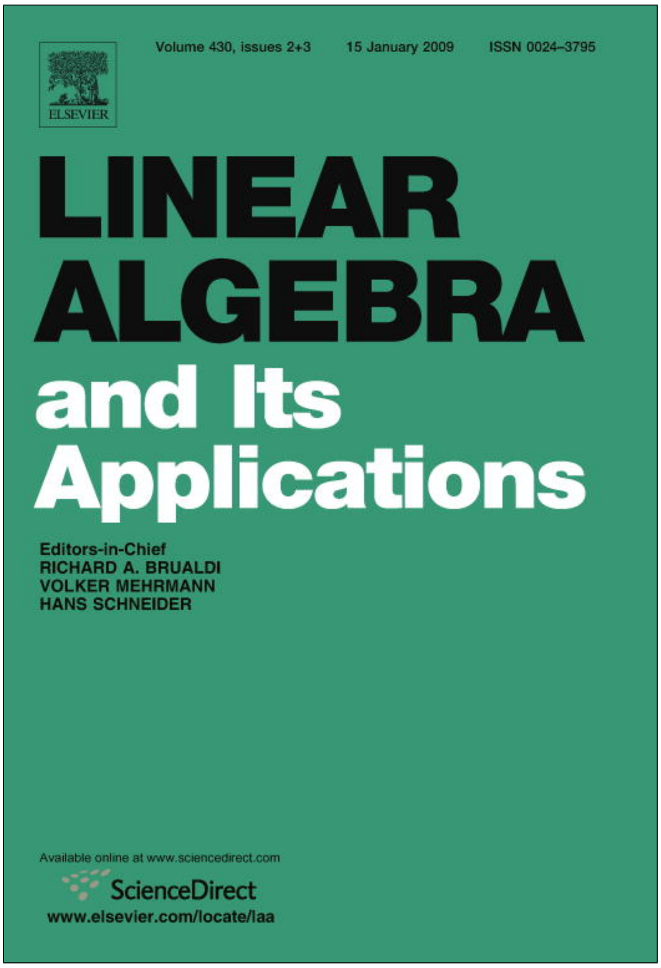
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On the optimal complex extrapolation of the complex Cayley transform

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Abstract

The *Cayley transform*, $F := \mathscr{F}(A) = (I + A)^{-1}(I - A)$, with $A \in \mathbb{C}^{n,n}$ and $-1 \notin \sigma(A)$, where $\sigma(\cdot)$ denotes spectrum, and its extrapolated counterpart $\mathscr{F}(\omega A)$, $\omega \in \mathbb{C}\backslash\{0\}$ and $-1 \notin \sigma(\omega A)$, are of significant theoretical and practical importance (see, e.g. [A. Hadjidimos, M. Tzoumas, On the principle of extrapolation and the Cayley transform, Linear Algebra Appl., in press]). In this work, we extend the theory in [8] to cover the complex case. Specifically, we determine the optimal *extrapolation parameter* $\omega \in \mathbb{C}\backslash\{0\}$ for which the spectral radius of the *extrapolated Cayley transform* $\rho(\mathscr{F}(\omega A))$ is minimized assuming that $\sigma(A) \subset \mathscr{H}$, where $\mathscr{H}$ is the smallest closed convex polygon, and satisfies $O(0) \notin \mathscr{H}$. As an application, we show how a complex linear system, with coefficient a certain class of indefinite matrices, which the ADI-type method of Hermitian/Skew-Hermitian splitting fails to solve, can be solved in a “best” way by the aforementioned method.

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Keywords: Cayley transform; Extrapolation; Convex hull; Möbius transformation; Capturing circle; Visibility angle; Hermitian/Skew-Hermitian splitting

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1. Introduction and preliminaries

The *Cayley transform* and the *extrapolated Cayley tranform* are of significant theoretical interest and have many applications (see [4,8]). Their definitions are as follows:

Definition 1.1. Given

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

the *Cayley transform* $\mathscr{F}(A)$ is defined to be

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

Definition 1.2. Under the assumptions of Definition 1.1, we call *extrapolated* Cayley transform, with *extrapolation* parameter ω, the matrix function (1.2) where A is replaced by ωA

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

In what follows the definition and assumptions below are needed.

Definition 1.3. Let $A \in \mathbb{C}^{n,n}$ and $\sigma(A)$ be its spectrum. The *closed convex hull* of $\sigma(A)$, denoted by $\mathscr{H}(A)$ or simply by $\mathscr{H}$, is the smallest closed convex polygon such that $\sigma(A) \subset \mathscr{H}$.

Main Assumption 1: In the following it will be assumed that $O(0) \notin \mathscr{H}$.

In many cases, F_ω is the iteration matrix of an iterative method [8]. Therefore, $\rho(F_\omega)$ constitutes a measure of its convergence. Hence, it must be $\max_{a\in\sigma(A)\subset\mathscr{H}} \left|\frac{1-\omega a}{1+\omega a}\right| < 1$ and this holds if and only if (*iff*) Re $(\omega a) > 0$. So, we also make the following assumption:

Main Assumption 2: In what follows it will be assumed that

$$\text{Re}\,(\omega a) > 0 \quad \forall a \in \sigma(A) \subset \mathscr{H} \text{ and } \omega \in \mathbb{C}. \tag{1.4}$$

Our main objective in this paper is to solve the following problem.

Problem I: Based on the hypotheses of Definitions 1.1–1.3 and *Main Assumptions* 1 and 2, determine the *extrapolation parameter* ω that minimizes the spectral radius of the extrapolated Cayley transform, i.e.

$$\min_{\omega\in\mathbb{C}\backslash\{0\},\,-1\notin\sigma(\omega A)} \rho(F_\omega) \ = \min_{\omega\in\mathbb{C}\backslash\{0\},-1\notin\sigma(\omega A)} \ \max_{a\in\sigma(A)\subset\mathscr{H}} \left|\frac{1-\omega a}{1+\omega a}\right|. \tag{1.5}$$

This work is organized as follows. In Section 2, an analysis similar to but more complicated than that in [8] leads to an algorithm for the determination of the optimal ω which is identical to the one in [6,7]. However, the expressions for the optimal values involved are different from those in [6]. Next, in Section 3, the algorithm is briefly presented, where one of its main steps is improved over that in [6]. In Section 4, the proof of uniqueness of the solution which was not quite mathematically complete in [6] is given. Then, in Section 5, it is shown how a class of complex linear systems with indefinite matrix coefficient can be solved by the *ADI*-type method of Hermitian/Skew-Hermitian splitting [2], which linear systems the aforementioned method fails to solve. In Section 6, we give a number of concluding remarks, and finally, in an appendix, we present a Theorem in connection with the present improved form of our algorithm.

