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A Unified Convergence Theory for *LR* and *QR* Algorithms Applied to Symmetric Eigenvalue Problems.

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Sunto. – *In questo articolo si considera il problema degli autovalori matrici simmetriche definite positive. In particolare si deducono le proprietà di convergenza per il metodo QR senza shift ed il metodo LR di Cholesky sia in versione restoring che in versione non restoring, considerando le proprietà di convergenza di opportune successioni di matrici triangolari. Per generiche matrici si ottengono alcuni risultati circa la velocità di convergenza del metodo di Cholesky in funzione dello shift prescelto. Tali risultati seguono dall'assoluta convergenza di serie numeriche associate a successioni di matrici. Applicando tale teoria si ricavano proprietà di convergenza del metodo QR per il calcolo degli autovalori di matrici normali e del metodo QR per il calcolo dei valori singolari di matrici complesse. Per ogni metodo oltre alle successioni di matrici ad esso associate si considera una successione convergente di matrici diagonali. Le proprietà di convergenza dei metodi seguono poichè le serie di matrici definite dalla differenza dei termini delle due successioni sono assolutamente convergenti.*

Summary. – *In this paper we consider the eigenvalue problem for positive definite symmetric matrices. Convergence properties for the zero shift QR method and the shift LR Cholesky method both in restoring and in non restoring version are deduced from the convergence properties of triangular matrices sequences. For general matrices we obtain some results on the convergence speed of the Cholesky method as a function of the chosen shift. These results follow from the absolute convergence of numerical series associated to matrices sequences. Concerning this theory we derive also convergence properties of the QR method for the computation of the eigenvalues of normal matrices and of the QR method for the computation of the singular values of complex matrices. For each method, together with the sequences of associated matrices, we consider a convergent sequence of diagonal matrices. Convergence properties of the methods follow since the matrices series defined by the differences of the terms of the two sequences are absolutely convergent.*

1. – Introduction.

In many papers concerning the computation of eigenvalues and singular values of a complex matrix, an important rule is reserved to the methods based on the *LR* and *QR* factorizations. The relation between these methods is shown for example in [5] and [6], and, successively, investigated in [1] and [2]. In particular for positive definite symmetric matrices it is well known that two steps of the zero-shift Cholesky method are equivalent to one step of the zero-shift QR method (see [6]). Hence a proof of the convergence of the LR Cholesky method is also a convergence proof of the QR method and vice versa. The aim of this paper is to analyze the convergence properties of a particular sequence of triangular matrices, from which it is possible to deduce, throught an unique and simple methodology, the convergence property of the following methods:

1. The LR Cholesky method with shift for eigenvalues of Hermitian definite positive matrices both in restoring and non restoring versions;
2. The constant shift QR method for the computation of eigenvalues of the normal matrices;
3. The QR method for the computation of the singular values of general complex matrices.

Since we study the QR method without shift in this theory there is not the convergence proof of the QR method for symmetric tridiagonal matrices with the shift of Wilkinson (see [7]). We give some results on the convergence speed of Cholesky method related to the choice of the shift. These results concern however general matrices more than tridiagonal ones. The main difficulty in the study of the convergence of sequences of triangular matrices arises from the singular values of the initial matrix with multiplicity greater than 1. This implies that the positive definite symmetric matrices have multiple eigenvalues. The paper is organized as follows. Sections 2 and 3 are dedicated to the analysis of the convergence of a sequence of triangular matrices that is the unifying element of this theory. The main results are given in Theorems 2 and 3. In Section 4 the results obtained are applied to the study of the convergence of the LR Choesky method with shift (Theorem 4). The results about the convergence speed in the case of positive shift are deduced from Theorem 3 (see (38)). In Section 5 the results are applied to prove the convergence of the QR method for the computation of the eigenvalues of normal matrices and to prove the convergence of the QR method for the computation of the singular values of a complex matrix (see Theorems 5 and 5). Finally Section 6 is an appendix where some preliminary results used in Sections 2 and 3 are proved dealing in particular with the case of multiple eigenvalues.

2. – The iterative process and the convergence properties.

Starting from the non singular lower triangular complex matrix $L^{(0)}$ of order n, let us consider the following iterative process:

$$L^{(k+1)}L^{(k+1)*} = L^{(k)*}L^{(k)} - \mu_k^2 I, \qquad k = 0, 1, 2, \dots \tag{1}$$

$$0 \leqslant \mu_k < \sigma_{\min}(L^{(k)}) \tag{2}$$

$$L^{(k)} = [l_{i,j}^{(k)}].$$

We observe that the sequence generated from (1)-(2) is well defined and unique if we impose, for example, $l_{ii}^{(k)} > 0$, $\forall i$, (uniqueness of the Cholesky factorization).

Let $\sigma_i^{(k)}$, $i = 1, \ldots, n$, $k = 0, 1, 2, \ldots$, be the the singular values of $L^{(k)}$ ordered as usual in decreasing way:

$$\sigma_1^{(k)} \geqslant \sigma_2^{(k)} \geqslant \ldots \geqslant \sigma_n^{(k)}.$$

Then from (1) it follows

$$\sigma_i^{(k+1)2} = \sigma_i^{(k)2} - \mu_k^2, \qquad i = 1, \ldots, n. \tag{3}$$

Consequently we put

$$s_i = \lim_{k \to \infty} \sigma_i^{(k)}, \qquad i = 1, \ldots, n \tag{4}$$

and

$$\mu^2 = \sum_{k=0}^{\infty} \mu_k^2.$$

Then we obtain

$$\sigma_i^{(0)^2} = s_i^2 + \mu^2 \qquad i = 1, \ldots, n. \tag{5}$$

The real nonnegative number μ is the total shift and it results $s_n = 0$ if and only if $\mu = \sigma_n^{(0)}$.

The following theorem states convergence properties of the sequence $\{L^{(k)}\}$.

