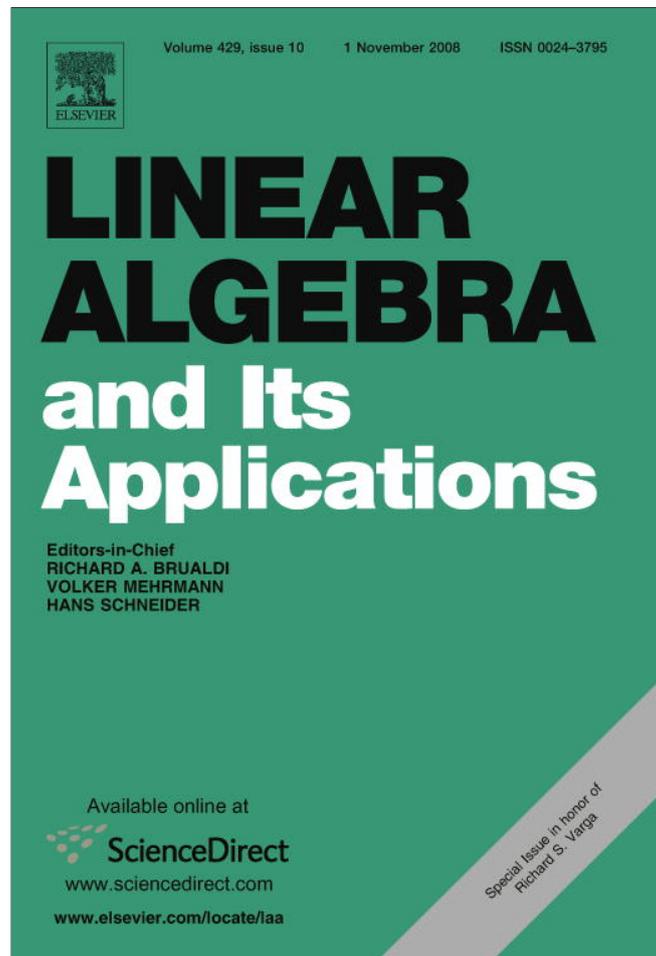


Provided for non-commercial research and education use.
Not for reproduction, distribution or commercial use.



This article appeared in a journal published by Elsevier. The attached copy is furnished to the author for internal non-commercial research and education use, including for instruction at the authors institution and sharing with colleagues.

Other uses, including reproduction and distribution, or selling or licensing copies, or posting to personal, institutional or third party websites are prohibited.

In most cases authors are permitted to post their version of the article (e.g. in Word or Tex form) to their personal website or institutional repository. Authors requiring further information regarding Elsevier's archiving and manuscript policies are encouraged to visit:

<http://www.elsevier.com/copyright>



ELSEVIER

Available online at www.sciencedirect.com

Linear Algebra and its Applications 429 (2008) 2465–2480

**LINEAR ALGEBRA
AND ITS
APPLICATIONS**

www.elsevier.com/locate/laa

The principle of extrapolation and the Cayley Transform[☆]

A. Hadjidimos^{a,*}, M. Tzoumas^b^a *Department of Computer and Communication Engineering, University of Thessaly, 10 Iasonos Street, GR-383 33 Volos, Greece*^b *Department of Mathematics, University of Ioannina, GR-451 10 Ioannina, Greece*

Received 14 September 2007; accepted 16 October 2007

Available online 11 December 2007

Submitted by D. Szyld

Dedicated to Professor Richard S. Varga on his 80th birthday with our gratitude for his fundamental contribution to the construction of the magnificent edifice of Matrix Iterative Analysis.

Abstract

The *Cayley Transform*, $F := (I + A)^{-1}(I - A)$, with $A \in \mathbb{C}^{n,n}$ and $-1 \notin \sigma(A)$, where $\sigma(\cdot)$ denotes spectrum, is of significant theoretical importance and interest and has many practical applications. E.g., in the solution of the Linear Complementarity Problem (LCP), in the solution of linear systems arising from the discretization of model problems elliptic PDEs by Alternating Direction Implicit (ADI) iterative methods, in the solution of complex linear systems by ADI-type methods of Hermitian/Skew Hermitian or Normal/Skew Hermitian Splittings, etc. In the present work we apply the principle of *Extrapolation* to generalize the *Cayley Transform* and determine in an optimal sense the *extrapolation* parameter involved so that problems in many practical applications are solved much more efficiently.

© 2007 Elsevier Inc. All rights reserved.

AMS classification: Primary 65F10*Keywords:* Cayley Transform; Extrapolation; Positive stable matrices; Möbius transformations; Convex hull; Capturing circle

[☆] Part of the work of this author was funded by the Program Pythagoras of the Greek Ministry of Education.

* Corresponding author. Tel.: +30 24210 74908; fax: +30 24210 74923.

E-mail addresses: hadjidim@inf.uth.gr (A. Hadjidimos), mtzoumas@cc.uoi.gr (M. Tzoumas).

1. Introduction and preliminaries

We begin our work with the definition of the *Cayley Transform*.

Definition 1.1. Given

$$A \in \mathbb{C}^{n,n}, \quad \text{with } -1 \notin \sigma(A), \quad (1.1)$$

the *Cayley Transform* is defined to be the following matrix function of A

$$F := \mathcal{F}(A) = (I + A)^{-1}(I - A). \quad (1.2)$$

Note. For properties of the Cayley Transform, theoretical applications to various classes of matrices, as e.g., M -matrices, inverses of M -matrices, and for other references, the reader is referred to the work by Fallatt and Tsatsomeros [10].

We generalize Definition 1.1 by putting ωA instead of A in (1.2), where ω is a nonzero complex number, as follows:

Definition 1.2. Under the assumptions of Definition 1.1, we call *Extrapolated Cayley Transform*, with *extrapolation* parameter ω , the matrix function

$$F_\omega := \mathcal{F}(\omega A) = (I + \omega A)^{-1}(I - \omega A), \quad \omega \in \mathbb{C} \setminus \{0\}, \quad -1 \notin \sigma(\omega A). \quad (1.3)$$

From now on we restrict to the following class of matrices.

Main Assumption: Unless otherwise stated, it will be assumed from now on that the matrix A in Definitions 1.1 and 1.2 has *real elements* and is *positive stable*, that is its eigenvalues $a \in \sigma(A)$ have positive real parts ($\operatorname{Re} a > 0$).

The Cayley Transform, its Extrapolated counterpart as well as their scalar analogues ($w = \frac{1-a}{1+a}$, $w = \frac{1-\omega a}{1+\omega a}$ which are Möbius transformations) appear in many practical applications. For example:

- (1) In the solution of the Linear Complementarity Problem (LCP) when the basic matrix A is, in addition, *real symmetric positive definite* and the LCP is solved by the Modulus Algorithm proposed by van Bokhoven [31].
- (2) In the solution of the problem of the determination of optimal *acceleration* parameter in the classical stationary Alternating Direction Implicit (ADI) iterative method for the solution of the linear system arising from the discretization of model problems elliptic PDE's (see, e.g., [27] and also [32] or [33]).
- (3) In a similar case as in the previous one for the solution of a *complex* linear system, with *positive stable* coefficient matrix, by an ADI-type method using (a) the Hermitian/Skew Hermitian Splitting introduced by Bai, Golub and Ng [1] or (b) the Normal/Skew Hermitian Splitting introduced by the same authors (see [12]).

More on the above applications will be given in Sections 5 and 6.

Since the Cayley Transform plays the role of the iteration matrix in the aforementioned problems, then by considering the Extrapolated Cayley Transform it would be expected that with an optimal choice of the extrapolation parameter we could achieve optimal convergence rates of the iterative schemes involved. So, we state and try to solve the following problem which constitutes the main objective of the present work.

