallel \leq \parallel G^k \parallel \parallel x^{(0)} \parallel \leq \parallel G \parallel^k \parallel x^{(0)} \parallel \rightarrow 0 \text{ as } k \rightarrow \infty$$

We have 
$$\sum_{k=1}^{\infty} G^{j} c = (I - G)^{-1} c$$

$$\lim_{k \to \infty} x^{(k)} = (I - G)^{-1}c$$



### Proof.

Second, suppose that  $\rho(G) \geq 1$ .

Select u and  $\lambda$ , so that  $Gu = \lambda u$   $|\lambda| \ge 1$   $u \ne 0$ .

Let c = u and  $x^{(0)} = 0$ .

By the Equation  $x^{(k)} = G^k x^{(0)} + \sum_{i=0}^{k-1} G^i c_i$ 

$$x^{(k)} = \sum_{j=0}^{k-1} G^j u = \sum_{j=0}^{k-1} \lambda^j u.$$

If  $\lambda = 1$ ,  $x^{(k)} = ku$ , and this diverges as  $k \to \infty$ .

If  $\lambda \neq 1$ , then  $x^{(k)} = (\lambda^k - 1)(\lambda - 1)^{-1}u$ , and this diverges also because

 $\lim_{k\to\infty} \lambda^k$  does not exist.

## COROLLARY 1 (Iterative Method Convergence Corollary)

The iteration formual  $Qx^{(k)}=(Q-A)x^{(k-1)}+b$ , will produce a sequence converging to the solution of Ax=b, for any  $x^{(0)}$ , if  $\rho(I-Q^{-1}A)<1$ 

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- Let us examine Gauss-Seidel iteration in more detail. It is defined by letting Q be the lower triangular part of A, including the diagonal.
- An algorithm for the Gauss-Seidel iteration follows:

input 
$$n$$
,  $(a_{ij})$ ,  $(b_i)$ ,  $(x_i)$ ,  $M$  for  $k=1$  to  $M$  do for  $i=1$  to  $n$  do  $x_i \leftarrow (b_i - \sum_{\substack{j=1 \ j \neq i}}^n a_{ij}x_j)/a_{ii}$  end do output  $k$ ,  $(x_i)$  end do

## THEOREM 6 (Theorem on Gauss-Seidel Method Convergence)

If A is diagonally dominant, then the Gauss-Seidel method converges for any starting vector.

#### Proof.

By Corollary 1, it suffices to prove that  $\rho(I-Q^{-1}A)<1$ . To this end, let  $\lambda$  be any eigenvalue of  $I-Q^{-1}A$ . Let x be a corresponding eigenvector. We assume, that  $\parallel x \parallel_{\infty}=1$ . We have now  $(I-Q^{-1}A)x=\lambda x$  or  $Qx-Ax=\lambda Qx$ .

Since Q is the lower triangular part of A, including its diagonal,

$$-\sum_{j=i+1}^{n} a_{ij}x_j = \lambda \sum_{j=1}^{i} a_{ij}x_j \qquad (1 \le i \le n)$$

$$\lambda a_{ii} x_i = -\lambda \sum_{j=1}^{i-1} a_{ij} x_j - \sum_{j=i+1}^{n} a_{ij} x_j \qquad (1 \le i \le n)$$

Select an index i such that  $|x_i| = 1 \ge |x_j|$  for all j. Then,

$$|\lambda||a_{ii}| \le |\lambda| \sum_{j=1}^{i-1} |a_{ij}| + \sum_{j=i+1}^{n} |a_{ij}|$$

$$|\lambda| \le \{\sum_{j=i+1}^n |a_{ij}|\}\{|a_{ij}| - \sum_{j=1}^{i-1} |a_{ij}|\}^{-1} < 1$$

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# **Basic Concepts**

In the space of complex n-vectors.

- The conjugate transpose of y,  $y^* = (\bar{y_1}, \bar{y_2}, ..., \bar{y_n})$
- The inner product  $\langle x,y \rangle = y^*x = \sum_{i=1}^n x_i \bar{y}_i$
- $\langle x, x \rangle > 0$  (if  $x \neq 0$ )  $\langle x, \lambda y \rangle = \overline{\lambda} \langle x, y \rangle$  $\langle x, y \rangle = \overline{\langle y, x \rangle}$
- The conjugate transpose of A,  $A^* = (\bar{a_{ji}})$
- Hermitian:  $A^* = A$
- If A is Hermitian, then  $\langle Ax, y \rangle = \langle x, Ay \rangle$

## THEOREM 7 (Theorem on SOR Method Convergence)

In the SOR method, suppose that splitting matrix Q is chosen to be  $\alpha D-C$ , where  $\alpha$  is a real parameter, D is any positive definite Hermitian matrix, and C is any matrix safisfying  $C+C^*=D-A$ . If A is positive definite Hermitian, if Q is nonsigular, and if  $\alpha>1/2$ , then the SOR iteration converges for any starting vector.