THEOREM 1. – *The real nonnegative l_j, $j = 1, \ldots, n$, exist such that*

$$\lim_{k \to \infty} | l_{jj}^{(k)} | = l_j$$

and for each $i \neq j$, it results

$$\sum_{k=0}^{\infty} | l_{ij}^{(k)} |^2 < +\infty.$$

PROOF. – From (1), we obtain,

$$\sum_{i=1}^{j} | l_{ji}^{(k+1)} |^2 = \sum_{i=j}^{n} | l_{ij}^{(k)} |^2 - \mu_k^2, \qquad j = 1, \ldots, n. \tag{6}$$

For $j = 1$ in (6) we obtain

$$|l_{11}^{(k+1)}|^2 - |l_{11}^{(k)}|^2 + \mu_k^2 = \sum_{i=2}^{n} |l_{i1}^{(k)}|^2 . \tag{6}$$

Consequently, each of the $n-1$ series of the general term $|l_{i1}^{(k)}|^2$ has bounded partial sums and therefore they are convergent series. Then also the serie with general term $|l_{11}^{(k+1)}|^2 - |l_{11}^{(k)}|^2$ is convergent and therefore it exists

$$l_1 = \lim_{k \to \infty} |l_{11}^{(k)}| .$$

Now we observe that from (6) it follows:

$$|l_{jj}^{(k+1)}|^2 - |l_{jj}^{(k)}|^2 + \mu_k^2 + \sum_{i=1}^{j-1} |l_{ji}^{(k+1)}|^2 = \sum_{i=j+1}^{n} |l_{ij}^{(k)}|^2 \qquad j = 2, \ldots, n-1$$

and

$$\mu_k^2 + \sum_{j=1}^{n-1} |l_{nj}^{(k+1)}|^2 = |l_{nn}^{(k)}|^2 - |l_{nn}^{(k+1)}|^2 .$$

The thesis can then be completed by induction on index j. ∎

REMARK 1. – *Let $G^{(k)}$ be, for $k = 0, 1, \ldots$, the diagonal and unitary matrices such that the diagonal elements of $G^{(k)} L^{(k)}$ are real positive ($G^{(k)} \equiv I$ if we have selected $l_{ii}^{(k)}$, $i = 1, \ldots, n$, real positive). Then, from Theorem 2 it results*

$$\lim_{k \to \infty} G^{(k)} L^{(k)} = \Lambda . \tag{7}$$

Where $\Lambda = \mathrm{diag}(l_1, \ldots, l_n)$ and l_i, $i = 1, \ldots, n$, are defined in Theorem 1.

REMARK 2. – *Since the singular values of $G^{(k)} L^{(k)}$ are the same of $L^{(k)}$, it exists a permutation matrix P such that*

$$\Lambda = PSP^T$$

where $S = \mathrm{diag}(s_1, \ldots, s_n)$. Putting

$$S^{(k)} = \begin{pmatrix} \sigma_1^{(k)} & & 0 \\ & \ddots & \\ 0 & & \sigma_n^{(k)} \end{pmatrix},$$

let

$$\Lambda^{(k)} = \begin{pmatrix} l_1^{(k)} & & 0 \\ & \ddots & \\ 0 & & l_n^{(k)} \end{pmatrix}$$

such that

$$\Lambda^{(k)} = PS^{(k)} P^T .$$

We observe that

$$\exists k,\; l_i^{(k)} = l_j^{(k)} \;\Leftrightarrow\; \forall k,\; l_i^{(k)} = l_j^{(k)} \;\Leftrightarrow\; l_i = l_j .$$

Now we are about to prove the absolute convergence of the series $l_{ij}^{(k)}$. Before we consider two preliminary lemmas.

LEMMA 1. – *For all i, j such that $l_i \neq l_j$, we have*

$$\sum_{k=0}^{\infty} |l_{ij}^{(k)}| < +\infty .$$

PROOF. – From (1) we deduce

$$\sum_{h=1}^{j} l_{ih}^{(k+1)} \bar{l}_{jh}^{(k+1)} = \sum_{h=i}^{n} l_{hj}^{(k)} \bar{l}_{hi}^{(k)}, \qquad j < i = 2, \ldots, n . \tag{8}$$

Then

$$l_{ij}^{(k+1)} \bar{l}_{jj}^{(k+1)} - l_{ij}^{(k)} \bar{l}_{ii}^{(k)} + \delta_k = 0$$

and, from Theorem 1

$$\sum_{k=0}^{\infty} |\delta_k| < \infty .$$

From hypotheses and from Theorem 1 both sequences $|l_{jj}^{(k)}|$ and $|l_{ii}^{(k)}|$ converge to different limits. Hence the thesis follows from the convergence properties of a more general sequence satisfying a two terms recurrence relation (see Lemma 10). ■

REMARK 3. – *Before proving next lemma we recall the following result* (*see* [4]). *If*

$$\sigma_1(A) \geq \sigma_2(A) \geq \ldots \geq \sigma_n(A)$$

and

$$\sigma_1(B) \geqslant \sigma_2(B) \geqslant \ldots \geqslant \sigma_n(B)$$

are the singular values of complex matrices of order n A and B respectively, then

$$|\sigma_i(A) - \sigma_i(B)| \leqslant \|A - B\|_2 \leqslant \sum_{r,\, s=1}^{n} |a_{rs} - b_{rs}| \qquad i = 1, \ldots, n.$$

Moreover if B is a complex matrix obtained from A setting as zero row or a column of A then

$$\sigma_i(A) \geqslant \sigma_i(B) \geqslant \sigma_{i+1}(A) \qquad i = 1, \ldots, n-1\,.$$

LEMMA 2. – *For all* i, j, *such that* $i > j$, $l_i = l_j$

$$\sum_{k=0}^{\infty} |l_{pq}^{(k)}| < +\infty \qquad p = 1, \ldots, i-1, \;\; q = 1, \ldots, p-1, \quad (\textit{if } i > 2),$$

we have

$$\sum_{k=0}^{\infty} |l_{ij}^{(k)}| < +\infty\,.$$

PROOF. – For every r, such that $r \neq j$, $r \neq i$ and $l_r = l_i$ we want to annihilate the element $l_{ir}^{(k)}$, if $r < i$, or the element $l_{ri}^{(k)}$ and $l_{rj}^{(k)}$ otherwise, preserving exactly two singular values equal to $l_i^{(k)}$. From Remark 2 and from the second part of Remark 2 this is obtained zeroing the r-th column or the r-th row respectively. The matrix $B^{(k)}$ obtained after this process converges, when $k \to \infty$, to a diagonal matrix C. This matrix is obtained from Λ in the same way and it possesses exactly two singular values equal to l_i. Now let $A^{(k)}$ be obtained from $B^{(k)}$ zeroing the rows and columns i and j but not the elements $l_{ii}^{(k)}$, $l_{ij}^{(k)}$ and $l_{jj}^{(k)}$. The singular values of

$$E^{(k)} = \begin{pmatrix} l_{jj}^{(k)} & 0 \\ l_{ij}^{(k)} & l_{ii}^{(k)} \end{pmatrix}$$

are also the singular values of $A^{(k)}$ (see Lemma 9), convergent to l_i. From hypothesis and Lemma 1 it results

$$\sum_{k=0}^{\infty} \sum_{r,\, s=1}^{n} |a_{rs}^{(k)} - b_{rs}^{(k)}| < +\infty\,.$$