Problem I. For $A \in \mathbb{R}^{n,n}$ positive stable, determine the Extrapolation Parameter $\omega (> 0)$ that minimizes the spectral radius of the Extrapolated Cayley Transform, i.e.

$$\min_{\omega > 0} \rho(F_\omega) = \min_{\omega > 0} \max_{a \in \sigma(A)} \left| \frac{1 - \omega a}{1 + \omega a} \right| (< 1). \tag{1.4}$$

Note. The extrapolation parameter is considered to be real to simplify matters. Furthermore, since $\operatorname{Re} a > 0$, it is taken to be positive in order to always guarantee the validity of the strict inequality

$$\max_{a \in \sigma(A)} \left| \frac{1 - \omega a}{1 + \omega a} \right| < 1. \tag{1.5}$$

2. The solution to the minimax Problem I

To go on with our analysis we introduce some further notation. For the positive stable matrix $A \in \mathbb{R}^{n,n}$ let \mathcal{H} be the *convex hull* of $\sigma(A)$, that is the smallest convex polygon that contains $\sigma(A)$ in the closure of its interior. Note that since A is *real positive stable*, $\sigma(A)$ will be symmetric with respect to (*wrt*) the positive real semiaxis and so will be \mathcal{H} .

To solve Problem I we seek first the solution to the more general optimization problem stated below.

Problem II. Determine the extrapolation parameter ω that solves the minimax problem

$$\min_{\omega > 0} \max_{a \in \mathcal{H}} \left| \frac{1 - \omega a}{1 + \omega a} \right| (< 1). \tag{2.1}$$

For this we study the function in (2.1)

$$w := w(a) = \frac{1 - \omega a}{1 + \omega a}, \quad a \in \mathcal{H}, \quad \omega > 0. \tag{2.2}$$

This function is a Möbius transformation [16], has no *poles*, since $\operatorname{Re}(1 + \omega a) > 0$, and maps the point a onto the point w . Since $\det \begin{pmatrix} 1 & -\omega \\ \omega & 1 \end{pmatrix} = 2\omega > 0$, w is not the constant function. In addition, it possesses an inverse transformation given by

$$w^{-1}(w(a)) = a = \frac{1 - w}{\omega(1 + w)}, \quad w = w(a), \quad a \in \mathcal{H}, \quad \omega > 0. \tag{2.3}$$

As is readily checked, the inverse function in (2.3) is also a Möbius transformation, has no poles, is not the constant function and maps back w onto its pre-image a .

To realize how the two transformations (2.2) and (2.3) work and draw useful conclusions, consider a certain $\omega > 0$ and let \mathcal{C}_ω be the circle with center $O(0, 0)$ and radius

$$\rho := \rho(\mathcal{C}_\omega) = \max_{a \in \mathcal{H}} |w(a)| (< 1). \tag{2.4}$$

Note that due to the definition of ρ in (2.4), \mathcal{C}_ω will capture¹ $w(\mathcal{H})$ and will pass through a boundary point of it. Therefore, in view of the nature of the two Möbius transformations (2.2) and (2.3) (real coefficients, and **no** poles), \mathcal{C}_ω must be the image of a circle \mathcal{C} . In other words

¹ From now on the word “captures” will mean “contains in the closure of its interior”.

$\mathcal{C}_\omega \equiv w(\mathcal{C})$. To see how these two circles \mathcal{C}_ω and \mathcal{C} are related and draw some further conclusions regarding \mathcal{C} , we begin with the equation for \mathcal{C}_ω , namely

$$\mathcal{C}_\omega := |w| = \rho.$$

We square both members of it, use the expression for w , from the Möbius transformation in (2.2), go through a series of successive equivalences

$$\begin{aligned} |w| = \rho &\Leftrightarrow |w|^2 = \rho^2 \Leftrightarrow w\bar{w} = \rho^2 \\ &\Leftrightarrow \frac{1-\omega a}{1+\omega a} \cdot \frac{1-\omega\bar{a}}{1+\omega\bar{a}} = \rho^2 \Leftrightarrow \omega^2(1-\rho^2)a\bar{a} - \omega(1+\rho^2)(a+\bar{a}) + (1-\rho^2) = 0 \\ &\Leftrightarrow a\bar{a} - \frac{(1+\rho^2)}{\omega(1-\rho^2)}(a+\bar{a}) + \frac{1}{\omega^2} = 0 \\ &\Leftrightarrow a\bar{a} - \frac{(1+\rho^2)}{\omega(1-\rho^2)}(a+\bar{a}) + \left(\frac{(1+\rho^2)}{\omega(1-\rho^2)}\right)^2 = \left(\frac{(1+\rho^2)}{\omega(1-\rho^2)}\right)^2 - \frac{1}{\omega^2} \\ &\Leftrightarrow \left|a - \frac{(1+\rho^2)}{\omega(1-\rho^2)}\right|^2 = \left(\frac{2\rho}{\omega(1-\rho^2)}\right)^2 \\ &\Leftrightarrow \left|a - \frac{(1+\rho^2)}{\omega(1-\rho^2)}\right| = \frac{2\rho}{\omega(1-\rho^2)} \Leftrightarrow |a - c| = R \end{aligned}$$

and end up with the equation of a circle \mathcal{C} , where

$$\mathcal{C} := |a - c| = R, \tag{2.5}$$

with c and R being given by

$$c := \frac{1+\rho^2}{\omega(1-\rho^2)}, \quad R := \frac{2\rho}{\omega(1-\rho^2)} \quad (c > R \geq 0). \tag{2.6}$$

Consequently, because of the above equivalences, we have that

$$\mathcal{C}_\omega = w(\mathcal{C}) \Leftrightarrow \mathcal{C} = w^{-1}(\mathcal{C}_\omega). \tag{2.7}$$

It can be observed that the circle \mathcal{C} possesses four basic properties: (1) It has its center on the positive real semiaxis ($c > 0$ since $0 \leq \rho < 1$). (2) It lies in the open right half complex plane ($c > R$). (3) It captures \mathcal{H} ($\mathcal{H} \subset \mathcal{C}$) since \mathcal{C}_ω captures $w(\mathcal{H})$ ($w(\mathcal{H}) \subset \mathcal{C}_\omega \equiv w(\mathcal{C})$). (4) It passes through a vertex of \mathcal{H} ; this is because \mathcal{C}_ω passes through a boundary point of $w(\mathcal{H})$, hence \mathcal{C} must pass through a boundary point of \mathcal{H} . But since \mathcal{C} is a circle that captures \mathcal{H} , with the latter being a convex polygon, the boundary point in question must be a vertex of it.

Definition 2.1. A circle \mathcal{C} satisfying the above four properties will be called a *capturing circle* (*cc*) of \mathcal{H} .

Theorem 2.1. Let $A \in \mathbb{R}^{n,n}$ be positive stable, $\sigma(A)$ be its spectrum and \mathcal{H} be the convex hull of $\sigma(A)$. Then, there are infinitely many capturing circles (*cc*) of \mathcal{H} .

Proof. Let $P_i, i = 1(1)k$, be the vertices of \mathcal{H} in the first quadrant of the complex plane in increasing order of their abscissas and consider the perpendicular bisectors of $OP_i, i = 1(1)k$. Let $K_i(c_i, 0), i = 1(1)k$, be their intersections with the positive real semiaxis. Then, the circle with center the point $K(c, 0)$, such that $c \in (\max_{i=1(1)k} c_i, +\infty)$, and radius $R = \max_{i=1(1)k} (K P_i)$ is a *cc* of \mathcal{H} . Consequently, there are infinitely many *cc*'s of a given \mathcal{H} . \square

Note. The notion of a cc of \mathcal{H} constitutes a particular case of the one defined in [14] (see also [15]).

One more consequence of the analysis so far is the validity of the following statement.

