CG-Method as an Iterative Method, Preconditioning

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Preconditioning CG-Method

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Preconditioning CG-Method

Consider the linear system of a symmetric positive definite matrix A

$$Ax = b$$

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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{1}$$

with $\tilde{A} = C^{-T}AC^{-1}$ s.p.d., $\tilde{b} = C^{-T}b$ and $\tilde{x} = Cx$. Applying CG-method to (1) it yields:

Input: Given
$$\tilde{x}_0 \in \mathbb{R}^n$$
 and $\tilde{r}_0 = b - A\tilde{x}_0 = \tilde{p}_0$. Set $k = 0$.
1: repeat
2: Compute $\tilde{\alpha}_k = \tilde{p}_k^T \tilde{r}_k / \tilde{p}_k^T C^{-T} A C^{-1} \tilde{p}_k$;
3: Compute $\tilde{x}_{k+1} = \tilde{x}_k + \tilde{\alpha}_k \tilde{p}_k$;
4: Compute $\tilde{r}_{k+1} = \tilde{r}_k - \tilde{\alpha}_k C^{-T} A C^{-1} \tilde{p}_k$;
5: Compute $\tilde{\beta}_k = -\tilde{r}_{k+1}^T C^{-T} A C^{-1} \tilde{p}_k / \tilde{p}_k C^{-T} A C^{-1} \tilde{p}_k$;

6: Compute
$$\tilde{p}_{k+1} = \tilde{r}_{k+1} + \beta_k \tilde{p}_k$$
;

7: Set
$$k = k + 1$$
;

B: **until**
$$\tilde{r}_k = 0$$

Simplification: Let

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

Then

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

and

$$r_k = C^T C z_k \equiv M z_k.$$

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Algorithm: CG-method with preconditioner M

Input: Given x_0 and $r_0 = b - Ax_0$, solve $Mp_0 = r_0$. Set k = 0.

1: repeat

2: Compute
$$\alpha_k = p_k^T r_k / p_k^T A p_k$$
;

3: Compute
$$x_{k+1} = x_k + \alpha_k p_k$$
;

4: Compute
$$r_{k+1} = r_k - \alpha_k A p_k$$
;

5: **if** $r_{k+1} = 0$ **then**

7: **else**

8: Solve
$$Mz_{k+1} = r_{k+1}$$
;

9: Compute
$$\beta_k = -z_{k+1}^T A p_k / p_k A p_k$$
;

10: Compute
$$p_{k+1} = z_{k+1} + \beta_k p_k$$
;

11: end if

12: Set
$$k = k + 1$$
;

13: **until** $r_k = 0$

Additional cost per step: solve one linear system Mz = r for z. Advantage: $\operatorname{cond}(M^{-1/2}AM^{-1/2}) \ll \operatorname{cond}(A)_{z}$, and $z \in \mathbb{R}$

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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.,

$$0 = (r_i^T + \beta_{i-1} p_{i-1}^T) r_k = r_i^T r_k, \ i < k$$

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 $p_i^T C^{-1} A C^{-1} p_j = 0 \Leftrightarrow \tilde{r}_j^T \tilde{r}_j = 0$, $i \neq j$ and requires

$$z_{i}^{T}Mz_{j} = r_{i}^{T}M^{-1}MM^{-1}r_{j} = r_{i}^{T}M^{-1}r_{j}$$

= $(r_{i}^{T}C^{-1})(C^{-1}r_{j}) = \widetilde{r}_{i}^{T}\widetilde{r}_{j} = 0, \quad i \neq j.$

Consider the iteration (in two parameters):

$$x_{k+1} = x_{k-1} + \omega_{k+1} \left(\alpha_k z_k + x_k - x_{k-1} \right)$$
(2)

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

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

$$Mz_{k+1} = b - A \left(x_{k-1} + \omega_{k+1} \left(\alpha_k z_k + x_k - x_{k-1} \right) \right)$$

= $Mz_{k-1} - \omega_{k+1} \left[\alpha_k (M - N) z_k + M (z_{k-1} - z_k) \right]$ (3)

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

$$z_p^T M z_q = 0, \quad p \neq q, \ p, q = 0, 1, \dots, n-1.$$
 (4)

Since M > 0, there is some $k \le n$ such that $z_k = 0$. Thus, $x_k = x$, the iteration converges no more than n steps. We show that (4) holds by induction. Assume

$$z_p^T M z_q = 0, \quad p \neq q, \ p, q = 0, 1, \dots, k$$

holds until k.

