Robust dropping criteria for F-norm minimization based sparse approximate inverse preconditioning

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Abstract Drop tolerance criteria play a central role in Sparse Approximate Inverse preconditioning. Such criteria have received, however, little attention and have been treated heuristically in the following manner: If the size of an entry is below some empirically small positive quantity, then it is set to zero. The meaning of “small” is vague and has not been considered rigorously. It has not been clear how drop tolerances affect the quality and effectiveness of a preconditioner $M$. In this paper, we focus on the adaptive Power Sparse Approximate Inverse algorithm and establish a mathematical theory on robust selection criteria for drop tolerances. Using the theory, we derive an adaptive dropping criterion that is used to drop entries of small magnitude dynamically during the setup process of $M$. The proposed criterion enables us to make $M$ both as sparse as possible as well as to be of comparable quality to the potentially denser matrix which is obtained without dropping. As a byproduct, the theory applies to static F-norm minimization based preconditioning procedures, and a similar dropping criterion is given that can be used to sparsify a matrix after it has been computed by a static sparse approximate inverse procedure. In contrast to the adaptive procedure, dropping in the static procedure does not reduce the setup time of the matrix but makes the application of the sparser $M$ for Krylov iterations cheaper. Numerical experiments reported confirm the theory and illustrate the robustness and effectiveness of the dropping criteria.

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1 Introduction

Preconditioned Krylov subspace methods [34] are among the most popular iterative solvers for large sparse linear system of equations

\[ Ax = b, \]

where \( A \) is a nonsingular and nonsymmetric (non-Hermitian) \( n \times n \) matrix and \( b \) is an \( n \)-dimensional vector. Sparse approximate inverse (SAI) preconditioning aims to construct sparse approximations of \( A^{-1} \) directly and is nowadays one class of important general-purpose preconditioning for Krylov solvers. There are two typical kinds of SAI preconditioning approaches. One constructs a factorized sparse approximate inverse (FSAI). An effective algorithm of this kind is the approximate inverse (AINV) algorithm, which is derived from the incomplete (bi)conjugation procedure [4, 7]. The other is based on F-norm minimization and is inherently parallelizable. It aims to construct \( M \approx A^{-1} \) by minimizing \( \|AM - I\|_F \) for a specified pattern of \( M \) that is either prescribed in advance or determined adaptively, where \( \| \cdot \|_F \) denotes the F-norm of a matrix. A hybrid version, i.e., the factorized approximate inverse (FSAI) preconditioning based on F-norm minimization, has been introduced by Kolotilina and Yeremin [30]. FSAI is generalized to block form, called BFSAI in [25]. An adaptive algorithm in [24] is presented that generates automatically the nonzero pattern of the BFSAI preconditioner. In addition, the idea of F-norm minimization is generalized in [22] by introducing a sparse readily inverted target matrix \( T \). \( M \) is then computed by minimizing \( \|AM - T\|_{F,H} \) over a space of matrices with a prescribed sparsity pattern, where \( \| \cdot \|_{F,H} \) is the generalized F-norm defined by \( \|B\|_{F,H}^2 = \langle B, B \rangle_{F,H} = \text{trace}(B^T H B) \) with \( H \) being some symmetric (Hermitian) positive definite matrix, the superscript \( T \) denotes the transpose of a matrix or vector, and is replaced by the conjugate transpose for a complex matrix \( B \). A good comparison of factorized SAI and F-norm minimization based SAI preconditioning approaches can be found in [6]. SAIs have been shown to provide effective smoothers for multigrid; see, e.g., [11, 12, 35, 37]. For a comprehensive survey on preconditioning techniques, we refer the reader to [3].

In this paper, we focus on F-norm minimization based SAI preconditioning, where a central issue is to determine the sparsity pattern of \( M \) effectively. There has been much work on a-priori pattern prescriptions, see, e.g., [2, 13, 14, 23, 36]. Once the pattern of \( M \) or its envelop is given, the computation of \( M \) is straightforward by solving \( n \) independent least squares (LS) problems and \( M \) is then further sparsified generally. This is called a static SAI preconditioning procedure. Huckle [23] has compared different a-priori sparsity patterns and established effective upper bounds for the sparsity pattern of \( M \) obtained by the famous adaptive SPAI algorithm [20]. He shows that the patterns of \((I + A)^k\), \((I + |A| + |A^T|)^k A^T \) and \((A^T A)^k A^T \) for small \( k \)
can be good envelop patterns of a good $M$. These patterns are very useful for reducing communication times when distributing and then computing $M$ in a distributed parallel computing environment.

