Comparison Theorems for Splittings of M-matrices in (block) Hessenberg Form

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Abstract

Some variants of the (block) Gauss–Seidel iteration for the solution of linear systems with M-matrices in (block) Hessenberg form are discussed. Comparison results for the asymptotic convergence rate of some regular splittings are derived: in particular, we prove that for a lower-Hessenberg M-matrix $\rho(P_{GS}) \geq \rho(P_S) \geq \rho(P_{AGS})$, where P_{GS}, P_S, P_{AGS} are the iteration matrices of the Gauss–Seidel, staircase, and anti-Gauss–Seidel method. This is a result that does not seem to follow from classical comparison results, as these splittings are not directly comparable. It is shown that the concept of stair partitioning provides a powerful tool for the design of new variants that are suited for parallel computation.

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1 Introduction

Solving block Hessenberg systems is one of the key issues in numerical simulations of many scientific and engineering problems. Possibly singular M-matrix linear systems in block Hessenberg form are found in finite difference or finite element methods for partial differential equations, Markov chains, production and growth models in economics, and linear complementarity problems in operational research [14, 2]. Finite difference or finite element discretizations of PDEs usually produce matrices which are banded or block banded (e.g., block tridiagonal or block pentadiagonal) [16]. Discrete-state models encountered in several applications such as modeling and analysis of communication and computer networks can be conveniently represented by a discrete/continuous time Markov chain [14]. In many cases an appropriate numbering of the states yields a chain with block upper or lower Hessenberg structures (GI/M/1 and M/G/1 queues) or, in the intersection, a block tridiagonal generator or transition probability matrix, that is, a quasi-birth-and-death process (QBD). QBDs are also well suited for modeling various population processes such as cell growth, biochemical reaction kinetics, epidemics, demographic trends, or queuing systems, amongst others [10].

Active computational research in this area is focused on the development of techniques, methods and data structures, which minimize the computational (space and time) requirements for solving large and possibly sparse linear systems. One of such techniques is parallelization. Divide-and-conquer solvers for M-matrix linear systems in block banded or block Hessenberg form are described in [5, 7, 18]. A specialization of these algorithms based on cyclic reduction for block Toeplitz Hessenberg matrices is discussed in [4]. However, due to the communication costs these schemes typically scale well with processor count only for very large matrix block sizes. Iterative methods can provide an attractive alternative primarily because they simplify both implementation and sparsity treatment. The crux resides in the analysis of their convergence properties.

Among classical iterative methods, the Gauss–Seidel method has several interesting features. It is a classical result that on a nonsingular M-matrix the Gauss–Seidel method converges faster than the Jacobi method [2, Corollary 5.22]. The SOR method with the optimal relaxation parameter can be better yet, but, however, choosing an optimal SOR relaxation parameter is difficult for many problems. Therefore, the Gauss–Seidel method is very attractive in practice and it is also used as preconditioner in combination with other iterative schemes. A classical example is the multigrid method for partial differential equations, where using Gauss–Seidel or SOR as a smoother typically yields good convergence properties [20]. Parallel implementations of the Gauss–Seidel method have been designed for certain regular problems,for example, the solution of Laplace's equations by finite differences, by relying upon red-black coloring or more generally multi-coloring schemes to provide some parallelism [15]. In most cases, constructing efficient parallel true Gauss–Seidel algorithms is challenging and Processor Block (or localized) Gauss–Seidel is often used [17]. Here, each processor performs Gauss–Seidel as a subdomain solver for a block Jacobi method. While Processor Block Gauss–Seidel is easy to parallelize, the overall convergence can suffer. In order to improve the parallelism of Gauss–Seidel-type methods while retaining the same convergence rate, in [12] staircase splittings are introduced by showing that for consistently ordered matrices [16] the iterative scheme based on such partitionings splits into independent computations and at the same time exhibits the same convergence rate as the classical Gauss–Seidel iteration. An extension of this result for block tridiagonal matrices appeared in [1]. The use of a Krylov solver like BCG, GMRES and BiCGSTAB, for block tridiagonal systems complemented with a stair preconditioner which accounts for the structure of the coefficient matrix is proposed in [11].

A classical framework to study the convergence speed of iterative methods for linear systems $A\boldsymbol{x} = \boldsymbol{b}$ is that of *matrix splittings*: one writes $A = M - N$, with M invertible, and considers the iterative method

$$\boldsymbol{x}^{(\ell+1)} = P\boldsymbol{x}^{(\ell)} + M^{-1}\boldsymbol{b}, \quad \ell \geq 0, \tag{1}$$

where $P = M^{-1}N$ is the *iteration matrix*. Various results exist to compare the spectral radii of the iteration matrices of two splittings $A = M_1 - N_1 = M_2 - N_2$

under certain elementwise inequalities, such as

$$N_2 \geq N_1 \geq 0, \quad M_1^{-1} \geq M_2^{-1}, \quad \text{or} \quad A^{-1}N_2A^{-1} \geq A^{-1}N_1A^{-1}: \tag{2}$$

see for instance [2, 3, 21].