2. The solution to the minimax Problem I

To solve *Problem* I we seek the solution to the more general *Problem* II below. As will be seen *Problem* II is easier to solve and its solution is identical to that of *Problem* I.

Problem II: Under the Main Assumptions 1 and 2, determine the extrapolation parameter ω that solves the minimax problem

$$\min_{\omega\in\mathbb{C}}\max_{a\in\mathscr{H}}\left|\frac{1-\omega a}{1+\omega a}\right| \ (<1). \tag{2.1}$$

The function in (2.1)

$$w := w(a) = \frac{1-\omega a}{1+\omega a}, \quad a\in\mathscr{H}, \ \ \omega\in\mathbb{C}, \quad \mathrm{Re}(\omega a)>0 \tag{2.2}$$

is a Möbius transformation [9]. It has no *poles*, because $\mathrm{Re}(1+\omega a)>1$ ($\neq 0$), and is not a constant as is readily checked. Hence, it possesses an inverse Möbius transformation

$$w^{-1}(w(a)) = a = \frac{1-w}{\omega(1+w)}, \quad w=w(a), \ \ a\in\mathscr{H}, \ \ \omega\in\mathbb{C}, \ \ \mathrm{Re}\,(\omega a)>0, \tag{2.3}$$

which has no poles and is not the constant function.

It is reminded that a Möbius transformation is a conformal mapping, i.e. it is a one-to-one correspondence that preserves angles [9]. In general, it maps a disk onto a disk and a circle onto the circle of its image. To see how their elements are mapped via (2.2) or (2.3), let an $\omega\in\mathbb{C}$ (with $\mathrm{Re}(\omega a)>0$, $a\in\mathscr{H}$) and $\mathscr{C}_\omega$ be the circle with center $O(0)$ and radius

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

In view of (2.4), $\mathscr{C}_\omega$ will capture[2] $w(\mathscr{H})$ and will pass through a boundary point of it. Therefore, since (2.2) and (2.3) have **no** poles, $\mathscr{C}_\omega$ must be the image of a circle $\mathscr{C}$. To find out how $\mathscr{C}$ is derived from $\mathscr{C}_\omega$ and vice versa, we begin with

$$\mathscr{C}_\omega := |w| = \rho, \tag{2.5}$$

use (2.2), go through the equivalences

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

and, finally, we obtain

$$\mathscr{C} := |a-c| = R, \tag{2.6}$$

which is the equation of a circle $\mathscr{C}$, with center c and radius R given by

$$c := \frac{1+\rho^2}{\omega(1-\rho^2)}, \quad R := \frac{2\rho}{|\omega|(1-\rho^2)}. \tag{2.7}$$

[2] The word "*captures*" will mean "*contains in the closure of its interior*".

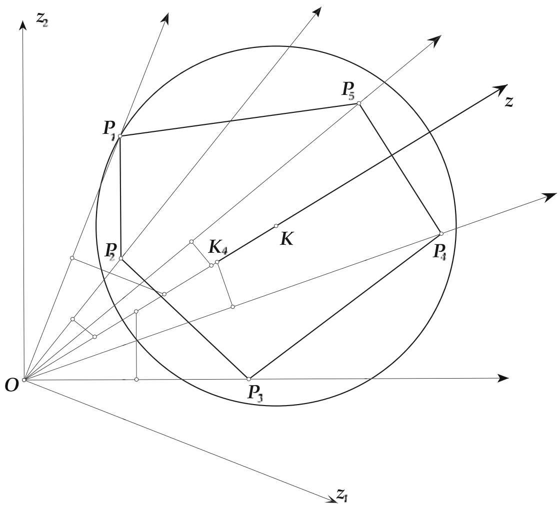

Fig. 1. One of the infinitely many *capturing circles*.

From the equivalences $\mathscr{C}_\omega = w(\mathscr{C}) \Leftrightarrow \mathscr{C} = w^{-1}(\mathscr{C}_\omega)$. Therefore, the circle $\mathscr{C}$ possesses the properties: (1) It leaves $O(0)$ strictly outside since $R < |c|$. (2) It captures $\mathscr{H}$ ($\mathscr{H} \subset \mathscr{C}$) since $\mathscr{C}_\omega$ captures $w(\mathscr{H})$ ($w(\mathscr{H}) \subset \mathscr{C}_\omega \equiv w(\mathscr{C})$). (3) It passes through at least one vertex of $\mathscr{H}$, because by (2.4) $\mathscr{C}_\omega$ captures $w(\mathscr{H})$ and passes through a boundary point of it. Hence, by the equivalences, $\mathscr{C}$ captures $\mathscr{H}$ and passes through a boundary point of it, that is a vertex.

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

Theorem 2.1 (see also Lemma 1 of [6]). *Let $A \in \mathbb{C}^{n,n}$, $\sigma(A)$ be its spectrum and $\mathscr{H}$ be the closed convex hull $\mathscr{H} \equiv \mathscr{H}(A)$, satisfying Definitions* 1.1–1.3 *and Main Assumptions* 1 *and* 2. *Then, there are infinitely many capturing circles (cc's) of $\mathscr{H}$.*

Proof. Let P_i, $i = 1, \ldots, l$, be the vertices of $\mathscr{H}$ and let $I := \{1, 2, , \ldots, l\}$. Let OP_i, $i = 1, \ldots, l$, be the semilines through the vertices of $\mathscr{H}$ and $OP_{i_1}, OP_{i_2}, i_1, i_2 \in I$, be the two extreme ones (Fig. 1). Then $\angle P_{i_1} O P_{i_2} < \pi$. Draw Oz_1, Oz_2 perpendicular to OP_{i_1}, OP_{i_2} at O so that $\angle P_{i_1} O P_{i_2} + \angle z_1 O z_2 = \pi$, and any semiline Oz within $\angle z_1 O z_2$. Draw also the perpendicular bisectors to OP_i, $i = 1, \ldots, l$, and let K_i be their intersections with Oz. The circle with center any $K \in Oz$ such that $(OK) > \max_{i \in I}(OK_i)$ and radius $R = \max_{i \in I}(KP_i)$ is a *cc* of $\mathscr{H}$. Consequently, given $\mathscr{H}$, there are infinitely many *cc*'s. $\square$

Note: The notion of a *cc* of $\mathscr{H}$ is a particular case of the one defined in [6] (see also [7]).

