An Implicit Algorithm for Computing the Minimal Geršgorin Set

S. Milićević[a], V. R. Kostić[b], Lj. Cvetković[b], A. Miedlar[c]

[a]*Department for Applied Fundamental Disciplines, Faculty of Technical Sciences, University of Novi Sad, Trg D. Obradovića 6, 21000 Novi Sad, Serbia.*
[b]*Department of Mathematics and Informatics, Faculty of Science, University of Novi Sad, Trg D. Obradovića 4, 21000 Novi Sad, Serbia.*
[c]*Department of Mathematics, University of Kansas, 1460 Jayhawk Blvd, Lawrence, KS 66045-7594, USA.*

Abstract. In this paper we present a new algorithm for the computation of the minimal Geršgorin set that can be considered an extension of the results from [5]. While the general approach to calculation of the boundary of the minimal Geršgorin set is kept, the core numerical calculation is changed. Namely, the problem is formulated in such a way that the eigenvalue computations are replaced by LU decompositions, allowing the algorithm to be used for larger matrices more efficiently. To illustrate the benefits, we compare both algorithms on several test matrices.

1. Introduction

While the research on minimal Geršgorin set (MGS) provided many interesting (theoretical) results, [7], one can not find in the literature many algorithms for computing this localization of the matrix spectrum. The reason for this probably lies in the fact that the boundary of the MGS is itself defined as an eigenvalue problem (of the same size as the given matrix). Thus, one may well ask why one would need to compute many eigenvalues in order to obtain (sometimes very crude) approximation of the spectrum. Nevertheless, the usefulness of the MGS is not solely based on the fact that it contains the spectrum of the matrix. It can be used for determining the stability of time dependent dynamical systems, [5]. In addition, it represents the optimality of the result on the set of extended family of equimodular matrices. Taking into account the previous argument, in this paper we wish to reformulate the boundary of the MGS in order to avoid the unnecessary eigenvalue computations and in such a way decrease the numerical cost of the computation of the MGS. To that end, we start with the algorithm eMGS from [5] that is summarized with some preliminaries in Section 2. Then, in Section 3, we provide the main results and we conclude the paper with numerical tests in Section 4.

2. Preliminaries

Given any matrix $A = [a_{ij}] \in \mathbb{C}^{n,n}$, $i, j \in \{1, 2, \ldots, n\}$, let $\sigma(A)$ denote its spectrum, i.e.,

$$\sigma(A) := \{\lambda \in \mathbb{C} : \det(\lambda I - A) = 0\}, \tag{1}$$

where I is the identity matrix of a size n, $n \in \mathbb{N}$. For any $\lambda \in \sigma(A)$, there exists $i \in \{1, 2, \ldots, n\}$ such that

$$\lambda \in \Gamma_i(A) := \left\{ z \in \mathbb{C} : |z - a_{ii}| \leq r_i(A) := \sum_{j \neq i}^{n} |a_{ij}| \right\}. \tag{2}$$

The set $\Gamma(A) := \bigcup_{i=1}^{n} \Gamma_i(A)$ is called *the Geršgorin set*, [7].

Given a positive vector $x = [x_1, x_2, \ldots, x_n] > 0$ and a diagonal matrix $X := diag(x) \in \mathbb{R}^{n,n}$, the Geršgorin disks for the matrix $X^{-1}AX$ are given by

$$\Gamma_i^{r^x}(A) := \left\{ z \in \mathbb{C} : |z - a_{ii}| \leq r_i^x(A) := \sum_{j \neq i}^{n} \frac{|a_{ij}|x_j}{x_i} \right\}, \quad \text{for } i \in \{1, 2, \ldots, n\}. \tag{3}$$

Moreover, the associated Geršgorin set is defined as

$$\Gamma^{r^x}(A) := \bigcup_{i=1}^{n} \Gamma_i^{r^x}(A). \tag{4}$$

The set

$$\Gamma^{\mathcal{R}}(A) := \bigcap_{x \in \mathbb{R}^n,\ x > 0} \Gamma^{r^x}(A) \tag{5}$$

is called *the minimal Geršgorin set* and $\sigma(A) \subseteq \Gamma^{\mathcal{R}}(A) \subseteq \Gamma(A)$.

The set $\Gamma^{\mathcal{R}}(A)$ is interesting because it gives, in a certain sense, the sharpest inclusion set for $\sigma(A)$ among all Geršgorin-type sets [4]. As it was mentioned in Introduction, some motivations for constructing the minimal Geršgorin set are provided in [5]. In the same paper, the numerical procedures for its computation are derived, the most advanced being the algorithm called eMGS based on the following characterization of the minimal Geršgorin set and the properties of its boundary.

Definition 2.1. *Given a matrix $A = [a_{ij}] \in \mathbb{C}^{n,n}$ and a scalar $z \in \mathbb{C}$, an essentially non-negative matrix $Q_A(z) = [q_{ij}(z)]$ is given by:*

$$q_{ii}(z) := -|z - a_{ii}| \quad \text{and} \quad q_{ij}(z) := |a_{ij}|, \quad \text{for } i, j \in \{1, 2, \ldots, n\}, \ i \neq j. \tag{6}$$

The real valued function

$$\nu_A(z) := \inf_{x > 0} \max_{i \in \{1,2,\ldots,n\}} (r_i^x(A) - |z - a_{ii}|), \tag{7}$$

can be obtained as the right-most eigenvalue of $Q_A(z)$.

Using the function $\nu_A(z)$, the set $\Gamma^{\mathcal{R}}(A)$ can be characterized by the following theorem.