Theorem 2.2. *The solutions to Problem II and Problem I are identical.*

Proof. From the preceding analysis we have that the following series of relations hold

$$\begin{aligned} \min_{\omega>0} \max_{a \in \mathcal{H}} \left| \frac{1 - \omega a}{1 + \omega a} \right| &= \min_{\omega>0} \max_{a \in \mathcal{H}} |w(a)| = \min_{\omega>0} \rho = \min_{\omega>0} \rho(\mathcal{C}_\omega) \\ &= \min_{\omega>0} \rho(w(\mathcal{C})) = \min_{\omega>0} \max_{a \in \sigma(A)} |w(a)| \\ &= \min_{\omega>0} \max_{a \in \sigma(A)} \left| \frac{1 - \omega a}{1 + \omega a} \right| = \min_{\omega>0} \rho(F_\omega). \end{aligned} \tag{2.8}$$

Specifically, the first expression is that of Problem II and is equal to the second one because of the definition of w in (2.2). The second expression is equal to the following two by the definition of ρ in (2.4). The fifth expression is equal to the previous one due to the fact that $\mathcal{C}_\omega \equiv w(\mathcal{C})$. The sixth expression is equal to its preceding one because \mathcal{C} captures \mathcal{H} and passes through a vertex of it and the latter is an element of $\sigma(A)$. The last but one expression is obtained from its previous one by (2.2) and the last expression is from equations (1.4) of Problem I. \square

By virtue of the analysis so far and Theorems 2.1 and 2.2, in order to solve Problem II it suffices to find out of the infinitely many cc's of \mathcal{H} the one that solves it. For this we have to find first how ω and $\rho = \rho(\mathcal{C}_\omega)$ of \mathcal{C}_ω are obtained from elements of \mathcal{C} . This is given in the following statement.

Theorem 2.3. *Let \mathcal{C} be a cc of \mathcal{H} , $K(c, 0)$ and R be its center and radius and \mathcal{C}_ω be its image via (2.2). Then, the extrapolation parameter ω and the radius ρ of \mathcal{C}_ω are given by the expressions*

$$\omega = \frac{1}{\sqrt{c^2 - R^2}}, \quad \rho = \rho(\mathcal{C}_\omega) = \frac{\sqrt{c + R} - \sqrt{c - R}}{\sqrt{c + R} + \sqrt{c - R}}. \tag{2.9}$$

Proof. From the expressions for c and R of \mathcal{C} in (2.6), which give them in terms of ω and ρ , we form the ratio $\frac{R}{c}$ to obtain $\frac{R}{c} = \frac{2\rho}{1+\rho^2}$. Solving for $\rho \in (0, 1)$ we take

$$\rho = \frac{c - \sqrt{c^2 - R^2}}{R},$$

the right side of which is readily proved to be an equivalent expression to the right side of the second equation in (2.9). The expression for ω is easily obtained by solving either of the ones in (2.6) and using the expression for ρ just found. \square

A simple statement follows that will be very useful.

Lemma 2.1. *Let the function*

$$f(x) := \frac{\sqrt{1+x} - \sqrt{1-x}}{\sqrt{1+x} + \sqrt{1-x}} \tag{2.10}$$

be defined in the interval $[0, 1)$. Then, $f(x)$ is continuously increasing in $[0, 1)$. Moreover, for $x \in [d, e) \subseteq [0, 1)$, $f(x)$ attains its minimum value at the minimum value of $x = d$.

Proof. Differentiating $f(x)$ wrt x it is readily obtained that $\frac{\partial f}{\partial x} > 0$ from which the conclusion follows. The second part is a consequence of the first one. \square

Now we can prove our key theorem.

Theorem 2.4. Under the notation and assumptions of Theorem 2.3, the solution to Problem II in (2.1) is equivalent to the determination of the optimal capturing circle (cc) \mathcal{C}^* of \mathcal{H} so that the ratio $\frac{R}{c}$ is a minimum.

Proof. The rightmost expression for ρ in (2.9) is written as follows:

$$\rho = \frac{\sqrt{1 + \frac{R}{c}} - \sqrt{1 - \frac{R}{c}}}{\sqrt{1 + \frac{R}{c}} + \sqrt{1 - \frac{R}{c}}} \equiv f\left(\frac{R}{c}\right). \tag{2.11}$$

So, ρ is minimized whenever $f(\frac{R}{c})$ is. By Lemma 2.1, $f(\frac{R}{c})$ attains its minimum value at the minimum of $\frac{R}{c}$ and the statement is proved. \square

The problem of minimization of the ratio $\frac{R}{c}$ of Theorem 2.4 for all cc's of \mathcal{H} is identical to the same problem in the classical extrapolation of a first order stationary iterative scheme solved completely in [14] for the complex case (see also [15]), using Apollonius circles [8], where the issues of existence and uniqueness are established. It is also identical to the analogous problem of the classical extrapolation in [17,18,13] for the real case, solved earlier, where, however, the issue of uniqueness is not quite clear.

We mention, in passing, that the problem in the classical extrapolation for $A \in \mathbb{C}^{n,n}$ and \mathcal{H} the convex hull of $\sigma(A)$, with $O \notin \mathcal{H}$, may be stated as follows:

Problem III. Determine $\omega \in \mathbb{C}$ that solves the minimax problem

$$\min_{\omega \in \mathbb{C}} \max_{a \in \mathcal{H}} |1 - \omega a|, \quad a \in \sigma(A) \subset \mathcal{H} \text{ and } O \notin \mathcal{H}. \tag{2.12}$$

If $A \in \mathbb{R}^{n,n}$ and $\sigma(A)$ is in the open right half complex plane, Problem III becomes:

Problem III'. Determine $\omega > 0$ that solves the minimax problem

$$\min_{\omega > 0} \max_{a \in \mathcal{H}} |1 - \omega a|, \quad a \in \sigma(A) \subset \mathcal{H}. \tag{2.13}$$

Consequently, the following statement is valid.

Theorem 2.5. The optimal cc \mathcal{C}^* of \mathcal{H} determined in the classical extrapolation of Problem III' is identical to the one determined in the case of the extrapolation of Problem II.

Although \mathcal{C}^* for the classical extrapolation and the extrapolation in the present work are identically the same, the values for the optimal parameters ω^* and $\rho(\mathcal{C}_{\omega^*})$ are **completely different**.

Having determined \mathcal{C}^* of \mathcal{H} using the Algorithm in the next section, the values of ω^* and $\rho(\mathcal{C}_{\omega^*})$ are determined by the theorem below which is obtained directly from Theorem 2.3.

Theorem 2.6. *Let \mathcal{C}^* be the optimal cc of \mathcal{H} obtained by using the Algorithm in the next section and let $K^*(c^*, 0)$ and R^* be its center and radius, respectively. Then the solution to the optimization Problem II in (2.1) is given by*

$$\min_{\omega > 0} \max_{a \in \mathcal{H}} \left| \frac{1 - \omega a}{1 + \omega a} \right| = \rho(\mathcal{C}_{\omega^*}) = \frac{\sqrt{c^* + R^*} - \sqrt{c^* - R^*}}{\sqrt{c^* + R^*} + \sqrt{c^* - R^*}}, \quad \text{with } \omega^* = \frac{1}{\sqrt{c^{*2} - R^{*2}}}. \quad (2.14)$$

Since Problem II refers to a real case it will be much simpler if its solution is given directly by an appropriate interpretation of the Algorithm in [14] as this is done in the next section.

3. The algorithm and the elements of \mathcal{C}^*

Let $A \in \mathbb{R}^{n,n}$ be positive stable and \mathcal{H} be the convex hull of its spectrum $\sigma(A)$. Then, the determination of the optimal cc \mathcal{C}^* of \mathcal{H} , of Theorem 2.4, is achieved as follows:

3.1. The algorithm

Step 1. Let $P_i(\beta_i, \gamma_i)$, $0 < \beta_i < \beta_{i+1}$, $i = 1(1)k - 1$, $\gamma_i \geq 0$, $i = 1(1)k$, be the k vertices of \mathcal{H} , in the first quadrant of the complex plane.