In this paper, we consider the solution of M-matrix linear systems in (block) Hessenberg form, and we show new comparison results between matrix splittings that hold for this special structure. In particular, for a lower Hessenberg invertible M-matrix A we prove the inequalities

$$\rho(P_{GS}) \geq \rho(P_S) \geq \rho(P_{AGS}),$$

where $\rho(A)$ denotes the spectral radius of A and P_{GS}, P_S, P_{AGS} are the iteration matrices of the Gauss–Seidel method, the staircase splitting method and the anti-Gauss–Seidel method, respectively. The first inequality fosters the use of stair partitionings for solving Hessenberg linear systems in parallel. The second inequality says that the anti-Gauss–Seidel method —also called Reverse Gauss–Seidel in [19] and Backward Gauss–Seidel in [16]— gives the better choice in terms of convergence speedup. Comparison results for more general splittings including some generalizations of staircase partitionings are also obtained.

The remarkable feature of these results is that they do not seem to arise from classical comparison results or from elementwise inequalities of the form (2) between the matrices that define the splittings: M_{GS} is lower triangular and M_{AGS} is upper triangular, so they are far from being comparable.

Another reason why our results are counterintuitive is that the intuition behind inequalities of the form (2) and classical comparison theorems (such as Theorem 1 in the following) suggests that one should put "as much of the matrix A as possible" into M to get a smaller radius: so it is surprising that on a lower Hessenberg matrix AGS, in which M only has $2n-1$ nonzeros, works better than GS, in which M has $\frac{n(n+1)}{2}$ nonzeros, and that this property holds irrespective of the magnitude of these nonzero items.

We give an alternative combinatorial proof of the inequality $\rho(P_{GS}) \geq \rho(P_{AGS})$, which adds a new perspective and shows an elementwise inequality that can be used to derive these bounds. Extensions to deal with possibly singular M-matrices and block Hessenberg structures are discussed. Finally, some numerical experiments confirm the results and give a quantitative estimate of the difference between these spectral radii.

2 Preliminaries

Let $A \in \mathbb{R}^{n\times n}$ be an invertible M-matrix.

A *regular splitting* of A is any pair (M, N), where M is an invertible M-matrix, $N \geq 0$, and $A = M - N$. In the terminology of Forsythe [6] a *linear stationary iterative method* for solving the system $A\boldsymbol{x} = \boldsymbol{b}$ can be described as (1). Let

$$A = M - N = M' - N'$$

be two regular splittings of A. We can derive two iterative schemes with iteration matrices $P = M^{-1}N$ and $P' = {M'}^{-1}N'$. When A is nonsingular, it is well known that the scheme (1) is convergent if and only if $\rho(P) < 1$, with $\rho(P)$ *the spectral radius* of P. Under convergence *the asymptotic rate of convergence* is also given by $\rho(P)$, and, therefore, it is interesting to compare $\rho(P)$ and $\rho(P')$. A classical result is the following.

Theorem 1 ([19]). *Let (M, N) and (M', N') be regular splittings of A. If $N \le N'$, then $\rho(M^{-1}N) \le \rho((M')^{-1}N')$.*

Another tool to obtain comparison results for matrix splittings is the exploitation of certain block partitionings of the matrix A.

Lemma 2. *Let*

$$M = \begin{bmatrix} M_{11} & 0 \\ A_{21} & M_{22} \end{bmatrix}, \quad N = \begin{bmatrix} N_{11} & -A_{12} \\ 0 & N_{22} \end{bmatrix}.$$

and

$$\hat{M} = \begin{bmatrix} M_{11} & A_{12} \\ 0 & M_{22} \end{bmatrix}, \quad \hat{N} = \begin{bmatrix} N_{11} & 0 \\ -A_{21} & N_{22} \end{bmatrix}.$$

be two regular splittings of $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{2,1} & A_{22} \end{bmatrix}$, with $A_{11}, M_{11}, N_{11} \in \mathbb{R}^{k\times k}$ and $A_{22}, M_{22}, N_{22} \in \mathbb{R}^{(n-k)\times(n-k)}$.

Then, $\hat{M}^{-1}\hat{N}$ and $M^{-1}N$ have the same eigenvalues (and, hence, the same spectral radius).

Proof. We shall prove that the polynomials

$$p(x) = \det(M)\det(xI - M^{-1}N) = \det(xM - N) = \det \underbrace{\begin{bmatrix} xM_{11} - N_{11} & A_{12} \\ xA_{21} & xM_{22} - N_{22} \end{bmatrix}}_{:=P(x)}$$

and

$$q(x) = \det(\hat{M})\det(xI - \hat{M}^{-1}\hat{N}) = \det(x\hat{M} - \hat{N}) = \det \underbrace{\begin{bmatrix} xM_{11} - N_{11} & xA_{12} \\ A_{21} & xM_{22} - N_{22} \end{bmatrix}}_{:=Q(x)}$$

coincide, hence they have the same zeros. For any $x \neq 0$ we have

$$P(x) = \operatorname{diag}(I_k, xI_{n-k}) \cdot Q(x) \cdot \operatorname{diag}(I_k, x^{-1}I_{n-k}).$$

The proof follows from the continuity of the determinant w.r.t. the matrix entries. $\square$

Corollary 3. *Let*

$$M' = \begin{bmatrix} M_{11} & 0 \\ M_{21} & M_{22} \end{bmatrix}, \quad N' = \begin{bmatrix} N_{11} & -A_{12} \\ N_{21} & N_{22} \end{bmatrix}.$$

and

$$\hat{M} = \begin{bmatrix} M_{11} & A_{12} \\ 0 & M_{22} \end{bmatrix}, \quad \hat{N} = \begin{bmatrix} N_{11} & 0 \\ -A_{21} & N_{22} \end{bmatrix}. \tag{3}$$

(where the blocks on the diagonal are square) be two regular splittings of A. Then, $\rho(\hat{M}^{-1}\hat{N}) \le \rho((M')^{-1}N')$.