Theorem 2.2. *([7, Proposition 4.3]) For any $A = [a_{ij}] \in \mathbb{C}^{n,n}$, $n \geq 2$, then $z \in \Gamma^{\mathcal{R}}(A)$ if and only if $\nu_A(z) \geq 0$. If $z \in \partial\Gamma^{\mathcal{R}}(A)$, then $\nu_A(z) = 0$.*

Theorem 2.3. *([7, Theorem 4.6]) For any irreducible matrix $A = [a_{ij}] \in \mathbb{C}^{n,n}$, $n \geq 2$, then $\nu_A(a_{ii}) > 0$, for every $i \in \{1, 2, \ldots, n\}$. Moreover, for each a_{ii} and each real θ, $0 \leq \theta \leq 2\pi$, let $\widehat{\rho_i}(\theta)$ be the smallest $\rho > 0$ for which*

$$\nu_A(a_{ii} + \widehat{\rho_i}(\theta)e^{i\theta}) = 0 \tag{8}$$

and there is a sequence of complex numbers $\{z_j\}_{j=1}^{\infty}$ with $\lim\limits_{j\to\infty} z_j = a_{ii} + \widehat{\rho_i}(\theta)e^{i\theta}$, such that $\nu_A(z_j) < 0$, $j \in \mathbb{N}$. Then,

the complex interval $[a_{ii} + te^{i\theta}]_{t=0}^{\widehat{\rho_i}(\theta)}$ is contained in $\Gamma^{\mathcal{R}}(A)$, i.e.,

$$\bigcup_{\theta=0}^{2\pi}[a_{ii} + te^{i\theta}]_{t=0}^{\widehat{\rho_i}(\theta)} \tag{9}$$

is a star-shaped *subset of* $\Gamma^{\mathcal{R}}(A)$.

Based on the previous theorems, the algorithm eMGS from [5] is obtained by fixing a diagonal entry $\xi = a_{ii}$ of a matrix as a center of the star-shaped subset whose boundary we wish numerically to approximate. Then, for different values of $\theta \in [0, 2\pi]$, the function $f_A^{\xi,\theta} : \mathbb{R} \to \mathbb{R}$ is defined by $f_A^{\xi,\theta}(t) := \nu_A(\xi + te^{i\theta})$, and the value $\rho(\theta)$ is computed as a zero of the function $f_A^{\xi,\theta}$ that is the closest to the center ξ via a Newton-like method. To that end, one needs to repeatedly compute function and derivative values. This is performed by computing the Perron eigenvalue $f_A^{\xi,\theta}(t)$ with left and right eigenvectors $x_A^{\xi,\theta}(t) > 0$ and $y_A^{\xi,\theta}(t) > 0$, respectively, i.e.,

$$\begin{aligned}
Q_A(\xi + te^{i\theta})x_A^{\xi,\theta}(t) &= f_A^{\xi,\theta}(t)x_A^{\xi,\theta}(t), \\
Q_A(\xi + te^{i\theta})^T y_A^{\xi,\theta}(t) &= f_A^{\xi,\theta}(t)y_A^{\xi,\theta}(t), \quad \text{and} \\
\frac{\partial}{\partial t} f_A^{\xi,\theta}(t) &= \frac{y_A^{\xi,\theta}(t)^T \frac{\partial}{\partial t} Q_A(\xi + te^{i\theta})x_A^{\xi,\theta}(t)}{y_A^{\xi,\theta}(t)^T x_A^{\xi,\theta}(t)}.
\end{aligned} \tag{10}$$

Once for fixed ξ and θ, $\rho(\theta)$ is computed, eMGS changes the angle θ in appropriate way to move along the boundary curve of a disjoint component of the minimal Geršgorin set, and, if needed changes the center ξ so that the whole curve can be passed using the following property.

Lemma 2.4. *([5]) Given an arbitrary irreducible matrix $A \in \mathbb{C}^{n,n}$, for every point $\omega \in \partial\Gamma^{\mathcal{R}}(A)$ there exists sufficiently small $\varepsilon > 0$ and an index $1 \le i \le n$ such that for all $\alpha \in [0, 1]$ and $z \in \mathbb{C}$ satisfying $|z - \omega| < \varepsilon$, $arg(z - a_{ii}) > arg(\omega - a_{ii})$ and $z \in \partial\Gamma^{\mathcal{R}}(A)$, it holds that $\alpha z + (1 - \alpha)a_{ii} \in \Gamma^{\mathcal{R}}(A)$.*

Once a closed boundary curve is constructed as a new polygon in the complex plane, the algorithm continues by checking if there are diagonal entries included in its exterior. In that case a new polygon is constructed around such a diagonal entry.

Finally, the important condition of irreducibility needed in the previous theorems can always be guaranteed since, for every $A \in \mathbb{C}^{n,n}$, $n \ge 2$, there always exists its normal reduced form

$$PAP^T = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ & A_{22} & \dots & A_{2m} \\ & & \ddots & \vdots \\ & & & A_{mm} \end{bmatrix},$$

where P is a permutation matrix and the diagonal blocks $A_{ii} \in \mathbb{C}^{n_i,n_i}$ are either 1×1 or irreducible $n_i \times n_i$ matrices, $n_i \ge 2$, $i \in \{1, 2, ..., m\}$. Thus, the computation of the minimal Geršgorin set for a general matrix can be obtained from the computations of the irreducible diagonal parts of its normal reduced form, as stated in the following theorem.