Step 2. If $k \geq 1$, find the point P_i which corresponds to the largest polar angle θ_i , that is

$$\max_{i=1(1)k} \tan \theta_i = \max_{i=1(1)k} \frac{\gamma_i}{\beta_i}. \quad (3.1)$$

If there are two vertices sharing the same polar angle go to the next Step; otherwise, let $\bar{i} \in \{1, 2, \dots, k\}$ be the index for which this happens and let $\mathcal{C}_{\bar{i}}$ be the circle that is tangent to the line $OP_{\bar{i}}$ at $P_{\bar{i}}$. If $\mathcal{C}_{\bar{i}}$ captures all the other vertices of \mathcal{H} , then it is the optimal cc \mathcal{C}_{ω^*} of \mathcal{H} (one-point optimal cc). If **no** such a cc \mathcal{C}_{ω^*} exists go on to the next Step.

Step 3. Determine the circles that pass through the pairs of vertices P_i, P_j , $i = 1(1)k - 1$, $j = i + 1(1)k$, and have centers on the real axis. Let $K_{i,j}(c_{i,j}, 0)$ and $R_{i,j}$ be their centers and radii, respectively. Discard those that either capture O or do not capture all the other vertices. From the rest the one that corresponds to the smallest ratio $\frac{R_{i,j}}{(OK_{i,j})}$ is the optimal cc \mathcal{C}_{ω^*} of \mathcal{H} (two-point optimal cc).

3.2. The elements of the optimal capturing circle

The following two points that refer mainly to the elements of the optimal cc \mathcal{C}^* of \mathcal{H} are made:

- (a) Let $\bar{i} \in \{1, 2, \dots, k\}$ be the index corresponding to the optimal one-point cc of \mathcal{H} . Then, its center and radius are readily found to be given by

$$K_i^*(c_i^*, 0), \quad c_i^* = \frac{\beta_i^2 + \gamma_i^2}{\beta_i}, \quad R_i^* = \frac{\gamma_i \sqrt{\beta_i^2 + \gamma_i^2}}{\beta_i}. \quad (3.2)$$

(b) To determine the *optimal two-point cc* of \mathcal{H} from the centers $K_{i,j}$ and radii $R_{i,j}$ of the $\binom{k}{2}$ possible candidates, we find the main elements of them, that is

$$c_{i,j} = \frac{(\beta_j^2 + \gamma_j^2) - (\beta_i^2 + \gamma_i^2)}{2(\beta_j - \beta_i)},$$

$$R_{i,j} = \frac{\sqrt{[(\beta_j^2 + \gamma_j^2) + (\beta_i^2 + \gamma_i^2) - 2\beta_i\beta_j]^2 - 4\gamma_i^2\gamma_j^2}}{2(\beta_j - \beta_i)}. \quad (3.3)$$

We discard the circles for which $c_{i,j} \leq 0$ or $0 < c_{i,j} \leq R_{i,j}$. From the rest we find the *optimal cc* as the one that captures the other $k - 2$ vertices of \mathcal{H} and corresponds to the smallest ratio

$$\frac{R_{i,j}}{c_{i,j}} = \frac{\sqrt{[(\beta_j^2 + \gamma_j^2) + (\beta_i^2 + \gamma_i^2) - 2\beta_i\beta_j]^2 - 4\gamma_i^2\gamma_j^2}}{(\beta_j^2 + \gamma_j^2) - (\beta_i^2 + \gamma_i^2)} \left(= \frac{(K_{i,j}P_i)}{(OK_{i,j})} = \frac{(K_{i,j}P_j)}{(OK_{i,j})} \right). \quad (3.4)$$

Denoting by \bar{i}, \bar{j} the indices for the *optimal cc*, $\mathcal{C}_{\bar{i},\bar{j}}^*$, its center $K_{\bar{i},\bar{j}}^*(c_{\bar{i},\bar{j}}^*, 0)$ and radius $R_{\bar{i},\bar{j}}^*$ will be given by (3.3).

3.3. Numerical examples

In this section we give two examples that cover the two possible cases of the *one-point* and the *two-point optimal cc*'s.

Example 1. Let

$$A = \begin{bmatrix} 10 & 1 & 3 & -1 \\ 2 & 4 & -2 & -3 \\ -3 & 5 & 6 & 2 \\ 3 & 3 & 1 & 11 \end{bmatrix}. \quad (3.5)$$

The given matrix A is *positive stable* since its spectrum is found to be

$$\sigma(A) = \{5.30510873756331 \pm i4.04212646134389, \\ 10.19489126243668 \pm i2.49823942823383\},$$

with the spectral radius of the *Cayley Transform* being given by

$$\rho(F) = \rho((I + A)^{-1}(I - A)) = 0.83069047703163.$$

It is easily found that the hull \mathcal{H} has two vertices in the first quadrant

$$P_1(5.30510873756331, 4.04212646134389), \quad P_2(10.19489126243668, 2.49823942823383).$$

Of the two vertices P_1 has the largest *polar angle*. It is found out that $c_1 = 8.38492993214283$ and $R_1 = 5.08174034363009$. Observe that \mathcal{C}_1 captures P_2 since $(K_1P_2) = 3.08498950694183 <$

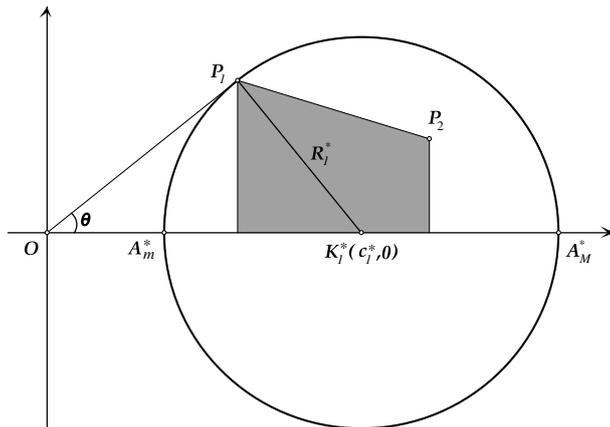


Fig. 1. Optimal elements of Example 1.

R_1 . Therefore the optimal cc is \mathcal{C}_1^* (see Fig. 1). The optimal value for the extrapolation parameter is found to be $\omega^* = 0.14993503870749$ and then the spectral radius of the optimal Extrapolated Cayley Transform is $\rho(F_{\omega^*}) = \rho(\mathcal{C}_{\omega^*}^*) = 0.33755657117885$.

Example 2. Let

$$A = \begin{bmatrix} 3.2674 & 0.8314 & 0.8577 & 0.3411 & 0.5209 & 0.4043 & 1.1564 & -0.7739 \\ 0.7801 & 2.9645 & 0.3279 & 0.3785 & 0.7860 & 0.2184 & 0.3424 & -0.3047 \\ -1.0629 & -0.2065 & 2.3540 & -0.7142 & 0.1065 & -0.5306 & 0.1741 & 0.3752 \\ 0.1682 & 0.7375 & 0.6341 & 2.0460 & 0.7078 & 1.0257 & 0.6017 & -0.9151 \\ 1.1390 & -0.4606 & 0.2989 & 0.0356 & 2.1130 & 0.4592 & 0.4386 & -0.1482 \\ -0.4309 & -0.1225 & -0.0049 & -0.0385 & 0.0966 & 2.0106 & -1.3353 & 1.0215 \\ -0.5356 & -0.0203 & -0.4978 & 0.5677 & 0.3314 & 0.1871 & 2.7104 & 0.4236 \\ -0.3741 & -0.2861 & -0.9002 & 0.6656 & -0.0451 & -1.1603 & -0.9873 & 4.8030 \end{bmatrix}.$$