From a result on lower triamgular matrices of order 2 (see Lemma 8) it is

$$(9)\quad |l_{ij}^{(k)}| \leqslant |\sigma_1(E^{(k)}) - \sigma_2(E^{(k)})| \leqslant |\sigma_1(E^{(k)}) - l_i^{(k)}| + |\sigma_2(E^{(k)}) - l_i^{(k)}|\,.$$

Using (9) for k large, and from the first part of Remark 3 the thesis follows. ■

We end this section with the announced convergence theorem, taking in mind that we denote by $|A|$ the matrix whose elements are $|a_{ij}|$.

THEOREM 2. – *Referring to sequence* $L^{(k)}$ *defined in* (1) *and* (2) *and to matrices* $G^{(k)}$ *and* Λ *defined in Remarks* 2 *and* 3 *respectively, it results*

$$\sum_{k=0}^{\infty} |G^{(k)} L^{(k)} - \Lambda^{(k)}| < +\infty\,.$$

PROOF. – From Lemmas 1 and 2, using induction on i

$$(10)\qquad \sum_{k=0}^{\infty} |l_{ij}^{(k)}| < +\infty\,, \qquad j = 1, \ldots, i-1\,.$$

Through let

$$A^{(k)} = \operatorname{diag}\left(|l_{11}^{(k)}|, \ldots, |l_{nn}^{(k)}|\right).$$

From (10), using, for k large, the first part of Remark 3, with $A = A^{(k)}$ and $B = G^{(k)} L^{(k)}$ it follows

$$\sum_{k=0}^{\infty} \left| l_i^{(k)} - |l_{ii}^{(k)}| \right| < +\infty \qquad i = 1, \ldots, n. \qquad ■$$

For Section 4 it is useful the following result.

COROLLARY 1. – *In the same hypotheses of Theorem* 2

$$\sum_{k=0}^{\infty} |L^{(k)} L^{(k)*} - \Lambda^{(k)^2}| < \infty\,.$$

PROOF. – It follows from Theorem 2 considering the entries (i, j), for every i, j, of matrix $L^{(k)} L^{(k)*} - \Lambda^{(k)2}$. ■

The result given in Theorem 2 is stronger than (7). Nevertheless in the next section we shall improve (7) in

$$(11)\qquad \lim_{k \to \infty} \frac{|l_{ii}^{(k)}| - l_i^{(k)}}{l_i^{(k)}} = 0 \qquad i = 1, \ldots, n\,.$$

Moreover, putting

$$\xi_i^{(k)^2} = \sum_{h=k+1}^{\infty} |l_{ni}^{(h)}|^2 \qquad i = 1, \ldots, n-1$$

it is obvious that, from Theorem 1,

$$\lim_{k \to \infty} \xi_i^{(k)} = 0 .$$

We want to prove the following relation

$$\lim_{k \to \infty} \frac{\xi_i^{(k)}}{l_n^{(k)}} = 0 . \tag{12}$$

These results improve (7) if $l_i = 0$ or $l_n = 0$. But it happens when $s_n = 0$, i.e. μ_k is sufficiently close to $\sigma_n(L^{(k)})$, (for example see [7]).

3. – Further convergence properties.

In this section we start proving (11) and (12) as a consequence of the more general Theorem 3. Finally we shall give some general condition so that

$$l_1 \geq l_2 \geq \ldots \geq \ldots l_n . \tag{13}$$

REMARK 4 (*See* [4]). – *Let A be an n order complex matrix, σ_i and λ_i be respectively the i-th singular value and eigenvalue of A ordered as*

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n$$

and

$$|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n| .$$

Then

$$\prod_{i=1}^{k} |\lambda_i| \leq \prod_{i=1}^{k} \sigma_i \qquad k = 1, \ldots, n.$$

Moreover if A is a order n complex triangular matrix. Then

$$\sigma_1(A) = \sigma_{\max}(A) \geq \max_i |a_{ii}| \geq \min_i |a_{ii}| \geq \sigma_n(A) = \sigma_{\min}(A).$$

THEOREM 3. – *Referring to the sequence $L^{(k)}$ defined in* (1) *and* (2), *and to $\Lambda^{(k)}$ defined in Remark* 2, *it results*

$$\sum_{k=0}^{\infty} \left| \frac{|l_{ii}^{(k)}| - l_i^{(k)}}{l_i^{(k)}} \right| < +\infty \qquad i = 1, \ldots, n \tag{14}$$

and

(15) $$\sum_{k=0}^{\infty} \frac{\xi_i^{(k)2}}{l_n^{(k)2}} < +\infty .$$

PROOF. – Let

$$J = \{i \in \{1, \ldots, n\} \,|\, l_i = 0\} .$$

If $J = \emptyset$ (14) is a consequence of Theorem 2, otherwise first we observe that for every $j \in J$, $l_j^{(k)} = \sigma_{\min}(L^{(k)})$ (see Remark 2). Hence from Remark 3, $\forall i \in J$,

$$|l_{ii}^{(k)}| \prod_{p \notin J} |l_{pp}^{(k)}| \leqslant |l_i^{(k)}| \prod_{p \notin J} l_p^{(k)}, \qquad |l_{ii}^{(k)}| \geqslant l_i^{(k)} .$$

Then if m is the number of indexes that do not belong to J, $\forall\, k\; \exists\, h$ such that

$$0 \leqslant \frac{|l_{ii}^{(k)}|}{l_i^{(k)}} - 1 \leqslant \frac{l_h^{(k)m}}{|l_{hh}^{(k)m}|} - 1 \leqslant c \big|\, |l_{hh}^{(k)}| - l_h^{(k)} \,\big| \leqslant c \sum_{r=1}^{n} \big|\, |l_{rr}^{(k)}| - l_r^{(k)} \,\big| .$$

Since every $l_{rr}^{(k)}$ converge to a non zero limit, the constant c can be chosen indipendent from k. Then (14) is a consequence of Theorem 2.