Lemma 2.5. *([5]) Given an arbitrary matrix $A = [a_{ij}] \in \mathbb{C}^{n,n}$, let $A_{ii} \in \mathbb{C}^{n_i,n_i}$ denote the i-th diagonal block of its normal reduced form, $n_i \ge 1$, $i \in \{1, 2, ..., m\}$. Then*

$$\Gamma^{\mathcal{R}}(A) = \bigcup_{i=1}^{m} \Gamma^{\mathcal{R}}(A_{ii}).$$

Here we omit further technical details needed for the full understanding and implementation of the eMGS algorithm, and refer the reader to [5].

For a Z-matrix $A = [a_{ij}] \in \mathbb{R}^{n,n}$ ($a_{ij} \leq 0$, $i, j \in \{1, 2, ..., n\}$, $i \neq j$), the following statements are equivalent:

- A is a nonsingular M-matrix.

- $A^{-1} \geq 0$.

- There exists a vector $x \in \mathbb{R}^n$, $x \geq 0$, such that $Ax > 0$.

- The real part of each eigenvalue of A is positive.

To end the preliminaries, in the following, we will use the well-known formula for inversion of a block matrix. Namely, if a matrix M is partitioned into four blocks, i.e., $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$, where matrices A and D are square and A and $E := D - CA^{-1}B$ are nonsingular, using the Schur complement, we have

$$M^{-1} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} + A^{-1}BE^{-1}CA^{-1} & -A^{-1}BE^{-1} \\ -E^{-1}CA^{-1} & E^{-1} \end{bmatrix}, \tag{11}$$

and

$$\det(M) = \det(A)\det(E). \tag{12}$$

3. Algorithm iMGS

In this section, we present the original results that are the basis for the construction of a new algorithm for numerical approximation of the minimal Geršgorin set. This new algorithm will be called an implicit algorithm, abbreviated **iMGS**, as the main idea is to avoid explicit computation of Perron eigentriplets within the algorithm **eMGS**, from the previous section, by replacing function $f_A^{\xi,\theta}$ with a new function $h_A^{\xi,\theta}$ that reveals Perron eigenvalue implicitly through the solution of a structured system of linear equations. The motivation for this approach to significantly reduce the overall number of expensive eigenvalue computations can be found in the idea of the implicit determinant method given in [3] and [6].

Given an arbitrary irreducible matrix $A \in \mathbb{C}^{n,n}$, a complex number ξ and a real $0 \leq \theta < 2\pi$, let us fix a vector $c \in \mathbb{R}^n$, $c > 0$ and for every $t \geq 0$ construct a system of linear equations

$$\underbrace{\begin{bmatrix} -Q_A(\xi + t e^{i\theta}) & -c \\ -c^T & 0 \end{bmatrix}}_{M_A^{\xi,\theta}(t)} \begin{bmatrix} x_A^{\xi,\theta}(t) \\ g_A^{\xi,\theta}(t) \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \tag{13}$$

where $Q_A(\xi + t e^{i\theta})$ is given by Definition 2.1. Assuming that $M_A^{\xi,\theta}(t)$ is nonsingular, (13) can be uniquely solved, and Cramer's rule provides that

$$g_A^{\xi,\theta}(t) := -\frac{\det(-Q_A(\xi + t e^{i\theta}))}{\det(M_A^{\xi,\theta}(t))}, \tag{14}$$

defines a function that becomes zero whenever matrix $Q_A(z)$ becomes singular in a point $z = \xi + t e^{i\theta}$. In the following we see how $g_A^{\xi,\theta}$ can be used instead of a ν_A to characterize the boundary of the minimal Geršgorin set.

Theorem 3.1. *Given an arbitrary irreducible matrix $A \in \mathbb{C}^{n,n}$, a complex number ξ, a real $0 \leq \theta < 2\pi$ and $c \in \mathbb{R}^n$, $c > 0$ arbitrary positive vector, let $\widehat{t} > 0$ be maximal such that $\xi + t e^{i\theta} \in \Gamma^{\mathcal{R}}(A)$, for all $t \in [0, \widehat{t}]$. Then, there exists $\varepsilon > 0$ such that $M_A^{\xi,\theta}(t)$ is a nonsingular matrix for all $t \in [\widehat{t} - \varepsilon, \widehat{t} + \varepsilon]$. Consequently, (13) defines an ∞-differentiable functions $g_A^{\xi,\theta}$ and $x_A^{\xi,\theta}$ on $[\widehat{t} - \varepsilon, \widehat{t} + \varepsilon]$.*

Proof. First let us show that matrix $M_A^{\xi,\theta}(\widehat{t})$ is nonsingular. Assume that $M_A^{\xi,\theta}(\widehat{t})$ is singular. As the positions of zero entries outside the main diagonal of A and $Q_A(\xi + \widehat{t} e^{i\theta})$ are the same and $c > 0$, the fact that the matrix A is irreducible implies the irreducibility of matrices $Q_A(\xi + \widehat{t} e^{i\theta})$ and $M_A^{\xi,\theta}(\widehat{t})$. Let $[v \; \alpha]^T$ be the right eigenvector of the matrix $M_A^{\xi,\theta}(\widehat{t})$ corresponding to the zero eigenvalue, i.e.,

$$\begin{bmatrix} -Q_A(\xi + \widehat{t} e^{i\theta}) & -c \\ -c^T & 0 \end{bmatrix} \begin{bmatrix} v \\ \alpha \end{bmatrix} = 0 \begin{bmatrix} v \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{15}$$