One more consequence of our analysis is the validity of the following statement.

Theorem 2.2. *Under the Main Assumptions* 1 *and* 2, *the solutions to Problem* II *and Problem* I *are identical*.

Proof. In view of the preceding analysis the following series of relations hold:

$$\max_{a\in\mathscr{H}}\left|\frac{1-\omega a}{1+\omega a}\right| = \max_{a\in\mathscr{H}}|w(a)| = \rho = \rho(C_\omega)$$
$$= \rho(w(\mathscr{C})) = \max_{a\in\sigma(A)}|w(a)| = \max_{a\in\sigma(A)}\left|\frac{1-\omega a}{1+\omega a}\right| = \rho(F_\omega). \tag{2.8}$$

Equalities (2.8) are analogous to those of Theorem 2.2 in [8] and their proof is omitted. □

To solve *Problem* II it suffices to find which of the *cc*'s of $\mathscr{H}$ is the one that minimizes ρ. The following two theorems constitute a decisive step in this direction.

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

$$\omega = \frac{|c|}{c\sqrt{|c|^2-R^2}}, \quad \rho = \frac{R}{|c|+\sqrt{|c|^2-R^2}}. \tag{2.9}$$

Proof. From (2.7) we obtain $\frac{R}{|c|} = \frac{2\rho}{1+\rho^2}$. Solving for $\rho \in (0, 1)$, we take the second equation in (2.9). ω is obtained from the first equation in (2.7) using the expression for ρ found. □

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

Proof. ρ in (2.9) is written as $\rho = \frac{\frac{R}{|c|}}{1+\sqrt{1-\left(\frac{R}{|c|}\right)^2}}$. Differentiating with respect to (*wrt*) $\frac{R}{|c|} \in [0, 1)$ we obtain

$$\frac{\mathrm{d}\rho}{\mathrm{d}\left(\frac{R}{|c|}\right)} = \frac{1}{\sqrt{1-\left(\frac{R}{|c|}\right)^2}\left(1+\sqrt{1-\left(\frac{R}{|c|}\right)^2}\right)} > 0.$$

Therefore, ρ strictly increases with $\frac{R}{|c|} \in [0, 1)$ and is minimized in any subinterval of it, whenever $\frac{R}{|c|}$ is; that is at the left endpoint of the subinterval. □

Definition 2.2. We call visibility angle (*v.a.*) of a *cc* of $\mathscr{H}$ from the origin O the angle formed by the tangents from O to the *cc* in question.

If ϕ is the *v.a.* of a certain *cc* of $\mathscr{H}$ it can be observed that

$$\sin\left(\frac{\phi}{2}\right) = \frac{R}{|c|}. \tag{2.10}$$

Based on Definition 2.2 and Theorems 2.3 and 2.4 we come to the following conclusion.

Theorem 2.5. *Under the assumptions of Theorem 2.3 the ratio $\frac{R}{|c|}$ is minimized iff the corresponding v.a. ϕ is.*

In the trivial case $l = 1$, $\mathscr{H}$ shrinks to the point $P_1(z_1)$ ($\mathscr{H} \equiv P_1$). The *v.a.* of $\mathscr{H}$ is zero and from (2.10) $R = 0$. Then, from (2.9), the optimal values for ω (ω^*) and ρ (ρ^*) are

$$\omega^* = \frac{1}{z_1}, \quad \rho^* = 0. \tag{2.11}$$

In case $l \geq 2$, the class of *cc*'s among which the optimal one is to be sought is a subclass of that of Definition 2.1. For this we appeal to the following statement which makes use of Definition 2.2.

Theorem 2.6 (Lemma 3 of [6]). *The optimal cc passes through at least two vertices of* $\mathscr{H}$.

From our hypotheses and analysis it is ascertained that for a given $\mathscr{H}$ the optimal *cc* $\mathscr{C}^*$ will be given by the same algorithm that gives its analogue in the *classical extrapolation* ($\min_{\omega\in\mathbb{C}} \max_{a\in\mathscr{H}} |1 - \omega a|$) [6,7]. The algorithm in [6] is based on *Apollonius circles* [3], and in the next section, is presented in an improved form. One should mention that many researchers have contributed to the solution of the *classical extrapolation* for $A \in \mathbb{R}^{n,n}$, $\omega \in \mathbb{R}$. The more general solution was given by Hughes Hallett [10,11] and Hadjidimos [5]. In the *classical extrapolation* for $A \in \mathbb{C}^{n,n}$, $\omega \in \mathbb{C}$, a solution was also given by Opfer and Schober [12] by using *Lagrange multipliers* [1] when $\mathscr{H}$ is a straight-line segment or an ellipse.

Note that although $\mathscr{C}^*$ for the *classical extrapolation* and the present one are identically the same, the expressions for the optimal parameters ω^* and $\rho(\mathscr{C}_{\omega^*})$ are **completely different**.

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

Let $A \in \mathbb{C}^{n,n}$ and $\mathscr{H}$ be the closed convex hull of $\sigma(A)$ satisfying all the assumptions so far. Then, the determination of the *optimal cc* $\mathscr{C}^*$ of $\mathscr{H}$ is achieved by the following algorithm.

The Algorithm

Step 1. Let $P_i(z_i)$, $i = 1, \ldots, l$, be the l vertices of $\mathscr{H}$ and let $I := \{1, 2, \ldots, l\}$.

Step 2. If $l = 1$, the elements of $\mathscr{C}_1^*$ are given by $c_1^* = z_1$, $R_1^* = 0$ (2.11).

Step 3. If $l = 2$, the center $K_{1,2}^*(c_{1,2}^*)$ of $\mathscr{C}_{1,2}^*$ is found as the intersection of any two of the three lines: (i) the perpendicular bisector to P_1P_2, (ii) the bisector of $\angle P_1OP_2$, and (iii) the circle circumscribed to the triangle OP_1P_2. ($K_{1,2}^*$ is also the point on the perpendicular bisector to P_1P_2 whose ratio of distances from P_1 and O and also from P_2 and O is minimal.) The elements of $\mathscr{C}_{1,2}^*$ are given by

$$c_{1,2}^* = \frac{(|z_1| + |z_2|)z_1z_2}{|z_1|z_2 + z_1|z_2|}, \quad R_{1,2}^* = \frac{|z_1|\,|z_2|\,|z_2 - z_1|}{|z_1|z_2| + |z_1|z_2|} \tag{3.1}$$

(see [6,12] or [7]). The optimal *cc* $\mathscr{C}_{1,2}^*$ in this case will be called a *two-point optimal cc*.

