Mathematical Tripos Part IB: Easter Term 2003

Numerical Analysis – Lecture 5

5 Iterative methods for solving linear systems

5.1 Basic iterative schemes

The general *iterative* method for solving $Ax = b$ is a rule $x^{k+1} = f_k(x^0, x^1, \dots, x^k)$. We will consider the simplest ones: *linear, one-step, stationary* iterative schemes:

$$x^{k+1} = Hx^k + v, \qquad x^0, v \in \mathbb{R}^n. \tag{5.1}$$

Here one chooses H and v so that x^*, a solution of $Ax = b$, satisfies $x^* = Hx^* + v$, i.e. it is the fixed point of the iteration (5.1) (if the scheme converges). Standard terminology:

the *iteration matrix* H, the *error* $e^k := x^k - x^*$, the *residual* $r^k := Ae^k = Ax^k - b$.

For a given class of matrices A, we are interested in *convergent* methods, i.e. the methods such that $x^k \to x^* = A^{-1}b$ for every starting value x^0. Substracting $x^* = Hx^* + v$ from (5.1) we obtain

$$e^{k+1} = He^k = \cdots = H^{k+1}e^0,$$

i.e., a method is convergent if $e^k = H^k e^0 \to 0$ for any $e^0 \in \mathbb{R}^n$.

Scheme 5.1 (Splitting) This is the scheme

$$Mx^{k+1} = Nx^k + b, \qquad A =: M - N, \qquad M \text{ is non-singular}.$$

The simplest splitting is $A = L_0 + D + U_0$, where L_0, D and U_0 are portions of A: subdiagonal (strictly lower triangular), diagonal and superdiagonal (strictly upper triangular), respectively. We assume that no diagonal element of A is zero (to provide non-singularity of D and $(L_0 + D)$).

Method 5.2 (Jacobi)

$$Dx^{k+1} = -(L_0 + U_0)x^k + b, \qquad H_{\mathrm{J}} = -D^{-1}(L_0 + U_0).$$

Method 5.3 (Gauss–Seidel)

$$(L_0 + D)x^{k+1} = -U_0 x^k + b \qquad H_{\mathrm{GS}} = -(L_0 + U_0)^{-1}U_0.$$

Remark 5.4 There is no need to invert any matrix. Writing the original system $Ax = b$ as

$$\textstyle\sum_{j=1}^n a_{ij}x_j = b_i, \qquad i = \overline{1,n}\,,$$

the Jacobi method reads

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

while Gauss–Seidel becomes

$$x_i^{(k+1)} = -\frac{1}{a_{ii}}\left(\textstyle\sum_{j<i} a_{ij}x_j^{(k+1)} + \sum_{j>i} a_{ij}x_j^{(k)} - b_i\right), \qquad i = \overline{1,n}\,.$$

Scheme 5.5 (Iterative refinement) This is the scheme

$$x^{k+1} = x^k - S(Ax^k - b).$$

If $S = A^{-1}$, then $x^{k+1} = A^{-1}b = x^*$, so that one should choose S as an approximation to A^{-1}. The iteration matrix for this scheme is

$$H_{\mathrm{S}} = I - SA.$$

Remark 5.6 Any splitting can be viewed as an iterative refinement, e.g.,

$$\text{Jacobi:} \quad S = D^{-1}, \qquad \text{Gauss-Seidel:} \quad S = (L_0 + D)^{-1}.$$

Method 5.7 (Simple iteration)

$$x^{k+1} = x^k - \tau(Ax^k - b), \quad \tau \in \mathbb{R}.$$

5.2 Necessary and sufficient conditions for convergence

Definition 5.8 Let $A \in \mathbb{R}^{n\times n}$. The set $\sigma(A) := (\lambda_1, \dots, \lambda_n)$ of the eigenvalues of A is called the *spectrum* of A, and the value

$$\rho(A) := \max_i |\lambda_i|$$

is called the *spectral radius* of A.

Theorem 5.9 *Let $H \in \mathbb{R}^{n\times n}$. Then $\lim\limits_{k\to\infty} H^k z = 0$ for every $z \in \mathbb{R}^n$ if and only if $\rho(H) < 1$.*

Proof. 1) We commence with the case $\rho(H) \geq 1$ and wish to demonstrate that, for some *real* z, the vector $H^k z$ need not tend to 0. Let λ be an eigenvalue of (the real) H, real or complex, such that $|\lambda| = \rho(H) \geq 1$, and let w be a corresponding eigenvector, i.e., $Hw = \lambda w$. Then $H^k w = \lambda^k w$, and

$$\|H^k w\|_\infty = |\lambda|^k \|w\|_\infty \geq \|w\|_\infty =: \gamma > 0. \tag{5.2}$$

If w is real, we choose $z = w$, hence $H^k z \geq \gamma$, and this cannot tend to zero.

