CG-Method as an Iterative Method, Preconditioning

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前言

Consider the linear system of a symmetric positive definite matrix A

$$Ax = b. \tag{1}$$

Let C be a nonsingular symmetric matrix and consider a new linear system

$$\tilde{A}\tilde{x} = \tilde{b} \tag{2}$$

with $\tilde{A} = C^{-1}AC^{-1}$ s.p.d., $\tilde{b} = C^{-1}b$ and $\tilde{x} = Cx$.

Applying CG-method to (2) it yields:

Choose $\tilde{x}_0$, $\tilde{r}_0 = \tilde{b} - \tilde{A}\tilde{x}_0 = \tilde{p}_0$.

If $\tilde{r}_0 = 0$, stop, otherwise for $k = 0,\ 1,\ 2,\ \ldots,$

$$\left\{\begin{array}{ll} (a) & \tilde{\alpha}_k = \tilde{p}_k^T\tilde{r}_k/\tilde{p}_k^T C^{-1}AC^{-1}\tilde{p}_k, \\ (b) & \tilde{x}_{k+1} = \tilde{x}_k + \tilde{\alpha}_k\tilde{p}_k, \\ (c) & \tilde{r}_{k+1} = \tilde{r}_k - \tilde{\alpha}_k C^{-1}AC^{-1}\tilde{p}_k, \\ & \text{if } \ \tilde{r}_{k+1} = 0 \text{ stop; otherwise,} \\ (d) & \tilde{\beta}_k = -\tilde{r}_{k+1}^T C^{-1}AC^{-1}\tilde{p}_k/\tilde{p}_k C^{-1}AC^{-1}\tilde{p}_k, \\ (e) & \tilde{p}_{k+1} = \tilde{r}_{k+1} + \tilde{\beta}_k\tilde{p}_k. \end{array}\right. \tag{3}$$

前言

Simplification: Let

$$C^{-1}\tilde{p}_k = p_k, \quad x_k = C^{-1}\tilde{x}_k, \quad z_k = C^{-1}\tilde{r}_k.$$

Then

$$r_k = C\tilde{r}_k = C\left(\tilde{b} - \tilde{A}\tilde{x}_k\right) = C\left(C^{-1}b - C^{-1}AC^{-1}Cx_k\right) = b - Ax_k.$$

and

$$C^2\mathfrak{z}_k = r_k \Longleftrightarrow M\mathfrak{z}_k = r_k.$$

前言

[Preconditioned CG-method (PCG)]

$M = C^2$, choose $x_0 = C^{-1}\tilde{x}_0$, $r_0 = b - Ax_0$, solve $Mp_0 = r_0$.

If $r_0 = 0$ stop, otherwise for $k = 0,\ 1,\ 2, \ldots.,$

$$\left\{\begin{array}{ll} (a) & \alpha_k = p_k^T r_k / p_k^T A p_k, \\ (b) & x_{k+1} = x_k + \alpha_k p_k, \\ (c) & r_{k+1} = r_k - \alpha_k A p_k, \\ & \text{if } r_{k+1} = 0, \text{ stop; otherwise } M z_{k+1} = r_{k+1}, \\ (d) & \beta_k = -z_{k+1}^T A p_k / p_k^T A p_k, \\ (e) & p_{k+1} = z_{k+1} + \beta_k p_k. \end{array}\right. \tag{4}$$

Algorithm 4 is CG-method with preconditioner M. If $M = I$, then it is CG-method.

Additional cost per step: solve one linear system $Mz = r$ for z.

Advantage: $\text{cond}(M^{-1/2}AM^{-1/2}) \ll \text{cond}(A)$.

一、A new point of view of PCG

From [(II) Conjugate Gradient Method] (21) and Theorem 4.8 follows that $p_i{}^T r_k = 0$ for $i < k$,
i.e., $(r_i{}^T + \beta_{i-1} p_{i-1}{}^T) r_k = r_i{}^T r_k = 0$, $i < k$ and

$$p_i{}^T A p_j = 0, i \neq j.$$

That is, the CG method requires $r_i{}^T r_j = 0$, $i \neq j$. So, the PCG method satisfies $p_i{}^T C^{-1} A C^{-1} p_j = 0 \Leftrightarrow \tilde{r}_j^T \tilde{r}_j = 0, \quad i \neq j$ and requires

$$\begin{aligned} z_i^T M z_j &= r_i^T M^{-1} M M^{-1} r_j = r_i{}^T M^{-1} r_j \\ &= \left(r_i{}^T C^{-1}\right)\left(C^{-1} r_j\right) = \tilde{r_i}^T \tilde{r_j} = 0, \quad i \neq j. \end{aligned}$$

Consider the iteration (in two parameters):

$$x_{k+1} = x_{k-1} + \omega_{k+1} \left(\alpha_k z_k + x_k - x_{k-1}\right) \tag{5}$$

with α_k and ω_{k+1} being two undetermined parameters.

一、A new point of view of PCG

Let $A = M - N$. Then from $Mz_k = r_k \equiv b - Ax_k$ follows that

$$\begin{aligned} Mz_{k+1} &= b - A\left(x_{k-1} + \omega_{k+1}\left(\alpha_k z_k + x_k - x_{k-1}\right)\right) \\ &= Mz_{k-1} - \omega_{k+1}\left[\alpha_k (M-N) z_k + M(z_{k-1} - z_k)\right] \end{aligned} \qquad (6)$$

For PCG method $\{\alpha_k, \omega_{k+1}\}$ are computed so that

$$z_p{}^T M z_q = 0, \quad p \neq q,\ p, q = 0, 1, \cdots, n-1. \qquad (7)$$

Since $M > 0$, there is some $k \leq n$ such that $z_k = 0$. Thus, $x_k = x$, the iteration converges no more than n steps. We show that (7) holds by induction. Assume

$$z_p{}^T M z_q = 0, \quad p \neq q,\ p, q = 0, 1, \cdots, k \qquad (8)$$

holds until k.