Step 4. If $l \geqslant 3$, find the elements of the $\binom{l}{2}$ *two-point optimal cc*'s $\mathscr{C}_{i,j}$, $i = 1, \ldots, l-1$, $j = i+1, \ldots, l$, and from these the maximum ratio $\frac{R_{i,j}}{|c_{i,j}|}$. If the *optimal cc* that corresponds to the maximum ratio, let it correspond to the indices $\bar{i}$ and $\bar{j}$, captures $\mathscr{H}$, that is

$$|c_{\bar{i},\bar{j}} - z_k| \leqslant R_{\bar{i},\bar{j}} \quad \forall k \in I\backslash\{\bar{i}, \bar{j}\},$$

then this *two-point optimal cc* $\mathscr{C}^*_{\bar{i},\bar{j}}$ will be the *optimal cc* of $\mathscr{H}$.[3] If such a circle does **not** exist, then find the elements of the $\binom{l}{3}$ circles that are circumscribed to the triangles $P_iP_jP_k$, $i = 1,\ldots,k-2,\ j = i+1,\ldots,k-1,\ k = j+1,\ldots,l$, let them be $K_{i,j,k}(c_{i,j,k})$ and $R_{i,j,k}$, using the formulas

$$c_{i,j,k} = \frac{|z_i|^2(z_j - z_k) + |z_j|^2(z_k - z_i) + |z_k|^2(z_i - z_j)}{\overline{z_i}(z_k - z_l) + \overline{z_j}(z_k - z_i) + \overline{z_k}(z_i - z_j)},$$
$$R_{i,j,k} = \left|\frac{(z_i - z_j)(z_j - z_k)(z_k - z_i)}{\overline{z_i}(z_j - z_k) + \overline{z_j}(z_k - z_i) + \overline{z_k}(z_i - z_j)}\right|. \tag{3.2}$$

(see [6] or [7]). Discard all circles that may capture the origin, i.e. $|c_{i,j,k}| \leqslant R_{i,j,k}$, and, from the remaining ones all those that do not capture all the other vertices, i.e.

$$(R_{i,j,k} < |c_{i,j,k}| \text{ and}) \quad \exists m \in I\backslash\{i, j, k\} \text{ such that } R_{i,j,k} < |c_{i,j,k} - z_m|.$$

From the rest the one that corresponds to the smallest ratio $\frac{R_{i,j,k}}{(OK_{i,j,k})}$, let the associated vertices be $P_{\bar{i}}, P_{\bar{j}}, P_{\bar{k}}$, is the *three-point optimal cc* $\mathscr{C}^*_{\bar{i},\bar{j},\bar{k}}$ of $\mathscr{H}$.

4. Uniqueness of the optimal capturing circle

In this section, we give a complete theoretical proof of the uniqueness of the optimal *cc* of $\mathscr{H}$ which is not quite mathematically satisfactory as is presented in [6]. For this we will need the classical Theorem of the *Apollonius circle* and one of its corollaries.

Theorem 4.1 (Apollonius Theorem [3]). *The locus of the points M of a plane whose distances from two fixed points A and B of the same plane are at a constant ratio $\frac{(MA)}{(MB)} = \lambda \neq 1$ is a circle whose diameter has endpoints C and D that lie on the straight-line AB and separate internally and externally the straight-line segment AB into the same ratio λ, namely*

$$\frac{(CA)}{(CB)} = \frac{(DA)}{(DB)} = \lambda. \tag{4.1}$$

Corollary 4.1. *Under the assumptions of the Apollonius Theorem 4.1, any point M' strictly inside the Apollonius circle has distances from A and B whose ratio is strictly less than λ while any M'' strictly outside has distances with ratio strictly greater than λ. Specifically,*

$$\frac{(M'A)}{(M'B)} < \lambda, \quad \frac{(M''A)}{(M''B)} > \lambda. \tag{4.2}$$

Theorem 4.2. *Under the assumptions of Theorem 2.4 the optimal cc of $\mathscr{H}$ is unique.*

Proof. Let that there exist two *optimal cc*'s $\mathscr{C}_i$, with centers $K_i(c_i)$ and radii R_i, $i = 1, 2$ (see Fig. 2). Since both circles are *optimal cc*'s of $\mathscr{H}$, $\mathscr{H}$ lies in both of them. Hence $\mathscr{C}_1$ and $\mathscr{C}_2$ intersect each other, say at A and B. Let $\mathscr{S}$ be their closed common region defined by the arc $\widehat{AB}$ of $\mathscr{C}_1$ lying in $\mathscr{C}_2$ and by $\widehat{AB}$ of $\mathscr{C}_2$ lying in $\mathscr{C}_1$. $\mathscr{H}$ must have at least two vertices on each arc not excluding the case

[3] If there exists a *two-point optimal cc* of $\mathscr{H}$ it will correspond to the maximal ratio above. So, the previous known part of the Algorithm [6,7] is improved. The proof of our claim is given in the Appendix.

that two vertices, one from each arc, coincide at A and/or B. Let M_1 and M_2 be the intersections of the straight-line K_1K_2 with the arcs $\widehat{AB}$ so that $(K_iM_i) = R_i$, $i = 1, 2$. The optimality condition of the two circles gives $\frac{R_1}{|c_1|} = \frac{R_2}{|c_2|} = \lambda$ (<1) or, equivalently, $\frac{(K_1A)}{(K_1O)} = \frac{(K_2A)}{(K_2O)} = \lambda$. Hence, the points K_1 and K_2 must lie on the *Apollonius circle* $\mathscr{C}_{\mathscr{A}}$ whose diameter has endpoints C and D that separate the straight-line segment OA, internally and externally, at the same ratio λ, namely $\frac{(CA)}{(CO)} = \frac{(DA)}{(DO)} = \lambda$. For any point K strictly in the interior of the straight-line segment K_1K_2 it will be

$$(K_1K) + (KA) > R_1 = (K_1K) + (KM_1) \Leftrightarrow (KA) > (KM_1),$$
$$(K_2K) + (KA) > R_2 = (K_2K) + (KM_2) \Leftrightarrow (KA) > (KM_2).$$

These inequalities show that the circle with center K and radius (KA) captures $\mathscr{S}$, and therefore, $\mathscr{H}$. Also, the point K as lying strictly between K_1 and K_2 lies strictly in the interior of the *Apollonius circle* $\mathscr{C}_{\mathscr{A}}$ which, by Corollary 4.1, implies that $\frac{(KA)}{(KO)} < \lambda$. However, this constitutes a contradiction because we have just found a circle that captures $\mathscr{H}$ and has a *v.a.* $\phi\left(\sin\left(\frac{\phi}{2}\right) = \frac{(KA)}{(KO)} < \lambda\right)$ strictly less than that of the two *optimal cc*'s $\mathscr{C}_1$ and $\mathscr{C}_2$. □

5. Linear systems with indefinite coefficient matrix

5.1. Introduction

In a recent paper Bai et al. [2] introduced an *alternating direction implicit (ADI)*-type method [13] (see also [14] or [15]) using *Hermitian/Skew-Hermitian splittings* for the solution of complex linear algebraic systems with matrix coefficient (positive) definite.