If we choose

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

then, from (3),

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

and if we choose

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

then

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

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From (3) for j < k - 1 we have

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

But (3) holds for j < k - 1,

$$Mz_{j+1} = Mz_{j-1} - \omega_{j+1} \left(\alpha_j (M - N) z_j + M(z_{j-1} - z_j) \right).$$
 (5)

Multiplying (5) by z_k^T we get

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

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

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

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

Consider (2) 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

$$x_{k+1} = x_k + z_k = x_k + M^{-1}r_k.$$
(6)

Here z_k is referred to as a correction . Write A = M - N. Then (6) becomes

$$x_{k+1} = x_k + M^{-1}(b - Ax_k)$$

= $x_k + M^{-1}(b - (M - N)x_k)$
= $M^{-1}Nx_k + M^{-1}b.$ (7)

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),

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

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

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

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

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

Then with A = D - L - R we have

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

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(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 (2) 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.

Choices of M (Criterion):

(i)
$$\operatorname{cond}(M^{-1/2}AM^{-1/2})$$
 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.

SSOR (Symmetric Successive Over Relaxation):

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

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

Then from the iterations

$$M_{\omega} x_{i+1/2} = N_{\omega} x_i + \omega b,$$

$$M_{\omega}^T x_{i+1} = N_{\omega}^T x_{i+1/2} + \omega b,$$

follows that

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

It holds that

$$((1 - \omega)D + \omega L) (D - \omega L)^{-1} + I$$

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

Thus

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

then

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

$$\approx (D-L) D^{-1} (D-L^T), \ (\omega=1).$$
(8)

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

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

and

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

Then

$$\begin{aligned} & \operatorname{cond}\left(M(\omega)^{-1/2}AM(\omega)^{-1/2}\right) \leq \frac{1 + \frac{(2-\omega)^2}{4\omega} + \omega\delta}{2\omega} = \kappa(\omega) \\ & \text{for } \omega^* = \frac{2}{1+2\sqrt{(2\delta+1)/2\mu}}, \ \kappa(\omega^*) \text{ is minimal and } \kappa(\omega^*) = 1/2 + \sqrt{(1/2+\delta)\mu}. \end{aligned}$$
 Especially

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

Disadvantage : μ , δ in general are unknown.

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

$$A = LL^T - N, (9)$$

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

Reserved Pattern: $E \subset \{1, ..., n\} \times \{1, ..., n\}$ with $\int (i,i) \in E, \ i=1,\dots,n$

$$(i, j) \in E \implies (j, i) \in E$$

For a given reserved pattern E we constr

or a given reserved pattern ${\cal E}$ we construct the matrices ${\cal L}$ and ${\cal N}$ as in (9) with

(i)
$$A = LL^T - N,$$
(10a)

(ii) L: lower triangular with $l_{ii} > 0$ and $l_{ij} \neq 0 \Rightarrow (i, j) \in E(10b)$ (iii) $N = (n_{ij}), n_{ij} = 0, \text{ if } (i,j) \in E$ (10c) 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

$$A = L_1 \left(\begin{array}{cc} 1 & 0 \\ 0 & \overline{A}_1 \end{array} \right) L_1^T.$$

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

$$b_{j1} = \begin{cases} a_{j1}, & (j,1) \in E, \\ 0, & \text{otherwise}, \end{cases} \quad c_{j1} = b_{j1} - a_{j1} = \begin{cases} 0, & (j,1) \in E, \\ -a_{j1}, & \text{otherwise}. \end{cases}$$
(11)

Then

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

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

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

and

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

Then

$$A = L_1 B_1 L_1^T - C_1. (12)$$

Consequently, compute the Cholesky decomposition on B_1 :

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

Thus,

$$A = L_1 L_2 B_2 L_2^T L_1^T - L_1 C_2 L_1^T - C_1$$

and so on, hence

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

with

$$L = L_1 \cdots L_n \text{ and } N = C_1 + C_2 + \cdots + C_n.$$
 (13)

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Lemma 1

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

1 L is lower triangular with
$$l_{ii} > 0$$
, $l_{ii} \neq 0 \Longrightarrow (i, j) \in E$.

2
$$N = (n_{ij}), n_{ij} = 0, \text{ if } (i, j) \in E$$

▶ Proof

The Incomplete Cholesky decomposition may not exist, if

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

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

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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 (11)-(13) can be performed on A until the computation of l_{44} (see proof of Lemma 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.