Proof. By Lemma 2 and Theorem 1, $\rho(\hat{M}^{-1}\hat{N}) = \rho(M^{-1}N) \le \rho((M')^{-1}N')$. $\square$

3 Comparing the GS, AGS, and staircase splitting on Hessenberg matrices

Corollary 3 shows that a regular splitting with $M(1:k, k+1:n) = 0$ can be converted into one with $M(k+1:n, 1:k) = 0$ and $N(1:k, k+1:n) = 0$ by decreasing its spectral radius, that is, equivalently by improving its asymptotic rate of convergence. On a lower Hessenberg matrix, we can apply the lemma repeatedly for different values of k, since each superdiagonal block $M(1:k, k+1:n)$ contains only one nonzero that does not overlap with blocks with a different k. In this way we obtain comparison results for different regular splittings.

To be more specific, let $A \in \mathbb{R}^{n\times n}$ be a lower Hessenberg invertible M-matrix. Then

$$\begin{aligned} M_J &= \mathrm{diag}(A), & N_J &= M_J - A, & P_J &= M_J^{-1} N_J \\ M_{GS} &= \mathrm{tril}(A), & N_{GS} &= M_{GS} - A, & P_{GS} &= M_{GS}^{-1} N_{GS} \end{aligned}$$

are the customary Jacobi and Gauss–Seidel regular splittings. An easy modification of the Gauss–Seidel partitioning is the so called anti-Gauss–Seidel regular splitting defined by

$$M_{AGS} = \mathrm{triu}(A), \quad N_{AGS} = M_{AGS} - A, \quad P_{AGS} = M_{AGS}^{-1} N_{AGS}.$$

Alternative regular splittings are analyzed in the works [13, 12] which introduce the concept of stair partitioning of a matrix aimed at the design of fast parallel (preconditioned) iterative solvers. Let $\mathrm{tridiag}(A) = \mathrm{tridiag}(A_{i,i-1}, A_{i,i}, A_{i,i+1})$ be the tridiagonal matrix formed from the subdiagonal, diagonal and superdiagonal entries of A. The *stair matrix* of first order generated by A is the $n \times n$ matrix $S_1 = \mathcal{S}_1(A)$ filled with the entries of A according to the following rule:

$$S_1 = \mathrm{tridiag}(A)\,; \quad \texttt{for} \quad i = 1:2:n\,; \quad S_1(i, i-1) = 0\,; \quad S_1(i, i+1) = 0\,.$$

Analogously, the stair matrix of second order generated by A is the $n \times n$ matrix $S_2 = \mathcal{S}_2(A)$ defined by

$$S_1 = \mathrm{tridiag}(A)\,; \quad \texttt{for} \quad i = 2:2:n\,; \quad S_1(i, i-1) = 0\,; \quad S_1(i, i+1) = 0\,.$$

If $S = \mathcal{S}(A)$ is the stair matrix of the first or second order constructed from A then

$$M_S = S, \quad N_S = M_S - A, \quad P_S = M_S^{-1} N_S$$

gives a staircase regular splitting of A. The next result compares the asymptotic convergence rates of these splittings. Recall that the classical inequality

$$\rho(P_J) \geq \rho(P_{GS})$$

easily follows from Theorem 1.

Theorem 4. *Let A be a lower Hessenberg invertible M-matrix. Then,*

$$\rho(P_{GS}) \geq \rho(P_S) \geq \rho(P_{AGS}).$$

Proof. The proof consists in applying Corollary 3 repeatedly for all even values of k, and then for all odd values of k. We depict the transformations in the case $n = 7$. We show here the nonzero pattern of M, displaying in position i, j a symbol $\times$ to denote a nonzero entry $M_{ij} = A_{ij}$, and an empty cell to denote a zero entry $M_{ij} = 0$. The symbol $\mapsto$ is used to denote a transformation of M that reduces the spectral radius by Corollary 3.

$$
\begin{aligned}
M_{GS} = &\left[\begin{array}{c|cccccc}
\times & & & & & & \\ \hline
\times & \times & & & & & \\
\times & \times & \times & & & & \\
\times & \times & \times & \times & & & \\
\times & \times & \times & \times & \times & & \\
\times & \times & \times & \times & \times & \times & \\
\times & \times & \times & \times & \times & \times & \times
\end{array}\right]
\mapsto
\left[\begin{array}{ccc|cccc}
\times & \times & & & & & \\
& \times & & & & & \\
& \times & \times & & & & \\ \hline
& \times & \times & \times & & & \\
& \times & \times & \times & \times & & \\
& \times & \times & \times & \times & \times & \\
& \times & \times & \times & \times & \times & \times
\end{array}\right] \\
\mapsto &\left[\begin{array}{ccccc|cc}
\times & \times & & & & & \\
& \times & & & & & \\
& \times & \times & \times & & & \\
& & & \times & & & \\
& & & \times & \times & & \\ \hline
& & & \times & \times & \times & \\
& & & \times & \times & \times & \times
\end{array}\right]
\mapsto
\left[\begin{array}{ccccccc}
\times & \times & & & & & \\
& \times & & & & & \\
& \times & \times & \times & & & \\
& & & \times & & & \\
& & & \times & \times & \times & \\
& & & & & \times & \\
& & & & & \times & \times
\end{array}\right] = M_S.
\end{aligned}
$$