Specifically, let the linear system

$$Ax = b, \quad A \in \mathbb{C}^{n,n}, \quad \det(A) \neq 0, \quad b \in \mathbb{C}^n \tag{5.1}$$

with A *positive definite*, namely $\mathrm{Re}(z^H Az) > 0\ \forall z \in \mathbb{C}^n\backslash\{0\}$. Consider the splitting

$$A = B + C \quad \text{where } B = \frac{1}{2}(A + A^H), \quad C = \frac{1}{2}(A - A^H). \tag{5.2}$$

In (5.2), B is *Hermitian positive definite* and C is *Skew-Hermitian*. For the solution of (5.1) the following *ADI*-type method is adopted:

$$\begin{aligned}(rI + B)x^{(m+\frac{1}{2})} &= (rI - C)x^{(m)} + b,\\ (rI + C)x^{(m+1)} &= (rI - B)x^{\left(m+\frac{1}{2}\right)} + b, \quad m = 0, 1, 2, \ldots,\end{aligned} \tag{5.3}$$

where r is a positive *acceleration* parameter, I the unit matrix of order n and $x^{(0)} \in \mathbb{C}^n$ any initial approximation to the solution. Since B is Hermitian with positive eigenvalues and C Skew-Hermitian with purely imaginary eigenvalues, the operators $rI + B$ and $rI + C$ are invertible and so eliminating $x^{\left(m+\frac{1}{2}\right)}$ from Eq. (5.3) we obtain the iterative scheme

$$x^{(m+1)} = T_r x^{(m)} + c_r, \quad m = 0, 1, 2, \ldots, \tag{5.4}$$

where

$$T_r = (rI + C)^{-1}(rI - B)(rI + B)^{-1}(rI - C), \quad c_r = 2r(rI + C)^{-1}(rI + B)^{-1}. \tag{5.5}$$

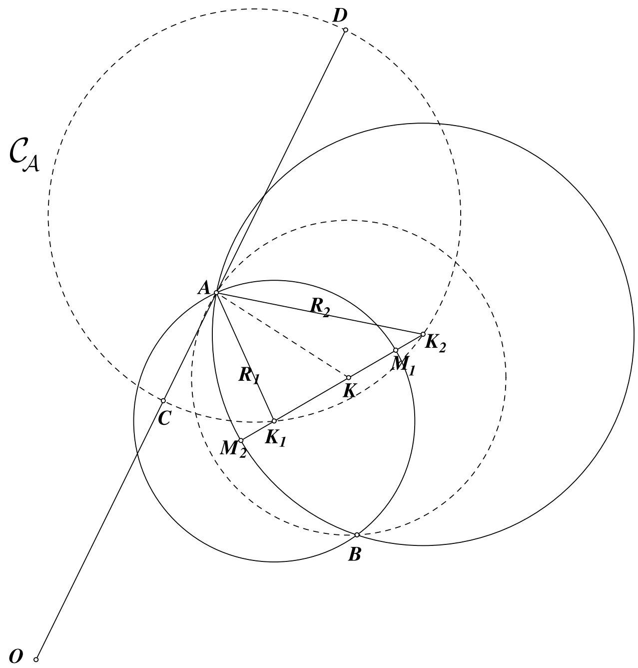

Fig. 2. The case of existence of two *optimal cc*'s.

Note that the matrices T_r and $\widetilde{T}_r = (rI - B)(rI + B)^{-1}(rI - C)(rI + C)^{-1}$ are similar. So,

$$\rho(T_r) = \rho(\widetilde{T}_r) \leqslant \|\widetilde{T}_r\|_2 \leqslant \|(rI - B)(rI + B)^{-1}\|_2 \|(rI - C)(rI + C)^{-1}\|_2. \tag{5.6}$$

Since C is Skew-Symmetric ($C^H = -C$) we have

$$\begin{aligned}\|(rI - C)(rI + C)^{-1}\|_2 &= \rho^{\frac{1}{2}}((rI + C)^{-H}(rI - C)^H(rI - C)(rI + C)^{-1})\\ &= \rho^{\frac{1}{2}}((rI - C)^{-1}(rI + C)(rI - C)(rI + C)^{-1})\\ &= \rho^{\frac{1}{2}}((rI - C)^{-1}(rI - C)(rI + C)(rI + C)^{-1})\\ &= \rho^{\frac{1}{2}}(I) = 1.\end{aligned} \tag{5.7}$$

Consequently, in view of (5.6) and (5.7), to obtain the "best" iterative scheme (5.3) we have to minimize the bound $\|(rI - B)(rI + B)^{-1}\|_2$ of the spectral radius $\rho(T_r)$ (or $\rho(\widetilde{T}_r)$). Recall that $(rI - B)(rI + B)^{-1}$ is Hermitian, and therefore,

$$\begin{aligned}\|(rI - B)(rI + B)^{-1}\|_2 &= \rho((rI - B)(rI + B)^{-1})\\ &= \max_{b\in\sigma(B)}\left|\frac{r-b}{r+b}\right| = \max_{b\in\sigma(B)}\left|\frac{1-\frac{1}{r}b}{1+\frac{1}{r}b}\right|.\end{aligned} \tag{5.8}$$

Let $b \in [b_1, b_2]$, where b_1 is a positive lower bound of $\sigma(B)$ and b_2 an upper bound. The minimum value of the right-hand side of (5.8) is attained at $r = r^* = \sqrt{b_1 b_2}$, as was found in [2] (see also [8,14,15]), and can also be found by the Algorithm of Section 3.