一、A new point of view of PCG

If we choose

$$\alpha_k = {z_k}^T M z_k \Big/ {z_k}^T (M - N) z_k,$$

then

$$z_k{}^T M z_{k+1} = 0$$

and if we choose

$$\omega_{k+1} = \left(1 - \alpha_k \frac{z_{k-1}^T N z_k}{z_{k-1}^T M z_{k-1}} \right)^{-1}, \qquad (9)$$

then

$$z_{k-1}^T M z_{k+1} = 0.$$

一、A new point of view of PCG

From (6) for $j < k-1$ we have

$$z_j{}^T M z_{k+1} = \alpha_k \omega_{k+1} z_j{}^T N z_k. \qquad (10)$$

But (6) holds for $j < k-1$,

$$M z_{j+1} = M z_{j-1} - \omega_{j+1} \left(\alpha_j (M-N) z_j + M(z_{j-1} - z_j) \right). \qquad (11)$$

Multiplying (11) by $z_k{}^T$ we get

$$z_k{}^T N z_j = 0.$$

Since $N = N^T$, it follows that

$$z_j{}^T M z_{k+1} = 0, \quad \text{for} \quad j < k-1.$$

Thus, we proved that $z_p{}^T M z_q = 0$, $p \neq q$, $p,\ q = 0, 1, \cdots, n-1$. ■

一、A new point of view of PCG

Consider (5) again

$$x_{k+1} = x_{k-1} + \omega_{k+1}(\alpha_k z_k + x_k - x_{k-1}).$$

Since $Mz_k = r_k = b - Ax_k$, if we set $\omega_{k+1} = \alpha_k = 1$, then

$$x_{k+1} = x_k + z_k = x_k + M^{-1} r_k. \tag{12}$$

Here z_k is referred to as a correction . Write $A = M - N$. Then (12) becomes

$$\begin{aligned} x_{k+1} &= x_k + M^{-1}(b - Ax_k) \\ &= x_k + M^{-1}(b - (M - N)x_k) \\ &= M^{-1}Nx_k + M^{-1}b. \end{aligned} \tag{13}$$

一、A new point of view of PCG

Recall the Iterative Improvement in Subsection

Solve $Ax = b$,

$r_k = b - Ax_k$,

$Az_k = r_k, \leftrightarrow Mz_k = r_k$.

$x_{k+1} = x_k + z_k$.

(i) **Jacobi method** $(\omega_{k+1} = \alpha_k = 1)$**:** $A = D - (L + R)$,

$$\begin{aligned} x_{k+1} &= x_k + D^{-1} r_k \\ &= x_k + D^{-1}(b - Ax_k) \\ &= D^{-1}(L + R)x_k + D^{-1}b \end{aligned}$$

(ii) **Gauss-Seidel** $(\omega_{k+1} = \alpha_k = 1)$**:** $A = (D - L) - R$,

$$\begin{aligned} x_{k+1} &= x_k + z_k \\ &= x_k + (D - L)^{-1}(b - Ax_k) \\ &= (D - L)^{-1} R x_k + (D - L)^{-1} b. \end{aligned}$$

一、A new point of view of PCG

(iii) **SOR-method** $(\omega_{k+1} = 1, \alpha_k = \omega)$: Solve $\omega A x = \omega b$. Write

$$\omega A = (D - \omega L) - ((1-\omega)D + \omega R) \equiv M - N.$$

Then with $A = D - L - R$ we have

$$\begin{aligned}
x_{k+1} &= (D-\omega L)^{-1}(\omega R + (1-\omega)D)x_k + (D-\omega L)^{-1}\omega b \\
&= (D-\omega L)^{-1}((D-\omega L) - \omega A)x_k + (D-\omega L)^{-1}\omega b \\
&= (I - (D-\omega L)^{-1}\omega A)x_k + (D-\omega L)^{-1}\omega b \\
&= x_k + (D-\omega L)^{-1}\omega(b - Ax_k) \\
&= x_k + \omega M^{-1} r_k \\
&= x_k + \omega z_k.
\end{aligned}$$

一、A new point of view of PCG

(iv) **Chebychev Semi-iterative method (later!)** $(\omega_{k+1} = c_{k+1}, \alpha_k = \gamma)$:

$$x_{k+1} = x_{k-1} + \omega_{k+1}\left(\gamma z_k + x_k - x_{k-1}\right).$$

We can think of the scalars ω_{k+1}, α_k in (5) as acceleration parameters that can be chosen to speed the convergence of the iteration $Mx_{k+1} = Nx_k + b$. Hence any iterative method based on the splitting $A = M - N$ can be accelerated by the Conjugate Gradient Algorithm so long as M (the preconditioner) is symmetric and positive definite.

一、A new point of view of PCG

Choices of M (Criterion):

(i) $\mathrm{cond}(M^{-1/2}AM^{-1/2})$ is nearly by 1, i.e.,
$M^{-1/2}AM^{-1/2} \approx I, A \approx M$.

(ii) The linear system $Mz = r$ must be easily solved. e.g. $M = LL^T$
(see Section 16.)

(iii) M is symmetric positive definite.

一、A new point of view of PCG

SSOR (Symmetric Successive Over Relaxation):

A is symmetric and $A = D - L - L^T$. Let

$$\begin{cases} M_\omega : \ = D - \omega L, \\ N_\omega : \ = (1-\omega)D + \omega L^T, \end{cases} \quad \text{and} \quad \begin{cases} M_\omega^T = D - \omega L^T, \\ N_\omega^T = (1-\omega)D + \omega L. \end{cases}$$

Then from the iterations

$$\begin{aligned} M_\omega x_{i+1/2} &= N_\omega x_i + \omega b, \\ M_\omega^T x_{i+1} &= N_\omega^T x_{i+1/2} + \omega b, \end{aligned}$$

follows that

$$\begin{aligned} x_{i+1} &= \left(M_\omega^{-T} N_\omega^T M_\omega^{-1} N_\omega\right) x_i + \tilde{b} \\ &\equiv G x_i + \omega \left(M_\omega^{-T} N_\omega^T M_\omega^{-1} + M_\omega^{-T}\right) b \\ &\equiv G x_i + M(\omega)^{-1} b. \end{aligned}$$

一、A new point of view of PCG

It holds that

$$
\begin{aligned}
&((1-\omega)D+\omega L)\,(D-\omega L)^{-1}+I \\
&=(\omega L-D-\omega D+2D)(D-\omega L)^{-1}+I \\
&=-I+(2-\omega)D(D-\omega L)^{-1}+I \\
&=(2-\omega)D(D-\omega L)^{-1},
\end{aligned}
$$

Thus

$$
M(\omega)^{-1}=\omega\left(D-\omega L^{T}\right)^{-1}(2-\omega)D(D-\omega L)^{-1},
$$

then

$$
\begin{aligned}
M(\omega) &= \frac{1}{\omega(2-\omega)}(D-\omega L)D^{-1}\left(D-\omega L^{T}\right) \qquad (14)\\
&\approx (D-L)D^{-1}\left(D-L^{T}\right),\ (\omega=1).
\end{aligned}
$$

一、A new point of view of PCG

For a suitable ω the condition number $\text{cond}(M(\omega)^{-1/2}AM(\omega)^{-1/2})$. Can be considered smaller than $\text{cond}(A)$. Axelsson(1976) showed (without proof): Let

$$\mu = \max_{x \neq 0} \frac{x^T D x}{x^T A x} \quad (\leq \text{cond}(A))$$

and

$$\delta = \max_{x \neq 0} \frac{x^T (LD^{-1}L^T - \frac{1}{4}D)x}{x^T A x} \geq \frac{1}{4}.$$

Then

$$\text{cond}\left(M(\omega)^{-1/2}AM(\omega)^{-1/2}\right) \leq \frac{1 + \frac{(2-\omega)^2}{4\omega} + \omega\delta}{2\omega} = \kappa(\omega)$$

for $\omega^* = \frac{2}{1+2\sqrt{(2\delta+1)/2\mu}}$, $\kappa(\omega^*)$ is minimal and $\kappa(\omega^*) = 1/2 + \sqrt{(1/2+\delta)\mu}$.