Hence, we obtain

$$Q_A(\xi + \widehat{t} e^{i\theta})v + c\alpha = 0 \tag{16}$$

and

$$c^T v = 0. \tag{17}$$

Using the Perron-Frobenius Theorem for essentially non-negative irreducible matrices [1], an eigenvalue $v_A(\xi + \widehat{t} e^{i\theta}) = 0$ of matrix $Q_A(\xi + \widehat{t} e^{i\theta})$ has a positive right and left eigenvector $\widehat{x}$ and $\widehat{y}$, respectively. Moreover, every right (left) eigenvector corresponding to the eigenvalue zero will be a scalar multiple of $\widehat{x}$ ($\widehat{y}$). Multiplying equation (16) by $\widehat{y}^T$, we obtain

$$\widehat{y}^T Q_A(\xi + \widehat{t} e^{i\theta})v + \widehat{y}^T c\alpha = 0 \implies \widehat{y}^T c\alpha = 0 \implies \alpha = 0, \tag{18}$$

which together with (16) implies that $Q_A(\xi + \widehat{t} e^{i\theta})v = 0$, i.e., $v \neq 0$ is the right eigenvector corresponding to the eigenvalue zero. Hence, there exists $\beta \neq 0$ that $v = \beta\widehat{x}$. Then, from (17), we obtain

$$\beta c^T \widehat{x} = 0 \implies c^T \widehat{x} = 0, \tag{19}$$

which is a contradiction. Therefore, $M_A^{\xi,\theta}(\widehat{t})$ has to be a nonsingular matrix. Moreover, using the continuity of $M_A^{\xi,\theta}(t)$ in parameter t, we conclude that there exists a sufficiently small $\varepsilon > 0$ such that for all $t \in [\widehat{t} - \varepsilon, \widehat{t} + \varepsilon]$, $M_A^{\xi,\theta}(t)$ is nonsingular and $g_A^{\xi,\theta}(t)$ and $x_A^{\xi,\theta}$ are ∞-differentiable functions for all $t \in [\widehat{t} - \varepsilon, \widehat{t} + \varepsilon]$. $\square$

Theorem 3.2. *Given an arbitrary irreducible matrix $A \in \mathbb{C}^{n,n}$, a complex number ξ, a real $0 \leq \theta < 2\pi$ and $c \in \mathbb{R}^n$, $c > 0$ a positive vector, let $\widehat{t} > 0$ be maximal such that $\xi + t e^{i\theta} \in \Gamma^{\mathcal{R}}(A)$, for all $t \in [0, \widehat{t}]$. Then, there exists $\varepsilon > 0$ such that:*

1. *For every $z = \xi + t e^{i\theta} \notin \Gamma^{\mathcal{R}}(A)$, $g_A^{\xi,\theta}(t)$ and $x_A^{\xi,\theta}(t)$ are well defined and positive.*
2. *$g_A^{\xi,\theta}(t) > 0$ for all $t \in (\widehat{t}, \widehat{t} + \varepsilon]$.*
3. *$g_A^{\xi,\theta}(\widehat{t}) = 0$.*
4. *$g_A^{\xi,\theta}(t) < 0$ for all $t \in [\widehat{t} - \varepsilon, \widehat{t})$.*
5. *The first and the second derivatives $\frac{\partial}{\partial t} g_A^{\xi,\theta}$, $\frac{\partial}{\partial t} x_A^{\xi,\theta}$ and $\frac{\partial^2}{\partial t^2} g_A^{\xi,\theta}$, $\frac{\partial^2}{\partial t^2} x_A^{\xi,\theta}$ are defined via the linear systems*

$$\begin{bmatrix} -Q_A(\xi + t e^{i\theta}) & -c \\ -c^T & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial t} x_A^{\xi,\theta}(t) \\ \frac{\partial}{\partial t} g_A^{\xi,\theta}(t) \end{bmatrix} = \begin{bmatrix} -D_A^{\xi,\theta}(t) x_A^{\xi,\theta}(t) \\ 0 \end{bmatrix}, \tag{20}$$

$$\begin{bmatrix} -Q_A(\xi + t e^{i\theta}) & -c \\ -c^T & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial^2}{\partial t^2} x_A^{\xi,\theta}(t) \\ \frac{\partial^2}{\partial t^2} g_A^{\xi,\theta}(t) \end{bmatrix} = \begin{bmatrix} -S_A^{\xi,\theta}(t) x_A^{\xi,\theta}(t) - 2D_A^{\xi,\theta}(t) \frac{\partial}{\partial t} x_A^{\xi,\theta}(t) \\ 0 \end{bmatrix}, \tag{21}$$

where the vector function $x(t)$ is defined as the solution of the linear system (13) and the entries of the diagonal matrices $D_A^{\xi,\theta}(t) := diag([d_1(t), d_2(t), \ldots, d_n(t)])$ and $S_A^{\xi,\theta}(t) := diag([s_1(t), s_2(t), \ldots, s_n(t)])$ are given by

$$d_i(t) := \frac{Re[(\xi - a_{ii}) e^{-i\theta}] + t}{|(\xi - a_{ii}) e^{-i\theta} + t|}, \tag{22}$$

$$s_i(t) := \frac{(Im[(\xi - a_{ii}) e^{-i\theta} + t])^2}{|(\xi - a_{ii}) e^{-i\theta} + t|^3}, \tag{23}$$

for $t \neq (\xi - a_{ii})e^{i(\pi-\theta)}$, $i \in \{1, 2, \ldots, n\}$.