For a general sparse matrix $A$, however, determining an effective sparsity pattern of $A^{-1}$ is nontrivial. A-priori sparse patterns may not capture positions of large entries in $A^{-1}$ effectively, or, they may capture the positions only when the patterns are unacceptably dense. Then the storage becomes a bottleneck and the time for the construction of the matrix is impractical. To cope with this difficulty, a number of researchers have proposed adaptive strategies that start with a simple initial pattern and successively augment or adaptively adjust this pattern until $M$ is satisfied with certain accuracy, i.e., $\|AM - I\| \leq \varepsilon$ for some norm, where $\varepsilon$ is fairly small, or a maximum number of augmentations is reached. This idea was first proposed by Cosgrove et al. [17], and developed by Grote and Huckle [20], Gould and Scott [19] and Chow and Saad [16]. From [6] it appears that the SPAI preconditioning proposed by Grote and Huckle [20] is more robust than the one proposed by Chow and Saad [16]. One of the key differences between these procedures is that they use different adaptive ways to generate sparsity patterns of $M$ by dropping entries of small magnitude so as to sparsify $M$. Recently, Jia and Zhu [27] have proposed a Power Sparse Approximate Inverse (PSAI) procedure that determines the sparsity pattern of $M$ in a new adaptive way. Furthermore, they have developed a practical PSAI algorithm with dropping, called PSAI($\text{tol}$), that dynamically drops the entries in $M$ whose magnitudes are smaller than a prescribed tolerance $\text{tol}$ during the process. Extensive numerical experiments in [26] demonstrate that the PSAI($\text{tol}$) is at least comparable to SPAI in [20].

As is well-known there are three goals for using dropping strategies in the SAI preconditioning procedure: (i) $M$ should be an effective preconditioner (ii) $M$ should be as sparse as possible so that it is cheap to set up and then to use in a Krylov solver, when its pattern is determined adaptively, and (iii) $M$ should be as sparse as possible so as to be cheap to use in a Krylov solver, when its sparsity pattern is prescribed. Apparently, dropping is a key step and plays a central role in designing a robust SAI preconditioning procedure. Chow [14] suggests a prefiltration strategy and drops the entries of $A$ itself that are below some tolerance before determining the pattern of $M$. This prefiltration idea is also adopted in, e.g., [28, 29, 36]. Instead of prefiltration, it may be more effective to apply the sparsification to $M$ after it has been computed, which is called postfiltration; see, e.g., [13, 37]. Wang and Zhang [38] have proposed a multistep static SAI preconditioning procedure that uses both prefiltration and postfiltration. Obviously, for a static SAI procedure, postfiltration cannot reduce the construction cost of $M$; rather, it only reduces the application cost of $M$ at each iteration of a Krylov solver. For an adaptive SAI procedure, a more effective approach is to dynamically drop entries of small magnitude as they are generated during the construction process. The approach is more appealing as it makes $M$ sparse throughout the whole setup process. As is clear, dropping is more important for an adaptive SAI procedure than for a static one since it reduces the setup time of $M$ for the former but not for the latter. For sparsification applied to FSAI, we refer the reader to [8, 9, 18, 31].

In this paper, we are concerned with drop tolerance strategies applied to the adaptive PSAI procedure. We have noticed that the drop tolerances used in the literature
are heuristic and empirical. One commonly takes some small quantities, say $10^{-3}$, as drop tolerances. Nevertheless, the mechanism for drop tolerances is by no means so simple. Empirically chosen tolerances are not necessarily robust, may not be effective, and might even lead to failure in preconditioning. Obviously, improperly chosen large tolerances may lead to a sparser but ineffective $M$, while tolerances that are too small may lead to a far denser but unnecessarily more effective preconditioner $M$ which is much more time consuming to apply. Our experiments confirm these statements, and illustrate that simply taking seemingly small tolerances, as suggested in the literature, may produce a numerical singular $M$, which can cause a Krylov solver to fail completely. Therefore, drop tolerance selection criteria deserve attention and it is desirable to establish a mathematical theory that can reveal intrinsic relationships between the drop tolerances and the quality of $M$. Such selection criteria enable the design of robust and effective SAI preconditioning procedures.

