Self-adaptive Extrapolated Gauss-Seidel Iterative Methods

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Abstract. In this paper, we consider a self-adaptive extrapolated Gauss-Seidel method for solving the Hermitian positive definite linear systems. Based on optimization models, self-adaptive optimal factor is given. Moreover, we prove the convergence of the self-adaptive extrapolated Gauss-Seidel method without any constraints on optimal factor. Finally, the numerical examples show that the self-adaptive extrapolated Gauss-Seidel method is effective and practical in iteration number.

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Key words: Hermitian positive definite, Gauss-Seidel iteration, self-adaptive, extrapolated, linear systems.

1 Introduction

Consider the large sparse system of linear equations

\[ Ax = b, \]

where \( A = (a_{ij}) \in \mathbb{C}^{n \times n} \) is a known nonsingular matrix and \( x, b \in \mathbb{C}^n \) are vectors. The splitting iterative method is one of the important way for solving the linear systems (1.1). For any splitting \( A = M - N \) with a nonsingular matrix \( M \), the basic splitting iterative method can be expressed as

\[ x^{(k+1)} = M^{-1}N x^{(k)} + M^{-1}b, \quad k = 0,1,\cdots. \]

Let \( T = M^{-1}N \) and \( c = M^{-1}b \). Then (1.2) can be also written as

\[ x^{(k+1)} = T x^{(k)} + c, \quad k = 0,1,\cdots. \]

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Consider the usual splitting of $A$,
\[ A = D - L - U, \] (1.4)
where $D$ is a diagonal matrix, $-L$ and $-U$ are the strictly lower and the strictly upper triangular parts of $A$, respectively. Taking $M = D - L$ in (1.2), the iteration (1.3) yields the classical Gauss-Seidel iterative method, and the iteration matrix of the Gauss-Seidel method is given by
\[ T = (D - L)^{-1}U. \] (1.5)

In order to accelerate the convergence of the Gauss-Seidel iterative method for solving the linear systems (1.1), Davod [4] presented the generalized Gauss-Seidel (GGS) iterative method, i.e., using the splitting $A = T_m - E_m - F_m$, where
\[ T_m = (t_{ij}) = \begin{cases} -a_{ij}, & \text{for } |i - j| \leq m, \\ 0, & \text{otherwise}. \end{cases} \]
So we can see that the GGS method is essentially block-type Gauss-Seidel method.

Gunawardena et. al [7] first introduced the modified Gauss-Seidel method with preconditioned technique. In particular, when coefficient matrix is an $M$-matrix, or a $Z$-matrix, or an $H$-matrix, many researchers [9, 13, 15, 20, 21, 23, 24] presented also the modifications and improvements of preconditioners to solve the linear systems (1.1). Recently, Kohno et. al [12], Kotakemori et. al [14] and Shen et. al [22] extended Gunawardena, Jain and Snyders’ works to more general cases and employed new different modified Gauss-Seidel methods by using the general preconditioner $P$ with various parameters. But these modifications and improvements of Gauss-Seidel iterative method are only theoretical and the numerical examples in those references are only small size problems, and the amount of calculation is rapidly increased with the problem size. And it is the most troubling that it is difficult in choosing many proper parameters for these methods.

With regard to parameters that have a significant effect on the convergence rate of the algorithm, Hadjidimos [8] considered the extrapolation and relaxation methods, Hadjidimos and Yeyios [10] proposed the extrapolated Gauss-Seidel method
\[ x^{(k+1)} = [(1 - \alpha)I + \alpha T]x^{(k)} + \alpha c, \] (1.6)

But the optimal parameters or the weighting matrices of all above-mentioned methods are determined in advance, they are not known to be good or bad, this influences the efficiency of these iterative methods. Fortunately, the papers [26] and [18] have applied...
the optimal model to compute the weight factors. Based on this strategy and the extrapolated methods [17], we consider the self-adaptive extrapolated Gauss-Seidel method for the Hermitian positive definite systems.

The rest of the paper is organized as follows. Next section is the preliminaries. In Section 3, We focus on to discuss the new algorithm and its convergence. Section 4 is devoted to the numerical experiments.

