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OPTIMAL ALTERNATING DIRECTION IMPLICIT PARAMETERS FOR NONSYMMETRIC SYSTEMS OF LINEAR EQUATIONS*

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Abstract. The determination of optimal parameters for the well-known alternating direction implicit (ADI) method leads to a minimization problem for rational functions of given degree l on compact sets E and F that contain the eigenvalues of the matrices involved. If E and F are real intervals, the solution of this problem was given by Zolotarev more than 100 years ago and by Wachspress in the 1960s. However, in the complex case, e.g., if the linear system arises from the discretization of non–self-adjoint elliptic differential equations, little is known about this problem. In this paper, two approaches to the Zolotarev problem in the complex plane are considered. First generalized Leja points are considered as an example for rational functions which are asymptotically minimal. In addition, for rectangular eigenvalue domains E and F, the exact minimal solutions for $l = 2$ are constructed and it is shown, by numerical examples, that the results obtained using the optimal parameters of degree 2 are comparable to those obtained with a much higher number of Leja points. Finally, the different strategies are compared for the model problem of a discretized convection diffusion equation.

Key words. iterative methods for nonsymmetric systems, optimal ADI parameters, rational Zolotarev problem in the complex plane, Leja points, convection-diffusion equation

AMS(MOS) subject classifications. 65F10, 30E10

1. Introduction.

An iterative method for the solution of large linear systems is the ADI (*Alternating Direction Implicit*) *method*, which was introduced by Peaceman and Rachford in 1955. The classical application of this method is the solution of discretized boundary value problems for elliptic partial differential equations. Writing the discretization in x- and y-direction into matrices H and V, respectively, leads to a linear system of equations

$$(H + V)\mathbf{u} = \mathbf{b} \tag{1.1}$$

where both H and V are sparse and possess a special structure. In particular, depending on the ordering of the unknown approximate values to the function $u(x, y)$ at the interior gridpoints rowwise or columnwise into the vector $\mathbf{u}$, H is a block diagonal matrix with tridiagonal blocks and V is block tridiagonal with diagonal blocks, or vice versa.

The iteration of the ADI method for solving the linear system (1.1) is given by

$$\begin{aligned} (H + \varphi I)\mathbf{u}^{(j+1/2)} &= (\varphi I - V)\mathbf{u}^{(j)} + \mathbf{b}\,, \\ (\psi I - V)\mathbf{u}^{(j+1)} &= (H + \psi I)\mathbf{u}^{(j+1/2)} - \mathbf{b}\,. \end{aligned} \tag{1.2}$$

The special block structure of the matrices H and V implies that, in each of the two halfsteps, we must solve a whole set of n linear systems of order n with tridiagonal matrices.

To improve the rate of convergence it is reasonable to change the parameters φ and ψ from step to step. For the *commutative case*, i.e., under the assumption $HV = VH$, the optimal choice of a whole set of parameters $\varphi_1, \cdots, \varphi_l, \psi_1, \cdots, \psi_l$

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leads to the *rational minimization problem*

$$\min_{r \in \mathbf{R}_{ll}} \frac{\max_{\lambda \in \sigma(V)} |r(\lambda)|}{\min_{\mu \in -\sigma(H)} |r(\mu)|}, \tag{1.3}$$

where $\mathbf{R}_{ll}$ denotes the set of all rational functions with denominator and numerator degree not exceeding l. However, the eigenvalues of H and V will usually not be given explicitly; but we can assume that we know disjoint compact sets E, F with $\sigma(V) \subseteq E$ and $-\sigma(H) \subseteq F$. Using this information, the rational minimization problem (1.3) turns into

$$\min_{r \in \mathbf{R}_{ll}} \frac{\max_{z \in E} |r(z)|}{\min_{z \in F} |r(z)|}. \tag{1.4}$$

The ADI method, applied to symmetric positive-definite systems, was extensively studied in the 1950s and in the 1960s (see, e.g., the books of Varga [18] and Wachspress [20]). Since we have real eigenvalues in this case, the sets E and F are disjoint real intervals. The problem of finding optimal parameters with respect to this information, i.e., the solution of the rational minimization problem (1.4) for the real case, was investigated by Wachspress in [19]. The optimal parameters were found by W. B. Jordan in terms of *elliptic functions* and presented in [19]. In 1977, Lebedev pointed out that, in the real case, (1.4) is equivalent to the third of four approximation problems which were solved by Zolotarev in the years 1868, 1877, and 1878 using *elliptic functions* (cf. Lebedev [11]; see also the review paper of Todd [17]). For the determination of the optimal ADI parameters in practice it was of great importance that, in [19], Wachspress was able to give a recursive algorithm for their computation for $l = 2^k$ which was independently discovered by Gastinel at the same time (again, see [17] for details and a complete historical overview).

During the last years there was an increasing interest in the solution of *non-self-adjoint problems* which lead to nonsymmetric linear systems. Thus, problem (1.4) was also studied for E and F being compact disjoint subsets of the complex plane. For complex domains, however, little is known by now about the *rational Zolotarev problem.*

The first to study this problem for the complex case was Gonchar in 1969 [9]. From his results it can be deduced that, for the minimal value in the rational Zolotarev problem (1.4)

$$\sigma_l(E, F) = \min_{r \in \mathbf{R}_{ll}} \frac{\max_{z \in E} |r(z)|}{\min_{z \in F} |r(z)|}, \tag{1.5}$$

there is a positive constant $\rho(E, F)$ such that

$$\lim_{l \to \infty} (\sigma_l(E, F))^{1/l} = \rho(E, F)^{-1}. \tag{1.6}$$

Examples of *asymptotically minimal* rational functions, i.e., sequences of rational functions $\{r_l\}_{l \in \mathrm{N}}$ with (1.6) being fulfilled, can be constructed by generalizations of the Fejér and Leja points which play an important role in connection with polynomial interpolation in the complex plane (see Gaier [7]). The *generalized Leja points* which were introduced by Bagby [1] in 1969 are very useful from a practical point of view since they are defined recursively and, thus, can be determined in a relatively efficient way.