Especially

$$\text{cond}\left(M(\omega^*)^{-1/2}AM(\omega^*)^{-1/2}\right) \leq \frac{1}{2} + \sqrt{(1/2+\delta)\text{cond}(A)} \sim \sqrt{\text{cond}(A)}.$$

Disadvantage : μ, δ in general are unknown.

二、Incomplete Cholesky Decomposition

Let A be sparse and symmetric positive definite. Consider the Cholesky decomposition of $A = LL^T$. L is a lower triangular matrix with $l_{ii} > 0$ $(i = 1, ..., n)$. L can be heavily occupied (fill-in). Consider the following decomposition

$$A = LL^T - N, \tag{15}$$

where L is a lower triangular matrix with prescribed reserved pattern E and N is "small".

Reserved Pattern: $E \subset \{1, ..., n\} \times \{1, ..., n\}$ with

$$\begin{cases} (i,i) \in E, \ i = 1, ..., n \\ (i,j) \in E \ \Rightarrow \ (j,i) \in E \end{cases}$$

For a given reserved pattern E we construct the matrices L and N as in (15) with

(i) $A \quad = LL^T - N,$ (16a)

(ii) $L:$ lower triangular with $l_{ii} > 0$ and $l_{ij} \neq 0 \ \Rightarrow \ (i,j) \in E$ (16b)

(iii) $N \quad = (n_{ij}), \ n_{ij} = 0,$ if $(i,j) \in E$ (16c)

二、Incomplete Cholesky Decomposition

First step: Consider the Cholesky decomposition of A,

$$A = \begin{pmatrix} a_{11} & a_1^T \\ a_1 & A_1 \end{pmatrix} = \begin{pmatrix} \sqrt{a_{11}} & 0 \\ a_1/\sqrt{a_{11}} & I \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \overline{A}_1 \end{pmatrix} \begin{pmatrix} \sqrt{a_{11}} & a_1^T/\sqrt{a_{11}} \\ 0 & I \end{pmatrix},$$

where $\overline{A}_1 = A_1 - a_1 a_1^T / a_{11}$. Then

$$A = L_1 \begin{pmatrix} 1 & 0 \\ 0 & \overline{A}_1 \end{pmatrix} L_1^T.$$

二、Incomplete Cholesky Decomposition

For the Incomplete Cholesky decomposition the first step will be so modified. Define $b_1 = (b_{21}, ..., b_{n1})^T$ and $c_1 = (c_{21}, ..., c_{n1})^T$ by

$$b_{j1} = \begin{cases} a_{j1}, & (j,1) \in E, \\ 0, & \text{otherwise}, \end{cases} \qquad c_{j1} = b_{j1} - a_{j1} = \begin{cases} 0, & (j,1) \in E, \\ -a_{j1}, & \text{otherwise}. \end{cases} \tag{17}$$

Then

$$A = \begin{pmatrix} a_{11} & b_1^T \\ b_1 & A_1 \end{pmatrix} - \begin{pmatrix} 0 & c_1^T \\ c_1 & 0 \end{pmatrix} = \tilde{B}_0 - C_1. \tag{18}$$

Compute the Cholesky decomposition on $\tilde{B}$, we get

$$\tilde{B}_0 = \begin{pmatrix} \sqrt{a_{11}} & 0 \\ b_1/\sqrt{a_{11}} & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & \bar{B}_1 \end{pmatrix} \begin{pmatrix} \sqrt{a_{11}} & b_1^T/\sqrt{a_{11}} \\ 0 & I \end{pmatrix} = L_1 B_1 L_1^T \tag{19}$$

and

$$\bar{B}_1 = A_1 - \frac{b_1 {b_1}^T}{a_{11}}. \tag{20}$$

二、Incomplete Cholesky Decomposition

Then

$$A = L_1 B_1 {L_1}^T - C_1. \tag{21}$$

Consequently, compute the Cholesky decomposition on B_1:

$$B_1 = L_2 B_2 L_2^T - C_2$$

Thus,

$$A = L_1 L_2 B_2 L_2^T L_1^T - L_1 C_2 L_1^T - C_1 \tag{22}$$

and so on, hence

$$A = L_1 \cdots L_n I L_n^T \cdots L_1^T - C_{n-1} - C_{n-2} - \cdots - C_1 \tag{23}$$

with

$$L = L_1 \cdots L_n \text{ and } N = C_1 + C_2 + \cdots + C_n. \tag{24}$$

二、Incomplete Cholesky Decomposition

Lemma 5.1

Let A be s.p.d. E be a reserved patten. Then there is at most a decomposition $A = LL^T - N$*, which satisfies the conditions:*

$$(16b) \;:\; L \text{ is lower triangular with } l_{ii} > 0,\; l_{ij} \neq 0 \Longrightarrow (i,j) \in E.$$

$$(16c) \;:\; N = (n_{ij}),\; n_{ij} = 0,\; \text{if } (i,j) \in E.$$

二、Incomplete Cholesky Decomposition

The Incomplete Cholesky decomposition may not exist, if

$$s_m := a_{mm} - \sum_{k=1}^{m-1} (l_{mk})^2 \leq 0.$$

Example 1

Let

$$A = \begin{bmatrix} 1 & -1 & 0 & 2 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -3 \\ 2 & 0 & -3 & 10 \end{bmatrix}.$$

The Cholesky decomposition of A follows $L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 2 & 2 & -1 & 1 \end{bmatrix}.$

二、Incomplete Cholesky Decomposition

Example 2

Consider the Incomplete Cholesky decomposition with patten

$$E = E(A) = \begin{bmatrix} \times & \times & 0 & \times \\ \times & \times & \times & 0 \\ 0 & \times & \times & \times \\ \times & 0 & \times & \times \end{bmatrix}.$$

Above procedures (17)-(24) can be performed on A until the computation of l_{44} (see proof of Lemma 5.1),

$$l_{44}^2 = a_{44} - l_{41}^2 - l_{42}^2 - l_{43}^2 = 10 - 9 - 4 = -3.$$

The Incomplete Cholesky decomposition does not exit for this pattern E.

