On Extrapolation of Complex Cayley Transform

Michael G. Tzoumas

University of Ioannina

Joint work with A. Hadjidimos

Contens

The structure of talk is the following

The Complex Cayley Transform

The *Cayley Transform* and the *Extrapolated Cayley Tranform* are of significant theoretical interest and have many applications.
The (Extrapolated) Cayley Transform appears in:

- The Linear Complementarity Problem (LCP) with Applications to Linear and Convex Quadratic Programming, Game Theory, Fluid Mechanics, Economics, etc.
- The determination of the optimal *acceleration parameter* in
    - Alternating Direction Implicit (ADI) Iterative Method [Peaceman/Rachford Jr. SINUM (1955)]
    - Solution of complex linear systems by
        - The HS Splitting [Z.-Z. Bai/Golub/M.K. Ng SIMAX (2003)]
        - The NS Splitting [Z.-Z. Bai/Golub/M.K. Ng NLAA (2006)]

Definitions

Their definitions (A.H./M.T. LAA 2008) are as follows:

Definition 1

Given

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

the Cayley Transform $\mathcal{F}(A)$ *is defined to be*

$$F := \mathcal{F}(A) = (I + A)^{-1}(I - A). \tag{2}$$

Definition 2

Under the assumptions of Definition **??**, *we call Extrapolated Cayley Transform, with extrapolation parameter* ω, *the matrix function where* A *is replaced by* ωA

$$F_\omega := \mathcal{F}(\omega A) = (I + \omega A)^{-1}(I - \omega A), \ -1 \notin \sigma(\omega A). \tag{3}$$

The Definitions

In many cases, F_ω is the iteration matrix of an iterative method. Therefore, $\rho(F_\omega)$ constitutes a measure of its convergence. Hence, it must be $\max_{a\in\sigma(A)\subset\mathcal{H}} \left|\frac{1-\omega a}{1+\omega a}\right| < 1$ and this holds *iff* $\mathrm{Re}\,(\omega a) > 0$.

Definition 3

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

We also make the following main assumptions:

$$i)\ 0 \notin \mathcal{H} \quad ii)\ \mathrm{Re}\,(\omega a) > 0,\ \forall\, a \in \sigma(A) \subset \mathcal{H}. \tag{4}$$

The Problem

Our main objective is to solve the following problem.

Problem 1

Based on the hypotheses of Definitions **??**, **??**, **??** *and Main Assumptions, determine the Extrapolation Parameter* ω *that minimizes the spectral radius of the Extrapolated Cayley Transform, i.e.*

$$\min_{\omega\in\mathbb{C}\setminus\{0\},\,-1\notin\sigma(\omega A)} \rho(F_\omega) = \min_{\omega\in\mathbb{C}\setminus\{0\},\,-1\notin\sigma(\omega A)} \max_{a\in\sigma(A)\subset\mathcal{H}} \left|\frac{1-\omega a}{1+\omega a}\right|. \quad (5)$$

Or equivalently, we have to solve the minmax problem

$$\min_{\omega\in\mathbb{C}} \max_{a\in\mathcal{H}} \left|\frac{1-\omega a}{1+\omega a}\right| \ (<1)\,. \quad (6)$$

The Solution

The previous function

$$w \ := \ w(a) \ = \ \frac{1-\omega a}{1+\omega a}, \quad a \in \mathcal{H}, \ \omega \in \mathbb{C}, \ \mathrm{Re}\,(\omega a) > 0, \tag{7}$$

is a Möbius transformation. It has no *poles* and is not a constant as is readily shown. Hence, it possesses an inverse Möbius transformation

$$w^{-1}(w(a)) \ = a \ = \ \frac{1-w}{\omega(1+w)}, \quad w = w(a), \ a \in \mathcal{H}, \ \omega \in \mathbb{C}, \ \mathrm{Re}\,(\omega a) > 0, \tag{8}$$

which has no poles and is not the constant function.
In general, a Möbius transformation maps a disk onto a disk and its circle onto the circle of its image.