Proof. 1. Let $z = \xi + t\,e^{i\theta} \notin \Gamma^{\mathcal{R}}(A)$, then $-Q_A(\xi + t\,e^{i\theta})$ is a nonsingular M-matrix, implying $(-Q_A(\xi + t\,e^{i\theta}))^{-1} \geq 0$ and $\det(-Q_A(\xi + t\,e^{i\theta})) > 0$. So, from (12),

$$\det(M_A^{\xi,\theta}(t)) = -\det(-Q_A(\xi + t\,e^{i\theta}))c^T(-Q_A(\xi + t\,e^{i\theta}))^{-1}c < 0 \tag{24}$$

and we obtain that $M_A^{\xi,\theta}(t)$ is nonsingular. Therefore, using a formula for the inversion of a block matrix (11), we have that

$$(M_A^{\xi,\theta}(t))^{-1} \begin{bmatrix} 0 \\ -1 \end{bmatrix} = \begin{bmatrix} (-Q_A(\xi + t\,e^{i\theta}))^{-1}cc^T(-Q_A(\xi + t\,e^{i\theta}))^{-1}c \\ c^T(-Q_A(\xi + t\,e^{i\theta}))^{-1}c \end{bmatrix} > 0,$$

implying that $g_A^{\xi,\theta}(t)$ and $x_A^{\xi,\theta}(t)$ are well defined and positive.

Items 2., 3. and 4. follow from the continuity of $\det(M_A^{\xi,\theta}(t))$ and the fact that $\det(-Q_A(\xi + \widehat{t}\,e^{i\theta})) = 0$.

5. Finally, we get the expressions for the derivatives. If $t \neq (\xi - a_{ii})e^{i(\pi-\theta)}$ for $i \in \{1, 2, ..., n\}$, the entries of $Q_A(\xi + t\,e^{i\theta})$ are ∞-differentiable functions in t and their first and second derivatives are given as

$$\frac{\partial}{\partial t}q_{ii}(\xi + t\,e^{i\theta}) = \frac{Re[(\xi - a_{ii}) e^{-i\theta}] + t}{|(\xi - a_{ii}) e^{-i\theta} + t|}, \qquad \frac{\partial}{\partial t}q_{ij}(\xi + t\,e^{i\theta}) = 0, \text{ for } j \neq i, \tag{25}$$

and

$$\frac{\partial^2}{\partial t^2}q_{ii}(\xi + t\,e^{i\theta}) = \frac{(Im[(\xi - a_{ii}) e^{-i\theta} + t])^2}{|(\xi - a_{ii}) e^{-i\theta} + t|^3}, \qquad \frac{\partial^2}{\partial t^2}q_{ij}(\xi + t\,e^{i\theta}) = 0, \text{ for } j \neq i, \tag{26}$$

for all $i, j \in \{1, 2, ..., n\}$. By differentiating (13) and using (25) and (26), we obtain (20) and (21). $\square$

Definition 3.3. *For a fixed $\xi \in \mathbb{C}$ and $0 \leq \theta < 2\pi$, define the functions:*
$\chi_A^{\xi,\theta}(t) := \min\left\{(x_A^{\xi,\theta}(t))_i : 1 \leq i \leq n\right\}$ *and* $h_A^{\xi,\theta}(t) := \min\left\{g_A^{\xi,\theta}(t), \chi_A^{\xi,\theta}(t)\right\}$, *for $t \geq 0$.*

Then, the following characterization of the minimal Geršgorin set holds.

Theorem 3.4. *Let be given an arbitrary irreducible matrix $A \in \mathbb{C}^{n,n}$ and its arbitrary diagonal entry $\xi = a_{kk}, k \in \{1, 2, ..., n\}$ and $z = \xi + t\,e^{i\theta}$, where $t \geq 0$ and $0 \leq \theta < 2\pi$. Then,*

- *$z \notin \Gamma^{\mathcal{R}}(A)$ if and only if $h_A^{\xi,\theta}(t) > 0$,*

- *$z \in \partial\Gamma^{\mathcal{R}}(A)$ such that $t = \widehat{\rho}_k(\theta)$ if and only if*

    i) $h_A^{\xi,\theta}(t) = g_A^{\xi,\theta}(t) = 0$,

    ii) $h_A^{\xi,\theta}(s_1) \leq 0$ holds for all $0 \leq s_1 \leq t$, and

    iii) for every $\varepsilon > 0$ there exists $s_2 \geq t$ such that $s_2 - \widehat{t} < \varepsilon$ and $h_A^{\xi,\theta}(s_2) > 0$,

- *if c is chosen to be a positive normalized ($\|c\|_2 = 1$) eigenvector of the Perron eigenvalue $\nu_A(\xi) > 0$ of $Q_A(\xi)$ and $M_A^{\xi,\theta}(0)$ is a nonsingular matrix, then $g_A^{\xi,\theta}(0) < 0$ and $x_A^{\xi,\theta}(0) > 0$.*

Proof. For the first item, we prove the equivalence. Assume that $z \notin \Gamma^{\mathcal{R}}(A)$, then, as it is shown in item 1. of Theorem 3.2, $h_A^{\xi,\theta}(t) > 0$. On the other hand, assume that $h_A^{\xi,\theta}(t) > 0$, then from the system (13), we get $-Q_A(z)x_A^{\xi,\theta}(t) = g_A^{\xi,\theta}(t)c > 0$, while $x_A^{\xi,\theta}(t) > 0$. But, this implies that $-Q_A(z)$ is a nonsingular M-matrix. So, $z \notin \Gamma^{\mathcal{R}}(A)$.