This sequence of transformations shows that $\rho(P_{GS}) \geq \rho(P_S)$. We then continue with odd values of k to obtain the anti–Gauss–Seidel splitting.

$$
\begin{aligned}
M_S = &\left[\begin{array}{cc|ccccc}
\times & \times & & & & & \\
& \times & & & & & \\ \hline
& \times & \times & \times & & & \\
& & & \times & & & \\
& & & \times & \times & \times & \\
& & & & & \times & \\
& & & & & \times & \times
\end{array}\right]
\mapsto
\left[\begin{array}{cccc|ccc}
\times & \times & & & & & \\
& \times & \times & & & & \\
& & \times & \times & & & \\
& & & \times & & & \\ \hline
& & & \times & \times & \times & \\
& & & & & \times & \\
& & & & & \times & \times
\end{array}\right] \\
\mapsto &\left[\begin{array}{cccccc|c}
\times & \times & & & & & \\
& \times & \times & & & & \\
& & \times & \times & & & \\
& & & \times & \times & & \\
& & & & \times & \times & \\
& & & & & \times & \\ \hline
& & & & & \times & \times
\end{array}\right]
\mapsto
\left[\begin{array}{ccccccc}
\times & \times & & & & & \\
& \times & \times & & & & \\
& & \times & \times & & & \\
& & & \times & \times & & \\
& & & & \times & \times & \\
& & & & & \times & \times \\
& & & & & & \times
\end{array}\right] = M_{AGS}.
\end{aligned}
$$

$\square$

Remark 5. *Theorem 4 extends straightforwardly to nonsingular M-matrices in block Hessenberg form by considering the corresponding block regular splittings.*

4 Comparing substitution splittings for Hessenberg matrices

Substitution splittings provide a generalization of the partitionings introduced in the previous section. A permutation $v = (i_1, i_2, \ldots, i_n)$ of $(1, 2, \ldots, n)$ is said a *substitution order* for $M \in \mathbb{R}^{n\times n}$ if $M_{ij} = 0$ whenever j comes after i in the list v. This property means that we can solve a system $Mx = b$ by substitution, computing unknowns x_i in the order of the list v, as in the following pseudocode:

```
for  i = i_1, i_2, ..., i_n
   solve for x_i in the ith row of Mx = b;
end
```

We call *substitution matrix* any matrix M that admits a substitution order. This includes lower triangular matrices (with order $[1, 2, \ldots, n]$), upper triangular matrices (with order $[n, n-1, \ldots, 1]$) and staircase partitionings (with order $[1, 3, \ldots, 2, 4, \ldots]$ or $[2, 4, \ldots, 1, 3, \ldots]$). Substitution splittings also comprise the generalized staircase partitionings described in [12]. More generally, it is not hard to see that M is a substitution matrix if and only if $\Pi M \Pi^T$ is lower triangular, where Π is the permutation matrix associated to v.

The following theorem generalizes the previous result on comparing splittings for Hessenberg matrices.

Theorem 6. *Let A be a lower Hessenberg invertible M-matrix, and let (M, N) be a regular splitting with a substitution matrix M. Then,*

$$\rho(M^{-1}N) \geq \rho(M_{AGS}^{-1} N_{AGS}).$$

Proof. First of all, note that it is sufficient to consider splittings of the form

$$M_{ij} = \begin{cases} 0 & j \text{ comes after } i \text{ in } v, \\ A_{ij} & \text{otherwise.} \end{cases} \tag{4}$$

for some permutation v. Indeed, if M' is another substitution matrix with the same v, then $N' \geq N$ and hence $\rho((M')^{-1}N') \geq \rho(M^{-1}N)$ by Theorem 1.

Take such a splitting (M, N), and suppose that $M_{k,k+1} \neq A_{k,k+1}$ for some $k \in \{1, 2, \ldots, n\}$. Then, $M_{k,k+1} = 0$, and we can apply Corollary 3 with the first block of size $k \times k$ and show that the splitting $(\hat{M}, \hat{N})$ as defined in in (3) has $\rho(\hat{M}^{-1}\hat{N}) \leq \rho(M^{-1}N)$.

We claim that $\hat{M}$ is a substitution matrix, too. Indeed, consider the permutation obtained by concatenating $v_2 = v \cap \{k+1, k+2, \ldots, n\}$ and $v_1 = v \cap \{1, \ldots, k\}$ (with this notation we mean that the entries in the ordered lists v_1, v_2 come in the same order as in v). Then, this is a substitution order for $\hat{M}$: indeed, if $i \in v_2$ and $j \in v_1$, then $\hat{M}_{ij} = 0$ by construction; while if i, j belong both to v_1 (resp. v_2), with i coming before j, then $\hat{M}_{ij} = M_{ij} = 0$.