The Solution

To see how their elements are mapped via the previous transform, let an $\omega \in \mathbb{C}$ and $\mathcal{C}_\omega$ be the circle with center $O(0)$ and radius

$$\rho \;:=\; \rho(\mathcal{C}_\omega) = \max_{a \in \mathcal{H}} |w(a)| \; (< 1). \tag{9}$$

In view of (**??**), $\mathcal{C}_\omega$ will capture[1] $w(\mathcal{H})$ and will pass through a boundary point of it. Therefore, $\mathcal{C}_\omega$ must be the image of a circle $\mathcal{C}$. To find out how $\mathcal{C}$ is derived from $\mathcal{C}_\omega$ and vice versa, we begin with

$$\mathcal{C}_\omega \;:= |w| = \rho \Leftrightarrow \cdots \Leftrightarrow |a - c| = R =: \mathcal{C}, \tag{10}$$

which is the equation of a circle, with center c and radius R given by

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

The Solution

$$c := \frac{1+\rho^2}{\omega(1-\rho^2)}, \quad R := \frac{2\rho}{|\omega|(1-\rho^2)}. \tag{11}$$

So, we can see that the circle $\mathcal{C}$ possesses the properties:

- leaves $O(0)$ strictly outside since $R < |c|$.
- captures $\mathcal{H}$ ($\mathcal{H} \subset \mathcal{C}$) since $\mathcal{C}_\omega$ captures $w(\mathcal{H})$ ($w(\mathcal{H}) \subset \mathcal{C}_\omega \equiv w(\mathcal{C})$), and
- passes through at least one vertex of $\mathcal{H}$, because by (**??**) $\mathcal{C}_\omega$ captures $w(\mathcal{H})$ and passes through a boundary point of it

Hence, equivalently, $\mathcal{C}$ captures $\mathcal{H}$ and passes through a boundary point of it, that is a vertex.

Definition and Theorems

Definition 4

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

Theorem: 1

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

Really, the circle with center any $K \in Oz$, where Oz is any ray within a specific angle, such that $(OK) > \max_{i\in I}(OK_i)$ and radius $R = \max_{i\in I}(KP_i)$ is a *cc* of $\mathcal{H}$.
In the following figure we can see one of these ones.

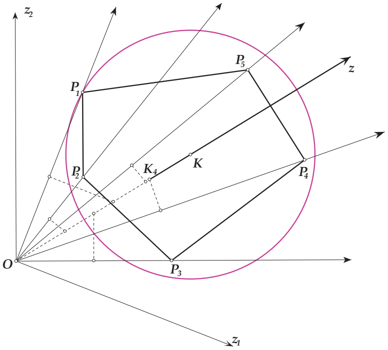


Figure: One of the infinitely many *capturing circles*

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

Theorem: 2

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

$$\omega = \frac{|c|}{c\sqrt{|c|^2 - R^2}}, \quad \rho = \frac{R}{|c| + \sqrt{|c|^2 - R^2}}. \tag{12}$$

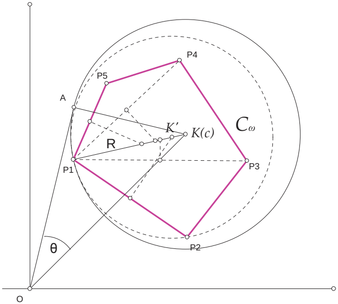
Theorem: 3

Under the assumptions of Theorem **??**, *the solution to our Problem is equivalent to the determination of the optimal cc* $\mathcal{C}^*$ *of* $\mathcal{H}$ *so that* $\frac{R}{|c|}$ *is a minimum.*

Theorem: 4

The optimal cc passes through at least two vertices of $\mathcal{H}$.

Indeed, if a circle passes through P_1 and captures all vertices of $\mathcal{H}$, then there exists a circle inside the previous one that passes through P_1 and from at least one (here from P_2) of the other vertices of H and has a smaller $\frac{R}{|c|}$.



So, one cc can be determined from two or three points (vertices of $\mathcal{H}$).

The *extrapolation problem* in a simpler case, ($\min_{\omega\in\mathbb{C}} \max_{a\in\mathcal{H}} |1-\omega a|$), was solved, in

- the Real Case
  by Hughes-Hallett Proceedings (1981), JCAM (1982) and
  A. Hadjidimos IJCM (1983)
- the Complex Case in
  - A.Hadjidimos, LAA (1984) ($\mathcal{H}$ was *line-segment or polygon*) and the solution was based on Apollonius Circles
  - Opfer/Schober LAA (1984) ($\mathcal{H}$ was *line-segment or ellipse*), and the solution was based on Lagrange Multipliers.

In our work only the Algorithm of the former case works, where one of its steps has been significantly improved.

We recall the classical Theorem of the *Apollonius circle*.

