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Optimal semi-iterative methods for complex SOR with results from potential theory

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Abstract We consider the application of semi-iterative methods (SIM) to the standard (SOR) method with complex relaxation parameter ω, under the following two assumptions: (1) the associated Jacobi matrix J is consistently ordered and weakly cyclic of index 2, and (2) the spectrum $\sigma(J)$ of J belongs to a compact subset Σ of the complex plane $\mathbb{C}$, which is symmetric with respect to the origin. By using results from potential theory, we determine the region of optimal choice of $\omega \in \mathbb{C}$ for the combination SIM–SOR and settle, for a large class of compact sets Σ, the classical problem of characterising completely all the cases for which the use of the SIM-SOR is advantageous over the sole use of SOR, under the hypothesis that $\sigma(J) \subset \Sigma$. In particular, our results show that, unless the outer boundary of Σ is an ellipse, SIM–SOR is always better and, furthermore, one of the best possible choices is an asymptotically optimal SIM applied to the Gauss–Seidel method. In addition, we derive the optimal complex SOR parameters for all ellipses which are symmetric with respect to the origin. Our work was motivated by recent results of M. Eiermann and R.S. Varga.

Dedicated to Professor Richard S. Varga in recognition of his substantial contributions to the subject of the paper.

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1 Introduction

For the solution of a non-singular linear system of algebraic equations

$$A\mathbf{x} = \mathbf{b}, \tag{1}$$

where $A \in \mathbb{C}^{n,n}$, $\mathbf{b} \in \mathbb{C}^n$, a splitting $A = M - N$ of A ($\det(M) \neq 0$) leads to the equivalent fixed point matrix equation

$$\mathbf{x} = T\mathbf{x} + \mathbf{c}, \quad T := M^{-1}N, \quad \mathbf{c} := M^{-1}\mathbf{b}. \tag{2}$$

The non-singularity of A and M guarantees that $1 \notin \sigma(T)$, where $\sigma(T)$ denotes the spectrum of the matrix T.

Equation (2) yields the following iterative scheme for the solution of (1)

$$\mathbf{x}_{m+1} = T\mathbf{x}_m + \mathbf{c}, \quad m = 0, 1, 2, \ldots, \ \ \mathbf{x}_0 \in \mathbb{C}^n. \tag{3}$$

It is well known that the sequence of vectors generated by (3) converges *for any* $\mathbf{x}_0$ to the unique solution of (1), if and only if $\rho(T) < 1$, where $\rho(T)$ denotes the spectral radius of the matrix T.

Let $\mathcal{P}$ be an infinite lower triangular matrix with elements from $\mathbb{C}$ and unit row sums, i.e. let

$$\mathcal{P} = \begin{bmatrix} \pi_{0,0} & & & \\ \pi_{1,0} & \pi_{1,1} & & \\ \pi_{2,0} & \pi_{2,1} & \pi_{2,2} & \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \tag{4}$$

where $\pi_{m,j} \in \mathbb{C}$, $m = 0, 1, 2, \ldots$, and $j = 0, 1, \ldots, m$, and

$$\sum_{j=0}^{m} \pi_{m,j} = 1, \quad m = 0, 1, 2, \ldots \tag{5}$$

Based on the iterative method (3), $\mathcal{P}$ induces a *semi-iterative method* (SIM), also called *polynomial acceleration method* (see, e.g. [24, ch. 5]), defined by a new sequence of vectors $\{\mathbf{y}_m\}_{m=0}^{\infty}$ of $\mathbb{C}^n$, in the following way. Starting with the infinite vector $[\mathbf{x}_0{}^{\mathrm{T}}\ \mathbf{x}_1{}^{\mathrm{T}}\ \mathbf{x}_2{}^{\mathrm{T}}\ \ldots]^{\mathrm{T}}$, the matrix $\mathcal{P}$ produces the infinite vector $[\mathbf{y}_0{}^{\mathrm{T}}\ \mathbf{y}_1{}^{\mathrm{T}}\ \mathbf{y}_2{}^{\mathrm{T}}\ \ldots]^{\mathrm{T}}$, via the relationship

$$\begin{bmatrix} \mathbf{y}_0 \\ \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \end{bmatrix} = (\mathcal{P} \otimes I) \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \end{bmatrix}, \tag{6}$$

where $\otimes$ stands for tensor product (see, e.g. [10, Sect. 52]) and I denotes the unit matrix of order n. That is, the semi-iterative method induced by $\mathcal{P}$ is given by

$$\mathbf{y}_m = \sum_{j=0}^{m} \pi_{m,j}\mathbf{x}_j, \quad m = 0, 1, 2, \ldots, \tag{7}$$

or, schematically,

$$\begin{aligned} \mathbf{x}_0 &\longrightarrow \mathbf{y}_0 = \pi_{0,0}\mathbf{x}_0, \\ \mathbf{x}_1 &\longrightarrow \mathbf{y}_1 = \pi_{1,0}\mathbf{x}_0 + \pi_{1,1}\mathbf{x}_1, \\ \mathbf{x}_2 &\longrightarrow \mathbf{y}_2 = \pi_{2,0}\mathbf{x}_0 + \pi_{2,1}\mathbf{x}_1 + \pi_{2,2}\mathbf{x}_2, \\ &\vdots \end{aligned} \tag{8}$$

We note that the consistency relations (5) ensure that if the initial vector $\mathbf{x}_0$, of the basic iteration (3), coincides with the unique solution $\mathbf{x}$ of (1), then $\mathbf{y}_m = \mathbf{x}$, for all $m \geq 0$.

The purpose of this paper is to study the asymptotic properties of SIM in cases when the basic iteration (3) is the standard successive over-relaxation (SOR) method with *complex relaxation parameter* ω, under certain conditions on the associated Jacobi matrix. More precisely, we consider

$$\mathbf{x}_{m+1} = \mathcal{L}_\omega \mathbf{x}_m + \mathbf{c}_\omega, \quad m = 0, 1, 2, \ldots, \tag{9}$$

where

$$\mathcal{L}_\omega := (D - \omega L)^{-1}[(1-\omega)D + \omega U], \quad \mathbf{c}_\omega := \omega(D - \omega L)^{-1}\mathbf{b}, \tag{10}$$

and $\omega \in \mathbb{C} \setminus \{0\}$. We recall that the matrices D, L and U are defined by the splitting

$$A = D - L - U, \tag{11}$$

so that D is a block diagonal matrix, thereafter assumed to be non-singular, and L, U are strictly lower and strictly upper triangular matrices, respectively. Regarding conditions on the corresponding block Jacobi matrix

$$J := D^{-1}(L + U),$$

we assume that J is *consistently ordered and weakly cyclic of index 2*; see, e.g. [24, Sect. 4.1]. This assumption implies the following results for the eigenvalues of J and $\mathcal{L}_\omega$ (see [29, Theorem 5.2.2] or [24, Theorem 4.4.5]):

1. The non-zero eigenvalues of J appear in opposite pairs of the same multiplicity.
2. *Young's fundamental relationship* holds between the eigenvalues λ of $\mathcal{L}_\omega$ and the eigenvalues μ of J:

$$(\lambda + \omega - 1)^2 = \omega^2\mu^2\lambda. \tag{12}$$

These two results should be coupled with the obvious implication $1 \notin \sigma(J)$ of the non-singularity of the matrices A and D. The above lead then naturally to the assumption that all the eigenvalues of the Jacobi matrix J are contained in an *inclusion* set Σ_μ, which is compact and symmetric with respect to the origin and such that $1 \notin \Sigma_\mu$. Our results, however, are derived under some extra conditions on Σ_μ. More precisely, in section 3, we require in addition that Σ_μ belongs to the class of sets $\mathbb{S}$, where

$\mathbb{S} := \{\Sigma \subset \mathbb{C} : \Sigma$ is compact containing more than one point, $1 \notin \Sigma$, and the line segment $[-a, a]$ lies on Σ, for any $a \in \Sigma\}$.