A is positive stable since its spectrum is

$$\sigma(A) = \{1.86276001393587, 2.01179239038023 \pm i0.65104401096444, 2.74937366128964 \pm i0.97219263735250, 0.353286710719112 \pm i0.82489924737867, 3.81807366834215\}$$

with the spectral radius of $F = (I + A)^{-1}(I - A)$ being $\rho(F) = 0.58489634288050$. Hence the vertices of \mathcal{H} in the first quadrant are

$$\begin{aligned} P_1(1.86276001393587, 0), & P_2(2.01179239038023, 0.65104401096444), \\ P_3(2.74937366128964, 0.97219263735250), & \\ P_4(3.53286710719112, 0.82489924737867), & P_5(3.81807366834215, 0). \end{aligned}$$

The vertex with the largest polar angle is P_3 . However, the circle that has center in the positive real semiaxis and is tangent to OP_3 at P_3 does not capture P_1 and P_2 . So, we are looking for a two-point optimal cc. For this we consider all $\binom{5}{2} = 10$ circles which pass through pairs of vertices $P_i, P_j, i = 1(1)4, j = i + 1(1)5$, and have centers on the real axis. Discarding the

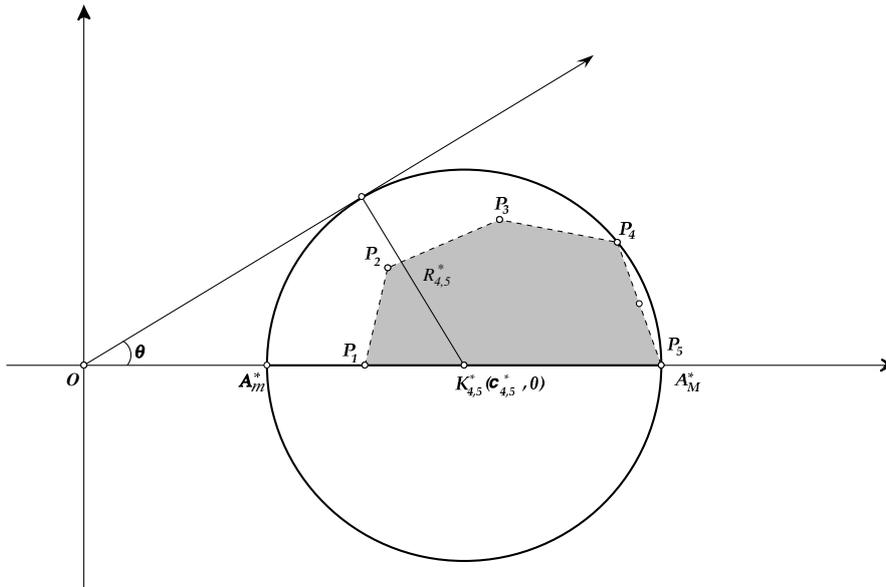


Fig. 2. Optimal elements of Example 2.

circles that either capture O or do not capture all the other vertices of \mathcal{H} , we select from the rest the unique one that corresponds to the smallest ratio $\frac{R}{c}$. Thus, the optimal cc is found to be $\mathcal{C}_{4,5}^*$, with $K_{4,5}^*(c_{4,5}^*, 0)$, $c_{4,5}^* = 2.48254767662753$, $R_{4,5}^* = 1.33552599171462$ and $\omega^* = 0.47785048804760$, where $\rho(F_{\omega^*}) = \rho(\mathcal{C}_{\omega^*}) = 0.29190214193811$ (see Fig. 2).

4. Special cases

In what follows we examine some special cases which may be of interest in applications. In each case we will show how the optimal cc of \mathcal{H} , \mathcal{C}^* , will be determined. In most of them not all the optimal values involved ($K^*(c^*, 0)$, R^* , ω^* , $\rho(\mathcal{C}_{\omega^*})$) will be found explicitly.

- (a) Let $\sigma(A) \subset [\beta_1 - \iota\gamma_1, \beta_1 + \iota\gamma_1]$, $\gamma_1 > 0$. Obviously, \mathcal{H} has only one vertex $P_1(\beta_1, \gamma_1)$ in the first quadrant and so c^* and R^* are given by (3.2) and then by (2.14) it is found that

$$\omega^* = \frac{1}{\sqrt{\beta_1^2 + \gamma_1^2}}, \quad \rho(\mathcal{C}_{\omega^*}) = \frac{\gamma_1}{\beta_1 + \sqrt{\beta_1^2 + \gamma_1^2}}. \tag{4.1}$$

- (b) Let $\sigma(A) \subset \mathcal{R}$, where \mathcal{R} is the rectangle with vertices $\beta_i \pm \iota\gamma$, $i = 1, 2$, and $\gamma > 0$. Of the two vertices of \mathcal{R} in the first quadrant P_1 has the largest polar angle and so we check if the circle with center $K_1\left(\frac{\beta_1 + \gamma^2}{\beta_1}, 0\right)$ and radius $R_1 = \frac{\gamma\sqrt{\beta_1^2 + \gamma^2}}{\beta_1}$, from (3.2), captures P_2 .

For this to happen there must hold $\frac{\beta_1 + \beta_2}{2} \leq \frac{\gamma\sqrt{\beta_1^2 + \gamma^2}}{\beta_1}$, in which case ω^* and $\rho(\mathcal{C}_{\omega^*})$ are given by the formulas in (4.1); otherwise $K_{1,2}\left(\frac{\beta_1 + \beta_2}{2}, 0\right)$, $R_{1,2} = \frac{1}{2}\sqrt{(\beta_2 - \beta_1)^2 + 4\gamma^2}$, from which

$$\omega^* = \frac{1}{\sqrt{\beta_1\beta_2 - \gamma^2}}, \quad \rho(\mathcal{C}_{\omega^*}) = \frac{\beta_1 + \beta_2 + \sqrt{(\beta_2 - \beta_1)^2 + 4\gamma^2} - 2\sqrt{\beta_1\beta_2 - \gamma^2}}{\beta_1 + \beta_2 + \sqrt{(\beta_2 - \beta_1)^2 + 4\gamma^2} + 2\sqrt{\beta_1\beta_2 - \gamma^2}}. \quad (4.2)$$

If $\gamma = 0$, then $K_{1,2}(\frac{\beta_1+\beta_2}{2}, 0)$, $R_{1,2} = \frac{\beta_2-\beta_1}{2}$, and

$$\omega^* = \frac{1}{\sqrt{\beta_1\beta_2}}, \quad \rho(\mathcal{C}_{\omega^*}) = \frac{\sqrt{\beta_2} - \sqrt{\beta_1}}{\sqrt{\beta_2} + \sqrt{\beta_1}}. \quad (4.3)$$

- (c) Let $\sigma(A) \subset \mathcal{T}$, where \mathcal{T} is an isosceles trapezium, a case examined in [15] in general terms. Let the vertices of \mathcal{T} in the first quadrant be $P_i(\beta_i, \gamma_i)$, $i = 1, 2$, with $\gamma_1, \gamma_2 > 0$ and $\gamma_1 \neq \gamma_2$. We distinguish two cases: (i) $\frac{\gamma_i}{\beta_i} > \frac{\gamma_j}{\beta_j}$, $i = 1, 2, j \in \{1, 2\} \setminus \{i\}$ or (ii) $\frac{\gamma_1}{\beta_1} = \frac{\gamma_2}{\beta_2}$.
- (i) Let P_i be the vertex with the largest polar angle so we find \mathcal{C}_i as in Step 3 of the Algorithm. Formulas (3.2) will give the center $K(c_i, 0)$ and the radius R_i of \mathcal{C}_i . If \mathcal{C}_i captures P_j , that is if and only if (iff) $2\gamma_i(\gamma_i\beta_j - \beta_i\gamma_j) \geq \beta_i[(\beta_i - \beta_j)^2 + (\gamma_i - \gamma_j)^2]$, then \mathcal{C}_i is the optimal cc of \mathcal{T} . Otherwise, the optimal cc of \mathcal{T} will be $\mathcal{C}_{1,2}^*$ whose center and radius will be given by formulas (3.3).
- (ii) If $\frac{\gamma_1}{\beta_1} = \frac{\gamma_2}{\beta_2}$, P_1, P_2 have the same polar angle and according to point (a) made after the Algorithm in Section 4, the optimal cc of \mathcal{T} will be $\mathcal{C}_{1,2}^*$ and its elements are found from (3.3).