For the second item, first observe that $i) - iii)$ imply that $t = \widehat{\rho_k}(\theta)$ as defined in Theorem 2.3. So, assume $z \in \partial\Gamma^{\mathcal{R}}(A)$ such that $t = \widehat{\rho_k}(\theta)$ and let $\varepsilon > 0$ and $0 \le s_1 \le t \le s_2$ and $s_2 - t < \varepsilon$. Then Theorem 3.2, item 3. gives $g_A^{\xi,\theta}(t) = 0$. Item 1. states that $x_A^{\xi,\theta}(s_2) > 0$, which with continuity implies $x_A^{\xi,\theta}(t) \ge 0$. So, we conclude $h_A^{\xi,\theta}(t) = 0$. Obviously, $ii)$ follows from the previous item and $iii)$ from the definition of $\widehat{\rho_k}(\theta)$.

For the third item, if c is a positive normalized eigenvector of Perron eigenvalue $\nu_A(\xi) > 0$ of $Q_A(\xi)$, then $Q_A(\xi)c = \nu_A(\xi)c$ and $c^T c = 1$. From the system (13) for $t = 0$, we obtain $-Q_A(\xi)x_A^{\xi,\theta}(0) = cg_A^{\xi,\theta}(0)$ and $-c^T x_A^{\xi,\theta}(0) = -1$. Because of the nonsigularity of $M_A^{\xi,\theta}(0)$, we get $g_A^{\xi,\theta}(0) = -\nu_A(\xi) < 0$ and $x_A^{\xi,\theta}(0) = c > 0$. $\square$

The results of the given theorems are the basis for the procedure iSearch which defines the implicit algorithm for computing the minimal Geršgorin set.

We formulate the modified Newton's method for computing the zeros of the function h_A, using an abbreviation $h_A(z) := h_A^{\xi,\theta}(t)$. First we define the sequence $\{t_k\}_{k\in\mathbb{N}}$ with

$$t_{k+1} := t_k + \gamma_k\Delta_k, \ k \in \mathbb{N}_0, \tag{27}$$

where $t_0 := 0$ and Δ_k is defined as

$$\Delta_k := \begin{cases} -\dfrac{g_A^{\xi,\theta}(t_k)}{\frac{\partial}{\partial t}g_A^{\xi,\theta}(t_k)}, & \text{if } \frac{\partial}{\partial t}g_A^{\xi,\theta}(t_k) > 0, \\[2ex] \Delta, & \text{otherwise} \end{cases}, \tag{28}$$

where $\Delta > 0$ is given parameter and

$$\gamma_k := \begin{cases} 1, & \text{if } h_A^{\xi,\theta}(t_{k+1}) \le 0, \\[2ex] \tau^{q_k}, & \text{otherwise} \end{cases}, \tag{29}$$

with parameter $\tau \in (0,1)$ arbitrarily fixed and $q_k \in \mathbb{N}$ being the smallest number such that

$$h_A^{\xi,\theta}(t_k + \tau^{q_k}\Delta_k) < 0 \quad \text{and} \quad h_A^{\xi,\theta}(t_k + \tau^{q_k-1}\Delta_k) > 0. \tag{30}$$

Additionally, if the convergence is achieved in $\widetilde{t}$, then we check if $h_A^{\xi,\theta}(\widetilde{t} + \varepsilon) > 0$ for a small tolerance $\varepsilon > 0$ and if not, we restart the sequence taking $t_0 := \widetilde{t} + \varepsilon$.

Theorem 3.5. *Given an arbitrary irreducible matrix $A \in \mathbb{C}^{n,n}$, a complex number ξ and a real $0 \le \theta < 2\pi$, a sequence $\{t_k\}_{k\in\mathbb{N}_0}$ defined by (27) is monotonically non-decreasing and it converges to $\widehat{t} > 0$ such that $\xi + \widehat{t}e^{i\theta} \in \partial\Gamma^{\mathcal{R}}(A)$. Furthermore, if $\dfrac{\partial^2}{\partial t^2}g_A^{\xi,\theta}(\widehat{t}) > 0$, the convergence is locally quadratic and otherwise, the convergence is linear with the convergence rate $\lim\sup_{k\to\infty}(1 - \tau^k)$.*

Proof. First we show that the sequence $\{t_k\}_{k\in\mathbb{N}_0}$ is well defined. From Theorem 3.4 (item 3.) follows $h_A^{\xi,\theta}(0) < 0$. From the definition of Δ_k, we have $\Delta_0 > 0$, since $\Delta_0 = 0$ implies that $g_A^{\xi,\theta}(t_0) = 0$. Thus $t_0 + \Delta_0 > 0$,

and the continuity of $h_A^{\xi,\theta}$ together with (30) implies that there exists $0 < \gamma_0 \leq 1$ such that $h_A^{\xi,\theta}(t_0 + \gamma_0\Delta_0) < 0$. So, we obtain $t_1 := t_0 + \gamma_0\Delta_0 > t_0$ such that $h_A^{\xi,\theta}(t_1) < 0$. By induction, we obtain that the sequence $\{t_k\}_{k\in\mathbb{N}}$ is well defined and that $h_A^{\xi,\theta}(t_k) < 0$ with $t_k > t_{k-1}$ for all $k \in \mathbb{N}$.

To prove the convergence of the monotonically increasing sequence $\{t_k\}_{k\in\mathbb{N}}$, it is enough to show that it is bounded above. Let's assume that $\{t_k\}_{k\in\mathbb{N}}$ is unbounded. Then for some $m \in \mathbb{N}$, there exists a subsequence $\{t_{k_m}\}$ such that $\lim_{m\to\infty} t_{k_m} = \infty$. Also, the fact $h_A^{\xi,\theta}(t_{k_m}) < 0$ implies that $z_m := \xi + t_{k_m} e^{i\theta} \in \Gamma^{\mathcal{R}}(A)$, for all $m \in \mathbb{N}$ and $\lim_{m\to\infty} |z_m| = \infty$. This is a contradiction because the minimal Geršgorin set is compact in $\mathbb{C}$. Therefore, the sequence is convergent and we denote its limit by $\widehat{t} = \lim_{k\to\infty} t_k$.