It will become apparent, though, from our work in the same section, that our analysis applies also to a wider class of sets than $\mathbb{S}$. In particular, it applies to the class

$\mathbb{S}' := \{\Sigma \subset \mathbb{C} : \Sigma$ is compact containing more than one point, it is symmetric with respect to the origin, it has connected outer boundary $\partial_\infty \Sigma$ and its polynomial convex hull $P_c(\Sigma)$ does not contain $1\}$.

Let Ω denote the unbounded component of the set $\overline{\mathbb{C}} \setminus \Sigma$. Then, by the *outer boundary* $\partial_\infty \Sigma$ of Σ we mean the boundary of Ω. Also, by the *polynomial convex hull* $P_c(\Sigma)$ of Σ we mean the compact set resulting from Σ by "filling up" its holes, i.e. $P_c(\Sigma) := \overline{\mathbb{C}} \setminus \Omega$. For the sake of simplicity, however, we work mainly under the assumption that

$$\sigma(J) \subset \Sigma_\mu, \quad \text{where} \quad \Sigma_\mu \in \mathbb{S}. \tag{13}$$

Our main objectives are as follows:

1. To investigate the classical question (see, e.g. [23] and [29, p 376]) whether the use of the combination SIM–SOR is advantageous over the sole use of SOR, in the sense of the asymptotic convergence rates of the associated sequences $\{\mathbf{y}_m\}_{m=0}^{\infty}$ and $\{\mathbf{x}_m\}_{m=0}^{\infty}$.
2. If so, to find the values of $\omega \in \mathbb{C}$ for which this advantage occurs and, furthermore, to indicate how a corresponding asymptotically optimal (AO) SIM, a notion to be defined precisely in section 2, can be constructed.

Our work was motivated by two recent papers of Eiermann and Varga [5,6] who considered the real case analogue (i.e. for $\omega \in \mathbb{R}$) of the following two special cases where

$$\Sigma_\mu = [-\beta, \beta], \quad 0 < \beta < 1 \tag{14}$$

and

$$\Sigma_\mu = [-\beta, \beta] \cup [-\mathrm{i}\alpha, \mathrm{i}\alpha], \quad 0 < \beta < 1, \ \alpha > 0. \tag{15}$$

One particular goal of the paper is to show that in both cases (14) and (15) the results of [5,6], regarding the comparison between an AOSIM-SOR and the optimal SOR, persist when the SOR relaxation parameter ω is allowed to take *complex values*. More precisely, in the case (14) there can be no advantage, in the asymptotic sense, by the use of the combination SIM–SOR and in the case (15) an AOSIM faster that the SOR can always be chosen. For more general inclusion sets Σ_μ we show in Theorem 6 that

if $\Sigma_\mu \in \mathbb{S}'$ and the outer boundary $\partial_\infty \Sigma_\mu$ of Σ_μ is an ellipse, then any AOSIM–SOR is equivalent to the optimal SOR and, furthermore, this is the only case for which the equivalence holds.

This leads, in particular, to the determination of the optimal complex SOR parameter ω for all ellipses which are symmetric with respect to the origin, a result which is, as far as we know, novel.

In cases where $\Sigma_\mu \in \mathbb{S}$ and $\partial_\infty \Sigma_\mu$ is not an ellipse, we show that the use of SIM–SOR is advantageous and a best choice would be an AOSIM based on the Gauss–Seidel (GS) method. (Recall that GS is the special case $\omega = 1$ of SOR.) More precisely, it follows from Corollary 2 and Theorem 6 that

> if $\Sigma_\mu \in \mathbb{S}$, then any AOSIM–GS is an AOSIM–SOR and if $\partial_\infty \Sigma_\mu$ is not an ellipse, then any AOSIM–SOR is better than the optimal SOR.

(In fact, we point out in section 3 that the above statement is also true for any $\Sigma_\mu \in \mathbb{S}'$.)

The paper is organised as follows: in section 2 we indicate how the convergence theory of SIM is related to the theory of Green functions and state the preparatory theorems needed for our subsequent work. In section 3 we prove the main results summarised above and make a number of remarks regarding AOSIM and comparisons with well-known results on the SOR and relevant theory.

2 From semi-iterative methods to Green functions

Consider the error vectors associated with the basic iterative method (3)

$$\mathbf{e}_m = \mathbf{x}_m - \mathbf{x}, \quad m = 0, 1, 2, \ldots .$$

Then, for any vector norm and the induced matrix norm, it holds that

$$\| \mathbf{e}_m \| = \| T^m \mathbf{e}_0 \| \leq \| T^m \| \| \mathbf{e}_0 \| \leq \| T \|^m \| \mathbf{e}_0 \| . \tag{16}$$

We recall that a SIM induced by $\mathcal{P}$ in (4) is defined by the sequence of vectors $\{\mathbf{y}_m\}_{m=0}^{\infty}$, given by (7). Thus, it can also be induced by the sequence of complex polynomials $\{p_m\}_{m=0}^{\infty}$, where

$$p_m(z) = \sum_{j=0}^{m} \pi_{m,j} z^j, \quad m = 0, 1, 2, \ldots, \tag{17}$$

with

$$p_m(1) = 1. \tag{18}$$

Note that in the identity case where $\pi_{m,j} = 0$, $j = 0, 1, \ldots, m-1$, and $\pi_{m,m} = 1$, (7) reduces to $\mathbf{y}_m = \mathbf{x}_m$, $m = 0, 1, 2, \ldots$, that is to the original iteration (3).

Let now ε_m be the error vector at the mth iteration of the SIM, i.e. let

$$\varepsilon_m := \mathbf{y}_m - \mathbf{x}, \quad m = 0, 1, 2, \ldots, \tag{19}$$

and recall that $1 \notin \sigma(T)$. Then, it follows easily from (7) and (17) and (18) that

$$\varepsilon_m = p_m(T)\varepsilon_0. \tag{20}$$

Thus, if P_n is the characteristic polynomial of the iteration matrix T and p_m is chosen so that

$$p_m(z) = z^{m-n}\frac{P_n(z)}{P_n(1)}, \quad m \geq n,$$

then, by virtue of the Cayley–Hamilton theorem we obtain, $p_m(T) = O$, and therefore $\varepsilon_m = \mathbf{0}$. In other words, the exact solution of (1) can be found after at most n iterations. The construction of the "exact" polynomial p_m, however, requires the exact knowledge of the spectrum $\sigma(T)$. To find the spectrum is, in principle, a much more involved problem than solving the corresponding linear system itself. Hence, it is more realistic to assume that a compact set Σ of $\mathbb{C}$ is available such that $\sigma(T) \subset \Sigma$, and $1 \notin \Sigma$. For regularity purposes, associated with the existence of the classical Green function considered below, we impose a bit more than compactness in the inclusion set Σ. More precisely, in this section we assume that Σ belongs to the class $\mathbb{M}$, where

> $\mathbb{M} := \{\Sigma \subset \mathbb{C} : \Sigma$ is a compact set consisting of a finite number of components, each of which contains more than one point $\}$.

Let Ω denote the component of $\overline{\mathbb{C}} \setminus \Sigma$ that contains the point at infinity, i.e. the unbounded component of $\overline{\mathbb{C}} \setminus \Sigma$. The assumption $\Sigma \in \mathbb{M}$ ensures that Ω possesses a (classical) *Green function g_Ω with pole at infinity.* This is the unique function satisfying the following three properties (see, e.g. [9, p 73] and [25, p 65]):

1. $g_\Omega(z)$ is positive and harmonic in $\Omega \setminus \{\infty\}$ and is bounded as z stays away from ∞,
2. $g_\Omega(z) - \log|z|$ is bounded around ∞,
3. $\lim_{z\to\zeta} g_\Omega(z) = 0$, for every $\zeta \in \partial\Omega$.

For the definition of the Green function associated with more general sets see, e.g. [20, p 106] and [22, p 108].