If w is complex, then $w = u + \mathrm{i}v$ with some real vectore u, v. But then at least one of the sequences $(H^k u), (H^k v)$ does not tend to zero. For if both do, then also $H^k w = H^k u + \mathrm{i}H^k v \to 0$, and this contradicts (5.2). This completes the proof of the 'only if' part of the theorem.

2) Now we turn to the 'if' case, i.e., $\rho(H) < 1$, where we assume for simplicity that H possesses n linearly independent eigenvectors (w_j) such that $Hw_j = \lambda_j w_j$. Linear independence means that every $z \in \mathbb{R}^n$ can be expressed as a linear combination of the eigenvectors, i.e., there exist $(c_j) \in \mathbb{C}$ such that $z = \sum_{j=1}^n c_j w_j$. Thus,

$$H^k z = \textstyle\sum_{j=1}^n c_j \lambda_j^k w_j, \qquad k = 0, 1, \dots$$

and since $|\lambda_j| \leq \rho(H) < 1$ we have $\lim_{k\to\infty} H^k z = 0$, as required. ∎

Theorem 5.10 *Let x^*, a solution of $Ax = b$, satisfy $x^* = Hx^* + v$ and we are given the scheme*

$$x^{k+1} = Hx^k + v, \qquad x^0, v \in \mathbb{R}^n. \tag{5.3}$$

Then $x^k \to x^*$ for any choice of x^0 if an only if $\rho(H) < 1$.

Proof. For the error $e^k := x^k - x^*$, substracting $x^* = Hx^* + v$ from (5.3), we obtain $e^{k+1} = He^k$, hence $e^k = H^k e^0$. Now, by Theorem 5.9, $e^k \to 0$ for any e^0 iff $\rho(H) < 1$. ∎

Theorem 5.11 *Let A be positive definite. Then the method of simple iteration*

$$x^{k+1} = x^k - \tau(Ax^k - b)$$

converges if and only if $\tau \in (0, \frac{2}{\rho(A)})$.

Proof. Let $\{\lambda_i\}$ be the spectrum of A. Then the spectrum of the iteration matrix H_τ is

$$\sigma(H_\tau) = \sigma(I - \tau A) = \{1 - \tau\lambda_i\}.$$

Since for a positive definite A we have $0 < \lambda_i \leq \rho(A)$, it follows that

$$\rho(H_\tau) < 1 \quad \Leftrightarrow \quad -1 < 1 - \tau\lambda_i < 1 \quad \Leftrightarrow \quad \tau \in (0, \tfrac{2}{\rho(A)}).$$ ∎

A non-trivial application of Theorem 5.10 is

Theorem 5.12 1) *If A is symmetric positive definite, then the Gauss-Seidel method converges.*
2) *If both A and $2D - A$ are positive definite, then the Jacobi method converges as well.*

Proof. Next year in Numerical Analysis II. ∎

5.3 Examples

Example 5.13 Jacobi and Gauss–Seidel methods for an approximate solution of

$$\begin{bmatrix} 4 & 2 & 1 \\ 2 & 5 & 2 \\ 1 & 2 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 5 \\ 4 \\ 7 \end{bmatrix} \quad \text{with the starting vector } x^{(0)} = (1,1,1)^T.$$

1) The Jacobi method:

$$\begin{aligned} x_1^{(k+1)} &= \tfrac{1}{4}\,(5 \qquad\quad -2x_2^{(k)} \quad -x_3^{(k)}) \\ x_2^{(k+1)} &= \tfrac{1}{5}\,(4 -2x_1^{(k)} \qquad\quad -2x_3^{(k)}) \\ x_3^{(k+1)} &= \tfrac{1}{6}\,(7 \;\; -x_1^{(k)} -2x_2^{(k)}) \end{aligned}$$

With $x^{(0)} = (1,1,1)^T$, the first two iterations are

$$\begin{aligned} x_1^{(1)} &= \tfrac{1}{4}\,(5-2\cdot 1-1\cdot 1) &&= \tfrac{1}{2} & \qquad & x_1^{(2)} &= \tfrac{1}{4}\,(5-2\cdot 0-1\cdot \tfrac{2}{3}) &&= \tfrac{13}{12} \\ x_2^{(1)} &= \tfrac{1}{5}\,(4-2\cdot 1-2\cdot 1) &&= 0 & \Rightarrow & x_2^{(2)} &= \tfrac{1}{5}\,(4-2\cdot \tfrac{1}{2}-2\cdot \tfrac{2}{3}) &&= \tfrac{1}{3} \\ x_3^{(1)} &= \tfrac{1}{6}\,(7-1\cdot 1-2\cdot 1) &&= \tfrac{2}{3} & & x_3^{(2)} &= \tfrac{1}{6}\,(7-1\cdot \tfrac{1}{2}-2\cdot 0) &&= \tfrac{13}{12} \end{aligned}$$