In applications we may have a convex region as the convex hull, instead of a polygon, whose (part of its) boundary consists of arcs of circles or ellipses as, e.g., in [5,4]. Then, the situation is tackled in a way analogous to that considered so far where a one- or two-point optimal cc is sought (see [15]).

- (d) Let $\sigma(A) \subset \mathcal{S}$ be the section of a circle symmetric wrt the positive real semiaxis. (A special case was treated in [15] and also in [5,4].) We distinguish two cases depending on whether the chord or the midpoint of the arc of \mathcal{S} is closer to the midpoint.

- (i) Let $P_1(\beta_1, \gamma_1)$ be the endpoint of the chord of \mathcal{S} in the first quadrant of the complex plane and $P_2(\beta_2, 0)$ be the midpoint of its arc. Consider the cc \mathcal{C}_1 whose elements are given by (3.2). For P_1 to have the largest polar angle of \mathcal{S} , \mathcal{C}_1 must capture P_2 . This

happens iff $c_1 + R_1 \geq \beta_2$ or $\frac{\sqrt{\beta_1^2 + \gamma_1^2}(\sqrt{\beta_1^2 + \gamma_1^2} + \gamma_1)}{\beta_1} \geq \beta_2$, and then \mathcal{C}_1^* is the one-point optimal cc. If the previous inequality is the other way then the optimal cc will be the two-point cc $\mathcal{C}_{1,2}^*$, the circle to which \mathcal{S} belongs, whose elements are

$$K_{1,2}^*(c_{1,2}^*, 0), \quad c_{1,2}^* = \frac{\beta_2^2 - (\beta_1^2 + \gamma_1^2)}{2(\beta_2 - \beta_1)}, \quad R_{1,2}^* = \frac{(\beta_2 - \beta_1)^2 + \gamma_1^2}{2(\beta_2 - \beta_1)}.$$

- (ii) This time the midpoint of the arc of \mathcal{S} is $P_1(\beta_1, 0)$ and the endpoint of the chord in the first quadrant is $P_2(\beta_2, \gamma_2)$. Now, the point of \mathcal{S} with the largest polar angle is P_2 iff

$c_2 - R_2 \leq \beta_1$ or $\frac{\sqrt{\beta_2^2 + \gamma_2^2}(\sqrt{\beta_2^2 + \gamma_2^2} - \gamma_2)}{\beta_2} \leq \beta_1$, the optimal cc will be the one-point cc \mathcal{C}_2^* .

If the inequality above is the other way then, as in the previous case, $\mathcal{C}_{1,2}^*$ is the circle to which \mathcal{S} belongs and its elements are

$$K_{1,2}^*(c_{1,2}^*, 0), \quad c_{1,2}^* = \frac{(\beta_2^2 + \gamma_2^2) - \beta_1^2}{2(\beta_2 - \beta_1)}, \quad R_{1,2}^* = \frac{(\beta_2 - \beta_1)^2 + \gamma_2^2}{2(\beta_2 - \beta_1)}.$$

(e) Let $\sigma(A) \subset \mathcal{S}$, where \mathcal{S} is a sector of a circle symmetric wrt to the positive real semiaxis. Since \mathcal{S} must be a convex region, the angle of \mathcal{S} is considered to be strictly less than π for otherwise we should consider a section of a circle examined in (d). We distinguish two subcases.

(i) Let $P_1(\beta_1, 0)$ be the center of the circle to which the sector belongs, $P_2(\beta_2, \gamma_2)$ be the endpoint of its chord and $P_3(\beta_3, 0)$ be the midpoint of its arc, where $\beta_3 = \beta_1 + \sqrt{(\beta_2 - \beta_1)^2 + \gamma_2^2}$. P_2 is the point with the largest polar angle and so if the cc through P_2, \mathcal{C}_2 , captures P_1 and P_3 it is the optimal one. For this to happen there must hold $c_2 - R_2 \leq \beta_1$ and $c_2 + R_2 \geq \beta_3$ or

$$\frac{\sqrt{\beta_2^2 + \gamma_2^2} \left(\sqrt{\beta_2^2 + \gamma_2^2} - \gamma_2 \right)}{\beta_2} \leq \beta_1 < \beta_1 + \sqrt{(\beta_2 - \beta_1)^2 + \gamma_2^2} \leq \frac{\sqrt{\beta_2^2 + \gamma_2^2} \left(\sqrt{\beta_2^2 + \gamma_2^2} + \gamma_2 \right)}{\beta_2}.$$

If either of the two extreme inequalities does not hold then the optimal cc is a two-point one. In such a case, observe that $\angle P_1 P_2 P_3 < \frac{\pi}{2}$, from the isosceles triangle $P_1 P_2 P_3$. This means that $\mathcal{C}_{1,3}$ cannot capture P_2 , since its diameter $P_1 P_3$ is strictly less than twice its median from P_2 . For the other two candidates we observe that $\mathcal{C}_{1,2}$ captures P_3 and $\mathcal{C}_{2,3}$ captures P_1 . The former because its center $K_{1,2}$ is such that $(K_{1,2} P_2) > (K_{1,2} P_3)$ since $\angle K_{1,2} P_3 P_2 = \angle P_1 P_2 P_3 > \angle K_{1,2} P_2 P_3$, and the latter because P_1 is the center of the sector and of $\mathcal{C}_{2,3}$. On the two candidates we observe the following: (α) If $\beta_1 \leq \frac{1}{2} \beta_3 = \frac{1}{2} (\beta_1 + \sqrt{(\beta_2 - \beta_1)^2 + \gamma_2^2})$ or, equivalently, $2\beta_1 \beta_2 \leq \beta_2^2 + \gamma_2^2$, then the circle $\mathcal{C}_{2,3}$ does capture the origin O . So it is not a cc; hence the optimal cc is $\mathcal{C}_{1,2}^*$. (β) If $2\beta_1 \beta_2 > \beta_2^2 + \gamma_2^2$, then $\mathcal{C}_{2,3}$ lies strictly in the open right half complex plane and is a possible candidate for the optimal cc. However, the two circles $\mathcal{C}_{2,3}$ and $\mathcal{C}_{1,2}$, have a common chord $P_2 P'_2$, where P'_2 is the symmetric of P_2 wrt the real axis, and the arc $P_2 P_1 P'_2$ of the latter circle lies in the closure of the interior of the former. This means that $\frac{R_{1,2}}{c_{1,2}} < \frac{R_{2,3}}{c_{2,3}}$. Consequently, by Theorem 2.4, the optimal cc of the sector \mathcal{S} is always $\mathcal{C}_{1,2}^*$.

(ii) This time it is $P_3(\beta_3, 0)$ the center of the sector, $P_2(\beta_2, \gamma_2)$, as before, the endpoint of its chord and $P_3(\beta_3, 0)$ its center, where $0 < \beta_1 = \beta_3 - \sqrt{(\beta_3 - \beta_2)^2 + \gamma_2^2}$. This case is examined in a similar way and so the determination of the optimal cc is omitted.

Note. In a similar way we can find the optimal elements of a circular zone that is a part of a circle which is defined by two chords perpendicular to the positive real semiaxis and the two arcs between them.

(f) Finally, we determine the optimal cc of an ellipse \mathcal{E} symmetric wrt the positive real semiaxis, with center $Q(c, 0)$ and $E_r (< c)$, E_i its real and imaginary semiaxes, as a special case of the one examined in [25]. Two cases are distinguished.

