# CG-Method as an Iterative Method, Preconditioning 

Tsung-Ming Huang

Department of Mathematics<br>National Taiwan Normal University

October 22, 2011

## Outline

(1) A new point of view of PCG
(2) Incomplete Cholesky Decomposition
(3) Chebychev Semi-Iteration Acceleration Method

Consider the linear system of a symmetric positive definite matrix $A$

$$
A x=b .
$$

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

$$
\begin{equation*}
\tilde{A} \tilde{x}=\tilde{b} \tag{1}
\end{equation*}
$$

with $\tilde{A}=C^{-T} A C^{-1}$ s.p.d., $\tilde{b}=C^{-T} b$ and $\tilde{x}=C x$.
Applying CG-method to (1) it yields:
Input: Given $\tilde{x}_{0} \in \mathbb{R}^{n}$ and $\tilde{r}_{0}=\tilde{b}-\tilde{A} \tilde{x}_{0}=\tilde{p}_{0}$. Set $k=0$.
1: repeat
2: $\quad$ Compute $\tilde{\alpha}_{k}=\tilde{p}_{k}^{T} \tilde{r}_{k} / \tilde{p}_{k}^{T} C^{-T} A C^{-1} \tilde{p}_{k}$;
3: $\quad$ 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: $\quad$ 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: $\quad$ Compute $\tilde{p}_{k+1}=\tilde{r}_{k+1}+\tilde{\beta}_{k} \tilde{p}_{k}$;
7: $\quad$ Set $k=k+1$;
8: until $\tilde{r}_{k}=0$

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

$$
\begin{aligned}
r_{k} & =C^{T} \tilde{r}_{k}=C^{T}\left(\tilde{b}-\tilde{A} \tilde{x}_{k}\right) \\
& =C^{T}\left(C^{-T} b-C^{-T} A C^{-1} C x_{k}\right) \\
& =b-A x_{k} .
\end{aligned}
$$

and

$$
r_{k}=C^{T} C z_{k} \equiv M z_{k}
$$

## Algorithm: CG-method with preconditioner $M$

Input: Given $x_{0}$ and $r_{0}=b-A x_{0}$, solve $M p_{0}=r_{0}$. Set $k=0$.

## 1: repeat

2: $\quad$ Compute $\alpha_{k}=p_{k}^{T} r_{k} / p_{k}^{T} A p_{k}$;
3: $\quad$ Compute $x_{k+1}=x_{k}+\alpha_{k} p_{k}$;
4: $\quad$ Compute $r_{k+1}=r_{k}-\alpha_{k} A p_{k}$;
5: if $r_{k+1}=0$ then
Stop;
else
Solve $M z_{k+1}=r_{k+1}$;
Compute $\beta_{k}=-z_{k+1}^{T} A p_{k} / p_{k} A p_{k}$;
10: $\quad$ Compute $p_{k+1}=z_{k+1}+\beta_{k} p_{k}$;
11: end if
12: $\quad$ Set $k=k+1$;
13: until $r_{k}=0$
Additional cost per step: solve one linear system $M z=r$ for $z$.
Advantage: $\quad \operatorname{cond}\left(M^{-1 / 2} A M^{-1 / 2}\right) \ll \operatorname{cond}(A)$.

## 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.,

$$
0=\left(r_{i}^{T}+\beta_{i-1} p_{i-1}^{T}\right) r_{k}=r_{i}^{T} r_{k}, i<k
$$

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 $p_{i}^{T} C^{-1} A C^{-1} p_{j}=0 \Leftrightarrow \tilde{r}_{j}^{T} \tilde{r}_{j}=0, \quad i \neq j$ and requires

$$
\begin{aligned}
z_{i}^{T} M z_{j} & =r_{i}^{T} M^{-1} M M^{-1} r_{j}=r_{i}^{T} M^{-1} r_{j} \\
& =\left(r_{i}^{T} C^{-1}\right)\left(C^{-1} r_{j}\right)=\widetilde{r}_{i}^{T} \widetilde{r_{j}}=0, \quad i \neq j
\end{aligned}
$$

Consider the iteration (in two parameters):

$$
\begin{equation*}
x_{k+1}=x_{k-1}+\omega_{k+1}\left(\alpha_{k} z_{k}+x_{k}-x_{k-1}\right) \tag{2}
\end{equation*}
$$

with $\alpha_{k}$ and $\omega_{k+1}$ being two undetermined parameters.