To prove (15) we observe that from (6) with $j = n$, and from (3) it is

$$\sum_{i=1}^{n-1} |l_{ni}^{(h+1)}|^2 = |l_{nn}^{(h)^2}| - |l_{nn}^{(h+1)^2}| - \mu_h^2 =$$
$$= (|l_{nn}^{(h)^2}| - l_n^{(h)^2}) - (|l_{nn}^{(h+1)^2}| - l_n^{(h+1)2}).$$

From the definition it follows

$$\xi_i^{(k)^2} \leqslant |l_{nn}^{(k)2}| - l_n^{(k)^2} \qquad i = 1, \ldots, n-1 .$$

Hence, dividing for $l_n^{(k)}$, (15) follows from (14), taking in mind that

$$\sup_k \frac{|l_{nn}^{(k)}| + l_n^{(k)}}{l_n^{(k)}} = 2 + \sup_k \frac{|l_{nn}^{(k)}| - l_n^{(k)}}{l_n^{(k)}} < +\infty . \qquad \blacksquare$$

To prove (13) first it is necessary to find the singular values decomposition (briefly SVD) of every matrix $L^{(k)}$ in sequence (1). For this purpose let $U^{(-1)}$ and $U^{(0)}$ be two unitary matrices such that

(16) $$U^{(-1)*} L^{(0)} U^{(0)} = S^{(0)} \qquad \text{(the SVD of L}^{(0)}\text{)}.$$

Having observed that

$$U^{(0)} = L^{(0)*} U^{(-1)} S^{(0)-1},$$

we define the following sequence of matrices:

$$U^{(k)} = L^{(k)*}\, U^{(k-1)} S^{(k)-1}, \qquad k = 0, 1, \dots \tag{17}$$

If $U^{(k-1)}$ and $U^{(k)}$ are unitary matrices the equation (17) it is equivalent to

$$U^{(k-1)*} L^{(k)}\, U^{(k)} = S^{(k)} \tag{18}$$

that is the SVD of $L^{(k)}$. Hence the following lemma holds.

LEMMA 3. – *All the matrices defined by equation* (17) *are unitary.*

PROOF. – By induction, supposing that $U^{(k-1)}$ and $U^{(k)}$ are unitary from (18) we observe that

$$U^{(k)*} L^{(k)*} L^{(k)}\, U^{(k)} = S^{(k)2}$$

and, from (1)

$$U^{(k)*} L^{(k+1)} L^{(k+1)*}\, U^{(k)} = S^{(k+1)2}.$$

Then, using the definition for $U^{(k+1)}$

$$U^{(k+1)*}\, U^{(k+1)} = S^{(k+1)^{-1}} \big(U^{(k)*} L^{(k+1)*} L^{(k+1)}\, U^{(k)}\big)\, S^{(k+1)^{-1}} =$$
$$= S^{(k+1)^{-1}} S^{(k+1)^2} S^{(k+1)^{-1}} = I\,. \qquad \blacksquare$$

From here to the end of the paper given a complex matrix A of order n we shall denote by A_{ii}, $i = 1, \dots, n$, the leading submatrix of order i, hence the leading minors of A are just $\det A_{ii}$.

THEOREM 4. – *Referring to sequence defined in* (1) *and* (2), *and to matrices Λ and S defined in Remarks* 1 *and* 2 *respectively, if matrix $U^{(0)}$ in* (16) *has non-zero leading minors, it results $S = \Lambda$.*

PROOF. – If $U_{ii}^{(0)}$, for $i = 1, \dots, n$, are the principal minors there exists $c > 0$ such that

$$|\det U_{ii}^{(0)}| \geqslant c, \qquad \forall i\,.$$

Now from

$$L^{(k)}\, U^{(k)} = U^{(k-1)} S^{(k)}$$

it follows

$$\prod_{h=1}^{i} |l_{hh}^{(k)}|\, |\det U_{ii}^{(k)}| = |\det U_{ii}^{(k-1)}| \prod_{h=1}^{i} |\sigma_h^{(k)}|\,.$$

Consequently from Remark 4, we have

$$|\det U_{ii}^{(k)}| \geqslant c > 0, \qquad \forall k \geqslant 1.$$

Having seen that

$$U^{(k)*} L^{(k)*} L^{(k)} U^{(k)} = S^{(k)^2}$$

the thesis is a consequence of a general results on the sequences of diagonalizable matrices given in Lemma 7. ■

4. – The LR Cholesky method.

Let A be an Hermitian definite positive matrix of order n. The Cholesky method in the no restoring version for the computation of the eigenvalues $\lambda_1(A) \geqslant \lambda_2(A) \geqslant \ldots \geqslant \lambda_n(A) > 0$ is the following:

$$A^{(k)} - z_k I = L^{(k)} L^{(k)*} \quad \text{(Cholesky factorization)} \quad A^{(0)} = A \tag{19}$$

$$A^{(k+1)} = L^{(k)*} L^{(k)} \qquad k = 0, 1, 2, \ldots \tag{20}$$

where $L^{(k)}$ is a lower triangular matrix. While in the Cholesky LR method in the restoring version (20) is replaced by

$$A^{(k+1)} = L^{(k)*} L^{(k)} + z_k I, \qquad k = 0, 1, 2, \ldots \tag{21}$$

Putting

$$\begin{aligned} &\lambda_i^{(k)} = \lambda_i(A^{(k)}) \qquad i = 1, \ldots, n \\ &\lambda_1^{(k)} \geqslant \lambda_2^{(k)} \geqslant \ldots \geqslant \lambda_n^{(k)} > 0, \\ &\lambda_i^{(0)} = \lambda_i = \lambda_i(A), \qquad i = 1, \ldots, n, \end{aligned} \tag{22}$$

the shift z_k is such that

$$0 \leqslant z_k < \lambda_n(A^{(k)}). \tag{23}$$

In non restoring version it results evidently

$$A^{(k+1)} = L^{(k)^{-1}} A^{(k)} L^{(k)} - z_k I \qquad k = 0, 1, 2, \ldots \tag{24}$$

while in restoring one it is

$$A^{(k+1)} = L^{(k)-1} A^{(k)} L^{(k)} \qquad k = 0, 1, 2, \ldots \tag{25}$$

In the first case we have

$$\lambda_i^{(k+1)} = \lambda_i^{(k)} - z_k, \qquad k = 0, 1, 2, \ldots \qquad i = 1, \ldots, n$$

while in the second one it is $\lambda_i^{(k)} = \lambda_i$, for $i = 1, \ldots, n$ and $k = 0, 1, 2, \ldots$.