Now take

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

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

M-matrices, H-matrices.

Definition 5

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

Lemma 6

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.

▶ Proof

Theorem 7

Let A be a symmetric M-matrix. Then the Incomplete Cholesky method described in (11)-(13) is executable and yields a decomposition $A = LL^T - N$, which satisfies (10).

▶ Proof

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Definition 8

 $A \in \mathbb{R}^{n \times n}$. Decomposition A = M - N is called regular, if $M^{-1} \ge 0$, $N \ge 0$ (regular splitting).

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Let $A^{-1} \ge 0$ and A = M - N is a regular decomposition. Then $\rho(M^{-1}N) < 1$. i.e., the iterative method $Mx_{k+1} = Nx_k + b$ for Ax = b is convergent for all x_0 .

Proof: Since $T = M^{-1}N \ge 0$, $M^{-1}(M - N) = M^{-1}A = I - T$, it follows that

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

Then

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

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

If $A^{-1} \ge 0$ and $A = M_1 - N_1 = M_2 - N_2$ are two regular decompositions with $0 \le N_1 \le N_2$, then it holds $\rho(M_1^{-1}N_1) \le \rho(M_2^{-1}N_2)$.

Proof: Let A = M - N, $A^{-1} \ge 0$. Then

$$\rho(M^{-1}N) = \rho((A+N)^{-1}N) = \rho([A(I+A^{-1}N)]^{-1}N)$$
$$= \rho((I+A^{-1}N)^{-1}A^{-1}N) = \frac{\rho(A^{-1}N)}{1+\rho(A^{-1}N)}.$$

$$[\lambda \rightarrow rac{\lambda}{1+\lambda} \text{ monotone for } \lambda \geq 0].$$

Because $0 \le N_1 \le N_2$ it follows $\rho(A^{-1}N_1) \le \rho(A^{-1}N_2)$. Then

$$\rho(M_1^{-1}N_1) = \frac{\rho(A^{-1}N_1)}{1 + \rho(A^{-1}N_1)} \le \frac{\rho(A^{-1}N_2)}{1 + \rho(A^{-1}N_2)} = \rho(M_2^{-1}N_2),$$

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

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If A is a symmetric M-matrix, then the decomposition $A = LL^T - N$ according to Theorem 7 is a regular decomposition.

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

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).

Other preconditioning:

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

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

Theorem 12 (Generalization)

Let A be an $n \times n$ matrix and E be an arbitrary reserved pattern with $(i,i) \in E$, i = 1, 2, ..., 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).

Chebychev Semi-Iteration Acceleration Method

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

$$x = Tx + f, \ T = M^{-1}N \text{ and } f = M^{-1}b.$$
 (14)

The basic iterative method of (14) is

$$x_{k+1} = Tx_k + f. (15)$$

How to modify the convergence rate?

Definition 13

The iterative method (15) 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.

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,

$$W(I-T)W^{-1} = M^{1/2}M^{-1}AM^{-1/2} = M^{-1/2}AM^{-1/2}$$
 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.

Lemma 15

If (15) is symmetrizable, then the eigenvalues μ_i of T are real and satisfy

$$\mu_i < 1, \text{ for } i = 1, 2, \dots, n.$$
 (16)

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 (16) holds.

Definition 16

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

$$\begin{cases}
 u_0 = x_0, \\
 u_{k+1} = \alpha(Tu_k + f) + (1 - \alpha)u_k \\
 = (\alpha T + (1 - \alpha)I)u_k + \alpha f \equiv T_\alpha u_k + \alpha f.
 \end{cases}$$
(17)

is called an Extrapolation method of (15).

Remark 1

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

If (15) is symmetrizable and T has the eigenvalues satisfying $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_n < 1$, then it holds for $\alpha^* = \frac{2}{2-\mu_1-\mu_2} > 0$ that

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

Proof: Eigenvalues of T_{α} are $\alpha \mu_i + (1 - \alpha) = 1 + \alpha(\mu_i - 1)$. Consider the problem

$$\min_{\alpha} \max_{i} |1 + \alpha(\mu_{i} - 1)| = \min!$$

$$\iff |1 + \alpha(\mu_{n} - 1)| = |1 + \alpha(\mu_{1} - 1)|,$$

$$\iff 1 + \alpha(\mu_{n} - 1) = \alpha(1 - \mu_{n}) - 1 \text{ (otherwise } \mu_{1} = \mu_{n}\text{)}.$$