二、Incomplete Cholesky Decomposition

Example 3

Now take

$$E = \begin{pmatrix} \times & \times & 0 & 0 \\ \times & \times & \times & 0 \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \end{pmatrix} \Longrightarrow L \text{ exists and } L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -3 & 1 \end{pmatrix}.$$

二、Incomplete Cholesky Decomposition

Find the certain classes of matrices, which have no breakdown by Incomplete Cholesky decomposition. The classes are

M-matrices, H-matrices.

Definition 5.2

$A \in \mathbb{R}^{n\times n}$ *is an* M*-matrix. If there is a decomposition* $A = \sigma I - B$ *with* $B \geq 0$ $(B \geq 0 \Leftrightarrow b_{ij} \geq 0$ *for* $i, j = 1, ..., n)$ *and* $\rho(B) = \max\{|\lambda| : \lambda$ *is an eigenvalue of* $B\} < \sigma$. Equivalence: $a_{ij} \leq 0$ *for* $i \neq j$ *and* $A^{-1} \geq 0$.

二、Incomplete Cholesky Decomposition

Lemma 5.3

A is symmetric, $a_{ij} \leq 0$, $i \neq j$. Then the following statements are equivalent
(i) *A is an M-matrix.*
(ii) *A is s.p.d.*

Theorem 5.4

Let A be a symmetric M-matrix. Then the Incomplete Cholesky method described in (17)-(24) is executable and yields a decomposition $A = LL^T - N$, which satisfies (16).

二、Incomplete Cholesky Decomposition

Definition 5.5

$A \in \mathbb{R}^{n \times n}$. *Decomposition* $A = B - C$ *is called regular, if* $B^{-1} \geq 0$, $C \geq 0$ *(regular splitting)*.

二、Incomplete Cholesky Decomposition

Theorem 5.6

Let $A^{-1} \geq 0$ and $A = B - C$ is a regular decomposition. Then $\rho(B^{-1}C) < 1$. i.e., the iterative method $Bx_{k+1} = Cx_k + b$ for $Ax = b$ is convergent for all x_0.

Proof: Since $T = B^{-1}C \geq 0$, $B^{-1}(B - C) = B^{-1}A = I - T$, it follows that

$$(I - T)A^{-1} = B^{-1}.$$

Then

$$0 \leq \sum_{i=0}^{k} T^i B^{-1} = \sum_{i=0}^{k} T^i (I - T) A^{-1} = (I - T^{k+1}) A^{-1} \leq A^{-1}.$$

That is, the monotone sequence $\sum_{i=0}^{k} T^i B^{-1}$ is uniformly bounded. Hence $T^k B^{-1} \to 0$ for $k \to \infty$, then $T^k \to 0$ and $\rho(T) < 1$. ■

二、Incomplete Cholesky Decomposition

Theorem 5.7

If $A^{-1} \geq 0$ and $A = B_1 - C_1 = B_2 - C_2$ are two regular decompositions with $0 \leq C_1 \leq C_2$, then it holds $\rho({B_1}^{-1}C_1) \leq \rho({B_2}^{-1}C_2)$.

Proof: Let $A = B - C$, $A^{-1} \geq 0$. Then

$$\begin{aligned} \rho(B^{-1}C) &= \rho((A+C)^{-1}C) = \rho([A(I + A^{-1}C)]^{-1}C) \\ &= \rho((I + A^{-1}C)^{-1}A^{-1}C) = \frac{\rho(A^{-1}C)}{1 + \rho(A^{-1}C)}. \end{aligned}$$

$$[\lambda \to \frac{\lambda}{1+\lambda} \text{ monotone for } \lambda \geq 0].$$

Because $0 \leq C_1 \leq C_2$ it follows $\rho(A^{-1}C_1) \leq \rho(A^{-1}C_2)$. Then

$$\rho({B_1}^{-1}C_1) = \frac{\rho(A^{-1}C_1)}{1 + \rho(A^{-1}C_1)} \leq \frac{\rho(A^{-1}C_2)}{1 + \rho(A^{-1}C_2)} = \rho({B_2}^{-1}C_2),$$

since $\lambda \to \frac{\lambda}{1+\lambda}$ is monotone for $\lambda > 0$. ∎

二、Incomplete Cholesky Decomposition

Theorem 5.8

If A is a symmetric M-matrix, then the decomposition $A = LL^T - N$ *according to Theorem 5.4 is a regular decomposition.*

Proof: Because each $L_j^{-1} \geq 0$, it follows $(LL^T)^{-1} \geq 0$, (from $(I - le^T)^{-1} = (I + le^T)$, $l \geq 0$). $N = C_1 + C_2 + \cdots + C_{n-1}$ and all $C_i \geq 0$. ■

二、Incomplete Cholesky Decomposition

History:

(i) CG-method, Hestenes-Stiefel (1952).

(ii) CG-method as iterative method, Reid (1971).

(iii) CG-method with preconditioning, Concus-Golub-Oleary (1976).

(iv) Incomplete Cholesky decomposition, Meijerink-Van der Vorst (1977).

(v) Nonsymmetric matrix, H-matrix, Incomplete Cholesky decomposition, Manteufel (1979).

二、Incomplete Cholesky Decomposition

Other preconditioning:

(i) A blockform $A = [A_{ij}]$ with A_{ij} blocks. Take $M = \text{diag}[A_{11}, ..., A_{kk}]$.

(ii) Try Incomplete Cholesky decomposition: Breakdown can be avoided by two ways. If $z_i = a_{ii} - \Sigma_{k=1}^{i-1} l_{ik}^2 \leq 0$, breakdown, then either set $l_{ii} = 1$ and go on or set $l_{ik} = 0$, $(k = 1, .., i-1)$ until $z_i > 0$ (change reserved pattern E).

(iii) A is an arbitrary nonsingular matrix with all principle determinants $\neq 0$. Then $A = LDR$ exists, where D is diagonal, L and R^T are unit lower triangular. Consider the following generalization of Incomplete Cholesky decomposition.

二、Incomplete Cholesky Decomposition

Theorem 5.9

(Generalization) Let A *be an* $n \times n$ *matrix and* E *be an arbitrary reserved pattern with* $(i,i) \in E$, $i = 1, 2, \ldots, n$. *A decomposition of the form* $A = LDR - N$ *which satisfies:*

(i) L *is lower triangular,* $l_{ii} = 1$, $l_{ij} \neq 0$, *then* $(i,j) \in E$,

(ii) R *is upper triangular,* $r_{ii} = 1$, $r_{ij} \neq 0$, *then* $(i,j) \in E$,

(iii) D *is diagonal* $\neq 0$,

(iv) $N = (n_{ij})$, $n_{ij} = 0$ *for* $(i,j) \in E$.

is uniquely determined. (The decomposition almost exists for all matrices).