We now come to the problem of measuring the performance of a SIM induced by the lower triangular matrix $\mathcal{P}$ (4) or, equivalently, by the sequence of the associated normalized polynomials $\{p_m\}_{m=0}^{\infty}$ (17) and (18), and in view of the given data $\sigma(T) \subset \Sigma$. For this purpose, we consider the following *asymptotic convergence factor* (see, e.g. [4, Sect. 2] and [7, Sect. 5]):

$$\kappa(\Sigma, \mathcal{P}) := \limsup_{m\to\infty} \| p_m \|_\Sigma^{1/m}, \tag{21}$$

where $\|\cdot\|_\Sigma$ denotes the maximum norm on Σ. In fact, $\kappa(\Sigma, \mathcal{P})$ is a measure of the average asymptotic decay of the norms of the corresponding error vectors ε_m, see (20) and equation (26) below. This leads naturally to the *asymptotic convergence factor* $\kappa(\Sigma)$, associated with the inclusion set Σ. This is defined to be the best, i.e. the *smallest*, convergence factor $\kappa(\Sigma, \mathcal{P})$ we can hope to achieve by using a SIM, i.e.

$$\kappa(\Sigma) := \inf\{\kappa(\Sigma, \mathcal{P}),\ \mathcal{P} \text{ defines a SIM}\}. \tag{22}$$

Remark 1 If $1 \notin \Omega$, then it follows from the maximum modules principle that $\|p_m\|_\Sigma \geq 1$, for any polynomial satisfying $p_m(1) = 1$ and, therefore,

$$\kappa(\Sigma) = 1.$$

This would be the case, for example, when $\overline{\mathbb{C}} \setminus \Sigma$ consists of two components, and 1 lies in the bounded component.

In the complementary case where $1 \in \Omega$, the asymptotic convergence factor $\kappa(\Sigma)$ is given in terms of the Green function g_Ω of Ω.

Theorem 1 *Let* $\Sigma \in \mathbb{M}$*, let* Ω *denote the unbounded component of* $\overline{\mathbb{C}} \setminus \Sigma$ *and assume that* $1 \in \Omega$*. Then,*

$$\kappa(\Sigma) = \frac{1}{\exp(g_\Omega(1))} < 1. \tag{23}$$

This important result which provides the link between the study of SIM and potential theory was, essentially, established in [4] (see also [8, p 160]) by applying the theory of *maximally convergent polynomials* of Walsh [25, ch VI] to the analytic function $1/(1-z)$ on Σ. (For a step by step guide from potential theory to iterative methods we refer the reader to [2].) This theory ensures, in addition, the existence of a sequence of polynomials for which the infimum in (22) is attained. In accordance, we say that a SIM induced by $\mathcal{P}$ is AOSIM if

$$\kappa(\Sigma, \mathcal{P}) = \kappa(\Sigma). \tag{24}$$

This leads to the following characterisation for an AOSIM.

Corollary 1 *Under the assumptions of Theorem* 1*, a SIM induced by* $\mathcal{P}$ *is AOSIM with respect to* Σ*, if and only if*

$$\kappa(\Sigma, \mathcal{P}) = \frac{1}{\exp(g_\Omega(1))}. \tag{25}$$

Another interesting characterisation of an AOSIM, valid at least in cases where Ω is simply connected, is stated in [7, Corollary 13]. Namely,

$$\kappa(\Sigma, \mathcal{P}) = \sup_{\sigma(T) \subset \Sigma} \left\{ \limsup_{m \to \infty} \left(\sup_{\varepsilon_0 \neq \mathbf{0}} \frac{\| \varepsilon_m \|}{\| \varepsilon_0 \|} \right)^{1/m} \right\}, \tag{26}$$

where the quantity inside the braces is independent of the particular vector norm used.

In the case where the domain Ω is simply connected, the asymptotic convergence factor $\kappa(\Sigma)$ can also be given in terms of an associated conformal map. To see this let

$$\Phi : \Omega \to \Delta := \{w : |w| > 1\} \tag{27}$$

be any conformal map such that

$$\Phi(z) = cz + \mathcal{O}(1), \quad c \neq 0, \; z \to \infty, \tag{28}$$

and note that the normalisation (28) determines Φ uniquely apart from rotations, hence the value of $|\Phi(z)|$, $z \in \Omega$ is uniquely defined. Then, it can be easily verified that the function $\log|\Phi(z)|$ satisfies the three defining properties of the Green function g_Ω and thus, from the uniqueness of the Green function,

$$g_\Omega(z) = \log|\Phi(z)|. \tag{29}$$

This observation and Theorem 1 lead, in this case, to the relation,

$$\kappa(\Sigma) = \frac{1}{|\Phi(1)|}. \tag{30}$$

In the following two theorems we consider the behaviour of the Green function under polynomial and meromorphic mapping.

Theorem 2 *Assume that $\Sigma \in \mathbb{M}$ and let p be a polynomial of exact degree d. If Ω and Ω' denote, respectively, the unbounded components of $\overline{\mathbb{C}}\backslash\Sigma$ and $\overline{\mathbb{C}}\backslash p^{-1}(\Sigma)$, then*

$$g_\Omega(p(z)) = d g_{\Omega'}(z), \quad z \in \Omega'. \tag{31}$$

Proof The result follows immediately from the first part of the proof of Theorem 5.2.5 in [20] by observing that our assumption $\Sigma \in \mathbb{M}$, in conjunction with Theorem 4.4.9 of [20], imply that Ω is a regular domain. (See also [22, p 165].) □

Theorem 3 *Let Σ_1 and Σ_2 be two sets in the class $\mathbb{M}$, let Ω_1 and Ω_2 denote, respectively, the unbounded components of $\overline{\mathbb{C}}\backslash\Sigma_1$ and $\overline{\mathbb{C}}\backslash\Sigma_2$, and assume that $f : \Omega_1 \to \Omega_2$ is a meromorphic function such that $f(\infty) = \infty$. Then:*

(i) It holds,

$$g_{\Omega_2}(f(z)) \geq g_{\Omega_1}(z), \quad z \in \Omega_1, \tag{32}$$

with equality if f is a conformal map from Ω_1 onto Ω_2, i.e. if f is injective and $f(\Omega_1) = \Omega_2$.

(ii) If there exists a point $z_0 \in \Omega_1 \setminus \{\infty\}$ such that

$$g_{\Omega_2}(f(z_0)) = g_{\Omega_1}(z_0),$$

then

$$g_{\Omega_2}(f(z)) = g_{\Omega_1}(z), \quad \textit{for all } z \in \Omega_1. \tag{33}$$

Furthermore, f is injective and $f(\Omega_1) = \Omega_2$.

Proof Both (i) and (ii) follow at once from Theorems 4.4.4 and 4.4.10 of [20], by observing that our assumptions on Σ_1 and Σ_2 imply that Ω_1 and Ω_2 are regular domains; see also the proof of Theorem 2. □

We end this section, by presenting a result that characterises all sets $\Sigma \in \mathbb{M}$ for which there exists no SIM scheme based on the iteration (3) that decreases further the associated asymptotic convergence factor $\rho(\Sigma)$ of (3) defined by the available data $\sigma(T) \subset \Sigma$, i.e. by

$$\rho(\Sigma) := \max_{\sigma(T)\subset\Sigma}\{|\lambda| : \lambda \in \sigma(T)\} = \max\{|\lambda| : \lambda \in \Sigma\}.$$

Theorem 4 *Assume that* $\Sigma \in \mathbb{M}$, *let* Ω *denote the unbounded component of* $\overline{\mathbb{C}} \setminus \Sigma$ *and suppose that* $1 \in \Omega$. *Then, it holds*

$$\kappa(\Sigma) = \rho(\Sigma), \tag{34}$$

if and only if the boundary $\partial\Omega$ *of* Ω, *coincides with the circle* $\{z : |z| = \rho(\Sigma)\}$.