Let $A=M-N$. Then from $M z_{k}=r_{k} \equiv b-A x_{k}$ follows that

$$
\begin{align*}
M z_{k+1} & =b-A\left(x_{k-1}+\omega_{k+1}\left(\alpha_{k} z_{k}+x_{k}-x_{k-1}\right)\right) \\
& =M z_{k-1}-\omega_{k+1}\left[\alpha_{k}(M-N) z_{k}+M\left(z_{k-1}-z_{k}\right)\right] \tag{3}
\end{align*}
$$

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

$$
\begin{equation*}
z_{p}^{T} M z_{q}=0, \quad p \neq q, p, q=0,1, \ldots, n-1 \tag{4}
\end{equation*}
$$

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 (4) holds by induction. Assume

$$
z_{p}^{T} M z_{q}=0, \quad p \neq q, p, q=0,1, \ldots, k
$$

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

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

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 $j<k-1$,

$$
\begin{equation*}
M z_{j+1}=M z_{j-1}-\omega_{j+1}\left(\alpha_{j}(M-N) z_{j}+M\left(z_{j-1}-z_{j}\right)\right) \tag{5}
\end{equation*}
$$

Multiplying (5) by $z_{k}^{T}$ we get

$$
z_{k}^{T} N z_{j}=0
$$

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

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

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

Consider (2) again

$$
x_{k+1}=x_{k-1}+\omega_{k+1}\left(\alpha_{k} z_{k}+x_{k}-x_{k-1}\right)
$$

Since $M z_{k}=r_{k}=b-A x_{k}$, if we set $\omega_{k+1}=\alpha_{k}=1$, then

$$
\begin{equation*}
x_{k+1}=x_{k}+z_{k}=x_{k}+M^{-1} r_{k} . \tag{6}
\end{equation*}
$$

Here $z_{k}$ is referred to as a correction. Write $A=M-N$. Then (6) becomes

$$
\begin{align*}
x_{k+1} & =x_{k}+M^{-1}\left(b-A x_{k}\right) \\
& =x_{k}+M^{-1}\left(b-(M-N) x_{k}\right) \\
& =M^{-1} N x_{k}+M^{-1} b . \tag{7}
\end{align*}
$$

## Recall the Iterative Improvement in Subsection

Solve $A x=b$,
$r_{k}=b-A x_{k}$,
$A z_{k}=r_{k}, \leftrightarrow M z_{k}=r_{k}$.
$x_{k+1}=x_{k}+z_{k}$.
(i) Jacobi method $\left(\omega_{k+1}=\alpha_{k}=1\right): A=D-(L+R)$,

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

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

$$
\begin{aligned}
x_{k+1} & =x_{k}+z_{k} \\
& =x_{k}+(D-L)^{-1}\left(b-A x_{k}\right) \\
& =(D-L)^{-1} R x_{k}+(D-L)^{-1} b .
\end{aligned}
$$

(iii) SOR-method $\left(\omega_{k+1}=1, \alpha_{k}=\omega\right)$ : $\quad$ 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

$$
\begin{aligned}
x_{k+1} & =(D-\omega L)^{-1}(\omega R+(1-\omega) D) x_{k}+(D-\omega L)^{-1} \omega b \\
& =(D-\omega L)^{-1}((D-\omega L)-\omega A) x_{k}+(D-\omega L)^{-1} \omega b \\
& =\left(I-(D-\omega L)^{-1} \omega A\right) x_{k}+(D-\omega L)^{-1} \omega b \\
& =x_{k}+(D-\omega L)^{-1} \omega\left(b-A x_{k}\right) \\
& =x_{k}+\omega M^{-1} r_{k} \\
& =x_{k}+\omega z_{k}
\end{aligned}
$$

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

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

We can think of the scalars $\omega_{k+1}, \alpha_{k}$ in (2) as acceleration parameters that can be chosen to speed the convergence of the iteration $M x_{k+1}=N x_{k}+b$. 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) cond $\left(M^{-1 / 2} A M^{-1 / 2}\right)$ is nearly by 1 , i.e., $M^{-1 / 2} A M^{-1 / 2} \approx I, A \approx M$.
(ii) The linear system $M z=r$ must be easily solved. e.g. $M=L L^{T}$ (see Section 16.)
(iii) $M$ is symmetric positive definite.

## SSOR (Symmetric Successive Over Relaxation):

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

$$
\left\{\begin{array} { l } 
{ M _ { \omega } : = D - \omega L , } \\
{ N _ { \omega } : = ( 1 - \omega ) D + \omega L ^ { T } , }
\end{array} \quad \text { and } \quad \left\{\begin{array}{l}
M_{\omega}^{T}=D-\omega L^{T}, \\
N_{\omega}^{T}=(1-\omega) D+\omega L .
\end{array}\right.\right.
$$

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

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

It holds that

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

Thus

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

then

$$
\begin{align*}
M(\omega) & =\frac{1}{\omega(2-\omega)}(D-\omega L) D^{-1}\left(D-\omega L^{T}\right)  \tag{8}\\
& \approx(D-L) D^{-1}\left(D-L^{T}\right),(\omega=1)
\end{align*}
$$

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

$$
\mu=\max _{x \neq 0} \frac{x^{T} D x}{x^{T} A x}(\leq \operatorname{cond}(A))
$$

and

$$
\delta=\max _{x \neq 0} \frac{x^{T}\left(L D^{-1} L^{T}-\frac{1}{4} D\right) x}{x^{T} A x} \geq-\frac{1}{4}
$$

Then

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

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

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

Disadvantage : $\mu, \delta$ in general are unknown.