Hence in the non restoring algorithm it is

$$\lambda_i^{(k)} = \lambda_i^{(0)} - \sum_{h=0}^{k-1} z_h, \qquad k = 1, 2, \ldots, \quad i = 1, 2, \ldots, n \tag{26}$$

and it is necessary to introduce the total shift $z \leqslant \lambda_n$,

$$z = \sum_{k=0}^{\infty} z_k. \tag{27}$$

Hence it results

$$\lim_{k \to \infty} \lambda_i^{(k)} = \hat{\lambda}_i, \qquad i = 1, 2, \ldots, n$$

where

$$\hat{\lambda}_i = \lambda_i - z\,. \tag{28}$$

In the case of restoring algorithm we observe that at step $k+1$ there is no reason to choose a shift smaller than the one taken at step k since the shift has be to chosen as close as possible to λ_n. Then having no other choice one can take $z_{k+1} = z_k$. Then replacing (27) we introduce $z \leqslant \lambda_n$ as

$$z = \lim_{k \to \infty} z_k. \tag{29}$$

In the non restoring case we put

$$D = \operatorname{diag}(\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_n) \tag{30}$$

and

$$D^{(k)} = \operatorname{diag}(\lambda_1^{(k)}, \lambda_2^{(k)}, \ldots, \lambda_n^{(k)})\,. \tag{31}$$

In the other case we introduce simply

$$D = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)\,. \tag{32}$$

To relate the LR Cholesky shift method with the sequence (1) defined in Section 2, we observe that from (19), with $k+1$ replacing k, (20) and (21):

$$L^{(k+1)} L^{(k+1)*} = L^{(k)*} L^{(k)} - z_{k+1} I \tag{33}$$

$$L^{(k+1)} L^{(k+1)*} = L^{(k)*} L^{(k)} - (z_{k+1} - z_k)\, I, \quad k = 0, 1, \ldots \;\; z_{k+1} - z_k \geqslant 0 \tag{34}$$

in the non restoring and restoring versions respectively.

The two sequences (33) and (34) are like (1) and the diagonal elements of each triangular matrix are real positive. In (33), from (20), we have

$$\sigma_i^2(L^{(k)}) = \lambda_i^{(k+1)}, \qquad i = 1, \ldots, n$$

while in (34), from (21)

$$\sigma_i^2(L^{(k)}) = \lambda_i - z_k, \qquad i = 1, \ldots, n .$$

Then referring to matrices $S^{(k)}$ and S of Remark 2 it results for the sequence (33)

$$(S^{(k)})^2 = D^{(k)} - z_k I, \qquad S^2 = D \tag{35}$$

while for sequence (34)

$$(S^{(k)})^2 = D - z_k I, \qquad S^2 = D - zI . \tag{36}$$

Now we show how the well-known convergence properties of Cholesky method in both versions can be derived using the theory exposed in Section 2. We start with the following theorem.

THEOREM 5. – *Let A be a positive definite Hermitian matrix with eigenvalues*

$$\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n .$$

The sequences defined by (19), (20), (23) *converge for $k \to \infty$ to a diagonal matrix. Similarly the sequence defined by* (19), (21) *and* (23) *converges to a diagonal matrix. In both the cases the limit matrix Γ verifies*

$$\Gamma = PDP^T \tag{37}$$

where P is a permutation matrix and D is given by (30) *for the first sequence and from* (32) *for the second one. In* (30) *$\widehat{\lambda}_i$ are given by* (28) *with z, total shift, defined by* (27).

PROOF. – The matrix sequence $L^{(k)}$ in (33), as in (34), converges, applying Remark 1 to a diagonal matrix Λ (different in the two cases). If (20) holds then $A^{(k)}$ converges to $\Gamma = \Lambda^2$, while if (21) holds, it converges to $\Gamma = \Lambda^2 + zI$, where z is defined by (29). The equation (37) follows from (35), or (36), and from Remark 2. ∎

Theorem 5 can be generalized in the following result.

THEOREM 6. – *In the same hypotheses of Theorem* 5, *let*

$$\Gamma^{(k)} = PD^{(k)}P^T$$

with $D^{(k)}$ defined by (31). *Hence for the sequence* (19), (20) *and* (23) *it is*

$$\sum_{k=0}^{\infty} |A^{(k)} - \Gamma^{(k)}| < +\infty ,$$

while for the other one it is

$$\sum_{k=0}^{\infty} |A^{(k)} - \Gamma| < +\infty .$$

PROOF. – Referring to matrix $\Lambda^{(k)}$ of Remark 2, if (35) holds then

$$\Lambda^{(k)^2} + z_k I = \Gamma^{(k)},$$

otherwise if (36) holds, it is

$$\Lambda^{(k)^2} + z_k I = \Gamma.$$

Then the thesis follows from (19) and from Corollary 1. ■

Also in the theory developed in Sections 2 and 3 we can give some general conditions such that $\Gamma = D$, that is $P = I$. It is well-known that for the LR method, when it converges, the limit matrix is a diagonal one with entries ordered in decreasing way (see [6]). In fact the following theorem holds.

THEOREM 7. – *Let Q be an unitary matrix such that*

$$Q^* AQ = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$$

and

$$\det Q_{ii} \neq 0 \qquad i = 1, \ldots, n-1 .$$

Then both for sequences (19), (20) *and* (23) *as for* (19), (21) *and* (23) *it is*

$$\lim_{k \to \infty} A^{(k)} = D$$

where D is given by (30) *for the sequence* (19), (20) *and* (23), *and by* (32) *for the sequence* (19), (21) *and* (23).