Proof Set $r := \rho(\Sigma)$ and note that our assumptions on Σ and Ω and Theorem 1 imply that (a) $r > 0$, (b) Ω possesses a Green function g_Ω, and (c) $\kappa(\Sigma) < 1$. Let $\Delta_r := \{z : |z| > r\}$ be the exterior of the circle $C_r := \{z : |z| = r\}$. Clearly, $\Delta_r \subset \Omega$. Also, as it can be checked easily, the Green function of Δ_r is given by

$$g_{\Delta_r}(z) = \log|z| - \log r. \tag{35}$$

If (34) holds, then $r < 1$, which gives $1 \in \Delta_r$, and in view of (23) and (35) we obtain $g_{\Delta_r}(1) = g_\Omega(1)$. Consider now the function $f(z) = z$. Obviously, $f : \Delta_r \to \Omega$ satisfies the assumptions of Theorem 3, with $z_0 = 1$. The required relation $C_r = \partial\Omega$ then follows because $f(\Delta_r) = \Omega$ and f is the identity map.

For the inverse result, assume that $\partial\Omega$ coincides with C_r, for some $r > 0$. Then $\Omega = \Delta_r$ and (34) follows at once from (23), by substituting g_{Δ_r} for g_Ω. □

3 Complex SIM–SOR

Now we turn our attention to the case where the SIM scheme (7) is applied to the SOR method (9) and (10) with relaxation parameter $\omega \in \mathbb{C} \setminus \{0\}$. We recall from section 1 that our assumptions on the associated Jacobi matrix $J = D^{-1}(L + U)$ imply that the non-zero eigenvalues μ of J appear in opposite pairs and are related to the eigenvalues λ of the SOR iteration matrix $\mathcal{L}_\omega$ through Young's relationship (12).

The requirement $|\omega - 1| < 1$ constitutes a necessary condition for the method to converge; see [14]. Furthermore, the above relationship, in conjunction with information on the spectrum $\sigma(J)$ of J can be used to determine, in certain cases, the optimal SOR parameter ω_b. The first result in this direction was obtained by Young, as early as 1950, in his Ph.D. Thesis [27] (see also [28, Theorem 6.2.3]), for a real relaxation parameter ω, under the assumption $\sigma(J) \subset [-\mu_1, \mu_1]$, $\mu_1 \in [0, 1)$. Kjellberg [15], and afterwards Kredell [16], considered the SOR with complex relaxation parameter ω, and Kredell was the first to obtain an optimal result in the complex case, as stated below.

Lemma 1 ([16, Theorem 4.1]) *Assume that* $\sigma(J) \subset [-\mu_1, \mu_1]$, *for some* $\mu_1 \in \mathbb{C}$ *such that* $1 \notin [-\mu_1, \mu_1]$. *Then,*

$$\min_{\omega \in \mathbb{C}} \rho(\mathcal{L}_\omega) = \rho(\mathcal{L}_{\omega_b}) = |\omega_b - 1|, \quad with \quad \omega_b := \frac{2}{1 + \sqrt{1 - \mu_1^2}}, \tag{36}$$

where $\Re(\sqrt{\cdot}\,) > 0$.

For $\mu_1 \in [0, 1)$ and $\omega \in \mathbb{R}$ the optimal result (36) reduces to that obtained by Young in [27]. It appears that the result of Lemma 1 is not widely known. For instance, it has been rediscovered recently in [21, Theorem 5.2], under the additional condition $|\mu_1| < 1$. We note in passing that the subject of [21] is the description and analysis of a generalized SOR algorithm for accelerating the convergence of an iteration method known as waveform relaxation. It is interesting to note that the performance of the specific algorithm is demonstrated to the solution of a differential algebraic system generated by spatial discretisation of the time-dependent semiconductor device equations. More recent results regarding the application of the SOR, as well as Krylov subspace acceleration methods, to the waveform relaxation can be found in [12,13,17]. For estimates associated with the l_2-norm of the error vector (19), we refer the reader to [19].

3.1 Three transformations

Kredell obtained his optimal result, for $\omega \in \mathbb{C} \setminus \{0, 1\}$, by decomposing the transformation

$$\mu \;\to\; \lambda, \tag{37}$$

induced by (12), into the following three transformations (an idea originally suggested by Kjellberg in [15]):

$$\mathbf{T}_1 : \quad \mu \to z = \tfrac{1}{2}\left(\alpha + \frac{1}{\alpha}\right)\mu, \quad \text{where } \alpha = \sqrt{\omega - 1}, \tag{38}$$

$$\mathbf{T}_2 : \quad z \to \zeta = z \pm \sqrt{z^2 - 1} \quad \Longleftrightarrow \quad z = \frac{1}{2}\left(\zeta + \frac{1}{\zeta}\right), \tag{39}$$

$$\mathbf{T}_3 : \qquad \zeta \to \lambda = \alpha^2 \zeta^2. \tag{40}$$

In (39) the equivalence sign indicates that the inverse transformation $\mathbf{T}_2^{-1}$ effects the mapping,

$$\mathbf{T}_2^{-1}(\zeta) = \frac{1}{2}\left(\zeta + \frac{1}{\zeta}\right), \tag{41}$$

which is known as the Joukowski transformation. Therefore, each of the two branches $\mathbf{T}_2^{+}(z) := z + \sqrt{z^2 - 1}$ and $\mathbf{T}_2^{-}(z) := z - \sqrt{z^2 - 1}$ of the double-valued function $\mathbf{T}_2$, maps conformally the unbounded domain $\overline{\mathbb{C}} \setminus [-1, 1]$, respectively, onto the exterior $\Delta_\zeta := \{\zeta : |\zeta| > 1\}$ and the interior $\mathbb{D}_\zeta := \{\zeta : |\zeta| < 1\}$ of the unit circle. This is done by choosing the value of the square root in both $\mathbf{T}_2^{+}$ and $\mathbf{T}_2^{-}$ so that $|z + \sqrt{z^2 - 1}| > 1$, for $z \in \overline{\mathbb{C}} \setminus [-1, 1]$. This choice gives, in particular,

$$\mathbf{T}_2^{\pm}(-z) = -\mathbf{T}_2^{\pm}(z) \quad \text{and} \quad \mathbf{T}_2^{+}(z)\mathbf{T}_2^{-}(z) = 1. \tag{42}$$

(See, e.g. [11, pp 296–298] for the details of the computation of $\sqrt{z^2 - 1}$.) For our purposes here, it is important to emphasize that the single-valued meromorphic function $\mathbf{T}_2^{-1}$ maps conformally each one of the domains Δ_ζ and $\mathbb{D}_\zeta$ onto $\overline{\mathbb{C}} \setminus [-1, 1]$ and takes continuously the unit circle $\{\zeta : |\zeta| = 1\}$ onto the interval $[-1, 1]$.

3.2 The associated parameter ν

It turns out that it is much more convenient for the purposes of our analysis and for the statement of our results to work with an associated parameter ν, rather than with the SOR relaxation parameter ω. This new parameter is related to ω by zeroing the discriminant of the quadratic equation in λ, which results from (12). More precisely, for any $\omega \in \mathbb{C} \setminus \{0, 1\}$ we associate two values of $\nu \in \mathbb{C} \setminus \{0\}$, via the equation

$$\omega^2 \nu^2 = 4(\omega - 1). \tag{43}$$

Equivalently, for any $\nu \in \mathbb{C} \setminus \{0\}$, we can find two values of $\omega \in \mathbb{C} \setminus \{0, 1\}$ that satisfy (43), namely $\omega^+ := \omega^+(\nu)$ and $\omega^- := \omega^-(\nu)$, where

$$\omega^+(\nu) := \frac{2}{1 + \sqrt{1 - \nu^2}} \quad \text{and} \quad \omega^-(\nu) := \frac{2}{1 - \sqrt{1 - \nu^2}}. \tag{44}$$

In (44) the square root is chosen so that $\sqrt{1 - \nu^2} = i\sqrt{\nu^2 - 1}$, if $\nu^2 \geq 1$ (hence $\nu \in \mathbb{R}$) and $\Re(\sqrt{\ \cdot\ }) > 0$, otherwise. For instance, with this terminology, Lemma 1 states that the choice $\nu = \mu_1$ and $\omega = \omega^+(\nu)$, yields the optimal SOR for the line segment $[-\mu_1, \mu_1]$.