From the construction of the sequence we have that $g_A^{\xi,\theta}(\widehat{t}) = 0$, when $\frac{\partial}{\partial t} g_A^{\xi,\theta}(\widehat{t})$ exists and is positive, or that $h_A^{\xi,\theta}(\widehat{t}) = 0$, otherwise. Finally, due to restarts we obtain that $z = \xi + \widehat{t}e^{i\theta}$ fulfills the second item of Theorem 3.4, and, therefore $z = \xi + \widehat{t}e^{i\theta} \in \partial\Gamma^{\mathcal{R}}(A)$.

Now, we prove the rate of local convergence. There are two cases.

If $\frac{\partial^2}{\partial t^2} g_A^{\xi,\theta}(\widehat{t}) > 0$, then $g_A^{\xi,\theta}$ is a locally convex function, and for sufficiently large $k \in \mathbb{N}$, $\gamma_k = 1$. This implies the quadratic convergence of modified Newton's method.

If $\frac{\partial^2}{\partial t^2} g_A^{\xi,\theta}(\widehat{t}) \leq 0$, then for sufficiently large $k \in \mathbb{N}$, $\frac{\partial}{\partial t} g_A^{\xi,\theta}(t_k) > 0$, and, thus, from (27) and (28), we obtain:

$$\widehat{t} - t_{k+1} = \widehat{t} - t_k - \gamma_k\Delta_k = \widehat{t} - t_k + \gamma_k \frac{g_A^{\xi,\theta}(t_k)}{\frac{\partial}{\partial t} g_A^{\xi,\theta}(t_k)}.$$

Using quadratic Taylor expansion for $g_A^{\xi,\theta}$, there exists $t^* \in (\widehat{t} - t_k, \widehat{t})$ such that

$$0 = g_A^{\xi,\theta}(\widehat{t}) = g_A^{\xi,\theta}(t_k) + \frac{\partial}{\partial t} g_A^{\xi,\theta}(t_k)(\widehat{t} - t_k) + \frac{1}{2}\frac{\partial^2}{\partial t^2} g_A^{\xi,\theta}(t^*)(\widehat{t} - t_k)^2.$$

So,

$$\widehat{t} - t_{k+1} = \hat{t} - t_k - \gamma_k \frac{\frac{\partial}{\partial t} g_A^{\xi,\theta}(t_k)(\widehat{t} - t_k) + \frac{1}{2}\frac{\partial^2}{\partial t^2} g_A^{\xi,\theta}(t^*)(\widehat{t} - t_k)^2}{\frac{\partial}{\partial t} g_A^{\xi,\theta}(t_k)} =$$

$$(\widehat{t} - t_k)(1 - \gamma_k - \frac{\frac{1}{2}\gamma_k \frac{\partial^2}{\partial t^2} g_A^{\xi,\theta}(t^*)(\widehat{t} - t_k)}{\frac{\partial}{\partial t} g_A^{\xi,\theta}(t_k)}),$$

and consequently,

$$\limsup_{k\to\infty} \frac{\widehat{t} - t_{k+1}}{\widehat{t} - t_k} = \limsup_{k\to\infty}(1 - \tau^k). \quad \square$$

Now, one can easily adapt the algorithm eMGS from [5] using Theorem 3.5 and compute $\widehat{t}$ using the sequence defined by (27)-(30) instead of using the procedure eSearch given there. In such a way, we obtain the approximation of the points of the boundary of the minimal Geršgorin set with $\{\omega_{i,j}\}_{j=1}^{m_i}$, $i \in \{1, 2, ..., k\}$, where k is a number of components of $\Gamma^{\mathcal{R}}(A)$ for the fixed maximal distance between the approximation and the boundary of the minimal Geršgorin $\varepsilon_1 > 0$ and the distance between successive two points bounded by ε_2, i.e., $\text{dist}(\omega_{i,j}, \partial\Gamma^{\mathcal{R}}(A)) < \varepsilon_1$ and $|\omega_{i,j} - \omega_{i,j+1}| < \varepsilon_2$, where $\omega_{i,m_i+1} := \omega_{i,1}$.

4. Numerical examples

In this section we test the iMGS algorithm on three examples and compare results with the results of the eMGS algorithm. We notice that the performance of iMGS is significantly faster. Both algorithms are implemented in MATLAB version R2015b and tested on 2.7 GHz Intel® Core™ i5 machine.

Example 4.1. *In the first example we tested iMGS and eMGS on the cyclic matrix of size $n = 4$:*

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & i & 1 \\ 1 & 0 & 0 & -i \end{bmatrix},$$

setting the parameters of both algorithms to be $\varepsilon_1 = 10^{-12}$, $\varepsilon_2 = 0.0254$ and $\tau = 2$. The corresponding CPU time for eMGS vs iMGS is 6.0824s vs 0.4451s, which was needed for (in total) 10902 Perron eigevalue computations for eMGS and 13934 linear system solves for iMGS. Figure 1(a) shows the minimal Geršgorin set of the matrix A using iMGS. Its zoomed version is presented in Figure 1(b).