Theorem: 5

(Apollonius Theorem) 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

$$\frac{(CA)}{(CB)} = \frac{(DA)}{(DB)} = \lambda. \tag{13}$$

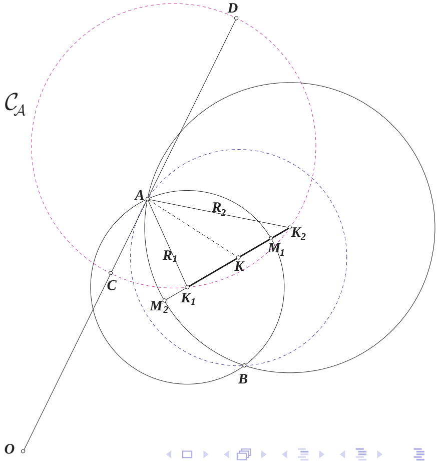
So,

Theorem: 6

Under the assumptions of Theorem **??** *the optimal cc of* $\mathcal{H}$ *is unique.*

Indeed, if we assume that there are two optimal *cc*, then we find a new circle, that captures the region AM_1BM_2 (which includes the polygon), and

$$\frac{KA}{KO} < \frac{K_1A}{K_1O} = \frac{K_2A}{K_2O}$$



If $l = 2$, we can prove that the point $K^*_{1,2}$ 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, is the center of *cc* of P_1 and P_2 and this 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.
The elements of $\mathcal{C}^*_{1,2}$ are given by

$$c^*_{1,2} = \frac{(|z_1| + |z_2|)z_1z_2}{|z_1|z_2 + z_1|z_2|}, \quad R^*_{1,2} = \frac{|z_1||z_2||z_2 - z_1|}{|z_1|z_2| + |z_1|z_2|}. \qquad (14)$$

The optimal *cc* $\mathcal{C}^*_{1,2}$ in this case will be called a *two-point optimal cc*.

Back

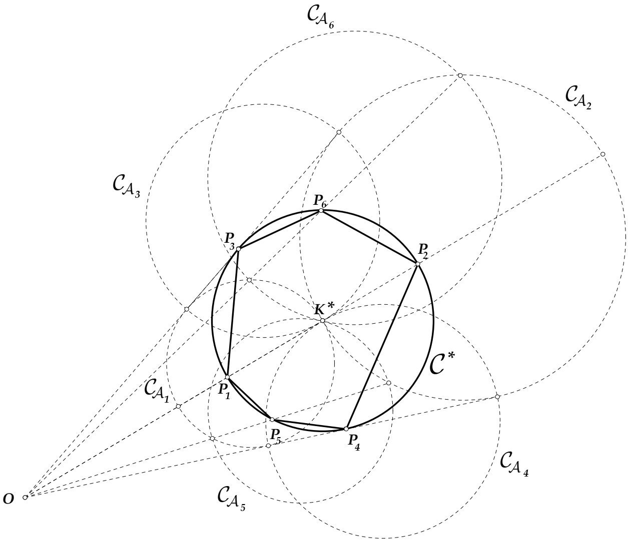
Theorem: 7

Let $\mathcal{H}$ have vertices P_i, $i = 1(1)l$, $l \geq 3$. Then, if the optimal cc of $\mathcal{H}$ is determined by an optimal two-point cc it will be the unique one that corresponds to the maximum ratio $\frac{R_{i,j}}{|c_{i,j}|}$, $i = 1(1)l - 1$, $j = i + 1(1)l$.

Remark 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 **??**.

We can see this in following figure.


$\mathcal{C}_{\mathcal{A}_6}$
$\mathcal{C}_{\mathcal{A}_2}$
$\mathcal{C}_{\mathcal{A}_3}$
P_6
P_3
P_2
K^*
$\mathcal{C}^*$
$\mathcal{C}_{\mathcal{A}_1}$
P_1
P_5
P_4
$\mathcal{C}_{\mathcal{A}_4}$
O
$\mathcal{C}_{\mathcal{A}_5}$

If $l = 3$ and does not exist a two-point *cc*, then the *cc* is a three-point *cc*. This is circumscribed to the triangles $P_1P_2P_3$, the elements of $\mathcal{C}^*_{1,2,3}$ ($K_{1,2,3}(c_{1,2,3})$ and $R_{1,2,3}$), are given by using the formulas

$$c_{1,2,3} = \frac{|z_1|^2(z_2 - z_3) + |z_2|^2(z_3 - z_1) + |z_3|^2(z_1 - z_2)}{\overline{z_1}(z_3 - z_l) + \overline{z_2}(z_3 - z_1) + \overline{z_3}(z_i - z_2)}, \tag{15}$$

$$R_{i,2,3} = \left| \frac{(z_1 - z_2)(z_2 - z_3)(z_3 - z_1)}{\overline{z_1}(z_2 - z_3) + \overline{z_2}(z_3 - z_1) + \overline{z_3}(z_1 - z_2)} \right|.$$