We note the relation

$$(\omega^+ - 1)\,(\omega^- - 1) = 1, \tag{45}$$

which follows easily from the definition of ω^+ and ω^-. We also note that (43) gives,

$$\nu = 0 \Leftrightarrow \omega = 1, \tag{46}$$

i.e. for $\nu = 0$ the SOR reduces to the GS method.

The next lemma shows how the complex line segment $[-\nu, \nu]$ is transformed under the sequential application of the three mappings (38), (39) and (40). It also contains a result concerning the modulus of $\omega^+ - 1$ and $\omega^- - 1$.

Lemma 2 *Assume that $\nu \in \mathbb{C} \setminus \{0\}$. Then,*

$$[-\nu, \nu] \xrightarrow{\mathbf{T}_1} [-1, 1] \xrightarrow{\mathbf{T}_2} \{\zeta : |\zeta| = 1\} \xrightarrow{\mathbf{T}_3} \{\lambda : |\lambda| = |\omega - 1|\}. \tag{47}$$

In particular,

$$\{-\nu, \nu\} \xrightarrow{\mathbf{T}_1} \{-1, 1\} \xrightarrow{\mathbf{T}_2} \{-1, 1\} \xrightarrow{\mathbf{T}_3} \{\omega - 1\}. \tag{48}$$

Also,

$$|\omega^+ - 1| \leq 1, \quad |\omega^- - 1| \geq 1, \tag{49}$$

where equalities hold simultaneously if and only if $\nu^2 \geq 1$.

Proof With $\nu \neq 0$, set $\mu = \pm\nu$ and observe that (38) in view of (43) gives $z^2 = 1$. This and the fact that $\mathbf{T}_1$ is a linear map imply the results involving $\mathbf{T_1}$ in (47) and (48). The results for $\mathbf{T_2}$ follow easily from the properties of $\mathbf{T}_2$ discussed in section 3.1. Finally, the results concerning $\mathbf{T}_3$ follow at once from its definition in (40).

In order to derive (49), we set $W := \sqrt{1-\nu^2}$, $Z := 1-\omega^+$ and observe that from (44),

$$Z = \frac{W-1}{W+1} =: T(W), \tag{50}$$

where $\Re(W) \geq 0$. The results for $|\omega^+ - 1|$ follow from the fact that the function $T(W)$ is a Möbius transformation which maps the right half-plane $\Re(W) > 0$ onto the unit disk $|Z| < 1$, and the imaginary axis $\Re(W) = 0$ onto the unit circle $|Z| = 1$. Finally, the results for $|\omega^- - 1|$ follow at once from (45). □

3.3 Main results

We recall from section 1 the definition of the class of sets $\mathbb{S}$. We also recall that our main objective is to investigate the application of the SIM scheme to the SOR method (9) and (10) under the assumption (13). To this end, we let $\Omega_\mu := \overline{\mathbb{C}} \setminus \Sigma_\mu$ and observe that the definition of $\mathbb{S}$ ensures the existence of the Green function g_{Ω_μ} of Ω_μ and implies the relations

$$\kappa(\Sigma_\mu) = \frac{1}{\exp\left(g_{\Omega_\mu}(1)\right)} < 1. \tag{51}$$

For the purposes of our analysis and for $\omega \in \mathbb{C} \setminus \{0, 1\}$, we need to consider the sequential application of the three transformations (38), (39) and (40) to Σ_μ. We identify the resulting couples of sets as follows:

$\Sigma_z := \mathbf{T}_1(\Sigma_\mu)$ and $\Omega_z :=$ the unbounded component of $\overline{\mathbb{C}} \setminus \Sigma_z$.
$\Sigma_\zeta := \mathbf{T}_2(\Sigma_z)$ and $\Omega_\zeta :=$ the unbounded component of $\overline{\mathbb{C}} \setminus \Sigma_\zeta$.
$\Sigma_{\lambda,\omega} := \mathbf{T}_3(\Sigma_\zeta)$ and $\Omega_\lambda :=$ the unbounded component of $\overline{\mathbb{C}} \setminus \Sigma_{\lambda,\omega}$.

From the definition of $\mathbf{T}_1$, $\mathbf{T}_2$ and $\mathbf{T}_3$ and the discussion thereafter, it is easy to see that each of the three sets Σ_z, Σ_ζ and $\Sigma_{\lambda,\omega}$ belongs to the class $\mathbb{M}$ and thus, each of the associated unbounded domains Ω_z, Ω_ζ and Ω_λ possesses a Green function denoted, respectively, by g_{Ω_z}, g_{Ω_ζ} and g_{Ω_λ}. (We use $\Sigma_{\lambda,\omega}$, instead of Σ_λ, in order to emphasize that the shape of this set depends, apart from Σ_μ, also on ω.)

For $\omega = 1$, the SOR reduces to the GS method and Young's relationship (12) becomes $\lambda(\lambda - \mu^2) = 0$. In this case, only the transformation

$$\lambda = \mu^2, \tag{52}$$

has to be considered, since the case $\lambda = 0$ is also covered in (52) (recall that $0 \in \Sigma_\mu$). Accordingly, the set $\Sigma_{\lambda,1}$ is derived from Σ_μ by means of (52). Again, $\Sigma_{\lambda,1} \in \mathbb{M}$ and the corresponding unbounded domain Ω_λ possesses a Green function.

We note that, since the SOR is equivalent to the special SIM–SOR, where the defining matrix (4) of SIM reduces to the infinite identity matrix $\mathcal{I}$, the asymptotic convergence factor $\kappa(\Sigma_{\lambda,\omega})$ and the spectral radius $\rho(\mathcal{L}_\omega)$ are related by

$$\kappa(\Sigma_{\lambda,\omega}) \leq \kappa(\Sigma_{\lambda,\omega}, \mathcal{I}) = \limsup_{m\to\infty} \| z^m \|_{\Sigma_{\lambda,\omega}}^{1/m} = \rho(\mathcal{L}_\omega), \tag{53}$$

where here $\rho(\mathcal{L}_\omega)$ is understood in the "effective" sense:

$$\rho(\mathcal{L}_\omega) = \rho(\Sigma_{\lambda,\omega}) := \max\{|z| : z \in \Sigma_{\lambda,\omega}\}. \tag{54}$$

In this setting, the use of the combination SIM–SOR is advantageous over the sole use of the SOR, at least in the asymptotic sense, *only if*

$$\kappa(\Sigma_{\lambda,\omega}) < \min\{1, \rho(\mathcal{L}_\omega)\}; \tag{55}$$

see also [6, p 50]. Ideally, we would like to know before applying a SIM whether,

$$\min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega}) < \min\left\{1, \min_{\omega\in\mathbb{C}} \rho(\mathcal{L}_\omega)\right\}.$$

This latter inequality is the subject of Theorem 6 below, where by using the result of Theorem 4, we describe all sets Σ_μ in the class $\mathbb{S}'$ (a class wider than $\mathbb{S}$) for which,

$$\min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega}) = \min_{\omega\in\mathbb{C}} \rho(\mathcal{L}_\omega) \quad (< 1).$$

Before that, in Theorem 5, we show that the value of $\min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega})$ is given explicitly in terms of the Green function g_{Ω_μ}.