Another approach to the complex Zolotarev problem was given by Ellner and Wachspress in [6] (see also [21]). There it is shown that the optimal rational functions for the real case are also optimal for some "elliptic function domains" in the complex plane. The spectral regions are then approximated by domains of this type, which leads to "approximately optimal" parameters for this problem. This is in some sense similar to the technique of embedding the spectrum into an ellipse and then using Chebyshev polynomials, a technique which is commonly used for polynomial acceleration of iterative methods. The convergence rates obtained using these parameters are often rather promising, even though they are neither optimal nor asymptotically optimal for sets E and F occurring in practice.

For discretized *convection diffusion equations*, the optimal ADI parameters for $l = 1$ were determined by Chin, Manteuffel, and de Pillis in [4].

In [14], a *near-circularity criterion* for the rational Zolotarev problem is proved which can be used to derive lower bounds for the best possible value in (1.4) and to construct the minimal rational functions for small degrees.

The main purpose of this paper is to compare the asymptotically optimal generalized Leja points with the exact minimal solutions for small degrees and to point out that the minimum in (1.4) for $l = 2$ is comparable to the numbers obtained with Leja points of much higher order.

We start in §2 with the derivation of the rational minimization problem (1.4) for commuting matrices H and V with complex eigenvalues. In §3 we review some results on the asymptotic behavior of the rational Zolotarev problem assuming that the sets E and F are bounded by Jordan curves. Furthermore, we present a technique for the computation of the generalized Leja points for piecewise differentiable boundary curves. After that, in §4 the optimal parameters for $l = 2$ are constructed for E and F being rectangular domains. Finally, in §5, we compare the convergence of the ADI method with different choice of parameters for a model problem of a discretized elliptic boundary value problem and illustrate its performance in practice.

2. Optimal ADI parameters.

Consider again the iterative method (1.2) for matrices H and V that commute, i.e., $HV = VH$. This assumption is fulfilled, e.g., for discretized separable elliptic boundary value problems on rectangular domains. The asymptotic convergence of this method is characterized by the spectral radius of the iteration operator

$$T_{\varphi,\psi} = (V - \psi I)^{-1}(H + \psi I)(H + \varphi I)^{-1}(V - \varphi I)\,. \tag{2.1}$$

So, finding optimal parameters for the ADI method means that we have to choose φ and ψ such that $\rho(T_{\varphi,\psi})$ is minimized. Because of the commutativity, we have

$$T_{\varphi,\psi} = (V - \varphi I)(V - \psi I)^{-1}(H + \psi I)(H + \varphi I)^{-1} = r_1(V)(r_1(-H))^{-1} \tag{2.2}$$

with $r_1(z) = (z - \varphi)/(z - \psi)$.

Analogously, if we use a whole set of l parameters $\varphi_1, \cdots, \varphi_l, \psi_1, \cdots, \psi_l$, we get the iteration operator

$$\begin{aligned} &\prod_{j=1}^{l}(V - \psi_j I)^{-1}(H + \psi_j I)(H + \varphi_j I)^{-1}(V - \varphi_j I) \\ &= \prod_{j=1}^{l}(V - \varphi_j I)(V - \psi_j I)^{-1}(H + \psi_j I)(H + \varphi_j I)^{-1} = r_l(V)(r_l(-H))^{-1} \end{aligned} \tag{2.3}$$

where $r_l(z) = \prod_{j=1}^{l}(z-\varphi_j)/(z-\psi_j)$.

At this point, in the symmetric case, a theorem due to Frobenius is used which states that two symmetric commuting matrices possess a common basis of eigenvectors (cf. Varga [18, p. 220]). This implies that

$$\rho\left(r_l(V)(r_l(-H))^{-1}\right) = \max_{1\leq i\leq n} \frac{|r_l(\lambda_i)|}{|r_l(\mu_i)|} \tag{2.4}$$

where λ_i and μ_i are the corresponding eigenvalues to the (common) eigenvector $\mathbf{x}_i$ of H and V. If we do not take into account the way the eigenvalues of V are related to those of H, we get

$$\frac{\max_{\lambda\in\sigma(V)} |r_l(\lambda)|}{\min_{\mu\in-\sigma(H)} |r_l(\mu)|}$$

as best possible upper bound for the spectral radius of the ADI operator.

The same is, in principle, also true for H and V being nonsymmetric commuting matrices, as stated in the following theorem.

THEOREM 2.1. *Let $A, B \in \mathbf{R}^{n,n}$ be two arbitrary, not necessarily symmetric, matrices with $AB = BA$, then each eigenvalue of AB can be written as a product of eigenvalues of A and B. Moreover, for each eigenvalue λ of A, there is an eigenvalue μ of B such that $\lambda\mu \in \sigma(AB)$.*

Proof. The proof is an immediate consequence of the fact that for any commuting matrices A and B there exists a unitary matrix U such that $U^H AU$ and $U^H BU$ are both upper triangular (see, e.g., Marcus and Minc [12, p. 77]). ◻

Again, if we do not take into account which eigenvalue of B belongs to a specific eigenvalue of A, then we obtain

$$\frac{\max_{\lambda\in\sigma(V)} |r_l(\lambda)|}{\min_{\mu\in-\sigma(H)} |r_l(\mu)|} \tag{2.5}$$

as best possible upper bound for the spectral radius of the ADI operator. Since the eigenvalues of H and V will usually not be given explicitly, we have to use the information $\sigma(V) \subseteq E, \sigma(-H) \subseteq F$ with some disjoint compact sets $E, F \subseteq \mathbb{C}$, e.g., rectangles obtained from the application of Bendixson's theorem (cf. Stoer and Bulirsch [16, Thm. 6.9.15]). This leads to the problem of minimizing

$$\frac{\max_{z\in E} |r_l(z)|}{\min_{z\in F} |r_l(z)|} \tag{2.6}$$

among all rational functions r_l of degree l.