Hence we have obtained a new splitting with $\rho(\hat{M}^{-1}\hat{N}) \leq \rho(M^{-1}N)$ and a substitution matrix $\hat{M}$ that has one more superdiagonal nonzero element than M; we can repeat the process until we obtain M_{AGS}, which is the (unique) splitting of the form (4) with the maximal number of superdiagonal nonzero elements. □

Remark 7. *Theorem 6 also extends easily to nonsingular M-matrices $A = (A_{ij}) \in \mathbb{R}^{N \times N}$, $A_{i,i} \in \mathbb{R}^{n_i \times n_i}$, $\sum_{i=1}^{n} n_i = N$, in block Hessenberg form whenever we consider block regular splittings determined by substitution orders $v = (i_1, i_2, \ldots, i_n)$ acting on the block entries. Adaptations of Theorem 4 and Theorem 6 for upper and block upper invertible M-matrices are immediate.*

5 Singular Systems

The solution of homogeneous singular system $A\boldsymbol{x} = \mathbf{0}$ where A is a singular M-matrix in (block) Hessenberg form is of paramount importance for application in Markov chains. Linear stationary iterative methods of the type (1) have been successfully used for this problem. The rate of convergence of these iterative methods is governed by the quantity $\gamma(P) = \max\{|\lambda|\colon \lambda \in \sigma(P), \lambda \neq 1\}$ where $\sigma(P)$ is the spectrum of P. Under convergence conditions this quantity is called the asymptotic convergence factor of the iterative method (1) applied for the solution of homogeneous singular system $A\boldsymbol{x} = \mathbf{0}$.

For the sake of clarity, let A be an irreducible singular M-matrix in lower Hessenberg form. Recall that from Theorem 4.16 in [2] A has rank $n-1$ and, hence, $\dim\ker(A) = 1$ (see also [9] for a brief survey of properties of singular irreducible M-matrices). We assume, up to scaling, that $A = I - T$, where T is a column stochastic matrix (in particular, $T_{ij} \geq 0$ for all i, j). It holds $\boldsymbol{e}^T A = \mathbf{0}^T$ and, hence,

$$B = LA = \begin{bmatrix} A[1\colon n-1, 1\colon n-1] & A[1\colon n-1, n] \\ \mathbf{0}^T & 0 \end{bmatrix}, \quad L = \begin{bmatrix} I_{n-1} & \mathbf{0} \\ \boldsymbol{e}^T & 1 \end{bmatrix}$$

As A is irreducible, it follows that $A_{n-1} := A[1\colon n-1, 1\colon n-1]$ is a nonsingular lower Hessenberg M-matrix. This makes possible to construct Jacobi-like, Gauss–Seidel-like and staircase-like regular partitionings of A starting from their analogue for the matrix B. Specifically, let us denote

$$M_J' = L^{-1}(\mathrm{diag}(A_{n-1}) \oplus 1), \quad M_{GS}' = L^{-1}(\mathrm{tril}(A_{n-1}) \oplus 1),$$

and

$$M_{AGS}' = L^{-1}(\mathrm{triu}(A_{n-1}) \oplus 1), \quad M_S' = L^{-1}(\mathcal{S}(A_{n-1}) \oplus 1).$$

Theorem 4 implies the following.

Theorem 8. *Let A be an irreducible singular lower Hessenberg M-matrix. Then,*

$$\gamma({M_J'}^{-1} N_J) \geq \gamma({M_{GS}'}^{-1} N_{GS}') \geq \gamma({M_S'}^{-1} N_S') \geq \gamma({M_{AGS}'}^{-1} N_{AGS}').$$

6 A combinatorial argument for $\rho(P_{GS}) \geq \rho(P_{AGS})$

M-matrices and non-negative matrices are intimately related to Markov chains and transition probabilities; hence the reader may wonder if the results presented here admit an alternative combinatorial proof based on comparing probabilities of certain walks on a Markov chain. We present briefly such a proof for the inequality $\rho(P_{GS}) \geq \rho(P_{AGS})$, to highlight the ideas behind the argument.

Up to scaling, we may assume $A = I - T$, where $T \in \mathbb{R}^{n \times n}$ is a *substochastic matrix*, i.e., $T \geq 0$ and $T\mathbf{1} \leq \mathbf{1}$, where $\mathbf{1} \in \mathbb{R}^n$ is the vector of all ones. A *walk* on the graph with vertices $\{1, 2, \ldots, n\}$ (from i_0 to i_ℓ of length ℓ) is a sequence of consecutive edges (*transitions*) $\omega = ((i_0, i_1), (i_1, i_2), \ldots, (i_{\ell-1}, i_\ell))$. To a set of walks Ω we associate the transition probability matrix

$$\mathbb{P}[\Omega] = (\mathbb{P}[\Omega]_{ij}), \quad \mathbb{P}[\Omega]_{ij} = \sum_{\omega \in \Omega \text{ with } i_0 = i, i_\ell = j} T_{ii_1} T_{i_1 i_2} \cdots T_{i_{\ell-1} j}.$$