2) The Gauss–Seidel method:

$$\begin{aligned} x_1^{(k+1)} &= \tfrac{1}{4}\,(5 \qquad\quad -2x_2^{(k)} \quad -x_3^{(k)}) \\ x_2^{(k+1)} &= \tfrac{1}{5}\,(4-2x_1^{(k+1)} \qquad\quad -2x_3^{(k)}) \\ x_3^{(k+1)} &= \tfrac{1}{6}\,(7 \;\; -x_1^{(k+1)} -2x_2^{(k+1)}) \end{aligned}$$

With $x^{(0)} = (1,1,1)^T$, the first two iterations are

$$\begin{aligned} x_1^{(1)} &= \tfrac{1}{4}\,(5-2\cdot 1-1\cdot 1) &&= \tfrac{1}{2} & \qquad & x_1^{(2)} &= \tfrac{1}{4}\,(5-2\cdot \tfrac{1}{5}-1\cdot \tfrac{61}{60}) &&= \tfrac{43}{48} &&= 0.8958 \\ x_2^{(1)} &= \tfrac{1}{5}\,(4-2\cdot \tfrac{1}{2}-2\cdot 1) &&= \tfrac{1}{5} & \Rightarrow & x_2^{(2)} &= \tfrac{1}{5}\,(4-2\cdot \tfrac{43}{48}-2\cdot \tfrac{61}{60}) &&= \tfrac{7}{200} &&= 0.035 \\ x_3^{(1)} &= \tfrac{1}{6}\,(7-1\cdot \tfrac{1}{2}-2\cdot \tfrac{1}{5}) &&= \tfrac{61}{60} & & x_3^{(2)} &= \tfrac{1}{6}\,(7-1\cdot \tfrac{43}{48}-2\cdot \tfrac{7}{200}) &&= \tfrac{7241}{7200} &&= 1.0057 \end{aligned}$$

3) The exact solution is $x^* = (1,0,1)^T$.

4) Both methods converge (because A is diagonally dominant), the Gauss–Seidel method being much faster.

5.4 Exercises

Exercises with a $*$-mark are *not* subject to supervision! They are just for fun!

5.1. The iteration $x^{k+1} = Hx^k + b$ is applied for $k = 0, 1, \ldots$, where H is the real 2×2 matrix

$$H = \begin{bmatrix} \alpha & \gamma \\ 0 & \beta \end{bmatrix},$$

with γ large and $|\alpha| < 1$, $|\beta| < 1$. Calculate the elements of H^k and show that they tend to zero as $k \to \infty$. Further, establish the equation $x^k - x^* = H^k(x^0 - x^*)$, where x^* is defined by $x^* = Hx^* + b$. Thus deduce that the sequence $(x^k)_{k=0}^{\infty}$ converges to x^*.

5.2. For some choice of x^0 the iterative method

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} x^{k+1} + \begin{bmatrix} 0 & 0 & 0 \\ \xi & 0 & 0 \\ \eta & \zeta & 0 \end{bmatrix} x^k = b$$

is applied for $k = 0, 1, \ldots$, in order to solve the linear system

$$\begin{bmatrix} 1 & 1 & 1 \\ \xi & 1 & 1 \\ \eta & \zeta & 1 \end{bmatrix} x = b,$$

where ξ, η and ζ are constants. Find all values of the constants such that the sequence $(x^k)_{k=0}^{\infty}$ converges for every x^0 and b. Give an example of nonconvergence when $\xi = \eta = \zeta = -1$. Is the solution always found in at most two iterations when $\xi = \zeta = 0$?

5.3*. The complete proof of the 'if' case of Theorem 5.9 exploits the so-called Jordan normal form of the matrix H, namely $H = SJS^{-1}$, where J is a block diagonal matrix consisting of the Jordan blocks

$$J = \begin{bmatrix} \boxed{J_1} & & & \\ & \boxed{J_2} & & \\ & & \ddots & \\ & & & \boxed{J_r} \end{bmatrix}, \qquad J_i = \begin{bmatrix} \lambda_i & 1 & & \\ & \lambda_i & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{bmatrix}, \qquad J_i \in \mathbb{R}^{n_i \times n_i}, \qquad \textstyle\sum_i n_i = n.$$

Prove that $J_i^k \to 0$ if $|\lambda_i| < 1$. [*Hint*: Split $J_i = \lambda_i I + P$, notice that $P^\ell = 0$ for $\ell \geq n_i$, and evaluate the terms of expansion $(\lambda_i I + P)^k = \sum_{\ell=0}^{n_i-1} \binom{k}{\ell} \lambda_i^{k-\ell} P^\ell$.]