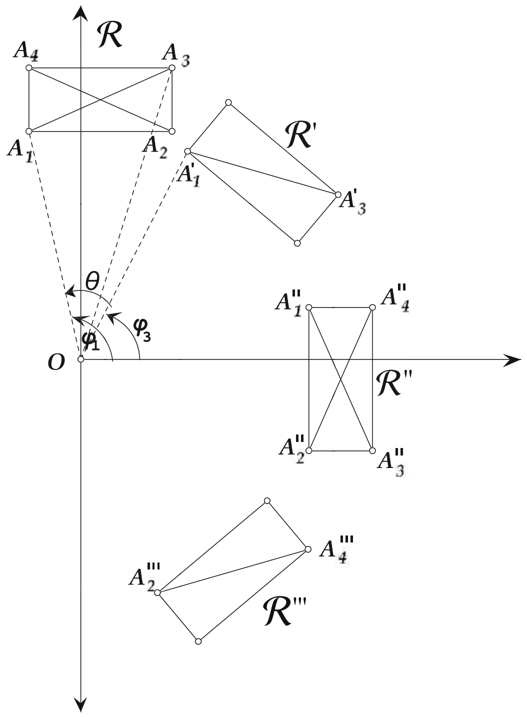

Fig. 3. The rectangles $\mathscr{R}$ and $e^{-\imath\theta}\mathscr{R}$ ($\mathscr{R}'$, $\mathscr{R}''$, $\mathscr{R}'''$).

5.2. *Cases of indefinite matrix coefficient*

The preceding analysis shows how to solve a complex linear system by the *ADI*-type method using the Hermitian/Skew-Hermitian splitting when the matrix coefficient A is *definite*. In what follows we show that there are cases where even if A is *indefinite* we can apply the previous method after a scalar preconditioning of the original system (5.1) (and of A).

Suppose that $\sigma(A) \subset \mathscr{R}$, where $\mathscr{R}$ is a rectangle, with vertices $A_1(\beta_1, \gamma_1)$, $A_2(\beta_2, \gamma_2)$, $A_3(\beta_3, \gamma_3)$, $A_4(\beta_4, \gamma_4)$ and with their coordinates satisfying

$$\begin{aligned} &\beta_1 \leqslant 0 \leqslant \beta_2,\ |\beta_1| + |\beta_2| > 0,\ \beta_3 = \beta_2,\ \beta_4 = \beta_1 \quad \text{and} \\ &0 < \gamma_1 < \gamma_4,\ \gamma_1 = \gamma_2,\ \gamma_3 = \gamma_4. \end{aligned} \tag{5.9}$$

(*Note*: The case, of having $\sigma(A) \subset \mathscr{R}'$ symmetric to $\mathscr{R}$ *wrt* the origin, is examined in an analogous way.) In (5.9), $\beta_1,\ \beta_2$ are the lower and upper bounds of $\sigma(B)$ and $\imath\gamma_1,\ \imath\gamma_4$, the purely imaginary ones of $\sigma(C)$ in (5.2). The rectangle $\mathscr{R}$ is illustrated in Fig. 3. To apply the *ADI*-type method (5.3) to the original system (5.1) we multiply both members of the system by $e^{-\imath\theta}$, $\theta > 0$, so that the new coefficient matrix $e^{-\imath\theta}A$ becomes *positive definite.* The angle θ takes values so that the projection of $e^{-\imath\theta}\mathscr{R}$ onto the real axis is on the *positive* real semiaxis. Let $r_i,\ \phi_i,\ i = 1, \ldots, 4,$ be the *polar radii* and the *polar angles* of the corresponding vertices of $\mathscr{R}$. It will be

$$r_i = \sqrt{\beta_i^2 + \gamma_i^2}, \quad \phi_i \ = \ \arccos\left(\frac{\beta_i}{r_i}\right), \ \ i = 1, \ldots, 4. \tag{5.10}$$

The projection of $e^{-\imath\theta}\mathscr{R}$ onto the real axis is defined by those of the "new positions" of the diagonal A_1A_3, for $\theta \in (\phi_1 - \frac{\pi}{2}, \frac{\pi}{2}]$, and by the corresponding ones of A_2A_4 for $\theta \in [\frac{\pi}{2}, \phi_2 + \frac{\pi}{2})$. The endpoints of these projections are

$$\begin{aligned} b_1(\theta) &= r_1\cos(\phi_1-\theta),\ b_2(\theta) = r_3\cos(\phi_3-\theta) \quad \text{for } \theta \in \left(\phi_1 - \frac{\pi}{2}, \frac{\pi}{2}\right], \\ b_1(\theta) &= r_2\cos(\phi_2-\theta),\ b_2(\theta) = r_4\cos(\phi_4-\theta) \quad \text{for } \theta \in \left[\frac{\pi}{2}, \phi_2 + \frac{\pi}{2}\right). \end{aligned} \tag{5.11}$$

Note that at $\theta = \frac{\pi}{2}$ we have

$$r_1\cos\left(\phi_1 - \frac{\pi}{2}\right) = r_2\cos\left(\phi_2 - \frac{\pi}{2}\right) \quad \text{and} \quad r_3\cos\left(\phi_3 - \frac{\pi}{2}\right) = r_4\cos\left(\phi_4 - \frac{\pi}{2}\right). \tag{5.12}$$

We follow the Algorithm of Section 3, with $\mathscr{H}$ being the positive real line segment $[b_1(\theta), b_2(\theta)]$. Therefore, the center $K(c)$ and the radius R of the *optimal cc* are given by $c = \frac{1}{2}(b_1(\theta) + b_2(\theta))$ and $R = \frac{1}{2}(b_2(\theta) - b_1(\theta))$, which are functions of $\theta \in (\phi_1 - \frac{\pi}{2}, \phi_2 + \frac{\pi}{2})$. Consequently, to find the *best optimal cc* we have to minimize $\frac{R}{c}$ given by

$$\frac{R}{c} = \frac{b_2(\theta) - b_1(\theta)}{b_2(\theta) + b_1(\theta)} = \begin{cases} \frac{r_3\cos(\phi_3-\theta) - r_1\cos(\phi_1-\theta)}{r_3\cos(\phi_3-\theta) + r_1\cos(\phi_1-\theta)} & \text{for } \theta \in \left(\phi_1 - \frac{\pi}{2}, \frac{\pi}{2}\right], \\ \frac{r_4\cos(\phi_4-\theta) - r_2\cos(\phi_2-\theta)}{r_4\cos(\phi_4-\theta) + r_2\cos(\phi_2-\theta)} & \text{for } \theta \in \left[\frac{\pi}{2}, \phi_2 + \frac{\pi}{2}\right). \end{cases} \tag{5.13}$$

Differentiating the first ratio in the right-hand side above we obtain

$$\frac{\mathrm{d}\left(\frac{r_3\cos(\phi_3-\theta) - r_1\cos(\phi_1-\theta)}{r_3\cos(\phi_3-\theta) + r_1\cos(\phi_1-\theta)}\right)}{\mathrm{d}\theta} = \frac{2r_1r_3\sin(\phi_3-\phi_1)}{(r_3\cos(\phi_3-\theta) + r_1\cos(\phi_1-\theta))^2} < 0,$$

so, the minimum is attained at $\theta = \frac{\pi}{2}$. Similarly, working with the other expression for $\frac{R}{c}$ we find out that its derivative is positive and so its minimum is assumed again at $\theta = \frac{\pi}{2}$.