We point out that dropping has been extensively used in other important preconditioning techniques such as ILU factorizations [15, 33]. Some effective selection criteria have been proposed for drop tolerances in, e.g., [10, 21, 32]. It is distinctive that the setup time of good sparse approximate inverses overwhelms the cost of Krylov solver iterations while this is not necessarily the case for ILU preconditioners. This is true in a parallel computing environment, though SPAI and PSAI$(tol)$ are inherently parallelizable. Therefore, SAI type preconditioners are particularly attractive for solving a sequence of linear systems with the same coefficient matrix, as has been addressed in the literature, e.g., [5], where BiCGStab preconditioned with the adaptive SPAI algorithm [20] and the factorized AINV algorithm [4, 7] are experimentally shown to be faster than BiCGStab preconditioned with ILU(0), even in the sequential computing environment when more than one linear systems is solved.

The goal of this paper is to establish a rigorous theory for the drop tolerance selection criteria used in PSAI. The quality and non-singularity of $M$ obtained by PSAI depends on, and can be very sensitive to, the drop tolerances. Based on our theory, we propose an adaptive dropping criterion that is used to drop entries of small magnitude dynamically during the setup process of $M$ by PSAI. The criterion aims to make $M$ as sparse as possible, while possessing comparable quality to a possibly much denser $M$ obtained by PSAI without dropping. As a byproduct, the theory applies to static $F$-norm minimization based SAI preconditioning procedures, and a similar dropping criterion is derived that runs postfiltration robustly after $M$ is computed by a static SAI procedure, making $M$ and its sparsification of comparable preconditioning quality. As has been noted already, however, as compared to adaptive SAI procedures, dropping in static SAI procedures does not reduce the setup time of the preconditioner, rather it reduces the cost of applying the sparser $M$ in the Krylov iteration.

Our numerical experiments illustrate that the drop tolerance criteria work well in general, and that the quality and effectiveness of $M$ depends critically on, and is sensitive to, these criteria. In particular, the reported numerical results demonstrate that (i) smaller tolerances are not necessary since they may make $M$ denser and more time consuming to construct, while not offering essential improvements in the quality of $M$, and (ii) larger tolerances may lead to a numerically singular $M$ so that preconditioning fails completely.
The paper is organized as follows. In Sect. 2, we review the Basic PSAI (BP-SAII) procedure without dropping and the PSAI(tol) procedure with dropping [27]. In Sect. 3, we present results and establish robust drop tolerance selection criteria. In Sect. 4, we test PSAI(tol) on a number of real world problems, justifying our theory and illustrating the robustness and effectiveness of our selection criterion for drop tolerances. We also test the three static F-norm minimization based SAI procedures with the patterns of \((I + A)^k\), \((I + |A| + |A^T|)^k\) and \((A^T A)^k A^T\) and illustrate the effectiveness of our selection criterion for drop tolerances. Finally concluding remarks are presented in Sect. 5.

2 PSAI algorithms

The BPSAI procedure is based on F-norm minimization and determines the sparsity pattern of \(M\) adaptively during the process. According to the Cayley–Hamilton theorem, \(A^{-1}\) can be expressed as a matrix polynomial of \(A\) of degree \(m - 1\) with \(m \leq n\):

\[
A^{-1} = \sum_{i=0}^{m-1} c_i A^i
\]

with \(A^0 = I\), the identity matrix, and \(c_i, i = 0, 1, \ldots, m - 1\), being certain constants.

Following [27], for \(i = 0, 1, \ldots, m - 1\), we shall denote by \(A^i(j, k)\) the entry of \(A^i\) in position \((j, k)\), \(j, k = 1, 2, \ldots, n\), and set \(\mathcal{J}_i^k = \{ j \mid A^i(j, k) \neq 0 \}\). For \(l = 0, 1, \ldots, l_{\text{max}}\), define \(\tilde{\mathcal{J}}_l^k = \bigcup_{i=0}^{l} \mathcal{J}_i^k\). Let \(M = [m_1, m_2, \ldots, m_n]\) be an approximate inverse of \(A\). BPSAI computes each \(m_k\), \(1 \leq k \leq n\), by solving the LS problem

\[
\min_{m_k} \| A(\cdot, \tilde{\mathcal{J}}_l^k) m_k(\tilde{\mathcal{J}}_l^k) - e_k \|_2, \quad l = 0, 1, \ldots, l_{\text{max}},
\]