So far, we have seen that there is no difference in the ADI minimization problem between the symmetric and the nonsymmetric case if H and V commute. However, there is a big difference for the noncommutative case. For A and B being symmetric, we have

$$\rho(AB) = \| AB \|_2 \leq \| A \|_2 \| B \|_2 = \rho(A)\rho(B)$$

and, thus, the expression (2.6) always gives an upper bound for the ADI spectral radius. Consider the matrices

$$A = \begin{pmatrix} 1 & \alpha \\ 0 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix}$$

which both have 1 as the only eigenvalue. The eigenvalues of

$$AB = \begin{pmatrix} 1+\alpha^2 & \alpha \\ \alpha & 1 \end{pmatrix}$$

are

$$\tau_{1/2} = 1 + \frac{\alpha^2}{2}\left(1 \pm \sqrt{1+\frac{4}{\alpha^2}}\right) .$$

This means that, for $\alpha \to \infty$, $\rho(AB) \to \infty$ and, thus, the minimization problem (1.4) makes no sense for the noncommutative case.

3. Asymptotically optimal parameters: generalized Leja points. As already mentioned in the Introduction, the rational minimization problem (1.4) was solved by Zolotarev for E and F being disjoint real intervals. As a starting point for the solution of this problem in the complex case we will now consider rational functions which solve this problem at least asymptotically. The main result about the asymptotic behavior of the rational Zolotarev problem is Theorem 3.1.

THEOREM 3.1. *Let the disjoint sets E and F both be bounded by Jordan curves. Then, for the minimal value in the rational Zolotarev problem* (1.4)

$$\sigma_l(E,F) = \min_{r\in\mathbf{R}_{ll}} \frac{\max_{z\in E}|r(z)|}{\min_{z\in F}|r(z)|} \tag{3.1}$$

there exists a positive constant $\rho(E,F)$ such that

$$\sigma_l(E,F) \geq \rho(E,F)^{-l} \tag{3.2}$$

and

$$\lim_{l\to\infty}(\sigma_l(E,F))^{1/l} = \rho(E,F)^{-1} . \tag{3.3}$$

The assertions of Theorem 3.1 can be deduced directly from results of Gonchar on the rate of growth of rational functions [9]. It should be noted that Gonchar's proof of this theorem is valid for much more general sets E and F. With our strong assumptions, we have the following analytic characterization of the number $\rho(E,F)$ which appears in Theorem 3.1. Since E and F are bounded by Jordan curves, the complementary region $D := \overline{\mathbb{C}}\backslash(E\cup F)$ is doubly connected and neither E nor F reduces to a single point. It is well known that, under these assumptions, there exists a conformal map Φ of D onto a circular annulus $\{w \in \mathbb{C} : 1 < |w| < \rho(E,F)\}$ (see, e.g., Henrici [10]). The number $\rho(E,F)$, which is uniquely determined and called the *modulus* of the doubly connected region D, coincides with the number appearing in (3.2) and (3.3).

Rational functions which are asymptotically minimal, i.e., sequences of rational functions $\{r_l\}_{l\in\mathbf{N}}, r_l \in \mathbf{R}_{ll}$ with the property

$$\lim_{l\to\infty}\left(\frac{\max_{z\in E}|r_l(z)|}{\min_{z\in F}|r_l(z)|}\right)^{1/l} = \rho(E,F)^{-1} , \tag{3.4}$$

can be obtained by a generalization of the concept of *uniformly distributed nodes*, which is important in connection with polynomial interpolation in the complex plane (see Gaier [7, Chap. II.2]).

In the sequel, we will consider a generalization of the Leja points that was proposed by Bagby in [1] for the rational Zolotarev problem. Another example of asymptotically minimal rational functions is generated by a generalization of the Fejér nodes. These generalized Fejér points are the "doubly connected special case" of a point set introduced by Walsh in [22]. This approach as well as the "Faber rationals" introduced by Ganelius [8] require the knowledge of the conformal map Ψ of the annulus $\{w \in \mathbb{C} : 1 < |w| < \rho(E,F)\}$ onto D, which is known explicitly only for very rare special cases, and the numerical determination of this mapping function is, in general, very expensive. In particular, for polygonal boundary curves—like, for example, for the rectangular domains obtained with Bendixson's theorem—we could think of using Däppen's implementation of the Schwarz–Christoffel map for the doubly connected case (cf. Henrici [10, paragraph 17.5]) which is described in [5].

The generalized Leja points are defined as follows. Given $\varphi_1 \in E$ and $\psi_1 \in F$ arbitrarily, for $l = 1, 2, \cdots$, the new points $\varphi_{l+1} \in E$, $\psi_{l+1} \in F$ are chosen recursively in such a way that, with

$$r_l(z) = \prod_{j=1}^{l} \frac{z - \varphi_j}{z - \psi_j} ,$$

the two conditions

$$\begin{aligned} &\max\nolimits_{z\in E} |r_l(z)| = |r_l(\varphi_{l+1})|, \\ &\min\nolimits_{z\in F} |r_l(z)| = |r_l(\psi_{l+1})| \end{aligned} \tag{3.5}$$

are fulfilled.

Bagby shows in [1] that the rational functions r_l obtained by this procedure are asymptotically minimal for the rational Zolotarev problem. Only slight modifications of the proof lead to the following more general formulation of this result (cf. [14, Thm. 2.5]), which we will use below.

THEOREM 3.2. *Let the points $\varphi_j \in \overline{\mathbb{C}}\backslash F$, $\psi_j \in \overline{\mathbb{C}}\backslash E$, $j = 1, \cdots, k$ be given arbitrarily. Starting with these points we carry out the recursive procedure described in* (3.5)*, i.e., we determine $\varphi_l \in E$, $\psi_l \in F$, $l = k+1, k+2, \cdots$, from*

$$\begin{aligned} &\max\nolimits_{z\in E} |r_l(z)| = |r_l(\varphi_{l+1})|, \\ &\min\nolimits_{z\in F} |r_l(z)| = |r_l(\psi_{l+1})| , \end{aligned} \tag{3.6}$$

where

$$r_l(z) = \prod_{j=1}^{l} \frac{z - \varphi_j}{z - \psi_j} .$$

The sequence of rational functions obtained in this way is asymptotically minimal for (1.4)*, i.e.,*

$$\lim_{l\to\infty} \left(\frac{\max_{z\in E} |r_l(z)|}{\min_{z\in F} |r_l(z)|} \right)^{1/l} = \rho(E,F)^{-1} \tag{3.7}$$

holds.