## Incomplete Cholesky Decomposition

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

$$
\begin{equation*}
A=L L^{T}-N \tag{9}
\end{equation*}
$$

where $L$ is a lower triangular matrix with prescribed reserved pattern $E$ and $N$ is "small".
Reserved Pattern: $E \subset\{1, \ldots, n\} \times\{1, \ldots, n\}$ with
$\left\{\begin{array}{l}(i, i) \in E, i=1, \ldots, n \\ (i, j) \in E \Rightarrow(j, i) \in E\end{array}\right.$
For a given reserved pattern $E$ we construct the matrices $L$ and $N$ as in (9) with
(i) $A=L L^{T}-N$,
(ii) $L$ : lower triangular with $l_{i i}>0$ and $l_{i j} \neq 0 \Rightarrow(i, j) \in E(10 \mathrm{~b})$
(iii) $N=\left(n_{i j}\right), n_{i j}=0$, if $(i, j) \in E$

First step: Consider the Cholesky decomposition of $A$,
$A=\left(\begin{array}{cc}a_{11} & a_{1}^{T} \\ a_{1} & A_{1}\end{array}\right)=\left(\begin{array}{cc}\sqrt{a_{11}} & 0 \\ a_{1} / \sqrt{a_{11}} & I\end{array}\right)\left(\begin{array}{cc}1 & 0 \\ 0 & \bar{A}_{1}\end{array}\right)\left(\begin{array}{cc}\sqrt{a_{11}} & a_{1}^{T} / \sqrt{a_{11}} \\ 0 & I\end{array}\right)$,
where $\bar{A}_{1}=A_{1}-a_{1} a_{1}^{T} / a_{11}$. Then

$$
A=L_{1}\left(\begin{array}{cc}
1 & 0 \\
0 & \bar{A}_{1}
\end{array}\right) L_{1}^{T}
$$

For the Incomplete Cholesky decomposition the first step will be so modified. Define $b_{1}=\left(b_{21}, \cdots, b_{n 1}\right)^{T}$ and $c_{1}=\left(c_{21}, \cdots, c_{n 1}\right)^{T}$ by

$$
b_{j 1}=\left\{\begin{array}{cc}
a_{j 1}, & (j, 1) \in E,  \tag{11}\\
0, & \text { otherwise },
\end{array} \quad c_{j 1}=b_{j 1}-a_{j 1}=\left\{\begin{array}{cl}
0, & (j, 1) \in E \\
-a_{j 1}, & \text { otherwise }
\end{array}\right.\right.
$$

Then

$$
A=\left(\begin{array}{cc}
a_{11} & b_{1}^{T} \\
b_{1} & A_{1}
\end{array}\right)-\left(\begin{array}{cc}
0 & c_{1}^{T} \\
c_{1} & 0
\end{array}\right)=\tilde{B}_{0}-C_{1}
$$

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

$$
\tilde{B}_{0}=\left(\begin{array}{cc}
\sqrt{a_{11}} & 0 \\
b_{1} / \sqrt{a_{11}} & I
\end{array}\right)\left(\begin{array}{cc}
I & 0 \\
0 & \bar{B}_{1}
\end{array}\right)\left(\begin{array}{cc}
\sqrt{a_{11}} & b_{1}^{T} / \sqrt{a_{11}} \\
0 & I
\end{array}\right)=L_{1} B_{1} L_{1}^{T}
$$

and

$$
\bar{B}_{1}=A_{1}-\frac{b_{1} b_{1}^{T}}{a_{11}}
$$

Then

$$
\begin{equation*}
A=L_{1} B_{1} L_{1}^{T}-C_{1} . \tag{12}
\end{equation*}
$$

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

$$
A=L_{1} \cdots L_{n} I L_{n}^{T} \cdots L_{1}^{T}-C_{n-1}-C_{n-2}-\cdots-C_{1}
$$

with

$$
\begin{equation*}
L=L_{1} \cdots L_{n} \text { and } N=C_{1}+C_{2}+\cdots+C_{n} \tag{13}
\end{equation*}
$$

## Lemma 1

Let $A$ be s.p.d. and $E$ be a reserved patten. Then there is at most a decomposition $A=L L^{T}-N$, which satisfies the conditions:
(1) $L$ is lower triangular with $l_{i i}>0, l_{i i} \neq 0 \Longrightarrow(i, j) \in E$.
(2) $N=\left(n_{i j}\right), n_{i j}=0$, if $(i, j) \in E$.