Theorem 5 *Assume that the Jacobi matrix J of* (11) *is consistently ordered and weakly cyclic of index* 2, *and suppose that the spectrum $\sigma(J)$ of J is contained in a compact set Σ_μ, where $\Sigma_\mu \in \mathbb{S}$. For $\nu \in \mathbb{C}$, let $\omega^+(\nu)$ and $\omega^-(\nu)$ be given by* (44). *Then the asymptotic convergence factor $\kappa(\Sigma_{\lambda,\omega})$ satisfies the following properties:*

(i) If $\nu \notin \Sigma_\mu$ and $\omega \in \{\omega^+(\nu), \omega^-(\nu)\}$ then

$$\frac{1}{\exp\left(2g_{\Omega_\mu}(1)\right)} < \kappa(\Sigma_{\lambda,\omega}) < 1. \tag{56}$$

(ii) If $\nu \in \Sigma_\mu$ and $\omega = \omega^+(\nu)$, then

$$\kappa(\Sigma_{\lambda,\omega}) = \frac{1}{\exp\left(2g_{\Omega_\mu}(1)\right)} < 1. \tag{57}$$

(iii) If $\nu \in \Sigma_\mu \setminus \{0\}$ and $\omega = \omega^-(\nu)$, then

$$\kappa(\Sigma_{\lambda,\omega}) = 1. \tag{58}$$

From the three cases of the above theorem and the fact that $0 \in \Sigma_\mu$ we get immediately the following result.

Corollary 2 *Let* $\mathcal{B} := \{\omega : \omega = \omega^{+}(\nu),\ \nu \in \Sigma_\mu\}$. *Then,*

$$\min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega}) = \{\kappa(\Sigma_{\lambda,\omega}),\ \omega \in \mathcal{B}\} = \frac{1}{\exp\left(2g_{\Omega_\mu}(1)\right)}. \tag{59}$$

In particular,

$$\min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega}) = \kappa(\Sigma_{\lambda,1}), \tag{60}$$

and therefore any asymptotically optimal SIM based on the GS method (AOSIM–GS) is an AOSIM–SOR.

Remark 2 We note the following regarding the assumptions and the consequences of Theorem 5.

(i) As it was indicated in section 3.2, we find it more instructive to state our hypotheses in terms of the parameter ν, rather than the conventional SOR parameter ω. The assumptions on ν can be easily converted to equivalent ones on ω by means of the Möbius transformation (50), for $\nu \neq 0$ or by (46) for $\nu = 0$.

(ii) It holds $\kappa(\Sigma_{\lambda,\omega}) < 1$, *if and only if* (a) $\nu \notin \Sigma_\mu$ and $\omega \in \{\omega^{+}(\nu), \omega^{-}(\nu)\}$ or (b) $\nu \in \Sigma_\mu$ and $\omega = \omega^{+}(\nu)$.

(iii) Corollary 2, in conjunction with (51), implies the relation

$$\kappa(\Sigma_{\lambda,1}) = \left(\kappa(\Sigma_\mu)\right)^2. \tag{61}$$

That is, an AOSIM–GS is twice as fast as any AOSIM based on the associated Jacobi iteration.

The proof of Theorem 5 will be facilitated by the following intermediate result.

Lemma 3 *Under the assumptions of Theorem* 5 *we have:*

(i) *If* $\nu \notin \Sigma_\mu$, *then* $\Omega_\zeta = \overline{\mathbb{C}} \setminus \Sigma_\zeta$ *and*

$$g_{\Omega_z}(\mathbf{T}_2^{-1}(\zeta)) > g_{\Omega_\zeta}(\zeta), \quad \zeta \in \Omega_\zeta \setminus \{\infty\}. \tag{62}$$

(ii) *If* $\nu \in \Sigma_\mu \setminus \{0\}$, *then the set* $\overline{\mathbb{C}} \setminus \Sigma_\zeta$ *consists of two components which are separated by the unit circle and*

$$g_{\Omega_z}(\mathbf{T}_2^{-1}(\zeta)) = g_{\Omega_\zeta}(\zeta), \quad \zeta \in \Omega_\zeta. \tag{63}$$

Proof Recall the definition $\mathbf{T}_2^{-1}(\zeta) = (1/2)(\zeta + 1/\zeta)$ and observe that $\mathbf{T}_2^{-1}$ is a meromorphic mapping from Ω_ζ onto Ω_z, such that $\mathbf{T}_2^{-1}(\infty) = \infty$. The results of the lemma follow easily from Lemma 2 and Theorem 3. The details are as follows.

Assume first that $\nu \notin \Sigma_\mu$. Then, the set $E := [-\nu, \nu] \setminus \left(\Sigma_\mu \cap [-\nu, \nu]\right)$ is non-empty and consists of two complex intervals (note that always $0 \in \Sigma_\mu$). Hence, from Lemma 2 we have that (a) $\mathbf{T}_1(E) = [-1, -\xi) \cup (\xi, 1]$ for some $0 \le \xi < 1$, and (b) the set $C_\zeta \setminus (\Sigma_\zeta \cap C_\zeta)$, where $C_\zeta := \{\zeta : |\zeta| = 1\}$, is non-empty. This implies that the set $\overline{\mathbb{C}} \setminus \Sigma_\zeta$ consists of a single component, i.e. $\Omega_\zeta = \overline{\mathbb{C}} \setminus \Sigma_\zeta$; see Figure 1. Therefore, the mapping $\mathbf{T}_2^{-1} : \Omega_\zeta \to \Omega_z$ cannot be injective in

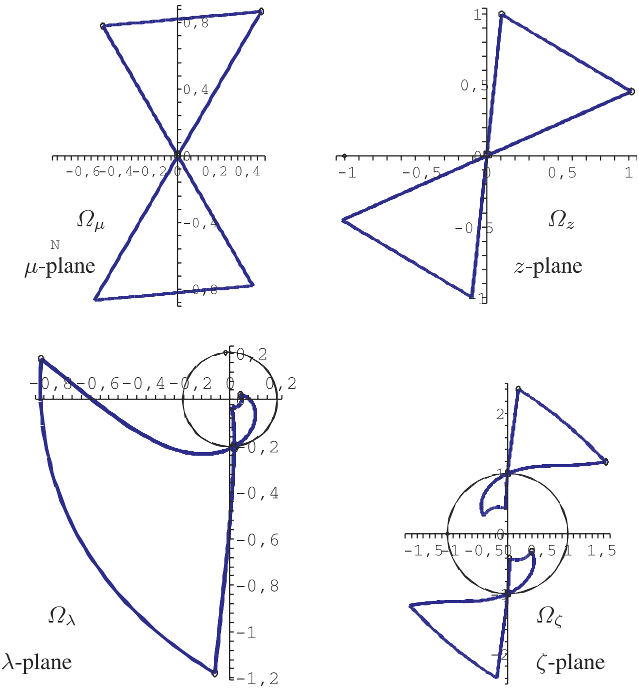

Fig. 1 The transformation $\mu \overset{\mathbf{T}_1}{\rightarrow} z \overset{\mathbf{T}_2}{\rightarrow} \zeta \overset{\mathbf{T}_3}{\rightarrow} \lambda$ of Σ_μ. Case: $\nu \notin \Sigma_\mu$ and $\omega = \omega^+(\nu)$. ($\nu = 0.9\mathrm{e}^{\mathrm{i}6\pi/5}$, denoted by "N" in the μ-plane)

this case, for if $\zeta \in \Omega_\zeta$ then also $1/\zeta \in \Omega_\zeta$ (see section 3.1, in particular (42)) and $\mathbf{T}_2^{-1}(\zeta) = \mathbf{T}_2^{-1}(1/\zeta)$. Theorem 3 then yields the strict inequality in (62): The equality sign is impossible for some $\zeta \in \Omega_\zeta \setminus \{\infty\}$, otherwise $\mathbf{T}_2^{-1}$ would have been injective.