For piecewise differentiable boundary curves the following strategy for the determination of the generalized Leja points in practice is near at hand. First, all the points on ∂E and ∂F, respectively, where the boundary is not differentiable have to be chosen as zeros, respectively as poles. After ensuring that the degrees in the numerator and denominator are equal, we compute the further points by the recursive procedure of (3.5). In practice this is now done by finding the local maximum of the function $|r(z)|^2$ on the boundary curve between two Leja points and then choosing the maximum of all these points as the new Leja point. Between two Leja nodes we can now determine the local maximum numerically by using the derivative of $|r(z)|^2$ with respect to the corresponding parametrization of the boundary, for example, with the one-dimensional minimization algorithm described in §10.3 in [13].

The generalized Leja points can be determined numerically in a relatively simple way for a large class of boundary curves ∂E and ∂F, and they have the very advantageous property that, once computed, points remain Leja points for all larger degrees. Moreover, the recursive construction automatically yields the value

$$\frac{\max_{z\in E}|r_l(z)|}{\min_{z\in F}|r_l(z)|}$$

in each step, and with this information we can increase the degree of the rational function until this value is less than a given bound.

4. Determination of the optimal parameters for $l = 2$. Assume that, using Bendixson's theorem (cf., e.g., [16, Thm. 6.9.15], we obtained the rectangle

$$E = \{z \in \mathbb{C} : \alpha \le \mathrm{Re} z \le \beta, |\mathrm{Im} z| \le \gamma\} \tag{4.1}$$

with $\sigma(H)$ and $\sigma(V)$ being contained in E. For convenience, we restrict ourselves to the case $F = -E$ here, i.e., we use the same eigenvalue bounds for the matrices H and V.

The optimal ADI parameter for $l = 1$ with respect to this information can be given explicitly. Because of the symmetry with respect to the origin we set $\psi = -\varphi$ and obtain the following solution of the minimization problem (1.4).

THEOREM 4.1. *The minimization problem*

$$\min_{\varphi\in\mathbb{R}} \frac{\max_{z\in E}|r_1(z)|}{\min_{z\in F}|r_1(z)|} \tag{4.2}$$

with

$$r_1(z) = \frac{z-\varphi}{z+\varphi} \tag{4.3}$$

is solved by

$$\varphi^* = \begin{cases} \sqrt{\alpha\beta-\gamma^2}, & \mathit{for}\ \gamma^2 \le \alpha(\beta-\alpha)/2\,; \\ \sqrt{\alpha^2+\gamma^2}, & \mathit{for}\ \gamma^2 \ge \alpha(\beta-\alpha)/2. \end{cases} \tag{4.4}$$

Proof. We have to minimize the expression

$$\max_{z\in E}\left|\frac{z-\varphi}{z+\varphi}\right| \max_{z\in -E}\left|\frac{z+\varphi}{z-\varphi}\right| = \max_{z\in E}\left|\frac{z-\varphi}{z+\varphi}\right|^2 . \tag{4.5}$$

Obviously,

$$\max_{z\in E}\left|\frac{z-\varphi}{z+\varphi}\right|^2 \ge \max_{z\in\{\alpha+i\gamma,\beta+i\gamma\}}\left|\frac{z-\varphi}{z+\varphi}\right|^2 . \tag{4.6}$$

The idea of the proof is to minimize the lower bound in (4.6) and then to show that for the optimal φ the maximum is attained at $\alpha + i\gamma$ or $\beta + i\gamma$.

Setting

$$f(\xi) = \frac{(\xi - \varphi)^2 + \gamma^2}{(\xi + \varphi)^2 + \gamma^2} ,$$

we have

$$\max_{z \in \{\alpha + i\gamma, \beta + i\gamma\}} \left| \frac{z - \varphi}{z + \varphi} \right|^2 = \max\{f(\alpha), f(\beta)\} .$$

It is easily seen that $f(\alpha) \leq f(\beta)$ for $\varphi \leq \sqrt{\alpha\beta - \gamma^2}$ and $f(\alpha) \geq f(\beta)$ for $\varphi \geq \sqrt{\alpha\beta - \gamma^2}$ and that $f(\xi)$ is minimized (with respect to φ) for $\varphi = \sqrt{\xi^2 + \gamma^2}$.

Thus, for $\gamma^2 \leq \alpha(\beta - \alpha)/2$, i.e., $\alpha\beta - \gamma^2 \geq \alpha^2 + \gamma^2$, the minimum is attained for $f(\alpha) = f(\beta)$ or $\varphi = \sqrt{\alpha\beta - \gamma^2}$ whereas for $\gamma^2 \leq \alpha(\beta - \alpha)/2$ or $\alpha\beta - \gamma^2 \leq \alpha^2 + \gamma^2$, the optimal choice is $\varphi = \sqrt{\alpha^2 + \gamma^2}$.

Now, all that is left to do to complete the proof is to show that for this optimal choice of the parameter

$$\max_{z \in E} \left| \frac{z - \varphi}{z + \varphi} \right|^2 = \max_{z \in \{\alpha + i\gamma, \beta + i\gamma\}} \left| \frac{z - \varphi}{z + \varphi} \right|^2 \tag{4.7}$$

holds. □

We are also able to construct the optimal parameters for $l = 2$, i.e., we have to consider rational functions of the form

$$r_2(z) = \frac{z^2 - \sigma_1 z + \sigma_0}{z^2 + \sigma_1 z + \sigma_0} . \tag{4.8}$$

For determining the optimal parameters $\sigma_1, \sigma_0 \in \mathbf{R}$ we first solve the *discrete problem*

$$\min \max_{z \in \{\alpha, \alpha + i\gamma, \beta + i\gamma\}} |r_2(z)|^2 \tag{4.9}$$

and then show that for the optimal rational function $r_2^*(z)$ the maximum is attained at one of these points.