## Proof

The Incomplete Cholesky decomposition may not exist, if

$$
s_{m}:=a_{m m}-\sum_{k=1}^{m-1}\left(l_{m k}\right)^{2} \leq 0
$$

## Example 2

Let

$$
A=\left[\begin{array}{cccc}
1 & -1 & 0 & 2 \\
-1 & 2 & -1 & 0 \\
0 & -1 & 2 & -3 \\
2 & 0 & -3 & 10
\end{array}\right]
$$

The Cholesky decomposition of $A$ follows $L=\left[\begin{array}{cccc}1 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 2 & 2 & -1 & 1\end{array}\right]$.

## Example 3

Consider the Incomplete Cholesky decomposition with patten

$$
E=E(A)=\left[\begin{array}{cccc}
\times & \times & 0 & \times \\
\times & \times & \times & 0 \\
0 & \times & \times & \times \\
\times & 0 & \times & \times
\end{array}\right]
$$

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 $E$.

## Example 4

Now take

$$
E=\left(\begin{array}{cccc}
\times & \times & 0 & 0 \\
\times & \times & \times & 0 \\
0 & \times & \times & \times \\
0 & 0 & \times & \times
\end{array}\right) \Longrightarrow L \text { exists and } L=\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
-1 & 1 & 0 & 0 \\
0 & -1 & 1 & 0 \\
0 & 0 & -3 & 1
\end{array}\right) .
$$

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

M-matrices, H -matrices.

## Definition 5

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

## Lemma 6

$A$ is symmetric, $a_{i j} \leq 0, i \neq j$. 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 $A=L L^{T}-N$, which satisfies (10).

# Definition 8 <br> $A \in \mathbb{R}^{n \times n}$. Decomposition $A=M-N$ is called regular, if $M^{-1} \geq 0$, $N \geq 0$ (regular splitting). 

## Theorem 9

Let $A^{-1} \geq 0$ and $A=M-N$ is a regular decomposition. Then $\rho\left(M^{-1} N\right)<1$. i.e., the iterative method $M x_{k+1}=N x_{k}+b$ for $A x=b$ is convergent for all $x_{0}$.

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

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

Then

$$
0 \leq \sum_{i=0}^{k} T^{i} M^{-1}=\sum_{i=0}^{k} T^{i}(I-T) A^{-1}=\left(I-T^{k+1}\right) A^{-1} \leq A^{-1}
$$

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

## Theorem 10

If $A^{-1} \geq 0$ and $A=M_{1}-N_{1}=M_{2}-N_{2}$ are two regular decompositions with $0 \leq N_{1} \leq N_{2}$, then it holds $\rho\left(M_{1}^{-1} N_{1}\right) \leq \rho\left(M_{2}^{-1} N_{2}\right)$.

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

$$
\begin{aligned}
\rho\left(M^{-1} N\right) & =\rho\left((A+N)^{-1} N\right)=\rho\left(\left[A\left(I+A^{-1} N\right)\right]^{-1} N\right) \\
& =\rho\left(\left(I+A^{-1} N\right)^{-1} A^{-1} N\right)=\frac{\rho\left(A^{-1} N\right)}{1+\rho\left(A^{-1} N\right)}
\end{aligned}
$$

$$
\left[\lambda \rightarrow \frac{\lambda}{1+\lambda} \text { monotone for } \lambda \geq 0\right]
$$

Because $0 \leq N_{1} \leq N_{2}$ it follows $\rho\left(A^{-1} N_{1}\right) \leq \rho\left(A^{-1} N_{2}\right)$. Then

$$
\rho\left(M_{1}^{-1} N_{1}\right)=\frac{\rho\left(A^{-1} N_{1}\right)}{1+\rho\left(A^{-1} N_{1}\right)} \leq \frac{\rho\left(A^{-1} N_{2}\right)}{1+\rho\left(A^{-1} N_{2}\right)}=\rho\left(M_{2}^{-1} N_{2}\right)
$$

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

## Theorem 11

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

Proof: Because each $L_{j}^{-1} \geq 0$, it follows $\left(L L^{T}\right)^{-1} \geq 0$, (from $\left.\left(I-l e^{T}\right)^{-1}=\left(I+l e^{T}\right), l \geq 0\right) . N=C_{1}+C_{2}+\cdots+C_{n-1}$ and all $C_{i} \geq 0$.