(2.1)

where \(\| \cdot \|_2\) is the vector 2-norm and the matrix spectral norm and \(e_k\) is the \(k\)th column of the \(n \times n\) identity matrix \(I\). We exit and output \(m_k\) when the minimum in (2.1) is less than a prescribed tolerance \(\varepsilon\) or \(l\) exceeds \(l_{\text{max}}\). We comment that \(m_k(\tilde{\mathcal{J}}_{l+1}^k)\) can be updated from the available \(m_k(\tilde{\mathcal{J}}_l^k)\) very efficiently; see [27] for details. The BPSAI procedure is summarized as Algorithm 1, in which \(a_k^l\) denotes the \(k\)th column of \(A^l\) and \(a_k^0 = e_k\). It is easily justified that if \(l_{\text{max}}\) steps are performed then the sparsity pattern of \(M\) is contained in that of \((I + A)^{l_{\text{max}}}\).

It is shown in [27, Theorem 1] that if \(A\) is irregularly sparse, that is, there is at least one column of \(A\) whose number of nonzero entries is considerably more than the average number of nonzero entries per column, then \(M\) may become dense very quickly as \(l\) increases. However, when most entries of \(A^{-1}\) are small, the corresponding entries of a good approximate inverse \(M\) for \(A^{-1}\) are small too, and thus contribute very little to \(A^{-1}\). Therefore, in order to control the sparsity of \(M\) and construct an effective preconditioner, we should apply dropping strategies to BPSAI. PSAI(tol) just serves this purpose. It aims to effectively determine an approximate sparsity pattern of \(A^{-1}\) and capture its large entries. At each while-loop in PSAI(tol), for the new
Algorithm 1 The BPSAI Algorithm

For $k = 1, 2, \ldots, n$, compute $m_k$:

1. Set $m_k = 0$, $l = 0$, $m^0 = e_k$ and take $\tilde{J}^k_0 = \{k\}$ as the initial sparsity pattern of $m_k$. Choose an accuracy requirement $\epsilon$ and the maximum $l_{\text{max}}$ of outer loops.

2. Solve (2.1) for $m_k$ and let $r_k = A m_k - e_k$.

3. while $\|r_k\|_2 > \epsilon$ and $l \leq l_{\text{max}} - 1$ do

4. $a_{l+1}^k = A a_l^k$, and augment the set $\tilde{J}_{l+1}^k$ by bringing in the indices of the nonzero entries in $a_{l+1}^k$.

5. $\hat{J} = \tilde{J}_{l+1}^k \setminus \tilde{J}_l^k$.

6. if $\hat{J} = \emptyset$ then

7. Set $l = l + 1$, and go to 3;

8. end if

9. Set $l = l + 1$

10. Solve (2.1) for updating $m_k$ and $r_k = A m_k - e_k$.

11. If $\|r_k\| \leq \epsilon$, then break.

12. end while

available $m_k$, entries of small magnitude below a prescribed tolerance $tol$ are dropped and only large ones are retained. We describe the PSAI($tol$) algorithm as Algorithm 2, in which the sparsity pattern of $m_k$ is denoted by $S^k_l$, $l = 0, 1, \ldots, l_{\text{max}}$, which are updated according to steps 9–11 of Algorithm 2. Hence, for every $k$, we solve the LS problem

$$\min_{m_k(S^k_l)} \| A(\cdot, S^k_l) m_k(S^k_l) - e_k \|_2, \quad l = 0, 1, \ldots, l_{\text{max}}. \quad (2.2)$$

Similar to BPSAI, $m_k(S^k_{l+1})$ can be updated from the available $m_k(S^k_l)$ very efficiently.