PROOF.

$$Q^* (A - z_0 I)\, Q = Q^* L^{(0)} L^{(0)*} Q = D .$$

The matrix $U^{(0)} = D^{-1/2} Q^* L^{(0)}$ is unitary and verifies

$$U^{(0)*} L^{(0)*} Q = D^{1/2}.$$

Hence

$$U^{(-1)} L^{(0)} U^{(0)} = D^{1/2}, \qquad Q = U^{(-1)}$$

is the SVD of $L^{(0)}$.

Now the leading minors of $U^{(0)}$ are not zero if and only if are not zero the leading minor of Q. The thesis is a consequence of the hypothesis on Q and of the theorem 4. ■

The strategies in the choice of the shift in LR and QR methods are well known, expecially for tridiagonal matrices (see [3], [5], [6] and [7]). In LR Cholesky method it is necessary required the bound given by (23) and it could be found $z = \lambda_n$. For example in restoring method, since the sequence $A^{(k)}$ is convergent it can be obtained using Gershgorin-type theorems (for general matrices). When at each step the shift is sufficiently close to the smallest eigenvalue so that $z = \lambda_n$, using Theorem 4 we could estimate the convergence to zero of the extradiagonal elements in the last column of $A^{(k)}$.

In fact

$$|a_{in}^{(k+1)}| = |a_{ni}^{(k+1)}| = |l_{ni}^{(k)}|\,|l_{nn}^{(k)}| \qquad i = 1, \dots, n-1 \tag{38}$$

and from Theorem 3 we could furnish an indication of how $a_{ni}^{(k+1)}$ approaches to zero.

5. – The QR method for eigenvalues and singular values.

Let A be an n order complex nonsingular matrix. It is well known that there exists the $A = QR$ factorization, with Q unitary matrix and R upper triangular matrix. The diagonal elements of R are defined up to a constant of modulus 1. The QR method to compute the eigenvalues of a complex matrix A is defined by the recursive scheme (see [6]):

$$\begin{aligned} &A^{(k)} - \mu_k I = Q^{(k)} R^{(k)} \qquad A^{(0)} = A \\ &A^{(k+1)} = R^{(k)} Q^{(k)} + \mu_k I, \qquad k = 0, 1, \dots \end{aligned} \tag{39}$$

Inside the theory developed in Sections 2 and 3 we can define also for the QR method a series of matrices absolutely convergent. A strong limit is that we have to consider only normal matrices and to take a constant shift. In fact the following theorem holds.

THEOREM 8. – *Let us suppose the shift in sequence* (39) *to be constant* (*i.e.* $\mu_k = \mu$ *for every* k) *and* A *to be a normal matrix* (*i.e.* $A^*A = AA^*$), *and to choose the diagonal elements of each* $R^{(k)}$, *real and definitely of the same sign* (*not necessarly the same for each index* i). *Then there exist real numbers* $r_1, \dots, r_n$ *such that, putting*

$$D = \operatorname{diag}(r_1, \dots, r_n),$$

we have

$$\sum_{k=0}^{\infty} |R^{(k)} - D| < +\infty . \tag{40}$$

The values $|r_i|$, *for* $i = 1, \ldots, n$, *are the singular values* $A - \mu I$ *(i.e. the moduli of eigenvalues of* $A - \mu I$*).*

PROOF. – If the shift is constant, from (39) we have

$$(A^{(k+1)} - \mu I)^* (A^{(k+1)} - \mu I) = R^{(k+1)*} R^{(k+1)}$$

$$(A^{(k+1)} - \mu I)(A^{(k+1)} - \mu I)^* = R^{(k)} R^{(k)*}.$$

From (39) it results

$$A^{(k+1)} = Q^{(k)*} A^{(k)} Q^{(k)},$$

and, since A is normal, also $A^{(k)}$ is normal for every k. Then

$$R^{(k+1)*} R^{(k+1)} = R^{(k)} R^{(k)*}.$$

Equation (40) follows from Theorem 2 with $L^{(k)} = R^{(k)*}$, $k = 0, 1, 2, \ldots$.

The rest of the thesis holds since, for every k, $R^{(k)}$ has the same singular values of $A - \mu I$. ■

As for the LR Cholesky method, the results shown in Section 3 give general conditions such that

$$|r_1| \geqslant |r_2| \geqslant \ldots \geqslant |r_n| . \tag{41}$$

In fact the following theorem holds.

THEOREM 5.9. – *In the same hypotheses of Theorem* 8, *let* $V^* A V = J$ *be the spectral decomposition of* A, *with diagonal elements of* J *ordered with the modulus in decreasing way. If* $\det V_{ii} \neq 0$, *for* $i = 1, 2, \ldots, n$, *then inequality* (41) *holds.*

PROOF. – It exists an unitary diagonal matrix Σ, such that, from (39)

$$V^* Q^{(0)} R^{(0)} V \Sigma = |J| .$$

Hence, putting $U^{(-1)} = (V\Sigma)^*$, $U^{(0)} = Q^{(0)*} V$, $U^{(-1)} L^{(0)} U^{(0)}$ is the SVD of $L^{(0)} = R^{(0)*}$. The thesis follows from Theorem 4 having observed that the leading minors of $U^{(0)}$ are non null if and only if so are the ones of V. ■

It is known (for example see [6]) that when QR method converges, the limit matrix is usually a block diagonal one. To obtain a similar result in this contest, we shall give in Section 6 a general theorem concerning sequences of matrices. Using this results it is possible to prove the following theorem.

THEOREM 10. – *In the same hypotheses of Theorems* 8 *and* 9, *if the sequence* $R^{(k)}$ *is such that*

$$|r_{ii}^{(k)}| = |r_{jj}^{(k)}| \Leftrightarrow r_{ii}^{(k)} = r_{jj}^{(k)},$$

then

$$\lim_{k\to\infty} A^{(k)} = \Omega \tag{42}$$

where Ω *is a block diagonal matrix whose eigenvalues are the same of* A. *If* λ_i *and* λ_j, $i \neq j$, *are eigenvalues of a diagonal block then*

$$|\lambda_i - \mu| = |\lambda_j - \mu|.$$

PROOF. – From (39) it is

$$A^{(k+1)} = R^{(k)} A^{(k)} R^{(k)-1}.$$

Since (40) holds, equation (42) follows from the more general Lemma 11. Since the entry (i, j) of matrix Ω is zero if $r_i \neq r_j$, and the moduli of r_i are the moduli of the eigenvalues of $A - \mu I$, the last of the thesis follows. ∎

We end the section proving that also for the convergence of the QR method for the singular values it is possible to apply the theory developed in Sections 2 and 3.