## 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 $A=\left[A_{i j}\right]$ with $A_{i j}$ blocks. Take $M=\operatorname{diag}\left[A_{11}, \cdots, A_{k k}\right]$.
(ii) Try Incomplete Cholesky decomposition: Breakdown can be avoided by two ways. If $z_{i}=a_{i i}-\Sigma_{k=1}^{i-1} l_{i k}^{2} \leq 0$, breakdown, then either set $l_{i i}=1$ and go on or set $l_{i k}=0,(k=1, \ldots, i-1)$ until $z_{i}>0$ (change reserved pattern $E$ ).
(iii) $A$ is an arbitrary nonsingular matrix with all principle determinants $\neq 0$. Then $A=L D R$ 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 $(i, i) \in E, i=1,2, \ldots, n$. A decomposition of the form $A=L D R-N$ which satisfies:
(i) $L$ is lower triangular, $l_{i i}=1, l_{i j} \neq 0$, then $(i, j) \in E$,
(ii) $R$ is upper triangular, $r_{i i}=1, r_{i j} \neq 0$, then $(i, j) \in E$,
(iii) $D$ is diagonal $\neq 0$,
(iv) $N=\left(n_{i j}\right), n_{i j}=0$ for $(i, j) \in E$.
is uniquely determined. (The decomposition almost exists for all matrices).

## Chebychev Semi-Iteration Acceleration Method

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

$$
\begin{equation*}
x=T x+f, T=M^{-1} N \text { and } f=M^{-1} b \tag{14}
\end{equation*}
$$

The basic iterative method of (14) is

$$
\begin{equation*}
x_{k+1}=T x_{k}+f . \tag{15}
\end{equation*}
$$

How to modify the convergence rate?

## Definition 13

The iterative method (15) is called symmetrizable, if there is a matrix $W$ with $\operatorname{det} W \neq 0$ and such that $W(I-T) W^{-1}$ is symmetric positive definite.

## Example 14

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,

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

(i): $M=\operatorname{diag}\left(a_{i i}\right)$ Jacobi method.
(ii): $M=\frac{1}{\omega(2-\omega)}(D-\omega L) D^{-1}\left(D-\omega L^{T}\right)$ SSOR-method.
(iii): $M=L L^{T}$ 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 $\mu_{i}$ of $T$ are real and satisfy

$$
\begin{equation*}
\mu_{i}<1, \text { for } i=1,2, \ldots, n \tag{16}
\end{equation*}
$$

Proof: Since $W(I-T) W^{-1}$ is s.p.d., the eigenvalues $1-\mu_{i}$ of $I-T$ are large than zero. Thus $\mu_{i}$ are real and (16) holds.

## Definition 16

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

$$
\left\{\begin{align*}
u_{0} & =x_{0}  \tag{17}\\
u_{k+1} & =\alpha\left(T u_{k}+f\right)+(1-\alpha) u_{k} \\
& =(\alpha T+(1-\alpha) I) u_{k}+\alpha f \equiv T_{\alpha} u_{k}+\alpha f
\end{align*}\right.
$$

is called an Extrapolation method of (15).

## Remark 1

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

## Theorem 17

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

$$
1>\rho\left(T_{\alpha^{*}}\right)=\frac{\mu_{n}-\mu_{1}}{2-\mu_{1}-\mu_{n}}=\min _{\alpha} \rho\left(T_{\alpha}\right) .
$$

Proof: Eigenvalues of $T_{\alpha}$ are $\alpha \mu_{i}+(1-\alpha)=1+\alpha\left(\mu_{i}-1\right)$. Consider the problem

$$
\begin{aligned}
& \min _{\alpha} \max _{i}\left|1+\alpha\left(\mu_{i}-1\right)\right|=\min ! \\
\Longleftrightarrow & \left|1+\alpha\left(\mu_{n}-1\right)\right|=\left|1+\alpha\left(\mu_{1}-1\right)\right| \\
\Longleftrightarrow & \left.1+\alpha\left(\mu_{n}-1\right)=\alpha\left(1-\mu_{n}\right)-1 \text { (otherwise } \mu_{1}=\mu_{n}\right) .
\end{aligned}
$$

This implies $\alpha=\alpha^{*}=\frac{2}{2-\mu_{1}-\mu_{n}}$, then $1+\alpha^{*}\left(\mu_{n}-1\right)=\frac{\mu_{n}-\mu_{1}}{2-\mu_{1}-\mu_{n}}$.

From (15) and (17) follows that

$$
u_{k}=\sum_{i=0}^{k} a_{k i} x_{i}, \text { and } \sum_{i=0}^{k} a_{k i}=1
$$

with suitable $a_{k i}$. Hence, we have the following idea:
Find a sequence $\left\{a_{k i}\right\}, k=1,2, \ldots, i=0,1,2, \ldots, k$ and $\sum_{i=0}^{k} a_{k i}=1$ such that

$$
u_{k}=\sum_{i=0}^{k} a_{k i} x_{i}, u_{0}=x_{0}
$$

is a good approximation of $x^{*}\left(A x^{*}=b\right)$. 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,

$$
\begin{align*}
d_{k} & =u_{k}-x^{*}=\sum_{i=0}^{k} a_{k i}\left(x_{i}-x^{*}\right)  \tag{18}\\
& =\sum_{i=0}^{k} a_{k i} T^{i} e_{0}=\left(\sum_{k i}^{k} a_{k i} T^{i}\right) e_{0} \\
& =\mathcal{P}_{k}(T) e_{0}=\mathcal{P}_{k}(T) d_{0}
\end{align*}
$$

where

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

is a polynomial in $\lambda$ with $\mathcal{P}_{k}(1)=1$.