LEMMA 4.2. *The minimum for* $\max\{|r_2(\alpha)|^2, |r_2(\alpha+i\gamma)|^2, |r_2(\beta+i\gamma)|^2\}$ *can only be reached for values of* σ_1, σ_0 *fulfilling one of the following four conditions*:

$$|r_2(\alpha)|^2 = |r_2(\alpha + i\gamma)|^2 \geq |r_2(\beta + i\gamma)|^2 ; \tag{4.10}$$

$$|r_2(\alpha + i\gamma)|^2 = |r_2(\beta + i\gamma)|^2 \geq |r_2(\alpha)|^2 ; \tag{4.11}$$

$$|r_2(\alpha)|^2 = |r_2(\beta + i\gamma)|^2 \geq |r_2(\alpha + i\gamma)|^2 ; \tag{4.12}$$

$$|r_2(\alpha)|^2 = |r_2(\alpha + i\gamma)|^2 = |r_2(\beta + i\gamma)|^2 . \tag{4.13}$$

Proof. Consider $|r_2(\alpha)|^2$, $|r_2(\alpha+i\gamma)|^2$, or $|r_2(\beta+i\gamma)|^2$ as functions of σ_1 and σ_0, i.e.,

$$f_1(\sigma_1,\sigma_0)=|r_2(\alpha)|^2,\quad f_2(\sigma_1,\sigma_0)=|r_2(\alpha+i\gamma)|^2,\quad f_3(\sigma_1,\sigma_0)=|r_2(\beta+i\gamma)|^2.$$

The minimum of any of these functions is zero and is attained for any pair of numbers (σ_1,σ_0) satisfying $\sigma_1=\alpha+\sigma_0/\alpha$ for f_1 and at the points $(\sigma_1,\sigma_0)=(2\alpha,\alpha^2+\gamma^2)$ and $(\sigma_1,\sigma_0)=(2\beta,\beta^2+\gamma^2)$ for f_2 and f_3, respectively. Moreover, these are the only local minimum points of these functions.

This implies that it is impossible for $\max\{|r_2(\alpha)|^2,|r_2(\alpha+i\gamma)|^2,|r_2(\beta+i\gamma)|^2\}$ to be minimized at points where the values of f_1, f_2 and f_3 are pairwise distinct—since there are σ_1,σ_0 in each neighborhood where the largest of these three functions is smaller—and, thus, the minimum can only be obtained if one of the four conditions (4.10), (4.11), (4.12), or (4.13) holds. $\square$

Each one of the first three conditions (4.10), (4.11), and (4.12) leads to a relation between σ_1^2 and σ_0. For (4.10), $|r_2(\alpha)|=|r_2(\alpha+i\gamma)|$ gives

$$\sigma_1^2=3\sigma_0+2\alpha^2-\gamma^2-\frac{\alpha^2(\alpha^2+\gamma^2)}{\sigma_0}, \tag{4.14}$$

whereas $|r_2(\alpha+i\gamma)|=|r_2(\beta+i\gamma)|$ of (4.11) leads to

$$\sigma_1^2=\frac{\sigma_0^3+\tau_2\sigma_0^2+\tau_1\sigma_0+\tau_0}{(\alpha\beta-\gamma^2)\sigma_0-(\alpha^2+\gamma^2)(\beta^2+\gamma^2)} \tag{4.15}$$

with $\tau_2=\alpha^2-\alpha\beta+\beta^2-\gamma^2$, $\tau_1=-\left(\gamma^4+2(\alpha^2+3\alpha\beta+\beta^2)\gamma^2+\alpha\beta(\alpha^2-\alpha\beta+\beta^2)\right)$ and $\tau_0=-(\alpha^2+\gamma^2)(\beta^2+\gamma^2)(\alpha\beta-\gamma^2)$ and $|r(\alpha)|=|r(\beta+i\gamma)|$ implies

$$\sigma_1^2=\frac{(\beta-\alpha)\sigma_0^3+\tau_2\sigma_0^2+\tau_1\sigma_0+\tau_0}{\alpha\left((\beta^2+\gamma^2-\alpha\beta)\sigma_0-\alpha(\beta-\alpha)(\beta^2+\gamma^2)\right)} \tag{4.16}$$

with $\tau_2=(2\alpha+\beta)\gamma^2+(\beta-\alpha)(\alpha^2-\alpha\beta+\beta^2)$, $\tau_1=(\beta-\alpha)\alpha\beta(\alpha\beta-\alpha^2-\beta^2)-\alpha\gamma^2(\gamma^2+2(\beta^2-\alpha^2-\alpha\beta))$ and $\tau_0=-\alpha^3(\beta^2+\gamma^2)(\beta^2+\gamma^2-\alpha\beta)$.

This means that each one of these three conditions leads us to a *one-dimensional minimization problem* which can be solved without much effort by standard algorithms like the "golden section search" algorithm (cf. [13, p. 277]).