### Proof.

We let  $G=I-Q^{-1}A$  and attempt to establish that the spectal radius of G satisfies  $\rho(G)<1$ . Let  $Gx=\lambda x$ , and y=(I-G)x.

$$y = x - Gx = x - \lambda x = Q^{-1}Ax$$
$$Q - A = (\alpha D - C) - (D - C - C^*) = \alpha D - D + C^*$$

We have

$$(\alpha D - C)y = Qy = Ay \tag{1}$$

$$(D - C - C^*)y = AGx \tag{2}$$

$$\alpha \langle Dy, y \rangle - \langle Cy, y \rangle = \langle Ax, y \rangle \tag{3}$$

$$\alpha \langle y, Dy \rangle - \langle y, Dy \rangle + \langle y, C^* y \rangle = \langle y, AGx \rangle \tag{4}$$

On adding Equations (3) and (4), We obtain

$$2\alpha \langle Dy, y \rangle - \langle y, Dy \rangle = \langle Ax, y \rangle + \langle y, AGx \rangle \tag{5}$$

## Proof.

$$(2\alpha - 1)\langle Dy, y \rangle = \langle Ax, y \rangle + \langle y, AGx \rangle$$

Since  $y = (1 - \lambda)x$  and  $Gx = \lambda x$ , Equation(5) yields

$$(2\alpha - 1)|1 - \lambda|^2 \langle Dx, x \rangle = (1 - \bar{\lambda})\langle Ax, x \rangle + \bar{\lambda}(1 - \lambda)\langle x, Ax \rangle = (1 - |\lambda|^2)\langle Ax, x \rangle$$
(6)

If  $\lambda \neq 1$ , the left side of the equation (6) is positive. Hence, the right side must also be positive, and  $|\lambda| < 1$ .

On the other hand, if  $\lambda = 1$ , then y = 0 from  $y = (1 - \lambda)x$  and Ax = 0.

This contradicts the condition  $\langle Ax, x \rangle > 0$  for any  $x \neq 0$ .

Thence,  $\rho(G) < 1$  and the SOR method converges.

A common choice for D and C in the SOR method is to let D be the diagonal of A and -C be the lower triangular part of A, excluding the diagonal.

4.6.7 Iteration Matrices

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Suppose that A is partitioned into  $A = D - C_L - C_U$ , where D = diag(A),  $C_L$  is the negitive of the strictly lower triangular part of A, and  $C_U$  is the negitive of the stictly upper triangular part of A.

$$Qx^{(k)} = (Q - A)x^{(k-1)} + b$$
  

$$x^{(k)} = (I - Q^{-1}A)x^{(k-1)} + Q^{-1}b$$
  

$$G = I - Q^{-1}A$$

#### Richardson:

$$\begin{cases} Q = I \\ G = I - A \end{cases}$$
$$x^{(k)} = (I - A)x^{(k-1)} + b$$

#### Jacobi

$$\begin{cases} Q = D \\ G = D^{-1}(C_L + C_U) \end{cases}$$
$$Dx^{(k)} = (C_L + C_U)x^{(k-1)} + b$$

#### **Gauss-Seidel**

$$\begin{cases} Q = D - C_L \\ G = (D - C_L)^{-1} C_U \end{cases}$$
$$(D - C_L)x^{(k)} = C_U x^{(k-1)} + b$$

#### SOR

$$\begin{cases} Q = \omega^{-1}(D - \omega C_L) \\ G = (D - \omega C_L)^{-1}(\omega C_U + (1 - \omega)D) \end{cases}$$
$$(D - \omega C_L)x^{(k)} = \omega(C_U x^{(k-1)} + b) + (1 - \omega)Dx^{(k-1)}$$

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Consider the iteration formula  $x^{(k)}=Gx^{(k-1)}+c$ We introduce a parameter  $\gamma\neq 0$  and embedded in a one-parameter family of iteration methods given by

$$x^{(k)} = \gamma (Gx^{(k-1)} + c) + (1 - \gamma)x^{(k-1)} = G_{\gamma}x^{k-1} + \gamma c$$

where

$$G_{\gamma} = \gamma G + (1 - \gamma)I$$

Then by taking a limit, we get  $x = \gamma(Gx + c) + (1 - \gamma)x$  or x = Gx + c.

## THEOREM 8 (Theorem on Eigenvalue of p(A))

If  $\lambda$  is an eigenvalue of a matrix A and if p is a polynomial, then  $p(\lambda)$  is an eigenvalue of p(A).

#### Proof.

Let  $Ax = \lambda x$  with  $x \neq 0$ . Then  $A^2x = \lambda Ax = \lambda^2 x$ , we have

$$A^k x = \lambda^k x$$

$$p(A)x = \sum_{k=0}^{m} c_k A^k x = \sum_{k=0}^{m} c_k \lambda^k x = p(\lambda)x$$



## THEOREM 9 (Theorem on Optimal Extrspolation Parameters)

If the only information avaliable about the eigenvalues of G is that they lie in the interval [a,b], and if  $1\notin [a,b]$ , then the best choice for  $\gamma$  is 2/(2-a-b). With this value of  $\gamma$ ,  $\rho(G_\gamma)\leq 1-|\gamma|d$ , where d is the distance from 1 to [a,b]

#### Proof.

The eigenvalues of G in an interval [a, b]

The eigenvalues of  $G_{\gamma} = \gamma G + (1 - \gamma)I$  in the interval

$$[\gamma a + 1 - \gamma, \gamma b + 1 - \gamma]$$

Since  $1 \notin [a, b]$ , a > 1 or b < 1

Since  $a \le b \le 1$ , it follows that  $\gamma > 0$  and d = 1 - b.

$$\gamma a + 1 - \gamma \le \lambda \le \gamma b + 1 - \gamma$$

$$\lambda \leq \gamma b + 1 - \gamma = 1 + \gamma (b - 1) = 1 - \gamma d$$

$$\lambda \ge \gamma a + 1 - \gamma = \gamma (a + b - 2) + 1 + \gamma (1 - b) = -1 + \gamma d$$

We have proved that 
$$-1 + \gamma d \le \lambda \le 1 - \gamma d$$