On the other hand, if $\nu \in \Sigma_\mu \setminus \{0\}$, then from Lemma 2 we see that (a) the line segment $[-1, 1]$ lies on Σ_z and, (b) the set $\overline{\mathbb{C}} \setminus \Sigma_\zeta$ consists of two components which are separated by the unit circle; see Figure 2. Thus, in this case, the unbounded component Ω_ζ is contained in $\Delta_\zeta = \{\zeta : |\zeta| > 1\}$, and consequently $\mathbf{T}_2^{-1}$ is a conformal map from Ω_ζ onto Ω_z, a property that yields (63), in view of Theorem 3(i). □

Proof (of Theorem 5) First, we note that if $\nu \neq 0$, then $\omega \notin \{0, 1\}$ and Theorem 2 applied to the linear map $\mathbf{T}_1$ gives the relation

$$g_{\Omega_\mu}(1) = g_{\Omega_z}\left(\frac{1}{2}\left(\alpha + \frac{1}{\alpha}\right)\right). \tag{64}$$

Also, since μ and λ are related by (12), we have $1 \in \overline{\mathbb{C}} \setminus \Sigma_{\lambda,\omega}$, otherwise it would have been $1 \in \Sigma_\mu$, contrary to our assumption $\Sigma_\mu \in \mathbb{S}$.

Assume now that $\nu \notin \Sigma_\mu$ and recall that in Lemma 3(i) we have established, under this assumption, the relation $\Omega_\zeta = \overline{\mathbb{C}} \setminus \Sigma_\zeta$; see also Figure 1. Hence,

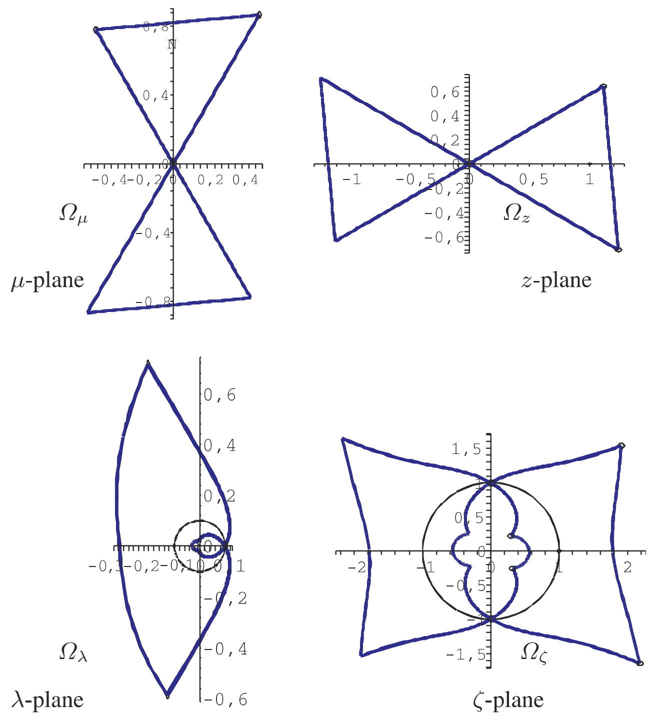

Fig. 2 The transformation $\mu \overset{\mathbf{T}_1}{\to} z \overset{\mathbf{T}_2}{\to} \zeta \overset{\mathbf{T}_3}{\to} \lambda$ of Σ_μ. Case: $\nu \in \Sigma_\mu \setminus \{0\}$ and $\omega = \omega^+(\nu)$ ($\nu = 0.7e^{i\pi/2}$, denoted by "N" in the μ-plane)

$\Omega_\lambda = \overline{\mathbb{C}} \setminus \Sigma_{\lambda,\omega}$ and therefore $1 \in \Omega_\lambda$. This leads, in view of Theorem 1, to

$$\kappa(\Sigma_{\lambda,\omega}) = \frac{1}{\exp\left(g_{\Omega_\lambda}(1)\right)} < 1. \tag{65}$$

Furthermore, we have the chain of relations

$$g_{\Omega_\lambda}(1) \overset{(a)}{=} 2g_{\Omega_\zeta}\left(\frac{1}{\alpha}\right) \overset{(b)}{<} 2g_{\Omega_z}\left(\frac{1}{2}\left(\alpha + \frac{1}{\alpha}\right)\right) \overset{(c)}{=} 2g_{\Omega_\mu}(1), \tag{66}$$

which follow from: (a) the application of Theorem 2 to the quadratic transformation $\mathbf{T}_3 : \Omega_\zeta \to \Omega_\lambda$, (b) inequality (62), and (c) equation (64). The result (56) then emerges at once from (65) by comparing the end parts of (66).

In order to establish parts (ii) and (iii) we consider first $\nu \in \Sigma_\mu \setminus \{0\}$. Then, from Lemma 3(ii) we see that the set $\overline{\mathbb{C}} \setminus \Sigma_\zeta$ consists of two components separated by the unit circle; see also Figure 2. In turn, the set $\overline{\mathbb{C}} \setminus \Sigma_{\lambda,\omega}$ consists of two components separated by the circle $\{\lambda : |\lambda| = |\omega - 1|\}$. If $\omega = \omega^-(\nu)$, then from Lemma 2, $|\omega - 1| > 1$ and thus 1 lies in the bounded component of $\overline{\mathbb{C}} \setminus \Sigma_{\lambda,\omega}$ (recall that $1 \notin \Sigma_\mu$). This, in conjunction with Remark 1, yields (58). If $\omega = \omega^+(\nu)$, then by the same lemma, we have $|\omega - 1| < 1$. Thus, in this case, 1 lies in Ω_λ. The result

(57) then follows from (65) and the chain of equalities

$$g_{\Omega_\lambda}(1) \overset{(a)}{=} 2g_{\Omega_\zeta}\left(\frac{1}{\alpha}\right) \overset{(b)}{=} 2g_{\Omega_z}\left(\frac{1}{2}\left(\alpha+\frac{1}{\alpha}\right)\right) \overset{(c)}{=} 2g_{\Omega_\mu}(1), \tag{67}$$

where now, in contrast to (66), equality holds in (b) due to (63).

Finally, if $\nu = 0$ then $\omega^+(\nu) = 1$ and, accordingly, the set $\Sigma_{\lambda,1}$ is derived from Σ_μ under the transformation (52). Thus, as above, $1 \in \Omega_\lambda$ and the application of Theorem 2.2 gives $g_{\Omega_\lambda}(1) = 2g_{\Omega_\mu}(1)$, which establishes (57) for $\nu = 0$ and $\omega = \omega^+(\nu)$. □

By inspecting the role of Lemma 3 in the proof of Theorem 5, in particular part (b) of both (66) and (67), we obtain the following corollary to Theorem 5.

Corollary 3 *It holds*

$$\kappa(\Sigma_{\lambda,\omega}) = \frac{1}{\exp\left(g_{\Omega_\lambda}(1)\right)} = \min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega}), \tag{68}$$

if and only if ω *is such that*

$$|\omega - 1| < 1 \quad \textit{and} \quad \Omega_\zeta \subset \{\zeta : |\zeta| > 1\}. \tag{69}$$

The above corollary suggests that our analysis can be applied to more general inclusion sets Σ_μ, provided we put suitable assumptions to ensure the existence of the Green functions involved and to be able to decide whether (69) holds true or not. For example, we can allow Σ_μ to include holes. More precisely, since for any $\Sigma \in \mathbb{M}$

$$\kappa(\Sigma) = \kappa(P_c(\Sigma)), \tag{70}$$

it is easy to verify that all the results of Theorem 5 remain valid for inclusion sets Σ_μ such that $P_c(\Sigma_\mu) \in \mathbb{S}$, provided we replace the conditions $\nu \notin \Sigma_\mu$, $\nu \in \Sigma_\mu$ and $\nu \in \Sigma_\mu \setminus \{0\}$ in the three cases (i), (ii) and (iii) of Theorem 5, respectively, by $\nu \notin P_c(\Sigma_\mu)$, $\nu \in P_c(\Sigma_\mu)$ and $\nu \in P_c(\Sigma_\mu) \setminus \{0\}$.