The last condition (4.13) where all three values are equal leads to the polynomial equation of order 4 for σ_0 given by

(4.17)

$$\sigma_0^4+(\alpha^2-4\alpha\beta+\beta^2+2\gamma^2)\sigma_0^3+\left[\gamma^4-5\alpha\beta\gamma^2+4\alpha^2\beta^2+(3\alpha^2+\beta^2)(\gamma^2-\alpha\beta)\right]\sigma_0^2$$
$$+(\alpha^2+\gamma^2)\left[\gamma^2(\alpha-\beta)\alpha+\alpha\beta(2\alpha\beta-\beta^2+\alpha^2)\right]\sigma_0-\alpha(\alpha^2+\gamma^2)^2(\beta^2+\gamma^2)=0\,.$$

The procedure for obtaining the optimal parameters for $l=2$ is as follows. Solve each one of the three minimization problems with respect to one parameter corresponding to (4.10), (4.11), and (4.12) above and verify if the conditions

$$|r_2(\alpha)|^2=|r_2(\alpha+i\gamma)|^2\ge|r_2(\beta+i\gamma)|^2 \quad \text{for (4.10)},$$
$$|r_2(\alpha+i\gamma)|^2=|r_2(\beta+i\gamma)|^2\ge|r_2(\alpha)|^2 \quad \text{for (4.11)},$$
$$|r_2(\alpha)|^2=|r_2(\beta+i\gamma)|^2\ge|r_2(\alpha+i\gamma)|^2 \quad \text{for (4.12)}$$

are fulfilled. Then, compute the solutions of equation (4.13) and take those parameters which give the minimal value of these four cases.

To finally justify our approach, we have to show that

$$|r_2(z)| \le \max\{|r_2(\alpha)|, |r_2(\alpha+i\gamma)|, |r_2(\beta+i\gamma)|\} \quad \text{for } z \in E \tag{4.18}$$

holds. Though we are not able to prove this for the general case, (4.18) was always fulfilled in our computational examples. For the important special case where $\beta = \alpha$, i.e., the spectra of H and V are contained in an interval of the complex plane (see the example in the following section), this is contained in the following theorem. Moreover, we are even able to give an explicit formula for the solution in this case.

THEOREM 4.3. *For $\alpha = \beta$, i.e.,*

$$E = \{z \in \mathbb{C} : \operatorname{Re} z = \alpha, |\operatorname{Im} z| \le \gamma\}, \tag{4.19}$$

the optimal rational function r_2^* is given by

$$r_2^*(z) = \frac{z^2 - \sigma_1^* z + \sigma_0^*}{z^2 + \sigma_1^* z + \sigma_0^*} \tag{4.20}$$

with

$$\sigma_1^* = \sqrt{4\alpha^2 + \gamma^2},$$
$$\sigma_0^* = \frac{1}{3}\sqrt{\alpha^2+\gamma^2}\left(\sqrt{\alpha^2+\gamma^2} + \sqrt{4\alpha^2+\gamma^2}\right),$$

and

$$\begin{aligned} \max_{z\in E} |r_2^*(z)| &= \max_{z \in \{\alpha, \alpha+i\gamma\}} |r_2^*(z)| = r_2^*(\alpha) \\ &= \frac{\sqrt{4\alpha^2+\gamma^2} + \sqrt{\alpha^2+\gamma^2} - 3\alpha}{\sqrt{4\alpha^2+\gamma^2} + \sqrt{\alpha^2+\gamma^2} + 3\alpha}. \end{aligned} \tag{4.21}$$

Proof. For any admissible rational function

$$r_2(z) = \frac{z^2 - \sigma_1 z + \sigma_0}{z^2 + \sigma_1 z + \sigma_0},$$

using (4.14) we get

$$\begin{aligned} \frac{d}{d\eta}|r_2(\alpha+i\eta)|^2 &= \frac{8\sigma_1\alpha\eta\left[\eta^4 + 2(\alpha^2+\sigma_0)\eta^2 + \alpha^4 - 2\sigma_0\alpha^2 - 3\sigma_0^2 + \sigma_0\sigma_1^2\right]}{\left[(\alpha^2 - \eta^2 + \sigma_1\alpha + \sigma_0)^2 + \eta^2(2\alpha+\sigma_1)^2\right]^2} \\ &= \frac{8\sigma_1\alpha\eta\left[\eta^4 + (\alpha^2+\sigma_0)(2\eta^2 - \gamma^2)\right]}{\left[(\alpha^2 - \eta^2 + \sigma_1\alpha + \sigma_0)^2 + \eta^2(2\alpha+\sigma_1)^2\right]^2}. \end{aligned}$$

This implies that there is a local maximum for $\eta = 0$ and only one further local extremum point for $\eta > 0$ which has to be a minimum.

In particular, the maximum is always attained for $z = \alpha$ and, since $r_2(\alpha) > 0$, it is sufficient to minimize $r_2(\alpha)$ with respect to σ_0 and σ_1. Setting

$$\frac{d}{d\sigma_0} r_2(\alpha) = \frac{d}{d\sigma_0}\frac{\alpha^2 - \sigma_1\alpha + \sigma_0}{\alpha^2 + \sigma_1\alpha + \sigma_0} = 0$$

(note that σ_1 depends on σ_0 via (4.14)) leads to

$$3\sigma_0^3 + (\alpha^2 - 2\gamma^2)\sigma_0^2 - 3\alpha^2(\alpha^2+\gamma^2)\sigma_0 - \alpha^4(\alpha^2+\gamma^2) = 0$$

with the (one) positive solution

$$\sigma_0^* = \frac{1}{3}\sqrt{\alpha^2+\gamma^2}\left(\sqrt{\alpha^2+\gamma^2} + \sqrt{4\alpha^2+\gamma^2}\right).$$

From (4.14) we obtain $\sigma_1^* = \sqrt{4\alpha^2+\gamma^2}$. □

5. Numerical results. We will test our methods for the following *model problem* which arises from the discretization of a *convection diffusion equation* (cf., e.g., Chin and Manteuffel [3]). Consider the boundary value problem

$$\begin{aligned} &-\Delta u + a(y)u_y + b(x)u_x + cu = f(x,y), \qquad (x,y) \in S,\\ &u(x,y) = g(x,y), \qquad (x,y) \in \partial S \end{aligned} \tag{5.1}$$

on the unit square $S := \{(x,y) \in \mathbf{R}^2 : 0 < y < 1, 0 < x < 1\}$ with the boundary ∂S. Here, the functions $a, b : [0,1] \to \mathbf{R}$ are assumed to be continuously differentiable, $f : S \cup \partial S \to \mathbf{R}$ and $g : \partial S \to \mathbf{R}$ to be continuous and c to be a nonnegative constant.