三、Chebychev Semi-Iteration Acceleration Method

Consider the linear system $Ax = b$. The splitting $A = M - N$ leads to the form

$$x = Tx + f,\ T = M^{-1}N \text{ and } f = M^{-1}b. \tag{25}$$

The basic iterative method of (25) is

$$x_{k+1} = Tx_k + f. \tag{26}$$

How to modify the convergence rate?

Definition 5.10

The iterative method (26) is called symmetrizable, if there is a matrix W with $\det W \neq 0$ and such that $W(I - T)W^{-1}$ is symmetric positive definite.

三、Chebychev Semi-Iteration Acceleration Method

Example 4

Let A and M be s.p.d., $A = M - N$ and $T = M^{-1}N$, then

$$I - T = I - M^{-1}N = M^{-1}(M - N) = M^{-1}A.$$

Set $W = M^{1/2}$. Thus,

$$W(I - T)W^{-1} = M^{1/2}M^{-1}AM^{-1/2} = M^{-1/2}AM^{-1/2} \text{ s.p.d.}$$

(i): $M = \text{diag}(a_{ii})$ Jacobi method.

(ii): $M = \frac{1}{\omega(2-\omega)}(D - \omega L)D^{-1}(D - \omega L^T)$ SSOR-method.

(iii): $M = LL^T$ Incomplete Cholesky decomposition.

(iv): $M = I \Rightarrow x_{k+1} = (I - A)x_k + b$ Richardson method.

三、Chebychev Semi-Iteration Acceleration Method

Lemma 5.11

If (26) is symmetrizable, then the eigenvalues μ_i of T are real and satisfy

$$\mu_i < 1, \text{ for } i = 1, 2, \ldots, n. \tag{27}$$

Proof: Since $W(I-T)W^{-1}$ is s.p.d., the eigenvalues $1-\mu_i$ of $I-T$ are large than zero. Thus μ_i are real and (27) holds. ■

Definition 5.12

Let $x_{k+1} = Tx_k + f$ be symmetrizable. The iterative method

$$\begin{cases} u_0 &= x_0, \\ u_{k+1} &= \alpha(Tu_k + f) + (1-\alpha)u_k \\ &= (\alpha T + (1-\alpha)I)u_k + \alpha f \equiv T_\alpha u_k + \alpha f. \end{cases} \tag{28}$$

is called an Extrapolation method of (26).

Remark 1

$T_\alpha = \alpha T + (1-\alpha)I$ is a new iterative matrix ($T_1 = T$). T_α arises from the decomposition $A = \frac{1}{\alpha}M - (N + (\frac{1}{\alpha} - 1)M)$.

三、Chebychev Semi-Iteration Acceleration Method

Theorem 5.13

If (26) is symmetrizable and T has the eigenvalues satisfying $\mu_1 \le \mu_2 \le \cdots \le \mu_n < 1$*, then it holds for* $\alpha^* = \frac{2}{2-\mu_1-\mu_2} > 0$ *that*

$$1 > \rho(T_{\alpha^*}) = \frac{\mu_n - \mu_1}{2 - \mu_1 - \mu_n} = \min_{\alpha} \rho(T_\alpha). \tag{29}$$

Proof: Eigenvalues of T_α are $\alpha\mu_i + (1-\alpha) = 1 + \alpha(\mu_i - 1)$. Consider the problem

$$\begin{aligned} & \min_{\alpha} \max_{i} |1 + \alpha(u_i - 1)| = \min! \\ \iff & |1 + \alpha(\mu_n - 1)| = |1 + \alpha(\mu_1 - 1)|, \\ \iff & 1 + \alpha(\mu_n - 1) = \alpha(1 - \mu_n) - 1 \text{ (otherwise } \mu_1 = \mu_n). \end{aligned}$$

This implies $\alpha = \alpha^* = \frac{2}{2-\mu_1-\mu_n}$, then $1 + \alpha^*(\mu_n - 1) = \frac{\mu_n-\mu_1}{2-\mu_1-\mu_n}$. ■

三、Chebychev Semi-Iteration Acceleration Method

From (26) and (28) follows that

$$u_k = \sum_{i=0}^{k} a_{ki} x_i, \text{ and } \sum_{i=0}^{k} a_{ki} = 1$$

with suitable a_{ki}. Hence, we have the following idea:

Find a sequence $\{a_{ki}\}$, $k = 1, 2, \ldots$, $i = 0, 1, 2, \ldots, k$ and $\sum_{i=0}^{k} a_{ki} = 1$ such that

$$u_k = \sum_{i=0}^{k} a_{ki} x_i, \; u_0 = x_0 \tag{30}$$

is a good approximation of x^* $(Ax^* = b)$. Hereby the cost of computation of u_k should not be more expensive than x_k.

三、Chebychev Semi-Iteration Acceleration Method

Error: Let

$$e_k = x_k - x^*, e_k = T^k e_0,\ e_0 = x_0 - x^* = u_0 - x^* = d_0. \qquad (31)$$

Hence,

$$\begin{aligned} d_k &= u_k - x^* = \sum_{i=0}^{k} a_{ki}(x_i - x^*) \qquad (32) \\ &= \sum_{i=0}^{k} a_{ki} T^i e_0 = (\sum_{ki}^{k} a_{ki} T^i) e_0 \\ &= \mathcal{P}_k(T) e_0 = \mathcal{P}_k(T) d_0, \end{aligned}$$

where

$$\mathcal{P}_k(\lambda) = \sum_{i=0}^{k} a_{ki} \lambda^i \qquad (33)$$

is a polynomial in λ with $\mathcal{P}_k(1) = 1$.

三、Chebychev Semi-Iteration Acceleration Method

Problem: Find $\mathcal{P}_k$ such that $\rho(\mathcal{P}_k(T))$ is small as possible.