Another example is the case when $\Sigma_\mu \in \mathbb{S}'$, where $\mathbb{S}'$ is defined in section 1. In this case, it is not difficult to verify that the validity of the results of Theorem 5 persists, provided we replace the conditions $\nu \notin \Sigma_\mu$, $\nu \in \Sigma_\mu$ and $\nu \in \Sigma_\mu \setminus \{0\}$ in (i), (ii) and (iii) of Theorem 5, respectively, by $\nu \in \mathbb{C}$ with $[-\nu, \nu] \cap \{\mathbb{C} \setminus P_c(\Sigma_\mu)\} \neq \emptyset$, $\nu \in \mathbb{C}$ with $[-\nu, \nu] \subset P_c(\Sigma_\mu)$ and $\nu \in \mathbb{C} \setminus \{0\}$ with $[-\nu, \nu] \subset P_c(\Sigma_\mu)$.

We turn now our attention to the problem of characterising all those sets Σ_μ in the class $\mathbb{S}'$ for which we have

$$\min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega}) = \min_{\omega\in\mathbb{C}} \rho(\mathcal{L}_\omega),$$

where $\rho(\mathcal{L}_\omega)$ is given by (54). To this end, let $E_{a,b,\theta}$ denote the ellipse with major and minor axes $[-a\mathrm{e}^{\mathrm{i}\theta}, a\mathrm{e}^{\mathrm{i}\theta}]$ and $[-b\mathrm{e}^{\mathrm{i}\theta+\pi/2}, b\mathrm{e}^{\mathrm{i}\theta+\pi/2}]$, respectively, where $a \geq b \geq 0$, $a > 0$ and $\theta \in [0, \pi)$. We note that $E_{a,b,\theta}$ is symmetric with respect to the origin. Also, let $\pm\mu_0$ denote the foci of $E_{a,b,\theta}$, i.e. let,

$$\pm\mu_0 = \pm c\,\mathrm{e}^{i\theta}, \quad \text{where} \quad c := \sqrt{a^2 - b^2}. \tag{71}$$

(The degenerate case where $E_{a,b,\theta}$ reduces to a line segment is covered by $b = 0$.) Then, we have the following.

Theorem 6 *Assume that the Jacobi matrix J of* (11) *is consistently ordered and weakly cyclic of index* 2*, and suppose that the spectrum $\sigma(J)$ of J is contained in a compact set Σ_μ, where $\Sigma_\mu \in \mathbb{S}'$. Then:*

(i) It holds,

$$\min_{\omega\in\mathbb{C}} \kappa(\Sigma_{\lambda,\omega}) = \min_{\omega\in\mathbb{C}} \rho(\mathcal{L}_\omega) \tag{72}$$

if and only if the outer boundary $\partial_\infty\Sigma_\mu$ of Σ_μ coincides with that of an ellipse $E_{a,b,\theta}$.

(ii) If $\partial_\infty\Sigma_\mu = E_{a,b,\theta}$, then

$$\min_{\omega\in\mathbb{C}} \rho(\mathcal{L}_\omega) = \rho(\mathcal{L}_{\omega_b}) = \left|\frac{a+b}{1+\sqrt{1-\mu_0^2}}\right|^2 < 1 \tag{73}$$

with

$$\omega_b := \omega^+(\mu_0) = \frac{2}{1+\sqrt{1-\mu_0^2}}, \tag{74}$$

where $\Re(\sqrt{\ \cdot\ }) > 0$.

Proof From the hypothesis $\Sigma_\mu \in \mathbb{S}'$, the discussion right after Corollary 3, in particular (70), it follows that we can further assume for our purposes here that $\Sigma_\mu = P_{\mathrm{c}}(\Sigma_\mu)$. It also follows from Corollary 2 that

$$\min_{\omega\in\mathbb{C}}\{\kappa(\Sigma_{\lambda,\omega})\} = \{\kappa(\Sigma_{\lambda,\omega}),\ \omega \in \mathcal{B}\} = \frac{1}{\exp\left(2g_{\Omega_\mu}(1)\right)} < 1, \tag{75}$$

where, as before, $\mathcal{B} := \{\omega : \omega = \omega^+(\nu),\ \nu \in \Sigma_\mu\}$. Finally, from (53) we get

$$\kappa(\Sigma_{\lambda,\omega}) \le \rho(\mathcal{L}_\omega), \quad \omega \in \mathbb{C} \setminus \{0\}. \tag{76}$$

Assume that (72) holds. Then from (75) and (76) we see that there exists an $\omega' \in \mathcal{B}$ such that $\kappa(\Sigma_{\lambda,\omega'}) = \rho(\mathcal{L}_{\omega'}) < 1$. Therefore, from Theorem 4 and (75), the boundary $\partial\Omega_\lambda$ of the corresponding domain Ω_λ is a circle centred at the origin with $1 \in \Omega_\lambda$. Hence, by considering the inverses of the transformations (38), (39) and (40), it is easy to verify that $\partial_\infty\Sigma_\mu$ is an ellipse $E_{a,b,\theta}$.

Assume now that $\partial_\infty\Sigma_\mu$ is an ellipse $E_{a,b,\theta}$ and not a circle, hence $\mu_0 \ne 0$. Then, setting $\nu = \mu_0$ and $\omega = \omega_b$ we see that

$$\frac{1}{\mu_0} = \pm\frac{1}{2}\left(\alpha + \frac{1}{\alpha}\right),$$

with α as in (38). Thus, by applying the transformations (38), (39) and (40) to the set Σ_μ we conclude that $\partial\Omega_\lambda$ is the circle $\{\lambda : |\lambda| = r\}$, with

$$r = \left|\frac{a+b}{1+\sqrt{1-\mu_0^2}}\right|^2. \tag{77}$$

By another application of the transformations (38), (39) and (40), this time to the ellipse which is confocal to $E_{a,b,\theta}$ and passes through 1, we get the inequality $r < 1$ (note that $E_{a,b,\theta}$ lies strictly in the interior of this confocal ellipse). The above, in conjunction with Theorem 4, give $\kappa(\Sigma_{\lambda,\omega_b}) = \rho(\mathcal{L}_{\omega_b}) = r$. and the required result (72) follows from (75) and (76), because $\omega_b \in \mathcal{B}$. This settles the inverse of part (i) of the theorem, as well as part (ii) in view of (77).

If $E_{a,b,\theta}$ is a circle (i.e. if $\mu_0 = 0$), then the corresponding results follow easily by working as above and using the quadratic transformation $\lambda = \mu^2$, in the place of the three transformations (38), (39) and (40). □

Clearly, Theorem 6 (ii) includes the result of Lemma 1 as the special case where $b = 0$. The real case analogues of (73) and (74) where $\theta = 0$ or $\theta = \pi/2$, were obtained by Wrigley [26], see also [29, pp 194–195]. Finally, for the special case where $E_{a,b,\theta}$ is a circle the relation (72) was first shown by Varga [23, Theorem 4].

In [12, pp 151–152], it is claimed that the result of Theorem 6 (ii) was previously proved by Hu et al. However, the authors of [12] give no reference for the proof, apart from stating that it is contained in "Working Notes". Unfortunately, we have not been able to get hold of a copy of these working notes from their authors.

We reiterate that our results in this section were derived under the assumption that nothing more apart form the information $\sigma(J) \subset \Sigma$, is known for the spectrum $\sigma(J)$ of the Jacobi matrix J. If, in addition, certain eigenvalues of J are explicitly known, then it is possible to improve the asymptotic convergence factor, see [1], [5] and [6].

We conclude by making a remark regarding the application of the SIM scheme to the SSOR method. This method is widely used as a preconditioner for the class of the Conjugate Gradient methods. We observe that if the Jacobi iteration matrix J is consistently ordered and weakly cyclic of index 2, then the relation connecting the eigenvalues μ of J and λ of the corresponding SSOR iteration matrix is (see [3,18])

$$(\lambda + \phi - 1)^2 = \phi^2\mu^2\lambda, \quad \text{with } \phi = \omega(2 - \omega). \tag{78}$$

The first equation is exactly Young's relationship, where now ϕ replaces ω. Therefore, all our theory applies to the combination SIM–SSOR, apart from the fact that the role of ω is now assumed by the parameter ϕ.

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