(a)

(b)
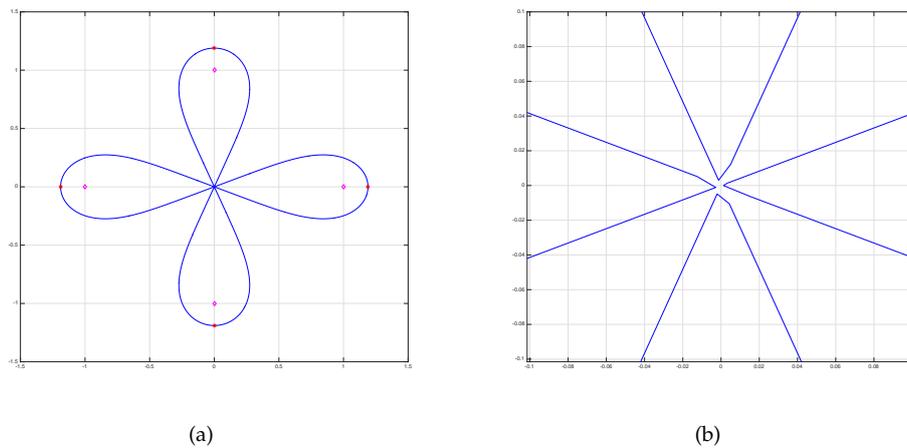
Figure 1: The minimal Geršgorin set of matrix A from Example 4.1: complete plot (a) and plot zoomed around the origin (b).

Example 4.2. *In the second example we used the Tolosa matrix tols340.mtx of size $n = 340$ from the Matrix Market repository [2]. This matrix is sparse, highly nonnormal of medium size. Parameters are set as $\varepsilon_1 = 10^{-12}$, $\varepsilon_2 = 31.2698$ and $\tau = 2$, which produces 3004 Perron eigenpair computations in 160.8012s for eMGS vs 1655 linear system solves in 3.0205s for iMGS. The result of iMGS is presented in Figure 2.*
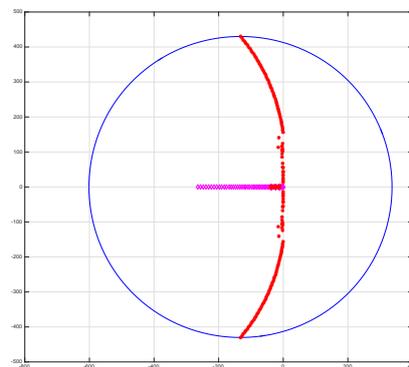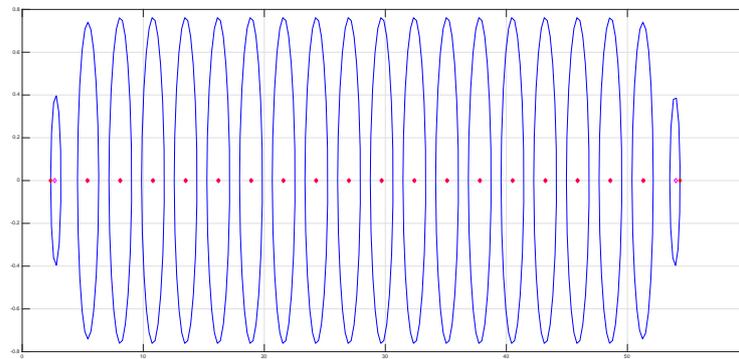

Figure 2: The minimal Geršgorin set of the Tolosa matrix of Example 4.2.

Example 4.3. *Our last example is a triangular matrix of the size* 20 :

$$
T_\mu = \begin{bmatrix}
\mu & 1 & 0 & \dots & 0 \\
1 & 2\mu & 1 & \ddots & \vdots \\
0 & 1 & 3\mu & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & 1 \\
0 & \dots & 0 & 1 & 20\mu
\end{bmatrix}.
$$

We tested eMGS and iMGS algorithm using value $\mu = 2.7$. *The parameters are set as* $\varepsilon_1 = 10^{-12}$, $\varepsilon_2 = 0.52$ *and* $\tau = 2$, *which produces 3463 Perron eigenpair computations in 13.8591s for eMGS vs 3890 linear system solves in 0.4415s for iMGS. The result of iMGS is presented in Figure 3.*

Figure 3: The minimal Geršgorin set of matrix $T_{2.7}$ of Example 4.3.

References

[1] A. Berman and R. Plemmons, Nonnegative Matrices in the Mathematical Sciences, 2014.
[2] B. Boisvert, R. Pozzo, K. Remington, B. Miller and R. Lipman, Matrix Market repository, http://math.nist.gov/MatrixMarket/.
[3] M. A. Freitag and A. Spence, A Newton-based method for the calculation of the distance to instability, Linear Algebra Appl., 435(12):3189-3205, 2011.
[4] V. Kostić, On general principles of eigenvalue localizations via diagonal dominance, Advances in Computational Mathematics, 41:55-75, 2015.
[5] V. Kostić, A. Miedlar and Lj. Cvetković, An algorithm for computing minimal Geršgorin sets, Numerical linear algebra with applications, 00:1-19, 2015.
[6] A. Spence and C. Poulton, Photonic band structure calculations using nonlinear eigenvalue techniques, J. Comput. Phys. 204 6581, 2005.
[7] R. S. Varga, Geršgorin na His Circles, Springer-Verlag, New York, 2004.
[8] R. S. Varga, Minimal Gershgorin sets, Pac. J. Math., 15:719-729, 1965.
[9] R. S. Varga, Lj. Cvetković and V. Kostić, Approximation of the minimal Geršgorin set of a square complex matrix, ETNA (Electronic Transactions on Numerical Analysis), 40:308-405, 2008.