Instead of writing the equation obtained from the discretization of this problem as a large linear system we will use the notation as a matrix equation $AX - XB = C$. We describe now how such a matrix equation is obtained from the discretization of (5.1) using central differences with stepsize $h = 1/(n+1)$. Our aim is to enumerate the elements u_{ij} of the unknown matrix X in such a way that u_{ij} stands for the approximate value of the function in the ith row and jth column of the mesh. Thus, we set $u_{ij} := u(x_j, y_i)$ with $x_j := jh$, $j = 1,\cdots,n$, $y_i := ih$, $i = 1,\cdots,n$. With respect to this numbering the multiplication of X from the left by the matrix

$$A = \begin{pmatrix} 2+\frac{c}{2}h^2 & -1+\frac{h}{2}a_1 & & \\ -1-\frac{h}{2}a_2 & \ddots & \ddots & \\ & \ddots & \ddots & -1+\frac{h}{2}a_{n-1} \\ & & -1-\frac{h}{2}a_n & 2+\frac{c}{2}h^2 \end{pmatrix} \tag{5.2}$$

just stands for applying the difference operator corresponding to the discretization in y-direction. Similarly, the multiplication from the right with

$$B = -\begin{pmatrix} 2+\frac{c}{2}h^2 & -1-\frac{h}{2}b_2 & & \\ -1+\frac{h}{2}b_1 & \ddots & \ddots & \\ & \ddots & \ddots & -1-\frac{h}{2}b_n \\ & & -1+\frac{h}{2}b_{n-1} & 2+\frac{c}{2}h^2 \end{pmatrix} \tag{5.3}$$

arises from the discretization in x-direction. Here, $a_i := a(y_i), i = 1,\cdots,n$ and $b_j := b(x_j), j = 1,\cdots,n$ denote the values of the functions a and b, respectively, at the gridpoints. The right-hand side consists of the discrete values of $f(x,y)$ and in the first and last row and column of the boundary values $g(x,y)$.

It is, of course, possible to write this matrix equation $AX - XB = C$ as a large linear system $(H+V)\mathbf{u} = \mathbf{b}$ of dimension n^2. If we put the coefficients of the unknown matrix X row by row into the vector

$$\mathbf{u} = (u_{11},\cdots,u_{1n},\cdots,u_{n1},\cdots,u_{nn})^T$$

we obtain a linear system of equations with the coefficient matrix

$$A \otimes I_n - I_n \otimes B^T = \begin{pmatrix} a_{11}I_n - B^T & a_{12}I_n & \cdots & a_{1n}I_n \\ a_{21}I_n & a_{22}I_n - B^T & \cdots & a_{2n}I_n \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1}I_n & a_{n2}I_n & \cdots & a_{nn}I_n - B^T \end{pmatrix} \tag{5.4}$$

where $\otimes$ denotes the standard *Kronecker product* (cf. Barnett [2, p. 165]). In our standard notation, $H = -I_n \otimes B^T$ and $V = A \otimes I_n$; hence, $\sigma(H) = -\sigma(B)$ and $\sigma(V) = \sigma(A)$.

To obtain useful bounds for the eigenvalues of A and B, instead of applying Bendixson's theorem (see, e.g. [16, Thm. 6.9.15]) directly, we should at first carry out the following similarity transformation.

It is easily seen, by looking at the characteristic polynomials of the principal submatrices, that the matrix A of (5.2) has the same eigenvalues as

$$\tilde{A} = \frac{2}{h^2} + \frac{c}{2} + \frac{1}{h^2}\begin{pmatrix} 0 & \tau_1 & & \\ \tau_1 & \ddots & \ddots & \\ & \ddots & \ddots & \tau_{n-1} \\ & & \tau_{n-1} & 0 \end{pmatrix} \tag{5.5}$$

with $\tau_i := ((1 - \frac{h}{2}a_i)(1 + \frac{h}{2}a_{i+1}))^{1/2}, i = 1, \cdots, n-1$. The coefficients of this matrix are either real or purely imaginary depending on the modulus of the *grid Reynolds numbers* $\sigma_i := \frac{h}{2}a_i$ being greater or less than 1. Splitting $\tilde{A}$ into its Hermitian and skew-Hermitian part leads to rectangular bounds for the spectrum which are much better than the direct application of Bendixson's theorem. Of course, the matrix B should be handled in the same way.

For linear systems of the special form (5.4) we have to solve a whole set of n linear systems with the coefficient matrix $B^T \in \mathbf{R}^{n,n}$ in the first halfstep of the ADI iteration (1.2) and, analogously, n linear sytems with the matrix $A \in \mathbf{R}^{n,n}$ in the second halfstep. Independently from the method used for solving these systems we have some kind of "natural" *parallelism* in the ADI method if we solve the n linear systems with the same coefficient matrix at the same time using n processors. One step of the block SOR method applied to this problem also requires the solution of n linear systems with the coefficient matrix B^T but this cannot be parallelized in the same way (cf. [15]).

Without taking into consideration the saving of computational time caused by parallelization it can be said that the ADI method needs about twice as many operations per iteration step as the SOR method. Thus, roughly speaking, the error reduction per halfstep of ADI has to be compared with one SOR step.