Note that $e^{-\imath\frac{\pi}{2}} = -\imath$, so the scalar preconditioner of A is $-\imath$ and the matrices $-\imath B$ and $-\imath C$ in (5.2) are now Skew-Hermitian and Hermitian, respectively.

In either case the "best" value of the acceleration parameter $r = r^*$ is given by

$$\begin{aligned} r^* &= \sqrt{\beta_1\left(\frac{\pi}{2}\right)\beta_2\left(\frac{\pi}{2}\right)} = \sqrt{r_1r_3\sin\phi_1\sin\phi_3} = \sqrt{\gamma_1\gamma_3} \\ &= \sqrt{r_2r_4\sin\phi_2\sin\phi_4} = \sqrt{\gamma_2\gamma_4}. \end{aligned} \tag{5.14}$$

5.3. *Special cases of indefinite matrix coefficient*

As a first special case let us consider the one where in (5.9) we have for the γ_i's that

$$\gamma_1 = \gamma_2 = \gamma_3 = \gamma_4 > 0. \tag{5.15}$$

So, the rectangle $\mathscr{R}$ reduces to a straight-line segment parallel to the real axis and intersecting the "positive" imaginary axis. Applying the theory of the previous paragraph we find that

$$b_2\left(\frac{\pi}{2}\right) = b_1\left(\frac{\pi}{2}\right), \quad r^* = \gamma_1$$

implying, from (5.13), (5.8) and (5.6), that $\rho(T_{r^*}) = 0$!

As a second special case we consider the one where again the rectangle $\mathscr{R}$ is restricted to a straight-line segment lying on the "positive" imaginary axis. Then, relations (5.9) become

$$\beta_1 = \beta_2 = \beta_3 = \beta_4 = 0, \quad 0 < \gamma_1 = \gamma_2 < \gamma_3 = \gamma_4. \tag{5.16}$$

In view of (5.16), from (5.10) we have that

$$r_1 = r_2 = \gamma_1, \quad r_3 = r_4 = \gamma_3, \quad \phi_1 = \phi_2 = \phi_3 = \phi_4 = \frac{\pi}{2}.$$

So, relations (5.13) give that

$$\frac{R}{c} = \frac{b_2(\theta) - b_1(\theta)}{b_2(\theta) + b_1(\theta)} = \frac{r_3 \cos\left(\frac{\pi}{2} - \theta\right) - r_1 \cos\left(\frac{\pi}{2} - \theta\right)}{r_3 \cos\left(\frac{\pi}{2} - \theta\right) + r_1 \cos\left(\frac{\pi}{2} - \theta\right)} = \frac{\gamma_3 - \gamma_1}{\gamma_3 + \gamma_1} \quad \forall \theta \in (0, \pi), \tag{5.17}$$

that is the ratio $\frac{R}{c}$ is independent of $\theta \in (0, \pi)$! Therefore

$$r^* = \sqrt{\gamma_1 \gamma_3} = \sqrt{\gamma_2 \gamma_4} \quad \forall \theta \in (0, \pi).$$

6. Concluding remarks

We close our work with a number of points:

(i) In case $\mathscr{H}$ is not a convex polygon but an ellipse $\mathscr{E}$, provided $O \notin \mathscr{E}$, a case studied explicitly in [12] for classical extrapolation, the *optimal cc* determined there is the same as the one in our case. It is understood, however, that the values of the *optimal parameters* ω^* and ρ^* are found by the formulas in (2.9).

(ii) *Optimal cc*'s and then corresponding *optimal* ω's and ρ's can be found for a convex region $(O \notin)\mathscr{S}$ capturing $\sigma(A)$, when $\mathscr{S}$ is a section, a sector or a zone of a circle or of an ellipse, by combining the idea in (i) with ours in [8] and in the present work.

(iii) In case $\mathscr{H}$ (or $\mathscr{E}$ or $\mathscr{S}$) is symmetric *wrt* the positive (negative) real semiaxis (as, e.g., when $A \in \mathbb{R}^{n,n}$ is *positive (negative) stable*) then, it is obvious that the *one-, two- or three-point optimal cc*, $\mathscr{C}^*$, will have center c on the positive (negative) real semiaxis. By (2.7), it is implied that ω^* will be positive (negative) real and a simplified Algorithm, in fact that in [10,11,6,7] and especially the one in [8], to determine the *optimal cc* of $\mathscr{H}$, etc. can be used.

(iv) In case an *optimal real extrapolation parameter* ω is desired, this is possible *iff* $\mathscr{H}$ (or $\mathscr{E}$ or $\mathscr{S}$) lies strictly to the right (left) of the imaginary axis. Then, we consider as the *convex hull* to work with, the *convex hull* of the union of $\mathscr{H} \cup \mathscr{H}'$ (or $\mathscr{E} \cup \mathscr{E}'$ or $\mathscr{S} \cup \mathscr{S}'$), where $\mathscr{H}'$, etc. is the symmetric of $\mathscr{H}$, etc. *wrt* the real axis, and we go on as in (iii) above.

Appendix A. Two-Point Optimal *cc* of $\mathscr{H}$ and Maximal v.a.