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

## Remark 2

Let $\|x\|_{W}=\|W x\|_{2}$. Then

$$
\begin{aligned}
\|T\|_{W} & =\max _{x \neq 0} \frac{\|T x\|_{W}}{\|x\|_{W}} \\
& =\max _{x \neq 0} \frac{\left\|W T W^{-1} W x\right\|_{2}}{\|W x\|_{2}} \\
& =\left\|W T W^{-1}\right\|_{2}=\rho(T)
\end{aligned}
$$

because $W T W^{-1}$ is symmetric. We take $\|\cdot\|_{W}$-norm on both sides of (18) and have

$$
\begin{align*}
\left\|d_{k}\right\|_{W} & \leq\left\|\mathcal{P}_{k}(T)\right\|_{W}\left\|d_{0}\right\|_{W}=\left\|W \mathcal{P}_{k}(T) W^{-1}\right\|_{2}\left\|d_{0}\right\|_{2}  \tag{19}\\
& =\left\|\mathcal{P}_{k}\left(W T W^{-1}\right)\right\|_{2}\left\|d_{0}\right\|_{W}=\rho\left(\mathcal{P}_{k}(T)\right)\left\|d_{0}\right\|_{W}
\end{align*}
$$

Replacement problem: Let $1>\mu_{n} \geq \cdots \geq \mu_{1}$ be the eigenvalues of $T$. Determine

$$
\begin{equation*}
\min \left[\left\{\max \left|\mathcal{P}_{k}(\lambda)\right|: \mu_{1} \leq \lambda \leq \mu_{n}\right\}: \operatorname{deg}\left(\mathcal{P}_{k}\right) \leq k, \mathcal{P}_{k}(1)=1\right] . \tag{20}
\end{equation*}
$$

Solution of (20): The replacement problem

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

has the solution

$$
Q_{k}(t)=T_{k}\left(\frac{2 t-b-a}{b-a}\right) / T_{k}\left(\frac{b+a}{a-b}\right)
$$

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 (20) can be transformed to [(II) Conjugate Gradient Method] (34) as

$$
\min \left[\max \left\{\tilde{P}_{k}(t) \mid 1-\mu_{1} \leq t \leq 1-\mu_{n}\right\}: \operatorname{deg}\left(\tilde{P}_{k}\right) \leq k, \tilde{P}_{k}(0)=1\right]
$$

Hence, the solution of (20) is given by

$$
\begin{equation*}
Q_{k}(t)=T_{k}\left(\frac{2 t-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right) / T_{k}\left(\frac{2-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right) \tag{21}
\end{equation*}
$$

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

$$
u_{k}=\sum_{i=0}^{k} a_{k i} x_{i}
$$

which is called the optimal Chebychev semi-iterative method.

Effective Computation of $u_{k}$ : Using recursion of $T_{k}$ :

$$
\left\{\begin{array}{l}
T_{0}(t)=1, \quad T_{1}(t)=t \\
T_{k+1}(t)=2 t T_{k}(t)-T_{k-1}(t)
\end{array}\right.
$$

we get

$$
T_{0}(t)=1, T_{1}(t)=t, T_{k+1}(t)=2 t T_{k}(t)-T_{k-1}(t)
$$

Transforming $T_{k}(t)$ to the form of $Q_{k}(t)$ as in (21) we get

$$
\begin{equation*}
Q_{0}(t)=1, Q_{1}(t)=\frac{2 t-\mu_{1}-\mu_{n}}{2-\mu_{1}-\mu_{n}}=p t+(1-p) \tag{22a}
\end{equation*}
$$

and

$$
\begin{equation*}
Q_{k+1}(t)=[p t+(1-p)] c_{k+1} Q_{k}(t)+\left(1-c_{k+1}\right) Q_{k-1}(t) \tag{22b}
\end{equation*}
$$

where

$$
\begin{equation*}
p=\frac{2}{2-\mu_{1}-\mu_{n}}, \quad c_{k+1}=\frac{2 T_{k}(1 / r)}{r T_{k+1}(1 / r)}, r=\frac{\mu_{1}-\mu_{n}}{2-\mu_{1}-\mu_{n}} . \tag{23}
\end{equation*}
$$