(i) $E_r < E_i$: Let OP_1 be the tangent to \mathcal{E} with $P_1(\beta_1, \gamma_1)$ being the point of contact. Obviously, P_1 has the largest polar angle. The coordinates of P_1 will satisfy the equations of the ellipse \mathcal{E} and of its tangent from O . Also, the coordinates of $O(0, 0)$ will satisfy the equation of OP_1 . So,

$$\frac{(\beta_1 - c)^2}{E_r^2} + \frac{\gamma_1^2}{E_i^2} = 1, \quad \frac{(0 - c)(\beta_1 - c)}{E_r^2} + \frac{0 \cdot \gamma_1}{E_i^2} = 1, \quad (4.4)$$

from which $\beta_1 = \frac{c^2 - E_r^2}{c}$, $\gamma_1 = \frac{E_i}{c} \sqrt{c^2 - E_r^2}$ are found. Therefore, for \mathcal{C}_1^* , we have

$$c_1^* = \frac{c^2 + E_i^2 - E_r^2}{c}, \quad R_1^* = \frac{E_i}{c} \sqrt{c^2 - E_r^2 + E_i^2}. \quad (4.5)$$

\mathcal{C}_1^* is indeed the optimal cc of \mathcal{E} since $R_1^* > E_r \Leftrightarrow (c + 1)(E_i^2 - E_r^2) (> 0)$.

(ii) $E_r > E_i$: The optimal cc is that which has center $K^*(c^*, 0)$, $c^* = c$, and radius $R^* = E_r$.

Note. The optimal parameters of a section, a sector or a zone of an ellipse \mathcal{E} symmetric wrt the positive real semiaxis are found in a similar way to that of the section, the sector and the zone of a circle.

5. The Linear Complementarity Problem (LCP)

The Linear Complementarity Problem (LCP) is met in many practical applications. For example, in linear and convex quadratic programming, in the problem of finding the Nash equilibrium point in a bimatrix game (see, e.g., Lemke [21] and Cottle and Dantzig [6]), in a number of problems in fluid mechanics (see, e.g., Cryer [9]), in problems in economics (see, e.g., Pantazopoulos [26] and Koulisianis and Papatheodorou [20]), etc. For more applications see, e.g., [23,2,7,24,11,3] and [28].

The LCP is defined in the following way:

Problem IV. Determine $x \in \mathbb{R}^{n,n}$, if it exists, satisfying the following conditions

$$r := Ax - b \geq 0, \quad x \geq 0, \quad x^T r = 0, \quad \text{with } A \in \mathbb{R}^{n,n}, \quad b \in \mathbb{R}^n \quad (b \not\leq 0) \quad (5.1)$$

(see, e.g., [2] and also [23,7] or [24]).

Note. We set $b \not\leq 0$ since otherwise (5.1) has the trivial solution $x = 0, r = -b \geq 0$.

A sufficient and necessary condition for LCP (5.1) to possess a unique solution, for all $b \in \mathbb{R}^n$, is that A is a P -matrix, that is all its principal minors are positive. For the proof see, e.g., [23,2,7,24,11,3] or [28]. In this section we focus on real symmetric positive definite matrices, which are both P -matrices, to guarantee uniqueness of the solution of (5.1), and positive stable as the analysis of the present work requires.

The problem in (5.1) can be solved by a direct or an iterative method. In this work we consider specifically the iterative method known as the Modulus Algorithm introduced by van Bokhoven [31] (see also Kappel and Watson [19] and Schäfer [29]). In it a new “unknown” z is introduced so that

$$x = |z| + z \quad \text{and} \quad r = |z| - z, \quad (5.2)$$

see, e.g., [24], where $|\cdot|$ denotes the vector whose components are the moduli of the corresponding components of the given one. Then, using (5.2) and replacing x and r in (5.1) it is readily obtained that

$$z = f(z) := F|z| + c, \quad (5.3)$$

where

$$z \in \mathbb{R}^n, \quad F = (I + A)^{-1}(I - A), \quad c = (I + A)^{-1}b, \quad (5.4)$$

and where, as is seen, the *Cayley Transform* appears and plays an important role.

For the iterative solution of (5.3) the simplest iterative scheme is the following

$$z^{(m+1)} = F|z^{(m)}| + c, \quad \text{with any } z^{(0)} \geq 0. \tag{5.5}$$

Under the assumptions on A so far, the convergence of (5.5) to the (unique) solution z^* of (5.3) is guaranteed (see, also [19] and [29]).

To accelerate the convergence of (5.5) we apply *extrapolation* to Problem IV. So, we multiply the first and the last relations in (5.1) by $\omega (> 0)$, the *extrapolation parameter*, and thus (5.1) becomes

$$\begin{aligned} (\omega r) &:= (\omega A)x - (\omega b) \geq 0, \quad x \geq 0, \\ x^T(\omega r) &= 0, \quad \text{with } \omega A \in \mathbb{R}^{n,n}, \quad \omega b \in \mathbb{R}^n \setminus \{0\} \ (\omega b \not\leq 0). \end{aligned} \tag{5.6}$$

Due to the positivity of ω , relations in (5.1) imply (5.6) and vice versa; also, the matrix properties of A are inherited by ωA .

The *extrapolated* iterative scheme based on (5.5) is constructed from (5.6) in the same way (5.5) is obtained from (5.3). Hence

$$z^{(m+1)} = F_\omega |z^{(m)}| + c_\omega, \quad \text{with any } z^{(0)} \geq 0, \tag{5.7}$$

where

$$F_\omega = (I + \omega A)^{-1}(I - \omega A), \quad c_\omega = (I + \omega A)^{-1}\omega b. \tag{5.8}$$

As is seen the *Extrapolated Cayley Transform* plays the role of the iteration matrix and it is our task to find the best value for the *extrapolation parameter* ω .

The *optimal extrapolation parameter* ω^* is found very easily since in this case \mathcal{H} is a line segment on the positive real semiaxis with endpoints the extreme eigenvalues of A (see Section 4, Case (b)). If the extreme eigenvalues of A are not known one can take $\|A\|_\infty$ as an upper bound of $\sigma(A)$. A positive lower bound can be found in many ways (see, e.g., [22] or [30]). Having found the extreme eigenvalues the optimal parameters are obtained from (4.3).

We present a simple example in which $z^{(0)}$ in (5.5) and (5.7) was taken to be the vector with all components equal to one, while the criterion for the iterations to stop was when two consecutive $x^{(m)}$'s ($x^{(m)} = z^{(m)} + |z^{(m)}|$) agreed to all 14 decimal places Matlab 7.0 gives.

Example. Let

$$A = \text{tridiag}(-1, 2, -1) \in \mathbb{R}^{9,9}, \quad b = [2 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1]^T,$$

where A is *symmetric positive definite* and its extreme eigenvalues are $\beta_1 = 4 \sin^2(\frac{\pi}{20})$ and $\beta_2 = 4 \cos^2(\frac{\pi}{20})$, with $\rho(F) = 0.82168115604716$. The number of iterations required to obtain the solution is **125** with $z^{(0)} = [1 \ 1 \ \dots \ 1]^T \in \mathbb{R}^9$. On the other hand, it is found that **93** iterations suffice to obtain the same solution when $\omega^* = 1.61803398874989$, with $\rho(F_{\omega^*}) = 0.72654252800536$. In both cases it is obtained that

$$\begin{aligned} x &= [1.00000000000000 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]^T, \\ r &= [0 \ 0.00000000000000 \ 1.00000000000000 \ 1.00000000000000 \ 1.00000000000000 \\ &\quad 1.00000000000000 \ 1.00000000000000 \ 1.00000000000000 \ 1.00000000000000]^T. \end{aligned} \tag{5.9}$$

6. Concluding remarks

Before we conclude our work we would like to make a number of points.