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

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From (15) and (17) follows that

$$u_k = \sum_{i=0}^k a_{ki} x_i$$
, 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, ..., i = 0, 1, 2, ..., k and $\sum_{i=0}^{k} a_{ki} = 1$ such that

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

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

Error: Let

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

Hence,

$$d_{k} = u_{k} - x^{*} = \sum_{i=0}^{k} a_{ki}(x_{i} - x^{*})$$

$$= \sum_{i=0}^{k} a_{ki}T^{i}e_{0} = (\sum_{ki}^{k} a_{ki}T^{i})e_{0}$$

$$= \mathcal{P}_{k}(T)e_{0} = \mathcal{P}_{k}(T)d_{0},$$
(18)

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where

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

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

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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 (18) and have

$$\begin{aligned} \|d_k\|_W &\leq \|\mathcal{P}_k(T)\|_W \|d_0\|_W = \|W\mathcal{P}_k(T)W^{-1}\|_2 \|d_0\|_2 \quad (19) \\ &= \|\mathcal{P}_k(WTW^{-1})\|_2 \|d_0\|_W = \rho(\mathcal{P}_k(T)) \|d_0\|_W. \end{aligned}$$

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

$$\min\left[\{\max|\mathcal{P}_k(\lambda)|:\mu_1 \le \lambda \le \mu_n\}: \deg(\mathcal{P}_k) \le k, \, \mathcal{P}_k(1) = 1\right].$$
(20)

Solution of (20): The replacement problem

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

has the solution

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

Let $\lambda = 1 - t$, then $1 - \mu_1 \le t \le 1 - \mu_n$, $P_k(\lambda) = P_k(1 - t) \equiv \tilde{P}_k(t)$ with $\tilde{P}_k(0) = 1$. The problem (20) can be transformed to [(II) Conjugate Gradient Method] (34) as

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

Hence, the solution of (20) is given by

$$Q_k(t) = T_k \left(\frac{2t - \mu_1 - \mu_n}{\mu_1 - \mu_n}\right) / T_k \left(\frac{2 - \mu_1 - \mu_n}{\mu_1 - \mu_n}\right).$$
 (21)

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.

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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 (21) we get

$$Q_0(t) = 1, \ Q_1(t) = \frac{2t - \mu_1 - \mu_n}{2 - \mu_1 - \mu_n} = pt + (1 - p)$$
 (22a)

and

$$Q_{k+1}(t) = [pt + (1-p)]c_{k+1}Q_k(t) + (1 - c_{k+1})Q_{k-1}(t),$$
(22b)

where

$$p = \frac{2}{2 - \mu_1 - \mu_n}, \ c_{k+1} = \frac{2T_k(1/r)}{rT_{k+1}(1/r)}, \ r = \frac{\mu_1 - \mu_n}{2 - \mu_1 - \mu_n}.$$
 (23)

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Recursion for u_k :

$$d_{k+1} = Q_{k+1}(T)d_0 = (pT + (1-p)I)c_{k+1}Q_k(T)d_0 + (1-c_{k+1})Q_{k-1}(T)d_0$$

$$x^* = (pT + (1-p)I)c_{k+1}x^* + (1-c_{k+1})x^* + p(I-T)x^*c_{k+1}.$$

Adding above two equations together we get

$$u_{k+1} = [pT + (1-p)I]c_{k+1}u_k + (1-c_{k+1})u_{k-1} + c_{k+1}pf$$

= $c_{k+1}p\{Tu_k + f - u_k\} + c_{k+1}u_k + (1-c_{k+1})u_{k-1}.$

Then we obtain the optimal Chebychev semi-iterative Algorithm.

[Optimal Chebychev semi-iterative Algorithm]

Let
$$r = \frac{\mu_1 - \mu_n}{2 - \mu_1 - \mu_n}, \ p = \frac{2}{2 - \mu_1 - \mu_n}, \ c_1 = 2$$

 $u_0 = x_0,$
 $u_1 = p(Tu_0 + f) + (1 - p)u_0$
For $k = 1, 2, \cdots,$
 $u_{k+1} = c_{k+1} \left[p(Tu_k + f) + (1 - p)u_k \right] + (1 - c_{k+1}) u_{k-1},$
 $c_{k+1} = (1 - r^2/4 c_k)^{-1}.$
(24)

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Remark 3

Here u_{k+1} can be rewritten as the three terms recursive formula with two parameters as in (2):

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

where
$$Mz_k = b - Au_k$$
.