The matrix entry $\mathbb{P}[\Omega]_{ij}$ can be interpreted as the probability of observing a walk from i to j belonging to Ω (conditioned on starting from $i_0 = i$) in an absorbing Markov chain [8] with transition matrix

$$\begin{bmatrix} T & \boldsymbol{e} \\ 0 & 1 \end{bmatrix} \in \mathbb{R}^{(n+1)\times(n+1)}, \quad \boldsymbol{e} = (I - T)\mathbf{1}.$$

We have added an additional absorbing state $n+1$ to account for the missing probability due to $T\mathbf{1} \leq \mathbf{1}$ not being an equality. Note that $\mathbb{P}[\Omega]$ defined in this way is a substochastic matrix only when the set Ω is prefix-free; otherwise it may contain entries larger than 1 due to repeating prefixes: e.g., when Ω contains both $((1,2))$ and $((1,2),(2,3),(3,2))$, then $\mathbb{P}[\Omega]_{12}$ contains a sum of probabilities of events that are not disjoint.

We write $T = D + L + U$, where $L = \operatorname{tril}(T)$ is associated with *downward* transitions, i.e., transitions from a level i to a level $j < i$, and symmetrically $U = \operatorname{triu}(T)$ is associated with *upward* transitions, i.e., transitions from a level i to a level $j > i$. The key combinatorial lemma is the following.

Lemma 9. *Let $A = I - T \in \mathbb{R}^{n\times n}$ (with T substochastic) be lower Hessenberg, and ω be a walk with non-zero probability. If ω contains k downward transitions, then it contains at least $k - n + 1$ upward transitions.*

Proof. Let us choose an integer h such that $1 \leq h < n$, and define

$s_h^{\uparrow}(\omega) =$ no. of transitions in ω from a state in $\{1, 2, \dots, h\}$ to one in $\{h+1, h+2, \dots, n\}$,

$s_h^{\downarrow}(\omega) =$ no. of transitions in ω from a state in $\{h+1, h+2, \dots, n\}$ to one in $\{1, 2, \dots, h\}$.

Clearly, once we reach $\{h+1, h+2, \dots, n\}$ we must leave it before entering it again, hence transitions of the two kinds alternate in ω, and thus

$$s_h^{\uparrow}(\omega) - 1 \leq s_h^{\downarrow}(\omega) \leq s_h^{\uparrow}(\omega) + 1.$$

We take the rightmost inequality and sum over h, to get

$$s^{\downarrow}(\omega) \leq \sum_{h=1}^{n-1} s_h^{\downarrow}(\omega) \leq \sum_{h=1}^{n-1} (s_h^{\uparrow}(\omega) + 1) = s^{\uparrow}(\omega) + (n-1).$$

Here, $s^{\uparrow}(\omega)$ is the total number of upward transitions in ω, which is equal to $\sum_{h=1}^{n-1} s_h^{\uparrow}(\omega)$ because in a lower Hessenberg matrix each upward transition with nonzero probability is of the form $(h, h+1)$ for some h. On the other hand, $s^{\downarrow}(\omega)$ is the number of downward transitions in ω, which is smaller or equal than the sum $\sum_{h=1}^{n-1} s_h^{\downarrow}(\omega)$, since each downward transition is counted in $s_h^{\downarrow}(\omega)$ for at least one choice of h, but may be counted in multiple ones: for instance, a transition from state 4 down to state 1 is counted in $s_1^{\downarrow}(\omega), s_2^{\downarrow}(\omega)$, and $s_3^{\downarrow}(\omega)$. □

From the lemma we can obtain an alternative proof of the following result.

Theorem 10. *Let $A = I - T \in \mathbb{R}^{n\times n}$ (with T substochastic) be lower Hessenberg. Then, $\rho(P_{GS}) \geq \rho(P_{AGS})$.*

Proof. By standard arguments for sojourn and hitting probabilities in Markov chains, we have

$$\begin{aligned} &\mathbb{P}[\text{walks of any length } \ell \text{ with 0 downward transitions}] \\ &\qquad = I + (D+U) + (D+U)^2 + (D+U)^3 + \cdots = (I - D - U)^{-1}, \end{aligned}$$

and

$$\begin{aligned}&\mathbb{P}[\text{walks with exactly } k \text{ downward transitions, ending with a downward transition}]\\&= (I-D-U)^{-1}L(I-D-U)^{-1}L(I-D-U)^{-1}L\cdots(I-D-U)^{-1}L = P_{AGS}^{k},\end{aligned}$$

where $P_{AGS} = (I-D-U)^{-1}L$ is the iteration matrix of the anti-Gauss–Seidel method. Similarly, when $k \geq n-1$, we have

$$\begin{aligned}&\mathbb{P}[\text{walks with } \textit{at least } k-n+1 \text{ upwards transitions}]\\&= (I-D-L)^{-1}U(I-D-L)^{-1}U(I-D-L)^{-1}U\cdots(I-D-L)^{-1}U(I+P+P^2+\dots)\\&\qquad = P_{GS}^{k-n+1}(I-P)^{-1},\end{aligned}$$

since a walk with at least $k-n+1$ upward transitions can be seen as a walk with exactly $k-n+1$ upward transitions, ending with one of them, followed by any walk. In view of Lemma 9, the following inequality hold component-wise

$$P_{AGS}^{k} \leq P_{GS}^{k-n+1}(I-P)^{-1}, \quad \text{for all } k \geq n-1, \tag{5}$$

and from (5) we get

$$\|P_{AGS}^{k}\|_{\infty}^{1/k} \leq \|P_{GS}^{k-n+1}\|_{\infty}^{1/k}\ \|(I-P)^{-1}\|_{\infty}^{1/k}.$$