The Algorithm

Step 1. Let $P_i(z_i),\ i = 1(1)l$, be the l vertices of $\mathcal{H}$ and let $I := \{1, 2, \ldots, l\}$.
Step 2. If $l = 1$, the elements of $\mathcal{C}_1^*$ are given by $c_1^* = z_1,\ \ R_1^* = 0$.
Step 3. If $l = 2$, the elements of $\mathcal{C}_{1,2}^*$ are given by (**??**)
Step 4. If $l \geq 3$, find the elements of the $\binom{l}{2}$ *two-point optimal cc*'s $\mathcal{C}_{i,j}$, $i = 1(1)l - 1,\ j = i + 1(1)l$, and from these the maximum ratio $\frac{R_{i,j}}{|c_{i,j}|}$. If the *optimal cc* that corresponds to the maximum ratio captures $\mathcal{H}$, that is

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

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

$$c_{i,j,k} = \frac{|z_i|^2(z_j - z_k) + |z_j|^2(z_k - z_i) + |z_k|^2(z_i - z_j)}{\overline{z_i}(z_k - z_l) + \overline{z_j}(z_k - z_i) + \overline{z_k}(z_i - z_j)}, \tag{16}$$

$$R_{i,j,k} = \left|\frac{(z_i - z_j)(z_j - z_k)(z_k - z_i)}{\overline{z_i}(z_j - z_k) + \overline{z_j}(z_k - z_i) + \overline{z_k}(z_i - z_j)}\right|. \tag{17}$$

Discard all circles that may capture the origin, i.e.

$$|c_{i,j,k}| \ \leq \ R_{i,j,k},$$

and, from the remaining ones all those that do not capture all the other vertices, i.e.

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

From the rest, the one that corresponds to the smallest ratio $\frac{R_{i,j,k}}{(OK_{i,j,k})}$, is the *three-point optimal cc* $\mathcal{C}^*_{\bar{i},\bar{j},\bar{k}}$ of $\mathcal{H}$.
Step 5. End of Algorithm.

Application: Linear System with Indefinite Coefficient Matrix

In 2003 Bai, Golub and Ng introduced an *Alternating Direction Implicit (ADI)*-type method using *Hermitian/Skew-Hermitian Splittings* for the solution of complex linear algebraic systems with matrix coefficient positive definite.
Consider the splitting

$$A = B + C, \tag{18}$$

where

$$B = \frac{1}{2}\left(A + A^H\right), \quad C = \frac{1}{2}\left(A - A^H\right)$$

B is *Hermitian* and C is *Skew-Hermitian*.

Back

For the solution of

$$Ax = b$$

the following *ADI*-type method is adopted

$$\begin{aligned} (rI + B)x^{(m+\frac{1}{2})} &= (rI - C)x^{(m)} + b, \\ (rI + C)x^{(m+1)} &= (rI - B)x^{(m+\frac{1}{2})} + b, \quad m = 0, 1, 2, \dots, \end{aligned} \tag{19}$$

where r is a positive *acceleration* parameter.
From equations (**??**) we obtain the iterative scheme

$$x^{(m+1)} = T_r x^{(m)} + c_r, \quad m = 0, 1, 2, \dots, \tag{20}$$

where

$$T_r = (rI+C)^{-1}(rI-B)(rI+B)^{-1}(rI-C), \quad c_r = 2r(rI+C)^{-1}(rI+B)^{-1}b. \tag{21}$$

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

$$\rho(T_r) = \rho(\widetilde{T}_r) \leq ||\widetilde{T}_r||_2 \leq ||(rI - B)(rI + B)^{-1}||_2 ||(rI - C)(rI + C)^{-1}||_2. \tag{22}$$

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

$$\begin{aligned} ||(rI - C)(rI + C)^{-1}||_2 &= \rho^{\frac{1}{2}} \left((rI + C)^{-H}(rI - C)^H(rI - C)(rI + C)^{-1} \right) = \\ &\rho^{\frac{1}{2}} \left((rI - C)^{-1}(rI + C)(rI - C)(rI + C)^{-1} \right) = \\ &\rho^{\frac{1}{2}} \left((rI - C)^{-1}(rI - C)(rI + C)(rI + C)^{-1} \right) = \rho^{\frac{1}{2}}(I) = 1. \end{aligned} \tag{23}$$

Consequently, we have to minimize the bound $||(rI-B)(rI+B)^{-1}||_2$ of the spectral radius $\rho(T_r)$ (or $\rho(\widetilde{T}_r)$). So

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

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 is attained at $r=r^*=\sqrt{b_1 b_2}$ (See R.S. Varga, Matrix Iterative Analysis, 2nd Edition, Springer, Berlin, 2000.) This can be also obtained by a simplified version of our Algorithm.