Remark 2

Let $\|x\|_W = \|Wx\|_2$. *Then*

$$\begin{aligned} \|T\|_W &= \max_{x \neq 0} \frac{\|Tx\|_W}{\|x\|_W} \\ &= \max_{x \neq 0} \frac{\|WTW^{-1}Wx\|_2}{\|Wx\|_2} \\ &= \|WTW^{-1}\|_2 = \rho(T), \end{aligned}$$

because WTW^{-1} *is symmetric. We take* $\|\cdot\|_W$*-norm on both sides of (32) and have*

$$\begin{aligned} \|d_k\|_W &\leq \|\mathcal{P}_k(T)\|_W \|d_0\|_W = \|W\mathcal{P}_k(T)W^{-1}\|_2 \|d_0\|_2 \qquad (34) \\ &= \|\mathcal{P}_k(WTW^{-1})\|_2 \|d_0\|_W = \rho(\mathcal{P}_k(T))\|d_0\|_W. \end{aligned}$$

三、Chebychev Semi-Iteration Acceleration Method

Replacement problem: Let $1 > \mu_n \geq \cdots \geq \mu_1$ be the eigenvalues of T. Determine

$$\min \left[\{\max |\mathcal{P}_k(\lambda)| : \mu_1 \leq \lambda \leq \mu_n\} : \deg(\mathcal{P}_k) \leq k,\ \mathcal{P}_k(1) = 1 \right]. \qquad (35)$$

Solution of (35): The replacement problem

$$\max\{|\mathcal{P}_k(\lambda)| : 0 < a \leq \lambda \leq b\} = \min!,\ \mathcal{P}_k(0) = 1$$

has the solution

$$Q_k(t) = T_k\left(\frac{2t - b - a}{b - a}\right) \Big/ T_k\left(\frac{b + a}{a - b}\right).$$

三、Chebychev Semi-Iteration Acceleration Method

Let $\lambda = 1 - t$,then $1 - \mu_1 \leq t \leq 1 - \mu_n$, $P_k(\lambda) = P_k(1-t) \equiv \tilde{P}_k(t)$ with $\tilde{P}_k(0) = 1$. The problem (35) can be transformed to [(II) Conjugate Gradient Method] (34) as

$$\mathtt{min}[\mathtt{max}\{\tilde{P}_k(t) | 1 - \mu_1 \leq t \leq 1 - \mu_n\} : \deg(\tilde{P}_k) \leq k, \tilde{P}_k(0) = 1]$$

Hence, the solution of (35) is given by

$$Q_k(t) = T_k\Big(\frac{2t - \mu_1 - \mu_n}{\mu_1 - \mu_n}\Big) \Big/ T_k\Big(\frac{2 - \mu_1 - \mu_n}{\mu_1 - \mu_n}\Big). \tag{36}$$

Write $Q_k(t) := \sum_{i=0}^{k} a_{ki} t^i$. Then we have

$$u_k = \sum_{i=0}^{k} a_{ki} x_i,$$

which is called the **optimal Chebychev semi-iterative method**.

三、Chebychev Semi-Iteration Acceleration Method

Effective Computation of u_k: Using recursion of T_k:

$$\begin{cases} T_0(t) = 1, \quad T_1(t) = t, \\ T_{k+1}(t) = 2tT_k(t) - T_{k-1}(t), \end{cases}$$

we get

$$T_0(t) = 1,\ T_1(t) = t,\ T_{k+1}(t) = 2tT_k(t) - T_{k-1}(t).$$

Transforming $T_k(t)$ to the form of $Q_k(t)$ as in (36) we get

$$Q_0(t) = 1,\ Q_1(t) = \frac{2t - \mu_1 - \mu_n}{2 - \mu_1 - \mu_n} = pt + (1-p) \tag{37a}$$

and

$$Q_{k+1}(t) = [pt + (1-p)]c_{k+1}Q_k(t) + (1 - c_{k+1})\,Q_{k-1}(t), \tag{37b}$$

where

$$p = \frac{2}{2 - \mu_1 - \mu_n},\ c_{k+1} = \frac{2T_k(1/r)}{rT_{k+1}(1/r)},\ r = \frac{\mu_1 - \mu_n}{2 - \mu_1 - \mu_n}. \tag{38}$$

三、Chebychev Semi-Iteration Acceleration Method

Recursion for u_k:

$$\begin{aligned} d_{k+1} &= Q_{k+1}(T)d_0 = (pT + (1-p)I)c_{k+1}Q_k(T)d_0 + (1-c_{k+1})Q_{k-1}(T) \\ x^* &= (pT + (1-p)I)c_{k+1}x^* + (1-c_{k+1})x^* + p(I-T)x^*c_{k+1}. \end{aligned}$$

Adding above two equations together we get

$$\begin{aligned} u_{k+1} &= [pT + (1-p)I]c_{k+1}u_k + (1-c_{k+1})u_{k-1} + c_{k+1}pf \\ &= c_{k+1}p\left\{Tu_k + f - u_k\right\} + c_{k+1}u_k + (1-c_{k+1})\,u_{k-1}. \end{aligned}$$

Then we obtain the optimal Chebychev semi-iterative Algorithm.

三、Chebychev Semi-Iteration Acceleration Method

[Optimal Chebychev semi-iterative Algorithm]

$$
\begin{aligned}
&\text{Let } r = \frac{\mu_1 - \mu_n}{2 - \mu_1 - \mu_n},\ p = \frac{2}{2 - \mu_1 - \mu_n},\ c_1 = 2 \\
&u_0 = x_0, \\
&u_1 = p(Tu_0 + f) + (1 - p)u_0 \\
&\text{For } k = 1, 2, \cdots, \\
&\quad u_{k+1} = c_{k+1}\left[p(Tu_k + f) + (1 - p)u_k\right] + (1 - c_{k+1})\, u_{k-1}, \\
&\quad c_{k+1} = (1 - r^2/4\, c_k)^{-1}.
\end{aligned} \tag{39}
$$

三、Chebychev Semi-Iteration Acceleration Method

Remark 3

Here u_{k+1} can be rewritten as the three terms recursive formula with two parameters as in (5):

$$
\begin{aligned}
u_{k+1} &= c_{k+1}\left[p\left(Tu_k + f\right) + (1-p)u_k\right] + \left(1 - c_{k+1}\right)u_{k-1} \\
&= c_{k+1}\left[pM^{-1}\left((M-A)u_k + b\right) + (1-p)u_k\right] + u_{k-1} - c_{k+1}u_{k-1} \\
&= c_{k+1}\left[u_k + pM^{-1}\left(b - Au_k\right) - u_{k-1}\right] + u_{k-1} \\
&= u_{k-1} + c_{k+1}(p\mathfrak{z}_k + u_k - u_{k-1}),
\end{aligned}
$$

where $Mz_k = b - Au_k$. ■

三、Chebychev Semi-Iteration Acceleration Method

Recursion for c_k: Since

$$c_1 = \frac{2t_0}{rT_1(1/r)} = \frac{2}{r \cdot \frac{1}{r}} = 2,$$

thus

$$T_{k+1}\left(\frac{1}{r}\right) = \frac{2}{r} T_k\left(\frac{1}{r}\right) - T_{k-1}\left(\frac{1}{r}\right)$$