Passing to the limit and using Gelfand's formula $\lim_{k\to\infty}\|M^k\|^{1/k} = \rho(M)$, we obtain $\rho(P_{AGS}) \leq \rho(P_{GS})$. □

Remark 11. *Equation* (5) *shows that this comparison theorem follows from an elementwise inequality, although a more complicated one than the ones considered in [3, 21].*

7 Numerical experiments

To verify the statements of the theorems and give a quantitative assessment of the difference between $\rho(P_{GS})$, $\rho(P_S)$, $\rho(P_{AGS})$, we plot them for various examples.

To obtain a random lower-Hessenberg M-matrix $A \in \mathbb{R}^{n\times n}$, we generate random non-negative $P \in \mathbb{R}^{n\times n}$, $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$ by drawing their entries uniformly and independently from $[0,1]$, and then we find the unique lower-Hessenberg matrix A such that

$$A\boldsymbol{u} = \boldsymbol{v} \quad \text{and} \quad A_{ij} = -P_{ij} \quad \text{for all } i \neq j,\ i \geq j-1.$$

In Matlab code:

```
P = tril(rand(n), 1);
P = P - diag(diag(P));
u = rand(n, 1);
v = rand(n, 1);
d = (v + P*u) ./ u;
A = diag(d) - P;
```

The condition $A\boldsymbol{u} = \boldsymbol{v}$ ensures that A is a nonsingular M-matrix, since any Z-matrix for which $A\boldsymbol{u} = \boldsymbol{v}$ for some $\boldsymbol{u} > 0, \boldsymbol{v} \geq 0, \boldsymbol{v} \neq 0$ is an M-matrix [2, Chapter 6, Condition I_{28}].

We show in Figure 1 the values of the three iteration radii for 50 random 5×5 lower Hessenberg matrices. One can confirm that the three values are alwasy in the order predicted by Theorem 4; moreover, the experiments reveal that while the difference between $\rho(P_{GS})$ and $\rho(P_S)$ if often minimal, the difference with $\rho(P_{AGS})$ is much more substantial.

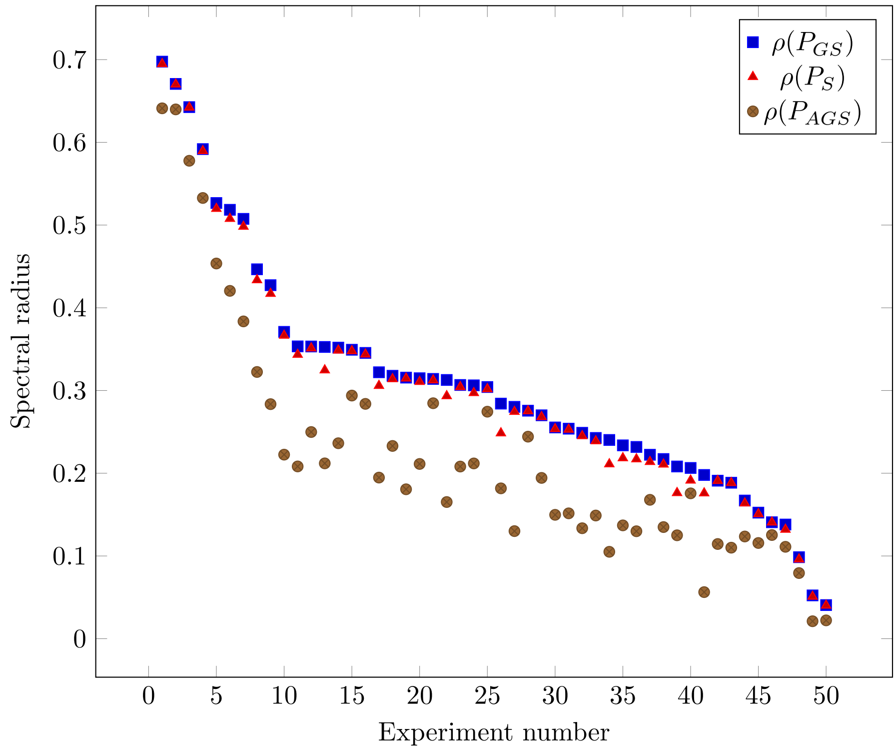

Fig. 1: Comparison of iteration radii for 50 random 5×5 lower Hessenberg M-matrices, sorted by decreasing value of $\rho(GS)$.