2 Preliminaries

In this section, we give some of the notations and lemmas which will be used in what follows.

As usual, $\mathbb{C}^{n\times n}$ is used to denote the $n \times n$ complex matrix set, and $\mathbb{C}^n$ the $n$-dimensional complex vector set. The matrix $A^H$ denotes the conjugate transpose of $A$. Similarly the conjugate transpose of a vector $x$ is denoted by $x^H$. A matrix $A \in \mathbb{C}^{n\times n}$ is called Hermitian positive definite (or semidefinite), if it is Hermitian and for all $x \in \mathbb{C}^n, x \neq 0$, it holds that $x^H A x > 0$ (or $x^H A x \geq 0$). If $A$ is Hermitian positive definite, the norm

$$
\|x\|_A = \|A^{1/2} x\|_2 = (Ax, x)^{1/2}
$$

(2.1)

is called the $A$-norm [5] or energy norms of the vector $x$.

**Lemma 2.1.** (Convergence, [25]) Let $A = D - E - E^H$ be an $n \times n$ Hermitian matrix with $D$ is Hermitian and positive definite and $D - E$ is nonsingular. Then, the Gauss-Seidel iterative method is convergent if and only if $A$ is positive definite.

**Lemma 2.2.** (Extrapolation, [10, 17]) The sufficient conditions for the convergence of the extrapolated Gauss-Seidel method (EGS) (1.6) are:

1. the original Gauss-Seidel method is convergent,
2. $0 < \alpha < 2/(1 + \rho(T))$, where $T$ is given by (1.5).

**Lemma 2.3.** ([11]) If a nonsingular $A$ is Hermitian positive definite, then there exists a unique Hermitian positive definite $B$ such that $B^2 = A$.

**Lemma 2.4.** (Cauchy-Schwarz inequality) If $(\cdot, \cdot)$ is an inner product on a vector space $V$ over the field $\mathbb{C}$, then

$$
|(x,y)|^2 \leq (x,x)(y,y), \text{ for all } x, y \in V.
$$

Equality occurs if and only if $x$ and $y$ are linear dependent, that is, $x = ay$ or $y = ax$ for some $a \in \mathbb{C}$.

**Lemma 2.5.** ([11]) Every vector norm $\|\cdot\|$ on $\mathbb{C}^n$ is a uniformly continuous function.
3 Self-adaptive EGS method

In this section, we give the self-adaptive extrapolated Gauss-Seidel method.

We assume that the symmetric positive definite matrix $A$ has the following splitting, as (1.4)

$$A = D - L - L^T,$$

and the iteration matrix of the Gauss-Seidel method is given by

$$T = (D - L)^{-1}L^T. \quad (3.2)$$

**Algorithm 3.1.** *(The Self-adaptive Extrapolated GS(SEGS) Iterative Method)*

Let $x^{(0)} \in \mathbb{C}^n$ be an arbitrary initial guess. For $k=0,1,2,\ldots$ until the sequence of iterations $\{x^{(k)}\}_{k=0}^\infty \subset \mathbb{C}^n$ converges, compute $x^{(k+1)}$ by the following scheme:

$$\tilde{x}^{(k)} = Tx^{(k)} + (D - L)^{-1}b, \quad (3.3)$$

$$x^{(k+1)} = \alpha \tilde{x}^{(k)} + (1 - \alpha)x^{(k)}, \quad (3.4)$$

where $\alpha$ is the solution of the following optimization model

$$\min_{\alpha} \frac{1}{2}(x^{(k)})^H A x^{(k)} - (x^{(k)})^H b. \quad (3.5)$$

Alternatively, (3.4) can be rewritten as:

$$x^{(k+1)} = x^{(k)} + \alpha_k (D - L)^{-1}r^{(k)}, \quad (3.6)$$

where

$$r^{(k)} = b - Ax^{(k)}, \quad (3.7)$$

and $\alpha_k$ is obtained by the optimization model (3.5). By simplified derivation, (3.5) yields the desired value of $\alpha_k$