(from [(II) Conjugate Gradient Method] (35)). It follows

$$\frac{1}{c_{k+1}} = \frac{rT_{k+1}\left(\frac{1}{r}\right)}{2T_k\left(\frac{1}{r}\right)} = 1 - \frac{r^2}{4}\left[\frac{2T_{k-1}\left(\frac{1}{r}\right)}{rT_k\left(\frac{1}{r}\right)}\right] = 1 - \frac{r^2}{4} c_k.$$

Then we have

$$c_{k+1} = \frac{1}{(1 - (r^2/4)\, c_k)} \quad \text{with} \quad r = \frac{\mu_1 - \mu_n}{2 - \mu_1 - \mu_n}. \tag{40}$$

三、Chebychev Semi-Iteration Acceleration Method

Error estimate: It holds

$$\|u_k - x^*\|_W \le \left| T_k\left(\frac{2-\mu_1-\mu_n}{\mu_1-\mu_n}\right)\right|^{-1} \|u_0 - x^*\|_W. \tag{41}$$

Proof: From (34) and (36) we have

$$\begin{aligned}
\|d_k\|_W &= \|Q_k(T)d_0\|_W \le \rho\left(Q_k(T)\right)\|d_0\|_W \\
&\le \max\left\{|Q_k(\lambda)| : \mu_1 \le \lambda \le \mu_n\right\}\|d_0\|_W \\
&\le \left| T_k\left(\frac{2-\mu_1-\mu_n}{\mu_1-\mu_n}\right)\right|^{-1} \|d_0\|_W.
\end{aligned}$$

三、Chebychev Semi-Iteration Acceleration Method

We want to estimate the quantity $q_k := |T_k(1/r)|^{-1}$ (see also Lemma 4.11). From [(II) Conjugate Gradient Method] (36),we have

$$
\begin{aligned}
T_k\left(\frac{1}{r}\right) &= \frac{1}{2}\left[\left(\frac{1+\sqrt{1-r^2}}{r}\right)^k + \left(\frac{1-\sqrt{1-r^2}}{r}\right)^k\right] \\
&= \frac{1}{2}\left[\frac{(1+\sqrt{1-r^2})^k + (1-\sqrt{1-r^2})^k}{(r^2)^{k/2}}\right] \\
&= \frac{1}{2}\left[\frac{(1+\sqrt{1-r^2})^k + (1-\sqrt{1-r^2})^k}{\left[(1+\sqrt{1-r^2})(1-\sqrt{1-r^2})\right]^{k/2}}\right] \\
&= \frac{1}{2}\left(c^{k/2} + c^{-k/2}\right) \geq \frac{1}{2c^{k/2}},
\end{aligned}
$$

where $c = \frac{1-\sqrt{1-r^2}}{1+\sqrt{1-r^2}} < 1$.

三、Chebychev Semi-Iteration Acceleration Method

Thus $q_k \le 2c^{k/2}$. Rewrite the eigenvalues of $I - T$ as $\lambda_i = 1 - \mu_i$, $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n > 0$. Then

$$r = \frac{\mu_n - \mu_1}{2 - \mu_1 - \mu_n} = \frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n} = \frac{\kappa - 1}{\kappa + 1}, \quad \kappa = \frac{\lambda_1}{\lambda_n}$$

Thus, from $c = \frac{1-\sqrt{1-r^2}}{1+\sqrt{1-r^2}} = \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^2$ follows

$$q_k \le 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k. \tag{42}$$

That is, after k steps of the Chebychev semi-iterative method the residual $\|u_k - x^*\|_W$ is reduced by a factor $2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k$ from the original residual $\|u_0 - x^*\|_W$.

三、Chebychev Semi-Iteration Acceleration Method

If $\mu_{\min} = \mu_1 = 0$, then $q_k = T_k\left(\frac{2-\mu_n}{\mu_n}\right)^{-1}$. Table 1 shows the convergence rate of the quantity q_k. All above statements are true, if we replace μ_n by $\mu_n^{'}$ ($\mu_n^{'} \geq \mu_n$) and μ_1 by $\mu_1^{'}$ ($\mu_1^{'} \leq \mu_1$), because λ is still in $[\mu_1^{'}, \mu_n^{'}]$ for all eigenvalue λ of T.

μ_n	k	q_4	j	$j^{'}$	q_8	j	$j^{'}$
0.8	5	0.0426	8	14	9.06(-4)	17–18	31
0.9	10	0.1449	9–10	18	1.06(-2)	22–23	43
0.95	20	0.3159	11–12	22	5.25(-2)	29–30	57
0.99	100	0.7464	14–15	29	3.86(-1)	47	95

Table: Convergence rate of q_k where $j : \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^j \approx q_4,\ q_8$ and $j^{'} : \mu_n^{j^{'}} \approx q_4,\ q_8$.

三、Chebychev Semi-Iteration Acceleration Method

Example 5

Let $1 > \rho = \rho(T)$. If we set $\mu_n^{'} = \rho, \mu_1^{'} = -\rho$, then p and r defined in (38) become $p = 1$ and $r = \rho$, respectively. Algorithm 45 can be simplified by

$$\begin{aligned} u_0 &= x_0, \\ u_1 &= Tu_0 + f, \\ u_{k+1} &= c_{k+1}(Tu_k + f) + (1 - c_{k+1})u_{k-1}, \\ c_{k+1} &= \left(1 - \left(\rho^2/4\right)c_k\right)^{-1} \quad \text{with } c_1 = 2. \end{aligned}$$

Also, Algorithm 45 can be written by the form of (43), by replacing T by $T_{\alpha^*} = T_p = (pT + (1-p)I)$ and it leads to

$$u_{k+1} = c_{k+1}\left(T_p u_k + f\right) + \left(1 - c_{k+1}\right)u_{k-1}. \qquad (44)$$

Here $p\mu_1 + (1-p) = \frac{\mu_1 - \mu_n}{2 - \mu_1 - \mu_n}$ and $p\mu_n + (1-p) = \frac{\mu_n - \mu_1}{2 - \mu_1 - \mu_n}$ are eigenvalues of T_p.

三、Chebychev Semi-Iteration Acceleration Method

Remark 4

(i) In (39) it holds $(r = \rho)$

$$c_2 > c_3 > c_4 > \cdots, \text{ and } \lim_{k\to\infty} c_k = \frac{2}{1+\sqrt{1-r^2}}. \quad \text{(Exercise!)}$$

(ii) If T *is symmetric, then by (36) we get*

$$\begin{aligned} \|Q_k(T)\|_2 &= \max\{|Q_k(\mu_i)| : \mu_i \text{ is an eigenvalue of } T\} \\ &\le \max\{|Q_k(\lambda)| : -\rho \le \lambda \le \rho\} \\ &= \left|T_k(1/\rho)\right|^{-1}, \quad (\rho = \rho(T)). \\ &= \frac{1}{c^{k/2}+c^{-k/2}} = \frac{(\omega_b-1)^{k/2}}{1+(\omega_b-1)^k}, \end{aligned} \tag{45}$$

where $c = \frac{1-\sqrt{1-\rho^2}}{1+\sqrt{1-\rho^2}} = \omega_b - 1$ *with* $\omega_b = \frac{2}{1+\sqrt{1-\rho^2}}$.