- (1) In the case of the LCP when A is real *symmetric positive definite* and one uses the *Stationary Extrapolated Modulus Algorithm* by van Bokhoven [31], or the generalized one by Kappel and Watson [19], the way described in the Example of the previous Section, one can also use a *Nonstationary Extrapolated Modulus Algorithm*. For the construction of a *nonstationary* method, we can recalculate the *extrapolation* parameter based on the appropriate submatrix of A as soon as one of the components, say the i th one, of either $x^{(k)}$ or $r^{(k)}$ is stabilized to zero. Obviously then, the convergence will be accelerated.
- (2) If A is also *symmetric*, then $|w|$ of w in (2.2) is written as

$$|w| = \left| \frac{1 - \omega a}{1 + \omega a} \right| = \left| \frac{\frac{1}{\omega} - a}{\frac{1}{\omega} + a} \right| = \left| \frac{r - a}{r + a} \right|, \quad r = \frac{1}{\omega}. \quad (6.1)$$

The solution to the minimax problem for the last expression in equalities (6.1) is associated with the determination of the optimal *acceleration parameter* r of the stationary ADI Method of the discretized Poisson equation in the unit square subject to Dirichlet boundary conditions using a 5-point discretization with equal mesh size in each co-ordinate direction. The *optimal* r , r^* , can be found in many textbooks, e.g., [32,33]. Obviously, from (4.3) it is obtained that

$$r^* = \frac{1}{\omega^*} = \sqrt{\beta_1 \beta_2}, \quad \min_{r>0} \max_{a \in \sigma(A)} \left| \frac{r - a}{r + a} \right| = \frac{\sqrt{\beta_2} - \sqrt{\beta_1}}{\sqrt{\beta_2} + \sqrt{\beta_1}}. \quad (6.2)$$

- (3) For the solution of a Complex Linear System whose matrix coefficient is *positive stable* by an ADI-type Method using the Hermitian/Skew Hermitian Splitting introduced in [1] the *acceleration* parameter r involved appears as in (2) above and can be determined in the same way as in the previous case.
- (4) Finally, for the solution of the Linear System in (3) if one uses the Normal/Skew Hermitian Splitting (see, e.g., [12]), where again the same expression to be optimized appears as before, \mathcal{H} is a rectangle. Therefore, the formulas for the optimal parameter and the spectral radii found there are the ones of Case (b) in Section 4. However, if some additional information on the spectrum is known the convergence can be improved further by using the Algorithm described in Section 3.

Acknowledgments

The authors are most grateful to an unknown referee for the many valuable comments he made on the previous version of the paper and for the rich bibliography he provided. They also thank Professor Michael Tsatsomeros for suggesting Ref. [10].

References

- [1] Z.-Z. Bai, G.H. Golub, M. Ng, Hermitian and skew-Hermitian splitting methods for non-Hermitian positive definite linear systems, *SIAM J. Matrix Anal. Appl.* 24 (2003) 603–626.
- [2] A. Berman, R.J. Plemmons, *Classics in Applied Mathematics*, SIAM, Philadelphia, 1994.
- [3] S. Billups, K. Murty, Complementarity Problems, *J. Comput. Appl. Math.* 124 (2000) 303–318.

- [4] M.-Q. Chen, C. Chiu, Region-dependent optimal m -stage Runge–Kutta schemes for solving a class of nonsymmetric linear systems, *Linear Algebra Appl.* 212/213 (1994) 523–546.
- [5] C. Chiu, Optimal one-stage and two-stage schemes for steady-state solutions of hyperbolic equations, *Appl. Numer. Math.* 11 (1993) 475–496.
- [6] R.W. Cottle, G.B. Dantzig, Complementarity Pivot theory of mathematical programming, *Linear Algebra Appl.* 1 (1968) 103–125.
- [7] R.W. Cottle, J.-S. Pang, R.E. Stone, *The Linear Complementarity Problem*, Academic Press, New York, 1992.
- [8] H.S.M. Coxeter, *Introduction to Geometry*. Wiley Classics Library, John Wiley & Sons, New York, 1989.
- [9] C.W. Cryer, The solution of a quadratic programming problem using systematic over-relaxation, *SIAM J. Control* 9 (1971) 385–392.
- [10] S.M. Fallatt, M.J. Tsatsomeros, On the Cayley Transform of positivity classes of matrices, *Electr. J. Linear Algebra* 9 (2002) 190–196.
- [11] M.C. Ferris, J.S. Pang, Engineering and economic applications of complementarity problems, *SIAM Rev.* 39 (1997) 669–713.
- [12] G.H. Golub, Solution of non-symmetric, real positive linear systems, Paper presented at the Milovy 2002 Conference on “Computational Linear Algebra with Applications”, August 5–9, 2002, Milovy, Czech Republic.
- [13] A. Hadjidimos, The optimal solution of the extrapolation problem of a first order scheme, *Intern. J. Comput. Math.* 13 (1983) 153–168.
- [14] A. Hadjidimos, The optimal solution to the problem of complex extrapolation of a first order scheme, *Linear Algebra Appl.* 62 (1984) 241–261.
- [15] A. Hadjidimos, On the equivalence of extrapolation and Richardson’s iteration and its applications, *Linear Algebra Appl.* 402 (2004) 165–192.
- [16] E. Hille, *Analytic Function Theory*, vol. 1, 4th ed., Blaisdel, New York, 1965.
- [17] A.J. Hughes Hallett, Some extensions and comparisons in the theory of Gauss–Seidel iterative technique for solving large equation systems, in: E.G. Charatsis (Ed.), *Proceedings of the Econometric Society European Meeting 1979*, North-Holland, Amsterdam, 1981, pp. 279–318.
- [18] A.J. Hughes Hallett, Alternative techniques for solving systems of nonlinear equations, *J. Comput. Appl. Math.* 8 (1982) 35–48.
- [19] N.W. Kappel, L.T. Watson, Iterative algorithms for the linear complementarity problem, *Int. J. Comput. Math.* 19 (1986) 273–297.
- [20] M.D. Koulisianis, T.S. Papatheodorou, Improving projected successive overrelaxation method for linear complementarity problems, *Appl. Numer. Math.* 45 (2003) 29–40.
- [21] C.E. Lemke, Bimatrix equilibrium points and mathematical programming, *Management Sci.* 11 (1965) 681–689.
- [22] E.M. Ma, C.J. Zarowski, On lower bounds for the smallest eigenvalue of a Hermitian matrix, *IEEE Trans. Inform. Theory* 41 (1995) 539–540.
- [23] O.L. Mangasarian, *Nonlinear Programming*, McGraw Hill, New York, 1969 (Reprint: SIAM Classics in Applied Mathematics 10, Philadelphia, 1994.)
- [24] K.G. Murty, *Linear Complementarity*, Linear and Nonlinear Programming, Internet Edition 1997.
- [25] G. Opfer, G. Schober, Richardson’s iteration for nonsymmetric matrices, *Linear Algebra Appl.* 58 (1984) 343–361.
- [26] K. Pantazopoulos, Numerical methods and software for the pricing of American financial derivatives, Ph.D. Thesis, Department of Computer Sciences, Purdue University, West Lafayette, IN, 1998.
- [27] D.W. Peaceman, H.H. Rachford Jr., The numerical solution of parabolic and elliptic differential equations, *SIAM J. Appl. Math.* 3 (1955) 28–41.
- [28] U. Schäfer, A linear complementarity problem with a P -matrix, *SIAM Rev.* 46 (2004) 189–201.
- [29] U. Schäfer, On the modulus algorithm for the linear complementarity problem, *Oper. Res. Lett.* 32 (2004) 350–354.
- [30] W. Sun, Lower bounds of the minimal eigenvalue of a Hermitian positive-definite matrix, *IEEE Trans. Inform. Theory* 46 (2000) 2760–2762.
- [31] W.M.G. van Bokhoven, *Piecewise-linear Modelling and Analysis*, Proefschrift, Eindhoven, 1981.
- [32] R.S. Varga, *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, NJ, 1962, Also: 2nd Edition, Revised and Expanded, Springer, Berlin, 2000.
- [33] D.M. Young, *Iterative Solution of Large Linear Systems*, Academic Press, New York, 1971.