## Recursion for $u_{k}$ :

$$
\begin{aligned}
d_{k+1} & =Q_{k+1}(T) d_{0}=(p T+(1-p) I) c_{k+1} Q_{k}(T) d_{0}+\left(1-c_{k+1}\right) Q_{k-1}(T) d_{0}, \\
x^{*} & =(p T+(1-p) I) c_{k+1} x^{*}+\left(1-c_{k+1}\right) x^{*}+p(I-T) x^{*} c_{k+1} .
\end{aligned}
$$

Adding above two equations together we get

$$
\begin{aligned}
u_{k+1} & =[p T+(1-p) I] c_{k+1} u_{k}+\left(1-c_{k+1}\right) u_{k-1}+c_{k+1} p f \\
& =c_{k+1} p\left\{T u_{k}+f-u_{k}\right\}+c_{k+1} u_{k}+\left(1-c_{k+1}\right) u_{k-1}
\end{aligned}
$$

Then we obtain the optimal Chebychev semi-iterative Algorithm.
[Optimal Chebychev semi-iterative Algorithm]

$$
\begin{aligned}
& \text { Let } r=\frac{\mu_{1}-\mu_{n}}{2-\mu_{1}-\mu_{n}}, p=\frac{2}{2-\mu_{1}-\mu_{n}}, c_{1}=2 \\
& u_{0}=x_{0} \\
& u_{1}=p\left(T u_{0}+f\right)+(1-p) u_{0} \\
& \text { For } k=1,2, \cdots, \\
& \quad u_{k+1}=c_{k+1}\left[p\left(T u_{k}+f\right)+(1-p) u_{k}\right]+\left(1-c_{k+1}\right) u_{k-1}, \\
& c_{k+1}=\left(1-r^{2} / 4 c_{k}\right)^{-1} .
\end{aligned}
$$

## Remark 3

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

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

where $M z_{k}=b-A u_{k}$.

Recursion for $c_{k}$ : Since

$$
c_{1}=\frac{2 t_{0}}{r T_{1}(1 / r)}=\frac{2}{r \cdot \frac{1}{r}}=2
$$

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

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

Then we have

$$
\begin{equation*}
c_{k+1}=\frac{1}{\left(1-\left(r^{2} / 4\right) c_{k}\right)} \text { with } r=\frac{\mu_{1}-\mu_{n}}{2-\mu_{1}-\mu_{n}} \tag{25}
\end{equation*}
$$

Error estimate: It holds

$$
\begin{equation*}
\left\|u_{k}-x^{*}\right\|_{W} \leq\left|T_{k}\left(\frac{2-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)\right|^{-1}\left\|u_{0}-x^{*}\right\|_{W} \tag{26}
\end{equation*}
$$

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

$$
\begin{aligned}
\left\|d_{k}\right\|_{W} & =\left\|Q_{k}(T) d_{0}\right\|_{W} \leq \rho\left(Q_{k}(T)\right)\left\|d_{0}\right\|_{W} \\
& \leq \max \left\{\left|Q_{k}(\lambda)\right|: \mu_{1} \leq \lambda \leq \mu_{n}\right\}\left\|d_{0}\right\|_{W} \\
& \leq\left|T_{k}\left(\frac{2-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)\right|^{-1}\left\|d_{0}\right\|_{W} .
\end{aligned}
$$

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

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

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

Thus $q_{k} \leq 2 c^{k / 2}$. 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

$$
\begin{equation*}
q_{k} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k} \tag{27}
\end{equation*}
$$

That is, after $k$ steps of the Chebychev semi-iterative method the residual $\left\|u_{k}-x^{*}\right\|_{W}$ is reduced by a factor $2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k}$ from the original residual $\left\|u_{0}-x^{*}\right\|_{W}$.

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 $\mu_{n}$ by $\mu_{n}^{\prime}\left(\mu_{n}^{\prime} \geq \mu_{n}\right)$ and $\mu_{1}$ by $\mu_{1}^{\prime}\left(\mu_{1}^{\prime} \leq \mu_{1}\right)$, because $\lambda$ is still in $\left[\mu_{1}^{\prime}, \mu_{n}^{\prime}\right]$ for all eigenvalue $\lambda$ of $T$.

| $\mu_{n}$ | $k$ | $q_{4}$ | $j$ | $j^{\prime}$ | $q_{8}$ | $j$ | $j^{\prime}$ |
| ---: | ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 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 $j^{\prime}: \mu_{n}^{j^{\prime}} \approx q_{4}, q_{8}$.