If A is an order n nonsingular complex matrix, starting from $QA = R$, with Q unitary and R upper tridiagonal matrix, the scheme of the method is the following

$$R^{(k+1)} = Q^{(k)} R^{(k)*}, \quad k = 0, 1, 2, \dots \qquad R^{(0)} = R \tag{43}$$

where each $Q^{(k)}$ is unitary and each $R^{(k)}$ is upper triangular. Then the following theorem holds.

THEOREM 11. – *If in the scheme* (43) *we impose that the diagonal elements of each* $R^{(k)}$ *are real positive, it results*

$$\lim_{k\to\infty} R^{(k)} = \mathrm{diag}(r_1, r_2, \dots, r_n) = \Lambda$$

and

$$\sum_{k=0}^{\infty} |R^{(k)} - \Lambda| < +\infty. \tag{44}$$

PROOF. – From (43) we have

$$R^{(k+1)^*} R^{(k+1)} = R^{(k)} R^{(k)^*}, \qquad k = 0, 1, 2, \ldots \tag{45}$$

and the thesis follows from Theorem 2. ■

The values r_i are clearly the singular values of A and of $R^{(k)}$, for every k, but to obtain the SVD of A it is necessary the following lemma.

LEMMA 4. – *Let* $\{h_m\}_{m \in N}$ *be an increasing sequence. Then the sequence*

$$\left\{ P_m := \prod_{i=1}^{m} Q^{(h_i)} \right\}_{m \in N}$$

is convergent.

PROOF. – First, we observe that $\|P^{(m)} - P^{(m-1)}\|_2 = \|Q^{(h_m)} - I\|_2$. From (43) we have

$$(R^{(k+1)} - R^{(k)^*}) R^{(k)^{-*}} = Q^{(k)} - I \, .$$

Since

$$\|R^{(k+1)} - R^{(k)}\|_2 \leq \|R^{(k+1)} - \Lambda\|_2 + \|R^{(k)} - \Lambda\|_2$$

$$\sup \|R^{(k)-1}\|_2 < \infty$$

and from (44) the thesis follows. ■

The construction of the SVD of A needs the following lemma.

LEMMA 5. – *Put*

$$U = \lim_{k \to \infty} Q^{(2k)} Q^{(2k-2)} \ldots Q^{(0)}$$

$$V = \lim_{k \to \infty} Q^{(2k-1)} Q^{(2k-3)} \ldots Q^{(1)}$$

we have

$$VRU^* = \Lambda$$

and

$$UR^* V^* = \Lambda \, .$$

PROOF. – The thesis is an immediate consequence of the following relations:

$$R^{(2k+1)} = Q^{(2k)} Q^{(2k-2)} \ldots Q^{(0)} R^* Q^{(1)^*} Q^{(3)^*} \ldots Q^{(2k-1)^*}, \qquad k = 1, 2, \ldots$$

$$R^{(2k)} = Q^{(2k-1)} Q^{(2k-3)} \ldots Q^{(1)} R Q^{(0)^*} Q^{(2)^*} \ldots Q^{(2k-2)^*}, \qquad k = 0, 1, \ldots \qquad ■$$

REMARK 5. – *Since* $A = Q^* R$, *it follows that*

$$A = (VQ)^* \Lambda U,$$

that however is not the SVD of A since the the singular values must be ordered in decreasing way.

The next lemma solves this question.

LEMMA 6. – *Let*

$$P^* AT = \Sigma$$

be the SVD of A. If the leading minors of T are non zero, $\Sigma = \Lambda$.

PROOF. – From $A = Q^* R$ then

$$(PQ)^* RT = \Sigma$$

is the SVD of R and

$$T^* R^* (PQ) = \Sigma$$

is the SVD of R^*.

Now, the leading minors of T are non zero if and only if PQ has non zero leading minors. From Theorem 4 it follows $\Sigma = \Lambda$. ■

6. – Appendix.

In this section we prove some preliminary results.

LEMMA 7. – *Let* $\{A^{(k)}\}$, $\{P^{(k)}\}$, $k = 0, 1, \dots$, *be two sequences of order n complex matrices such that*

1. $\lim_{k \to \infty} A^{(k)} = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$, $\lambda_i \in \mathbb{C}$, $i = 1, \dots, n$;
2. $P^{(k)}$ *is a bounded sequence*;
3. $\exists c > 0$ *such that*

$$\forall k \in N : \ |\det P_{ii}^{(k)}| \geq c, \qquad i = 1, 2, \dots, n;$$

where $\det P_{ii}^{(k)}$ *is the leading order i principal minor of* $P^{(k)}$;

4. $\forall k \in N$,

$$P^{(k)^{-1}} A^{(k)} P^{(k)} = \Lambda^{(k)},$$

where $\Lambda^{(k)}$ *is a diagonal matrix, and*

$$\lim_{k \to \infty} \Lambda^{(k)} = \Lambda = \mathrm{diag}(\gamma_1, \gamma_2, \dots, \gamma_n) \quad \gamma_i \in \mathbb{C}, i = 1, \dots, n.$$

Then

$$\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n).$$

PROOF. – For a suitable increasing sequence k_n let

$$\lim_{n \to \infty} P^{(k_n)} = P.$$

From 4. we have,

$$\lim_{n \to \infty} A^{k_n} P^{k_n} = \lim_{n \to \infty} P^{k_n} \Lambda^{k_n}.$$

Then

$$\operatorname{diag}(\lambda_1, \ldots, \lambda_i)\, P_{ii} = P_{ii} \operatorname{diag}(\gamma_1, \ldots, \gamma_i), \quad i = 1, \ldots, n\,.$$

From 3., $\det P_{ii} \neq 0\ \forall i$, and

$$\prod_{j=1}^{i} \lambda_j = \prod_{j=1}^{i} \gamma_j, \qquad i = 1, \ldots, n\,;$$

then, if $\det \Lambda \neq 0$,

$$\lambda_i = \gamma_i, \qquad i = 1, \ldots, n\,.$$

If $\det \Lambda = 0$ then the hypotheses are still valid for $A^{(k)} + \varepsilon I$, with ε such that $\det(\Lambda + \varepsilon I) \neq 0$. ■