In our model problem, the parameters for the ADI method often occur in complex conjugate pairs. To avoid complex calculations it seems useful to combine two successive iteration steps

$$\mathbf{u}^{(j+1)} = (V - \psi I)^{-1}(H + \varphi I)^{-1}[(H + \psi I)(V - \varphi I)\mathbf{u}^{(j)} + (\varphi - \psi)\mathbf{c}]$$

and

$$\mathbf{u}^{(j+2)} = (V - \overline{\psi} I)^{-1}(H + \overline{\varphi} I)^{-1}[(H + \overline{\psi} I)(V - \overline{\varphi} I)\mathbf{u}^{(j+1)} + (\overline{\varphi} - \overline{\psi})\mathbf{c}]\,.$$

With the abbreviations $(z-\varphi)(z-\overline{\varphi}) = z^2 - \sigma_1 z + \sigma_0$, $(z-\psi)(z-\overline{\psi}) = z^2 - \tau_1 z + \tau_0$, i.e., $\sigma_1 = 2\operatorname{Re}\varphi$, $\sigma_0 = |\varphi|^2$, and $\tau_1 = 2\operatorname{Re}\psi$, $\tau_0 = |\psi|^2$, we obtain

$$\begin{aligned}
\mathbf{u}^{(j+2)} &= (V^2 - \tau_1 V + \tau_0 I)^{-1}(H^2 + \sigma_1 H + \sigma_0 I)^{-1} \\
&\quad \cdot \Bigg[(H^2 + \tau_1 H + \tau_0 I)(V^2 - \sigma_1 V + \sigma_0 I)\mathbf{u}^{(j)} \\
&\quad + (\sigma_1 - \tau_1)\Bigg[\left(H + \frac{\sigma_0 - \tau_0}{\sigma_1 - \tau_1} I\right)\left(V - \frac{\sigma_0 - \tau_0}{\sigma_1 - \tau_1} I\right) \\
&\quad + \left(\left(\frac{\sigma_0 - \tau_0}{\sigma_1 - \tau_1}\right)^2 - \frac{\sigma_0\tau_1 - \tau_0\sigma_1}{\sigma_1 - \tau_1}\right) I \Bigg] \mathbf{c} \Bigg].
\end{aligned} \tag{5.6}$$

The systems that we have to solve in (5.6) for our model problem are no longer tridiagonal but pentadiagonal. However, these systems can be solved in a similar way by Gaussian elimination where, in general, we do not need any pivoting.

These observations imply that we should try to get the ADI parameters either real or in complex conjugate pairs. This is always the case if we determine the optimal parameters, e.g., for $l = 2$, by the technique presented in §4 if only the associated sets are symmetric with respect to the real line, but it is, in general, not true for the generalized Leja points of §3. Here, it is useful to take also the complex conjugate to each Leja point as a parameter.

Example. Consider the Dirichlet problem (5.1) for $a(y) = \delta(1+y)/2$ and $b(x) = \delta(1+x)/2$. Discretizing this problem by central differences leads to a matrix equation $AX - XB = C$ with

$$A = 2 + \begin{pmatrix} 0 & -1+\sigma_1 & & \\ -1-\sigma_2 & \ddots & \ddots & \\ & \ddots & \ddots & -1+\sigma_{n-1} \\ & & -1-\sigma_n & 0 \end{pmatrix} \tag{5.7}$$

and $B = -A^T$ where $\sigma_i := \frac{h}{2}\delta(1+ih)/2, i = 1, \cdots, n$. This means that the grid Reynolds numbers σ_i vary between $\frac{h}{2}\delta$ and $\frac{h}{4}\delta$. From the application of Bendixson's theorem to the corresponding matrix $\tilde{A}$ (cf. (5.5)) for $h = 0.01$ we get rectangles

$$E = \{z \in \mathbb{C} : \alpha \le \operatorname{Re} z \le \beta, |\operatorname{Im} z| \le \gamma\}$$

and $F = -E$ with the numbers α, β, γ listed in Table 5.1. There, σ is the maximum grid Reynolds number, i.e., $\sigma = \frac{h}{2}\delta$ in this example. The columns denoted by ADI/opt(1), ADI/opt(2), and ADI/Leja(22) contain the numbers

$$\left(\max_{z\in E} |r_l(z)|\right)^{1/l}$$

for the optimal 1 and 2 parameters and for 22 "symmetrized" Leja points—starting with the six points $\alpha, \alpha \pm i\gamma, \beta, \beta \pm i\gamma$ we computed the next eight points by the Leja recursion and, in addition, took the eight complex conjugate numbers as ADI parameters—being used where l denotes the number of the parameters. This can be seen as the "average convergence factor" per halfstep of the ADI method and, thus, is

TABLE 5.1
ADI *for the model problem.*

σ	α	β	γ	ADI/opt(1)	ADI/opt(2)	ADI/Leja(22)	SOR
0	0.0010	3.9990	0	0.9687	0.8355	0.6600	0.9150
1	0.3364	3.6636	0	0.5349	0.3822	0.3000	0.1750
1.2	0.4894	3.5106	1.1581	0.6630	0.6396	0.5866	0.5651
1.4	0.6852	3.3148	1.7815	0.6868	0.5944	0.5734	0.5684
1.6	0.9426	3.0574	2.3037	0.6713	0.5767	0.5378	0.5266
1.8	1.3110	2.6890	2.7806	0.6341	0.5349	0.4881	0.4580
2	2	2	3.2320	0.5572	0.4438	0.3607	0.3700
3	2	2	5.3321	0.6929	0.5886	0.5062	0.7429
4	2	2	7.3056	0.7630	0.6724	0.6034	0.9702
5	2	2	9.2512	0.8069	0.7282	0.6741	—

the number to be compared with the spectral radius of the SOR method. The optimal SOR parameter was computed by the procedure described in [15] and the spectral radius is taken from Table 1 in that paper.

In this example, for $\sigma \leq 1$ we have real, for $\sigma \geq 2$ complex intervals as eigenvalue domains. For $1 < \sigma < 2$ both the Hermitian and the skew-Hermitian parts of $\tilde{A}$ and $\tilde{B}$ (cf. (5.5)) do not vanish and, thus, E and F are rectangles.

Table 5.1 shows that the improvement using 22 Leja points instead of the 2 optimal parameters is surprisingly small compared to the improvement caused by using 2 instead of 1 parameter. Here, it can be observed that ADI is superior to SOR for very small grid Reynolds numbers (symmetrizable case) and for values of σ larger than 2. However, the ADI method should also be preferred for problems where the convergence of SOR is "theoretically faster" because of two reasons. First, the "natural parallelism" of the method described above can be used for implementations and, second, it can often be observed that the asymptotic convergence behavior is reached after relatively few ADI steps (cf. [14, Figs. 3.3 and 3.6]).

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