## Example 18

Let $1>\rho=\rho(T)$. If we set $\mu_{n}^{\prime}=\rho, \mu_{1}^{\prime}=-\rho$, then $p$ and $r$ defined in (23) become $p=1$ and $r=\rho$, respectively. Algorithm 46 can be simplified by

$$
\begin{aligned}
& u_{0}=x_{0} \\
& u_{1}=T u_{0}+f \\
& u_{k+1}=c_{k+1}\left(T u_{k}+f\right)+\left(1-c_{k+1}\right) u_{k-1}, \\
& c_{k+1}=\left(1-\left(\rho^{2} / 4\right) c_{k}\right)^{-1} \quad \text { with } c_{1}=2 .
\end{aligned}
$$

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

$$
\begin{equation*}
u_{k+1}=c_{k+1}\left(T_{p} u_{k}+f\right)+\left(1-c_{k+1}\right) u_{k-1} . \tag{29}
\end{equation*}
$$

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 $(r=\rho)$

$$
c_{2}>c_{3}>c_{4}>\cdots, \text { and } \lim _{k \rightarrow \infty} c_{k}=\frac{2}{1+\sqrt{1-r^{2}}} . \quad \text { (Exercise!) }
$$

(ii) If $T$ is symmetric, then by (21) we get

$$
\begin{align*}
\left\|Q_{k}(T)\right\|_{2} & =\max \left\{\left|Q_{k}\left(\mu_{i}\right)\right|: \mu_{i} \text { is an eigenvalue of } T\right\} \\
& \leq \max \left\{\left|Q_{k}(\lambda)\right|:-\rho \leq \lambda \leq \rho\right\} \\
& =\left|T_{k}(1 / \rho)\right|^{-1}, \quad(\rho=\rho(T)) \\
& =\frac{1}{c^{k / 2}+c^{-k / 2}}=\frac{\left(\omega_{b}-1\right)^{k / 2}}{1+\left(\omega_{b}-1\right)^{k}} \tag{30}
\end{align*}
$$

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

## Appendix

Proof: Let $A=L L^{T}-N=\bar{L} \bar{L}^{T}-\bar{N}$. Then
$a_{11}=l_{11}^{2}=\bar{l}_{11}^{2} \Longrightarrow l_{11}=l_{11}^{-}$(since $l_{11}$ is positive). Also,
$a_{k 1}=l_{k 1} l_{11}-n_{k 1}=\bar{l}_{k 1} l_{11}-\bar{n}_{k 1}$, so we have

$$
\begin{align*}
& \text { If }(k, 1) \in E \Longrightarrow n_{k 1}=\bar{n}_{k 1}=0 \Longrightarrow l_{k 1}=\bar{l}_{k 1}=a_{k 1} / l_{11}  \tag{31a}\\
& \text { If }(k, 1) \notin E \Longrightarrow l_{k 1}=\bar{l}_{k 1}=0 \Longrightarrow n_{k 1}=\bar{n}_{k 1}=-a_{k 1} \tag{31b}
\end{align*}
$$

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

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

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

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

and (31) follows that $n_{r m}=\bar{n}_{r m}$ and $l_{r m}=\bar{l}_{r m}(r \geq m)$.

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

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 $A=k I-\hat{A}$, $\tilde{B}_{0}=k I-\hat{B}_{0}$ with $\hat{A} \geq 0, \hat{B}_{0} \geq 0$, then $\hat{B}_{0} \leq \hat{A}$. By Perron-Frobenius Theorem ?? follows $\rho\left(\hat{B_{0}}\right) \leq \rho(\hat{A})<k$. This implies that $\tilde{B}_{0}$ is an M-matrix.
(ii): Thus $\tilde{B}_{0}$ is positive definite, hence $B_{1}=L_{1}^{-1} \tilde{B}_{0}\left(L_{1}^{-1}\right)^{T}$ is also positive definite. $B_{1}$ has nonpositive off-diagonal element, since $\overline{B_{1}}=\overline{A_{1}}-\frac{b_{1} b_{1} T}{a_{11}}$. Then $B_{1}$ is an M-matrix (by Lemma 6)

Claim: (22b)

$$
\begin{aligned}
Q_{k+1}(t)= & T_{k+1}\left(\frac{2 t-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right) / T_{k+1}\left(\frac{1}{r}\right) \\
= & \frac{1}{T_{k+1}(1 / r)}\left[2\left(\frac{2 t-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right) T_{k}\left(\frac{2 t-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)-T_{k-1}\left(\frac{2 t-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)\right] \\
= & \frac{2 T_{k}(1 / r)}{r T_{k+1}(1 / r)} r\left(\frac{2 t-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right) \frac{T_{k}\left(\frac{2 t-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)}{T_{k}(1 / r)} \\
& -\frac{T_{k-1}\left(\frac{2-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)}{T_{K+1}\left(\frac{2-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)} \frac{T_{k-1}\left(\frac{2-\mu_{1}-\mu_{n}}{\mu_{1}-\mu_{n}}\right)}{T_{k-1}(1 / r)} \\
= & c_{k+1}[p t+(1-p)] Q_{k}(t)-\left[1-c_{k+1}\right] Q_{k-1}(t)
\end{aligned}
$$

since

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

and

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