$$\alpha_k = \frac{\left((D - L)^{-1}r^{(k)}\right)^H r^{(k)}}{\left((D - L)^{-1}r^{(k)}\right)^H A (D - L)^{-1}r^{(k)}}$$

$$= \frac{\left((D - L)^{-1}r^{(k)}, r^{(k)}\right)}{\left((D - L)^{-1}r^{(k)}, A (D - L)^{-1}r^{(k)}\right)}. \quad (3.8)$$
Accordingly, the iteration matrix \( G_{\alpha_k} \) at the \( k \)-th step for the Algorithm 3.1 is

\[
\begin{align*}
G_{\alpha_k} &= \alpha_k T + (1 - \alpha_k) I \\
&= \alpha_k (D - L)^{-1} L^H + (1 - \alpha_k) (D - L)^{-1} (D - L) \\
&= (D - L)^{-1} \left( \alpha_k L^H + (1 - \alpha_k) (D - L) \right) \\
&= I - \alpha_k (D - L)^{-1} A.
\end{align*}
\]

If \( \alpha_k \) is independent on the iteration index \( k \), Algorithm 3.1 will be the extrapolated Gauss-Seidel method. From Lemma 2.1 and Lemma 2.2, we know that the extrapolated Gauss-Seidel method of the Hermitian positive definite matrix is convergent with \( 0 < \alpha < \frac{2}{1 + \rho(T)} \). But our Algorithm 3.1 will be proved convergence without any constraints on \( \alpha \).

**Theorem 3.1.** Let \( A \) be a Hermitian positive definite matrix. Then Algorithm 3.1 is convergent with respect to \( \| \cdot \|_A \) for any choice of the initial guess \( x^{(0)} \).

**Proof.** Let \( x^* \) be the unique solution of linear system of equations (1.1), \( x^{(k)} \) be the solution generated by the Algorithm 3.1 at the \( k \)-th step, and

\[
\varepsilon^{(k)} = x^{(k)} - x^*, \ k = 0, 1, 2, \ldots
\]

be the error at the \( k \)-th step of iteration. And the following can be obtain from (3.7),

\[
\begin{align*}
r^{(k)} &= b - Ax^{(k)} = Ax^* - Ax^{(k)} = -A\varepsilon^{(k)}. \quad (3.10)
\end{align*}
\]

Similar to (3.10),

\[
r^{(k+1)} = -A\varepsilon^{(k+1)}. \quad (3.11)
\]

For simplification, we define

\[
z^{(k)} = (D - L)^{-1} r^{(k)}. \quad (3.12)
\]
Due to the properties of the matrix \(A\) and the definition of \(A\)-norm (2.1), we have
\[
\|e^{(k+1)}\|_A^2 = \langle Ae^{(k+1)}, e^{(k+1)} \rangle = \left( -r^{(k+1)} , G_a \varepsilon^{(k)} \right) \\
= \left( -r^{(k)} + \alpha_k A (D-L)^{-1} r^{(k)} , \left( I - \alpha_k (D-L)^{-1} A \right) \varepsilon^{(k)} \right) \\
= \left( -r^{(k)} , \varepsilon^{(k)} \right) + \alpha_k \left( \left( r^{(k)} , (D-L)^{-1} A \varepsilon^{(k)} \right) + \left( A z^{(k)} , \varepsilon^{(k)} \right) \right) \\
- \alpha_k^2 \left( A z^{(k)} , (D-L)^{-1} A \varepsilon^{(k)} \right) \\
= \|e^{(k)}\|_A^2 + \frac{\left( z^{(k)} , r^{(k)} \right)}{(z^{(k)} , A z^{(k)})} \cdot \\
\left( r^{(k)} - z^{(k)} \right) + \frac{\left( z^{(k)} , r^{(k)} \right)}{(z^{(k)} , A z^{(k)})} \left( A z^{(k)} , -z^{(k)} \right) \\
= \|e^{(k)}\|_A^2 - \frac{\left( z^{(k)} , r^{(k)} \right)^2}{(z^{(k)} , A z^{(k)})}. \tag{3.13}
\]