From now on we denote by $M$ the preconditioners generated by either BPSAI or PSAI($tol$). We will distinguish them by $M$ and $M_d$, respectively when necessary. The non-singularity and quality of $M$ by BPSAI clearly depends on $\epsilon$, while the situation becomes much more complicated for $M_d$. We will consider these theoretical issues in the next section. At present it should be clear that for BPSAI the non-singularity and quality of $M$ is determined by $\epsilon$ and $l_{\text{max}}$, two parameters that control while-loop termination in Algorithm 1. On the one hand, a smaller $\epsilon$ will generally give rise to higher quality but possibly denser preconditioner $M$. As a result, more while-loops $l_{\text{max}}$ are used, so that the setup cost of $M$ is higher. We reiterate that it is also more expensive to apply a denser $M$ at each iteration of a Krylov solver. On the other hand, a bigger $\epsilon$ may generate a sparser but less effective $M$, so that the Krylov solvers use more iterations to achieve convergence. Unfortunately the selection of $\epsilon$ can only be empirical. As is standard in the literature, in numerical experiments we simply take $\epsilon$ to be a fairly small quantity, say $0.2 \sim 0.4$. 
Algorithm 2 The PSAI(tol) Algorithm

For $k = 1, 2, \ldots, n$, compute $m_k$:

1. Set $m_k = 0$, $l = 0$, $a_k^0 = e_k$ and $\mathcal{J}_0^k = \tilde{\mathcal{J}}_0^k = \{k\}$ as the initial sparsity pattern of $m_k$. Choose an accuracy requirement $\varepsilon$, drop tolerance $\text{tol}$ and the maximum $l_{\text{max}}$ of outer loops.

2. Solve (2.2) for $m_k$ and let $r_k = A_{m_k} - e_k$.

3. while $\|r_k\|_2 > \varepsilon$ and $l \leq l_{\text{max}} - 1$ do

4. $a_{k+1} = Aa_k^l$, and augment the set $\mathcal{J}_l^{k+1}$ by bringing in the indices of the nonzero entries in $a_{k+1}^l$.

5. $\mathcal{J} = \mathcal{J}_l^{k+1} \setminus \tilde{\mathcal{J}}_l^k$.

6. if $\mathcal{J} = \emptyset$ then

7. Set $l = l + 1$, and go to 3;

8. end if

9. $\mathcal{J}_{l+1}^k = \mathcal{J}_l^k \cup \mathcal{J}$

10. Solve (2.2) for $m_k$ and compute $r_k = A_{m_k} - e_k$. If $\|r_k\| \leq \varepsilon$, perform 11 and break.

11. Drop the entries of small magnitude in $m_k$ whose sizes are below $\text{tol}$ and delete the corresponding indices from $\mathcal{J}_{l+1}^k$.

12. Set $l = l + 1$

13. end while

3 Selection criteria for drop tolerances

First of all, we should keep in mind that all SAI preconditioning procedures are based on the basic hypothesis that the majority of entries of $A^{-1}$ are small, that is, there exist sparse approximate inverses of $A$. Mathematically, this amounts to supposing that there exists (at least) a sparse $M$ such that the residual $\|AM - I\| \leq \varepsilon$ for some fairly small $\varepsilon$ and some matrix norm $\|\cdot\|$. The size of $\varepsilon$ is a reasonable measure for the quality of $M$ as an approximation to $A^{-1}$. Generally speaking, the smaller $\varepsilon$, the more accurate $M$ as an approximation of $A^{-1}$.

In the following discussion, we will assume that BPSAI produces a nonsingular $M$ satisfying $\|AM - I\| \leq \varepsilon$ for some norm, given fairly small $\varepsilon$. We comment that this is definitely achieved for a suitable $l_{\text{max}}$. Under this assumption, keep in mind that $M$ may be relatively dense but have many entries of small magnitude. PSAI(tol) aims at dynamically dropping those entries of small magnitude below some absolute drop tolerance $\text{tol}$ during the setup of $M$ and computing a new sparser $M$, so as to reduce storage memory and computational cost of constructing and applying $M$ as a preconditioner. We are concerned with two problems. The first problem is how to select $\text{tol}$ to make $M$ nonsingular. As will be seen, since $\text{tol}$ varies dynamically for each $k$, $1 \leq k \leq n$, as $l$ increases from 0 to $l_{\text{max}}$ in Algorithm 2, we will instead denote it by $\text{tol}_k$ when computing the $k$th column $m_k$. The second is how to select the $\text{tol}_k$ which are required to meet two requirements: (i) $M$ is as sparse as possible; (ii) its approximation quality is comparable to that obtained by BPSAI in the sense that the residuals of two $M$ have very comparable sizes. With such sparser
it is expected that Krylov solvers preconditioned by BPASI and PSAI($tol$), respectively, will use a comparable number of iterations to achieve convergence. If so, PSAI($tol$) will be considerably more effective than BPASI provided that $M$ obtained by PSAI($tol$) is considerably sparser than that provided by BPASI. As far as we are aware, these important problems have not been studied rigorously and systematically in the context of SAI preconditioning. The establishment of robust selection criteria, $tol_k$, $k = 1, 2, \ldots, n$, for drop tolerances that meet the two requirements is significant but nontrivial.