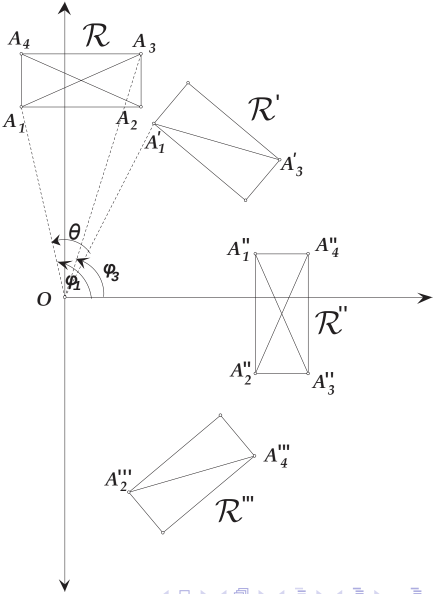
Suppose that $\sigma(A) \subset \mathcal{R}$, where $\mathcal{R}$ is a rectangle, and with its coordinates satisfying

$$\beta_1 \leq 0 \leq \beta_2,\ |\beta_1| + |\beta_2| > 0,$$

$$\beta_3 = \beta_2,\ \beta_4 = \beta_1$$

and $0 < \gamma_1 < \gamma_4,\ \gamma_1 = \gamma_2,\ \gamma_3 = \gamma_4.$

Back



To apply the *ADI*-type method to the original system we multiply both members of the system by $e^{-\imath\theta}$, $\theta > 0$,

$$e^{-\imath\theta} Ax = e^{-\imath\theta} b,$$

so that the new coefficient matrix $e^{-\imath\theta} A$ becomes *positive definite.* The angle θ takes values so that the projection of $e^{-\imath\theta}\mathcal{R}$ onto the real axis is on the *positive* real semiaxis.

The *polar radii* r_i and the *polar angles* ϕ_i, $i = 1(1)4$, of the corresponding vertices of $\mathcal{R}$ will be

$$r_i \;=\; \sqrt{\beta_i^2 + \gamma_i^2}, \quad \phi_i \;=\; \arccos\left(\frac{\beta_i}{r_i}\right), \qquad i = 1(1)4. \tag{24}$$

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

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

We follow our Algorithm, with $\mathcal{H}$ 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

$$c = \frac{1}{2}(b_1(\theta) + b_2(\theta)) \quad \text{and} \quad R = \frac{1}{2}(b_2(\theta) - b_1(\theta)),$$

which are functions of $\theta \in \left(\phi_1 - \frac{\pi}{2}, \phi_2 + \frac{\pi}{2}\right)$.
Consequently, to find the *best optimal cc* we have to minimize $\frac{R}{c}$ given by

$$\frac{R}{c} = \frac{b_2(\theta) - b_1(\theta)}{b_2(\theta) + b_1(\theta)} = \begin{cases} \frac{r_3 \cos(\phi_3 - \theta) - r_1 \cos(\phi_1 - \theta)}{r_3 \cos(\phi_3 - \theta) + r_1 \cos(\phi_1 - \theta)} & \text{for} \quad \theta \in \left(\phi_1 - \frac{\pi}{2}, \frac{\pi}{2}\right], \\ \frac{r_4 \cos(\phi_4 - \theta) - r_2 \cos(\phi_2 - \theta)}{r_4 \cos(\phi_4 - \theta) + r_2 \cos(\phi_2 - \theta)} & \text{for} \quad \theta \in \left[\frac{\pi}{2}, \phi_2 + \frac{\pi}{2}\right). \end{cases} \tag{26}$$

It can be obtained that the minimum is attained 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 (**??**) are now Skew-Hermitian and Hermitian, respectively.
So, the acceleration parameter $r = r^*$ is given by

$$r^* = \sqrt{\beta_1\left(\frac{\pi}{2}\right)\beta_2\left(\frac{\pi}{2}\right)} = \sqrt{r_1 r_3 \sin\phi_1 \sin\phi_3} = \sqrt{\gamma_1\gamma_3} = \sqrt{\gamma_2\gamma_4}. \quad (27)$$

As a special case let us consider the one, where the rectangle $\mathcal{R}$ 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 (**??**), (**??**) and (**??**), that

$$\rho(T_{r^*}) = 0 \ !$$