By Lemma 2.3, there exists a Hermitian positive definite matrix \(B = A^{1/2}\), such that
\[
\frac{\|e^{(k+1)}\|_A^2}{\|e^{(k)}\|_A^2} = 1 - \frac{\left( z^{(k)} , r^{(k)} \right)^2}{(z^{(k)} , A z^{(k)}) \langle Ae^{(k)} , \varepsilon^{(k)} \rangle} \\
= 1 - \frac{\left( z^{(k)} , -A z^{(k)} \right)^2}{(z^{(k)} , A z^{(k)}) \langle Ae^{(k)} , \varepsilon^{(k)} \rangle} \\
= 1 - \frac{\left( A^{1/2} z^{(k)} , A^{1/2} \varepsilon^{(k)} \right)^2}{\left( A^{1/2} z^{(k)} , A^{1/2} \varepsilon^{(k)} \right) \left( A^{1/2} \varepsilon^{(k)} , A^{1/2} \varepsilon^{(k)} \right)}. \tag{3.14}
\]

And in (3.14) the vectors \(A^{1/2} z^{(k)}\) and \(A^{1/2} \varepsilon^{(k)}\) are linear independent. If not, there exists a real \(\beta\), so
\[
z^{(k)} = \beta \varepsilon^{(k)},
\]
\[
\iff (D-L)^{-1} r^{(k)} = \beta A^{-1} r^{(k)},
\]
\[
\iff \beta \det(D-L) = \det(A), \quad \text{or} \quad r^{(k)} = 0.
\]

But on the account of (3.1) and (3.10) the equations (3.15) is, in general, not true, so we are done. This means that the equality does not hold for Cauchy-Schwarz inequality (2.2), namely
\[
0 < \frac{\left( A^{1/2} z^{(k)} , A^{1/2} \varepsilon^{(k)} \right)^2}{\left( A^{1/2} z^{(k)} , A^{1/2} \varepsilon^{(k)} \right) \left( A^{1/2} \varepsilon^{(k)} , A^{1/2} \varepsilon^{(k)} \right)} < 1. \tag{3.15}
\]
Then, it follows from (3.15) and (3.14)
\[ \frac{\| e^{(k+1)} \|_A}{\| e^{(k)} \|_A} < 1. \tag{3.16} \]
Consequently, by Lemma 2.5 there exist a positive number \( \rho < 1 \) such that
\[ \frac{\| e^{(k+1)} \|_A}{\| e^{(k)} \|_A} \leq \rho, \tag{3.17} \]
which is equivalent to
\[ \lim_{k \to \infty} e^{(k+1)} = 0. \]
Hence, we have proved this theorem.

**Remark 3.1.** For Algorithm 3.1, the optimization model in each iteration require the ‘exact’ solution. However, this may be very costly and impractical in actual implementations, particularly when the scale of the original problem is very large. To improve the computing efficiency of the Algorithm 3.1, similar to the Algorithm 4.2.1 of [16], we will employ a simple strategy to perform a new updating after \( k \) iteration steps.

4 Numerical experiments

In this section, we use three different numerical examples to show the feasibility and effectiveness of Algorithm 3.1 when it is used to find the solution of the linear systems (1.1) with Hermitian positive definite coefficient matrix. The results of all examples are compared with some of the better existing iterative methods. That is to say, we solve the system of linear equations (1.1) by Algorithm 3.1, the basic Gauss-Seidel (GS) method and the extrapolated Gauss-Seidel (EGS) method with some arbitrary values of \( \alpha \). Also, we solve the system of linear equations (1.1) by the GGS method presented by Davod [4].

For each example, we compare all the above methods from the view of the iteration numbers (denoted by IT) and in terms of the total CPU execution time (denoted by CPU). All timing results are reported in seconds. In the following tables, \( k \) stands for a new updating after \( k \) iteration steps.