In Figure 2, we investigate what happens as the matrices A get close to singular. For this experiment, rather than taking random $\boldsymbol{u}, \boldsymbol{v}$, we set $\boldsymbol{u} = \mathbf{1}$ and $\boldsymbol{v} = \eta\mathbf{1}$ for a certain scalar η. The first plot displays the three spectral radii; one sees that as η gets smaller they get closer to 1 (i.e., the iterative methods get slower) and the difference between them is harder to detect. For this reason, in a second plot we display the value of k needed to obtain $\rho(P)^k \leq 0.01$ (that is, $k = \frac{\log 0.01}{\log \rho(P)}$). This quantity gives an indication of the number of iterations required for the convergence of an iterative method, and is a more practical metric for this case. One can see that the benefits of the anti-Gauss–Seidel splitting in terms of convergence speed are present even in cases where the matrix is closer to singular.

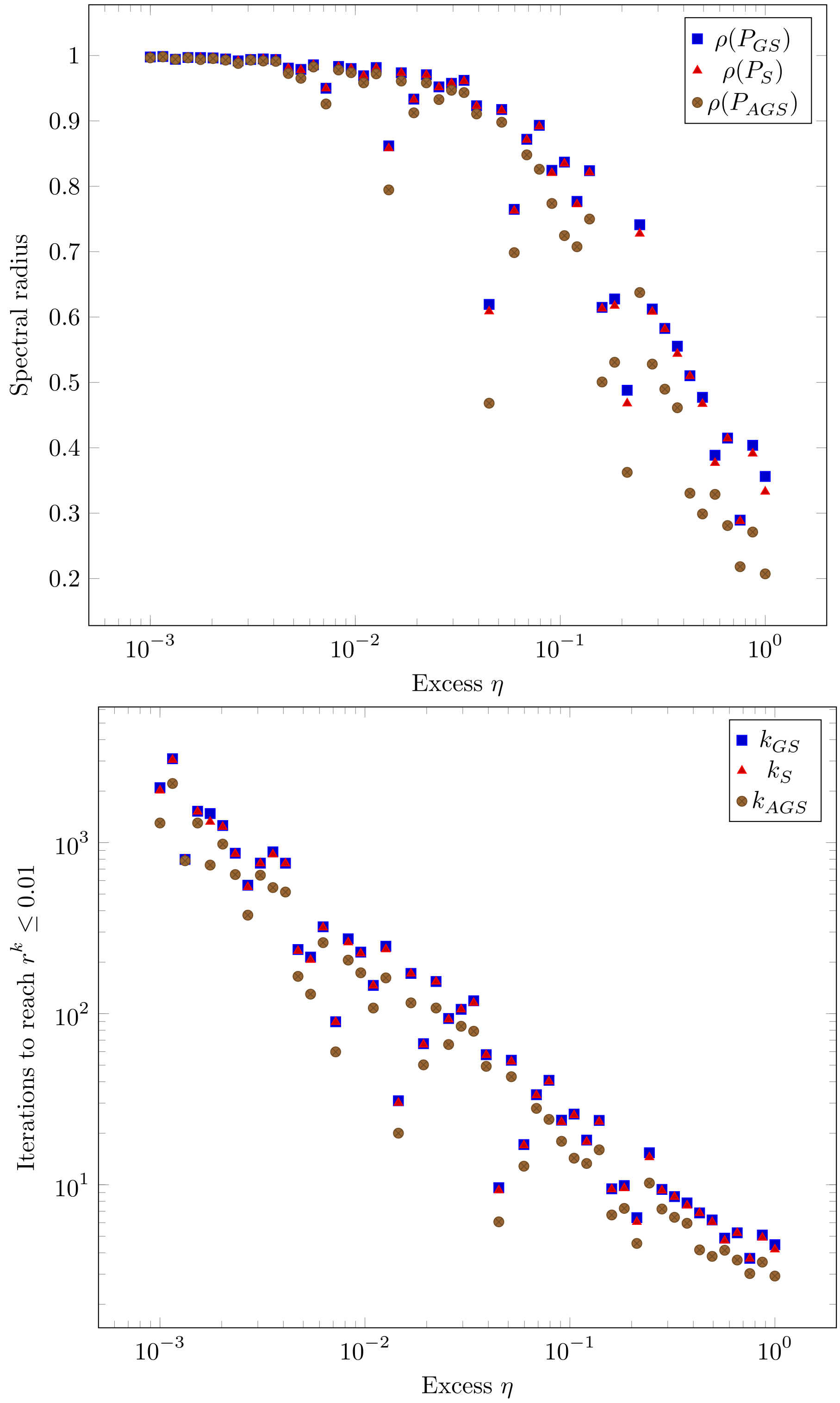

Fig. 2: Comparison of (a) iteration radii (b) power k needed to reach $\rho(P)^k \leq 0.01$, for 50 random 5×5 lower Hessenberg M-matrices with varying excess η.

8 Conclusions

In this paper we have shown that there is a hierarchy among matrix splittings for M-matrices in Hessenberg form, covering the Gauss–Seidel, anti-Gauss–Seidel, and staircase partitionings, together with some generalizations. These results encourage further investigation into comparison theorems for M-matrix splittings, suggesting that this classical topic is far from being completely analyzed and solved. Future work is concerned with the analysis of these generalizations for the design of efficient processor-oriented variants of staircase splitting methods for parallel computation. Another interesting topic is the comparison of classical stationary iterative methods and staircase splitting methods for semidefinite matrices, under suitable structures.

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