The first part of Step 4 of the Algorithm of Section 3 constitutes a major improvement over the corresponding part of the Algorithm presented in [6] (or [7]). To prove our claim in the associated footnote, a statement given as a theorem in [6] is needed. Specifically:

Lemma A.1. *Under the notation and assumptions in the beginning and in Step* 1 *of the Algorithm of Section 3, suppose that* $\mathscr{H}$ *is the straight-line segment* P_1P_2. *Let the optimal cc of* $\mathscr{H}$ *have center* $K^*_{1,2}$. $K^*_{1,2}$ *is defined as the unique point of contact of two Apollonius circles. The points of these circles have distances from* P_1 *and* O *and from* P_2 *and* O *with ratio equal to the minimal ratio of the distances of the points of the perpendicular bisector to* P_1P_2 *from the aforementioned pairs of points.*

Proof. For the proof see the Theorem in [6]. □

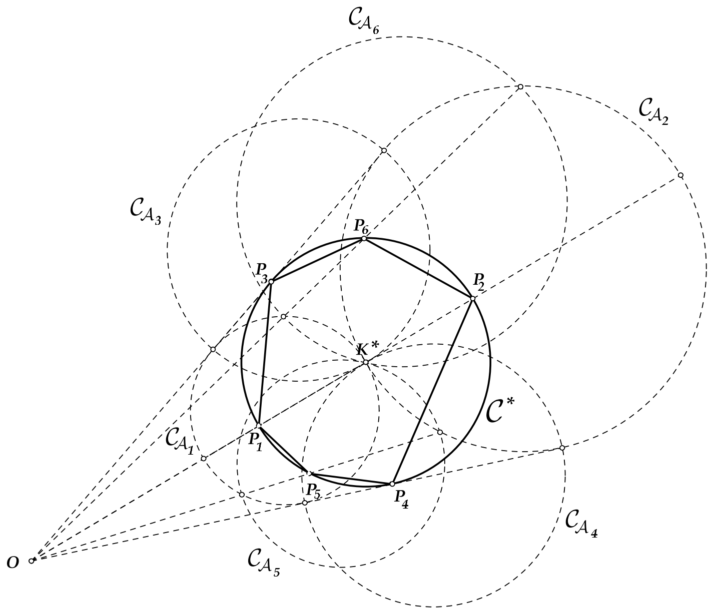

Fig. 4. Three characteristic pairs of *Apollonius circles* $\mathscr{C}_{\mathscr{A}_i}$, $i = 1, \ldots, 6$, are illustrated that share a common *two-point optimal cc* $\mathscr{C}^*$ of $\mathscr{H}$.

Theorem A.1. *Under the main assumptions of Lemma A.1, let $\mathscr{H}$ have vertices P_i, $i = 1, \ldots, l$, $l \geqslant 3$. Then, if the optimal cc of $\mathscr{H}$ is determined by an optimal two-point cc it will be the unique one that corresponds to the maximum ratio $\frac{R_{i,j}}{|c_{i,j}|}$, $i = 1, \ldots, l-1$, $j = i+1, \ldots, l$, or, equivalently, to the $\mathscr{C}_{i,j}$ corresponding to the maximum v.a.*

Proof. Consider all l *Apollonius circles* whose diameters have endpoints that divide internally and externally the straight-line segments OP_i, $i = 1, \ldots, l$, into two parts whose ratio of distances from P_i and O is $\lambda < 1$. As is known, from the Apollonius Theorem 4.1, every point on each of these l circles has distances from P_i and O that share the common ratio λ. Assume that λ varies increasing continuously in $[0, 1)$. For $\lambda = 0$, all l *Apollonius circles* are nothing but the points P_i. Increasing λ from the value 0, the two *Apollonius circles* of each pair, out of the $\binom{l}{2}$ ones, first will come into contact with each other for some value of λ, in general different for each pair, and then will intersect each other. Let $\bar{i}$ and $\bar{j}$ be the indices, $\bar{i} \in I$, $\bar{j} \in I \backslash \{\bar{i}\}$, of the vertices of $\mathscr{H}$ that define the pair of the *Apollonius circles* whose point of contact $K^*_{\bar{i},\bar{j}}(c^*_{\bar{i},\bar{j}})$ corresponds to the maximum value of $\lambda = \lambda^*$. We claim that the circle with center $K^*_{\bar{i},\bar{j}}$ and radius $R^*_{\bar{i},\bar{j}} = (K^*_{\bar{i},\bar{j}}P_{\bar{i}}) = (K^*_{\bar{i},\bar{j}}P_{\bar{j}})$, satisfying

$$\lambda^* = \frac{R^*_{\bar{i},\bar{j}}}{|c^*_{\bar{i},\bar{j}}|} \geqslant \frac{R_{i,j}}{|c_{i,j}|} \quad \forall i, j \in I \backslash \{\bar{i}, \bar{j}\}, \tag{A.1}$$

is the *optimal cc* of $\mathscr{H}$. Suppose there exists at least one of the *Apollonius circles* with $\lambda = \lambda^*$ corresponding to an index $i \in I \backslash \{\bar{i}, \bar{j}\}$ that leaves $K^*_{\bar{i},\bar{j}}$ strictly outside it. The fact that all the *two-point optimal cc*'s have been exhausted and **no** *two-point optimal cc* of $\mathscr{H}$ has been found contradicts our main assumption that the *optimal cc* of $\mathscr{H}$ is a *two-point optimal* one. That the *two-point optimal cc* $\mathscr{C}^*_{\bar{i},\bar{j}}$ corresponds to the largest *v.a.* comes from (2.10). $\square$

Remark A.1. It is possible to have more than one pair of *Apollonius circles* that share the point of contact $K^*_{\bar{i},\bar{j}}$ of Theorem A.1. In fact there can be as many as $\left[\frac{l}{2}\right]$ pairs, where the symbol $[\cdot]$ denotes integral part. However, all of these possible pairs will share the unique *two-point optimal cc* of $\mathscr{H}$.

Referring to Remark A.1, in Fig. 4 three such pairs of *Apollonius circles* are shown corresponding to the pairs of points (P_1, P_2), (P_3, P_4) and (P_5, P_6). If the vertices of $\mathscr{H}$ are $l > 6$, the points P_i, $i = 7, \ldots, l$, are supposed to be captured by the common *two-point optimal cc* $\mathscr{C}^* \equiv \mathscr{C}^*_{1,2} \equiv \mathscr{C}^*_{3,4} \equiv \mathscr{C}^*_{5,6}$, whose center is $K^* \equiv K^*_{1,2} \equiv K^*_{3,4} \equiv K^*_{5,6}$ and radius $R^* = (K^*P_1) = (K^*P_2) = (K^*P_3) = (K^*P_4) = (K^*P_5) = (K^*P_6)$, and **not** any two of them $P_i, P_j,\ i \neq j = 7, \ldots, l$, define a *two-point optimal cc* of $\mathscr{H}$.

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