In our implementations, the initial vector \( x^{(0)} \) is set to zero and the iteration is terminated when the current iterate satisfied
\[ \frac{\| b - Ax^{(k)} \|_2}{\| b \|_2} \leq 10^{-6}, \tag{4.1} \]
where \( \| \cdot \|_2 \) refers to \( L_2 \)-norm. In addition, all codes were run in MATLAB [version 7.12.0.635 (R2011a)] in double precision and all experiments were performed on a personal computer with 3.20GHz central processing unit [Intel(R) Pentium(R)(TM)2 CPU G2130], 4G memory and Microsoft Window 7 operating system (6.1).
Table 1: IT and CPU for SEGS, EGS, GGS and GS methods for Example 4.1.

<table>
<thead>
<tr>
<th>p</th>
<th>SEGS</th>
<th>EGS</th>
<th>GGS</th>
<th>GS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>k=3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>IT</td>
<td>83</td>
<td>351</td>
<td>262</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.004764</td>
<td>0.017525</td>
<td>0.012783</td>
</tr>
<tr>
<td>40</td>
<td>IT</td>
<td>141</td>
<td>1220</td>
<td>914</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.016766</td>
<td>0.113716</td>
<td>0.090983</td>
</tr>
<tr>
<td>60</td>
<td>IT</td>
<td>341</td>
<td>2546</td>
<td>1908</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.075822</td>
<td>0.486628</td>
<td>0.364732</td>
</tr>
<tr>
<td>80</td>
<td>IT</td>
<td>582</td>
<td>4294</td>
<td>3219</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.226410</td>
<td>1.356569</td>
<td>1.009542</td>
</tr>
<tr>
<td>100</td>
<td>IT</td>
<td>896</td>
<td>6439</td>
<td>4828</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.538224</td>
<td>3.297829</td>
<td>2.443553</td>
</tr>
<tr>
<td>120</td>
<td>IT</td>
<td>1216</td>
<td>8962</td>
<td>6721</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>1.197484</td>
<td>7.282420</td>
<td>5.268566</td>
</tr>
<tr>
<td>140</td>
<td>IT</td>
<td>1874</td>
<td>11849</td>
<td>8886</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>2.632422</td>
<td>13.892134</td>
<td>10.198586</td>
</tr>
</tbody>
</table>

Example 4.1 The test PDE problem we are considering in this Example is

\[-\Delta u \equiv - \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = f(x,y) \quad (4.2)\]

with \((x,y) \in \Omega\), where \(\Omega = (0,1) \times (0,1)\) is a square region. For the test problem, only the matrix \(A\), which is constructed from nine-point finite difference discretization of the given PDE (4.2), is of importance, so the right-hand side vector \(b\) is created artificially. Hence, the right-hand side function \(f(x,y)\) in Examples 4.1 is not relevant. So the coefficient matrix

\(A = \text{tridiag}(D,G,D) \in \mathbb{R}^{q \times q}\),

where

\(D = \text{tridiag}(-4,20,-4) \in \mathbb{R}^{p \times p}, G = \text{tridiag}(-1,-4,-1) \in \mathbb{R}^{p \times p}\).

and the right-hand side vector \(b\) is chosen so that \(b = Ae\) with \(e\) being the vector of all entries equal to 1. For this example, we set \(p = q\).

In Table 1 we list the iteration numbers and the CPU times in seconds with respect to SEGS, EGS, GGS and GS methods.

Example 4.2 Consider the following system of linear equations, for which \(A = (a_{kj}) \in \mathbb{C}^{n \times n}\) is defined as follows:

\[a_{kj} = \begin{cases} 
8, & \text{for } j = k; \\
-1, & \text{for } \max\{1,k-4\} \leq j \leq \{n,k+4\}, k \neq j; \\
0, & \text{otherwise.}
\]
We chose the right-hand side vector $b = (1, 1, \cdots, 1)^T$. The above coefficient matrix is ill-conditioned if $n$ is large.

The following Table 2 shows the iteration numbers and the CPU times in seconds.
Table 4: Comparison of computational results for Example 4.4.