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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

$$c_{k+1} = \frac{1}{(1 - (r^2/4)c_k)}$$
 with $r = \frac{\mu_1 - \mu_n}{2 - \mu_1 - \mu_n}$. (25)

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Error estimate: It holds

$$\|u_k - x^*\|_W \le \left|T_k\left(\frac{2-\mu_1-\mu_n}{\mu_1-\mu_n}\right)\right|^{-1} \|u_0 - x^*\|_W.$$
(26)

Proof: From (19) and (21) we have

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

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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

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

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

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

$$q_k \le 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^k.$$
(27)

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 $||u_0 - x^*||_W$.

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 μ'_n $(\mu'_n \ge \mu_n)$ and μ_1 by μ'_1 $(\mu'_1 \le \mu_1)$, because λ is still in $[\mu'_1, \mu'_n]$ for all eigenvalue λ of T.

μ_n	k	q_4	j	j^{\prime}	q_8	j	j^{\prime}
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 $j': \mu_n^{j'} \approx q_4, \ q_8$.

Let $1 > \rho = \rho(T)$. If we set $\mu'_n = \rho, \mu'_1 = -\rho$, then p and r defined in (23) become p = 1 and $r = \rho$, respectively. Algorithm 46 can be simplified by

$$u_{0} = x_{0},$$

$$u_{1} = Tu_{0} + f,$$

$$u_{k+1} = c_{k+1}(Tu_{k} + f) + (1 - c_{k+1})u_{k-1}$$

$$c_{k+1} = (1 - (\rho^{2}/4) c_{k})^{-1} \text{ with } c_{1} = 2.$$

Also, Algorithm 46 can be written by the form of (28), by replacing T by $T_{\alpha^*}=T_p=(pT+(1-p)I)$ and it leads to

$$u_{k+1} = c_{k+1} \left(T_p u_k + f \right) + \left(1 - c_{k+1} \right) u_{k-1}.$$
 (29)

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 .

Remark 4

(i) In (24) it holds
$$(r = \rho)$$

 $c_2 > c_3 > c_4 > \cdots$, and $\lim_{k \to \infty} c_k = \frac{2}{1 + \sqrt{1 - r^2}}$. (Exercise!)
(ii) If T is symmetric, then by (21) we get
 $||Q_k(T)||_2 = \max\{|Q_k(\mu_i)| : \mu_i \text{ is an eigenvalue of } T\}$
 $\leq \max\{|Q_k(\lambda)| : -\rho \leq \lambda \leq \rho\}$
 $= \left|T_k(1/\rho)\right|^{-1}, \quad (\rho = \rho(T)).$
 $= \frac{1}{c^{k/2} + c^{-k/2}} = \frac{(\omega_b - 1)^{k/2}}{1 + (\omega_b - 1)^k},$ (30)

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

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Appendix

Proof: Let
$$A = LL^T - N = \overline{L}\overline{L}^T - \overline{N}$$
. Then
 $a_{11} = l_{11}^2 = \overline{l}_{11}^2 \Longrightarrow l_{11} = \overline{l}_{11}$ (since l_{11} is positive). Also,
 $a_{k1} = l_{k1}l_{11} - n_{k1} = \overline{l}_{k1}l_{11} - \overline{n}_{k1}$, so we have
If $(k, 1) \in E \Longrightarrow n_{k1} = \overline{n}_{k1} = 0 \Longrightarrow l_{k1} = \overline{l}_{k1} = a_{k1}/l_{11}$, (31a)
If $(k, 1) \notin E \Longrightarrow l_{k1} = \overline{l}_{k1} = 0 \Longrightarrow n_{k1} = \overline{n}_{k1} = -a_{k1}$. (31b)
Suppose that $l_{k1} = \overline{l}_{k1} = n_{k1} = \overline{n}_{k1}$ for $k = i \cdots n$, $1 \le i \le m - 1$. Then

Suppose that $l_{ki} = \overline{l}_{ki}$, $n_{ki} = \overline{n}_{ki}$, for $k = i, \dots, n, 1 \le i \le m - 1$. 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 $l_{mm} = \overline{l}_{mm}$. 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 (31) follows that $n_{rm} = \bar{n}_{rm}$ and $l_{rm} = \bar{l}_{rm}$ $(r \ge m)$.

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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.

return

Proof: It is sufficient to show that the matrix B_1 constructed by (11)-(12) 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 6)

Claim: (22b)

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

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

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

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