LEMMA 8. – *Let*

$$E = \begin{pmatrix} \alpha & 0 \\ \beta & \gamma \end{pmatrix}$$

be a 2×2 *complex matrix and* $\sigma_1 \geqslant \sigma_2$ *be the singular values of E. Then*

$$|\beta| \leqslant \sigma_1 - \sigma_2.$$

PROOF. – From

$$\sigma_1^2 + \sigma_2^2 = \alpha^2 + \beta^2 + \gamma^2$$

and

$$\sigma_1 \sigma_2 = |\alpha\gamma|\,,$$

it follows

$$(\sigma_1 - \sigma_2)^2 = (|\alpha| - |\gamma|)^2 + \beta^2 \geqslant \beta^2. \qquad ■$$

LEMMA 9. – *Let $A = [a_{ij}]$ be a complex matrix of order n such that:*

$a_{pj} = a_{qj} = 0 \quad j = 1, \dots, n$ *except at the most for $j = p$, and $j = q$,*

$a_{ip} = a_{iq} = 0 \quad i = 1, \dots, n$ *except at the most for $i = q$, and $i = p$*

and $q > p$. Then the singular values of

$$E = \begin{pmatrix} a_{pp} & a_{pq} \\ a_{qp} & a_{qq} \end{pmatrix}$$

are also the singular values of A.

PROOF. – It is not difficult to construct a permutation matrix P, such that

$$PAP^T = \left(\begin{array}{c|c} E & O \\ \hline O & * \end{array} \right)$$

where « $*$ » denotes a not essential matrix. Then the thesis is a trivial consequence of the structure of PAP^T and of the property of invariance of the singular values under unitary transformations. ■

LEMMA 10. – *Let $\{y_n\}_{n \in N}$ be a complex sequence generated through the two terms recurrence relation*

$$\alpha_n y_{n+1} + \beta_n y_n + \delta_n = 0 ,$$

where $\alpha_n, \beta_n, \delta_n \in C$, $\forall n \in N$ and $y_0 \in \mathbb{C}$, also

1. $$\lim_{n \to \infty} |\alpha_n| = \alpha, \qquad \lim_{n \to \infty} |\beta_n| = \beta, \qquad \alpha \neq \beta ,$$

and

2. $$\sum_{n=0}^{\infty} |\delta_n| < +\infty$$

3. $$\sup_{n \in N} |y_n| < +\infty .$$

Then

$$\sum_{n=0}^{\infty} |y_n| < +\infty .$$

PROOF. – Fixed $\varepsilon < |\alpha - \beta|/2$, for large n we have:

$$\begin{array}{lll} \alpha - \varepsilon & \leqslant |\alpha_n| & \leqslant \alpha + \varepsilon \\ \beta - \varepsilon & \leqslant |\beta_n| & \leqslant \beta + \varepsilon \, . \end{array}$$

If $\alpha > \beta$, $\alpha - \varepsilon > 0$, from

$$|\alpha_n| \, |y_{n+1}| \leqslant |\beta_n| \, |y_n| + |\delta_n|$$

we have

$$(\alpha - \varepsilon) \, |y_{n+1}| \leqslant (\beta + \varepsilon) \, |y_n| + |\delta_n|$$

or, equivalentely

$$((\alpha - \varepsilon) - (\beta + \varepsilon)) \, |y_{n+1}| \leqslant (\beta + \varepsilon)(|y_n| - |y_{n+1}|) + |\delta_n| \, .$$

Then

$$|y_{n+1}| \leqslant ((\beta + \varepsilon)(|y_n| - |y_{n+1}|) + |\delta_n|)/h, \qquad h = \alpha - \beta - 2\varepsilon > 0,$$

from which the thesis follows.

Analogously, if $\beta > \alpha$, we have

$$(\beta - \varepsilon) \, |y_n| \leqslant (\alpha + \varepsilon) \, |y_{n+1}| + |\delta_n|$$

and

$$|y_n| \leqslant ((\alpha + \varepsilon)(|y_{n+1}| - |y_n|) + |\delta_n|)/h, \qquad h = \beta - \alpha - 2\varepsilon > 0,$$

from which also in this case the thesis follows. ■

LEMMA 11. – *Let* $\{P^{(k)}\}$ *be a sequence of nonsingular complex matrices of order* n *such that*

$$\sum_{k=0}^{\infty} |P^{(k)} - D| < +\infty$$

with $D = \mathrm{diag}(d_1, \ldots, d_n)$, $\det D \neq 0$, *and*

$$|d_i| = |d_j| \;\Leftrightarrow\; d_i = d_j \qquad \forall i, j \, .$$

Moreover for a fixed n *order complex matrix* A *the sequence* $\{A^{(k)}\}$ *generated by*

$$A^{(k+1)} = P^{(k)} A^{(k)} P^{(k)-1}, \qquad A^{(0)} = A$$

let be bounded.

Then the sequence $\{A^{(k)}\}$ *is convergent and*

$$d_i \neq d_j, \qquad i \neq j$$

implies that the entry (i, j) *in the limit matrix is zero.*

PROOF. – From

$$A^{(k+1)}P^{(k)} = P^{(k)}A^{(k)},$$

we have

$$a_{ij}^{(k+1)}p_{jj}^{(k)} - a_{ij}^{(k)}p_{ii}^{(k)} + \delta_k = 0, \qquad \forall (i,j),$$

where, from hypotheses

$$\sum_{k=0}^{\infty} |\delta_k| < +\infty .$$

From lemma 6, if $d_i \neq d_j$

$$\lim_{k\to\infty} a_{ij}^{(k)} = 0 .$$

Moreover, if $i=j$, for k large, $m < |p_{ii}^{(k)}|$ exists such that

$$\sum_{k=0}^{\infty} |a_{ii}^{(k+1)} - a_{ii}^{(k)}| < \frac{1}{m}\sum_{k=0}^{\infty} |\delta_k| .$$

Finally if $d_i = d_j$ for $i \neq j$, since

$$\sum_{k=0}^{\infty} |p_{ii}^{(k)} - p_{jj}^{(k)}| < +\infty ,$$

we have always

$$\sum_{k=0}^{\infty} |a_{ij}^{(k+1)} - a_{ij}^{(k)}| < +\infty . \qquad \blacksquare$$

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