<table>
<thead>
<tr>
<th>m</th>
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<th>EGS</th>
<th>GGS</th>
<th>GS</th>
</tr>
</thead>
<tbody>
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<td></td>
<td>k=2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>IT</td>
<td>155</td>
<td>343</td>
<td>293</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.009617</td>
<td>0.015375</td>
<td>0.014176</td>
</tr>
<tr>
<td>32</td>
<td>IT</td>
<td>487</td>
<td>1391</td>
<td>1191</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.057962</td>
<td>0.135159</td>
<td>0.118799</td>
</tr>
<tr>
<td>64</td>
<td>IT</td>
<td>2181</td>
<td>5556</td>
<td>4762</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>0.820887</td>
<td>1.658372</td>
<td>1.421410</td>
</tr>
<tr>
<td>96</td>
<td>IT</td>
<td>4337</td>
<td>12454</td>
<td>10674</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>3.657569</td>
<td>7.898573</td>
<td>6.892787</td>
</tr>
<tr>
<td>128</td>
<td>IT</td>
<td>7790</td>
<td>22069</td>
<td>18916</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>11.980302</td>
<td>25.932632</td>
<td>22.352691</td>
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<td>160</td>
<td>IT</td>
<td>12109</td>
<td>-</td>
<td>29483</td>
</tr>
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<td></td>
<td>CPU</td>
<td>32.774894</td>
<td>-</td>
<td>58.186521</td>
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<tr>
<td>192</td>
<td>IT</td>
<td>17903</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>CPU</td>
<td>68.103404</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Notes. the symbol “−” denotes that the iteration is failing.

with respect to SEGS, EGS, GGS and GS methods.

**Example 4.3** Consider linear equations with Hermitian positive definite coefficient matrix that rise in the reference [26], we choose $A = 0.1 \pi I + \mu K$ with $\mu = 0.02$, and the matrix $K$ possesses the form $K = I \otimes V + V \otimes E$ with

$$V = (m+1)^2 \text{tridiag}(-1,2,1) \in \mathbb{R}^{m \times m},$$

where $I$ is the identity matrix, and $\otimes$ is the Kronecker product symbol. Hence, $A$ is an $n \times n$ block-tridiagonal matrix, with $n = m^2$. We take the right-hand side vector $b = (1,1,\cdots,1)^T$.

Table 3 shows the iteration numbers and the CPU times in seconds with respect to SEGS, EGS, GGS and GS methods.

**Example 4.4** We consider the complex linear system $Ax = b$, with the Hermitian positive definite coefficient matrix $A = W + iT + (8-4i)I \in \mathbb{C}^{n \times n}$ being given by

$$W = \text{tridiag}(c,a,c) \in \mathbb{R}^{n \times n}, \quad T = I \otimes V_c + V_c \otimes I \in \mathbb{R}^{n \times n},$$

(4.3)

with

$$V_c = V - e_1 e_m^T + e_m e_1^T \in \mathbb{R}^{m \times m}$$
and

\[ V = \text{tridiag}(-1,2,1) \in \mathbb{R}^{m \times m}, \]
\[ e_1 = (1,0,\cdots,0)^T \in \mathbb{R}^m, \quad e_m = (0,\cdots,0,1)^T \in \mathbb{R}^m, \]
\[ a = (1,3,5,\cdots,2n-3,2n-1)^T \in \mathbb{R}^n, \]
\[ c = (-1,-2,\cdots,-(n-1))^T \in \mathbb{R}^{n-1}. \]

The right-hand side vector \( b \) is defined as \( b = Ax^\ast \), with \( x^\ast = (1,2,\cdots,n)^T \in \mathbb{R}^n \).

In Table 4 we report results for SEGS, EGS, GGS and GS methods.

We see from Tables 1–4 that for all methods, the iteration numbers and the CPU times grow with problem size. However, this growth is slower for SEGS than for other methods, such as GS, GGS and EGS with fixed extrapolated factors. The reason is that the stationary of weighting factors is deleted, the range for finding the optimal weighting factors is extended. Hence, we show that our SEGS method with fixed initial guess \( \alpha = 1 \) is practical and effective.

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