四、Appendix

Proof: Let $A = LL^T - N = \bar{L}\bar{L}^T - \bar{N}$. Then $a_{11} = l_{11}^2 = \bar{l}_{11}^2 \Longrightarrow l_{11} = \bar{l_{11}}$ (since l_{11} is positive). Also, $a_{k1} = l_{k1}l_{11} - n_{k1} = \bar{l}_{k1}l_{11} - \bar{n}_{k1}$, so we have

$$\text{If } (k,1) \in E \Longrightarrow n_{k1} = \bar{n}_{k1} = 0 \Longrightarrow l_{k1} = \bar{l}_{k1} = a_{k1}/l_{11}, \quad (46a)$$

$$\text{If } (k,1) \notin E \Longrightarrow l_{k1} = \bar{l}_{k1} = 0 \Longrightarrow n_{k1} = \bar{n}_{k1} = -a_{k1}. \quad (46b)$$

Suppose that $l_{ki} = \bar{l}_{ki}$, $n_{ki} = \bar{n}_{ki}$, for $k = i, \cdots, n$, $1 \le i \le m-1$. Then from

$$a_{mm} = l_{mm}^2 + \sum_{k=0}^{m-1} l_{mk}^2 = \bar{l}_{mm}^2 + \sum_{k=1}^{m-1} \bar{l}_{mk}^2$$

follows that $l_{mm} = \bar{l}_{mm}$. Also from

$$a_{rm} = l_{rm}l_{mm} + \sum_{k=1}^{m-1} l_{rk}l_{mk} - n_{rm} = \bar{l}_{rm}\bar{l}_{mm} + \sum_{k=0}^{m-1} \bar{l}_{rk}\bar{l}_{mk} - \bar{n}_{rm}$$

and (46) follows that $n_{rm} = \bar{n}_{rm}$ and $l_{rm} = \bar{l}_{rm}$ $(r \ge m)$. ∎

四、Appendix

Proof: (i) $\Rightarrow$ (ii): $A = \sigma I - B$, $\rho(B) < \sigma$. The eigenvalues of A have the form $\sigma - \lambda$, where λ is an eigenvalue of B and $|\lambda| < \sigma$. Since λ is real, so $\sigma - \lambda > 0$ for all eigenvalues λ, it follows that A has only positive eigenvalues. Thus (ii) holds.
(ii) $\Rightarrow$ (i): For $a_{ij} \leq 0$, $(i \neq j)$, there is a decomposition $A = \sigma I - B$, $B \geq 0$ (for example $\sigma = \max(a_{ii})$). Claim $\rho(B) < \sigma$. By Perron-Frobenius Theorem **??**, we have that $\rho(B)$ is an eigenvalue of B. Thus $\sigma - \rho(B)$ is an eigenvalue of A, so $\sigma - \rho(B) > 0$. Then (i) holds. ■

四、Appendix

Proof: It is sufficient to show that the matrix B_1 constructed by (17)-(21) is a symmetric M-matrix.
(i): We first claim: $\tilde{B}_0$ is an M-matrix. $A = \tilde{B}_0 - C_1 \leq \tilde{B}_0$, (since only negative elements are neglected). There is a $k > 0$ such that $A = kI - \hat{A}$, $\tilde{B}_0 = kI - \hat{B}_0$ with $\hat{A} \geq 0$, $\hat{B}_0 \geq 0$, then $\hat{B}_0 \leq \hat{A}$. By Perron-Frobenius Theorem **??** follows $\rho(\hat{B}_0) \leq \rho(\hat{A}) < k$. This implies that $\tilde{B}_0$ is an M-matrix.
(ii): Thus $\tilde{B}_0$ is positive definite, hence $B_1 = L_1^{-1}\tilde{B}_0(L_1^{-1})^T$ is also positive definite. B_1 has nonpositive off-diagonal element, since $\bar{B}_1 = \bar{A}_1 - \frac{b_1 b_1{}^T}{a_{11}}$. Then B_1 is an M-matrix (by Lemma 5.3) ■

四、Appendix

Claim: (37b)

$$
\begin{aligned}
Q_{k+1}(t) &= T_{k+1}\left(\frac{2t-\mu_1-\mu_n}{\mu_1-\mu_n}\right) \Big/ T_{k+1}\left(\frac{1}{r}\right) \\
&= \frac{1}{T_{k+1}(1/r)}\left[2\left(\frac{2t-\mu_1-\mu_n}{\mu_1-\mu_n}\right)T_k\left(\frac{2t-\mu_1-\mu_n}{\mu_1-\mu_n}\right) - T_{k-1}\left(\frac{2t-\mu_1-\mu_n}{\mu_1-\mu_n}\right)\right] \\
&= \frac{2T_k(1/r)}{rT_{k+1}(1/r)} r\left(\frac{2t-\mu_1-\mu_n}{\mu_1-\mu_n}\right)\frac{T_k\left(\frac{2t-\mu_1-\mu_n}{\mu_1-\mu_n}\right)}{T_k(1/r)} \\
&\quad - \frac{T_{k-1}\left(\frac{2-\mu_1-\mu_n}{\mu_1-\mu_n}\right)}{T_{K+1}\left(\frac{2-\mu_1-\mu_n}{\mu_1-\mu_n}\right)} \frac{T_{k-1}\left(\frac{2-\mu_1-\mu_n}{\mu_1-\mu_n}\right)}{T_{k-1}(1/r)} \\
&= c_{k+1}[pt+(1-p)]Q_k(t) - [1-c_{k+1}]Q_{k-1}(t),
\end{aligned}
$$

since

$$
r\left(\frac{2t-\mu_1-\mu_n}{\mu_1-\mu_n}\right) = \frac{2t-\mu_1-\mu n}{2-\mu_1-\mu_n} = pt+(1-p)
$$

and

$$
\begin{aligned}
1-c_{k+1} &= 1-\frac{2T_k(1/r)}{rT_{k+1}(1/r)} = \frac{rT_{k+1}(1/r)-2T_k(1/r)}{rT_{k+1}(1/r)} \\
&= \frac{-rT_{k-1}(1/r)}{rT_{k+1}(1/r)} = \frac{-T_{k-1}(1/r)}{T_{k+1}(1/r)}.
\end{aligned}
$$