Over the years the dropping reported in the literature has been empirical. One commonly applies a tolerance as follows: set $m_{jk}$ to zero if $|m_{jk}| < tol$, for some empirical value for $tol$, such as $10^{-3}$, see, e.g. [16, 27, 37, 38]. Due to the absence of mathematical theory, doing so is problematic, and one may either miss significant entries if $tol$ is too large or retain too many superfluous entries if $tol$ is too small. As a consequence, $M$ may be of poor quality, or while a good approximate inverse it may be unduly denser than desirable, leading to considerably higher setup and application costs.

For general purposes, we should take the size of $m_k$ into account when dropping a small entry $m_{jk}$ in $m_k$. Define $f_k$ to be the $n$-dimensional vector whose nonzero entries $f_{jk} = m_{jk}$ are those to be dropped in $m_k$. Precisely drop $m_{jk}$ in $m_k$ when

$$\frac{\|f_k\|}{\|m_k\|} \leq \mu_k, \quad k = 1, 2, \ldots, n$$

for some suitable norm $\| \cdot \|$, where $\mu_k$ is a relative drop tolerance that is small and should be chosen carefully based on some mathematical theory. For suitably chosen $\mu_k$, our ultimate goal is to derive corresponding drop tolerance selection criteria $tol_k$ that are used to adaptively detect and drop small entries $m_{jk}$ below the tolerance.

In what follows we establish a number of results that play a vital role in selecting the $\mu_k$ and $tol_k$ effectively. The matrix norm $\| \cdot \|$ denotes a general induced matrix norm, which includes the 1-norm and the 2-norm.

**Theorem 3.1** Assume that $\|AM - I\| \leq \varepsilon < 1$. Then $M$ is nonsingular. Define $M_d = M - F$. If $F$ satisfies

$$\|F\| < \frac{1 - \varepsilon}{\|A\|},$$

then $M_d$ is nonsingular.

**Proof** Suppose that $M$ is singular and let $w$ with $\|w\| = 1$ be an eigenvector associated with its zero eigenvalue(s), i.e., $Mw = 0$. Then for any induced matrix norm we have

$$\|AM - I\| \geq \|(AM - I)w\| = \|w\| = 1,$$

a contradiction to the assumption that $\|AM - I\| < 1$. So $M$ is nonsingular.

Since

$$M_d = M - F = M(I - M^{-1}F),$$

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from (3.2) we have

\[ \| M^{-1} F \| \leq \| M^{-1} \| \| F \| < (1 - \varepsilon) \frac{\| M^{-1} \|}{\| A \|}. \]  

(3.4)

On the other hand, since

\[ \| A \| - \| M^{-1} \| \leq \| A - M^{-1} \| \leq \| AM - I \| \| M^{-1} \| \leq \varepsilon \| M^{-1} \|, \]

we get

\[ (1 - \varepsilon) \| M^{-1} \| \leq \| A \| \leq (1 + \varepsilon) \| M^{-1} \|, \]

which means

\[ 1 - \varepsilon \leq \frac{\| A \|}{\| M^{-1} \|} \leq 1 + \varepsilon. \]  

(3.5)

Substituting (3.5) into (3.4), we have

\[ \| M^{-1} F \| < 1, \]

from which it follows that \( I - M^{-1} F \) in (3.3) is nonsingular and so is \( M_d \). □

Denote by \( M_d \) the sparse approximate inverse of \( A \) obtained by PSAI(\( tol \)). Then \( M_d \) aims to retain the entries \( m_{jk} \) of large magnitude and drop those of small magnitude in \( M \). The entries of small magnitude to be dropped are those nonzero ones in the matrix \( F \). So, \( M_d \) is generally sparser than \( M \), and the number of its nonzero entries is equal to that of \( M \) minus that of \( F \).

In order to get an \( M_d \) comparable to \( M \) as an approximation to \( A^{-1} \), we need to impose further restrictions on \( F \) and \( \varepsilon \), as indicated below.

**Theorem 3.2** Assume that \( \| AM - I \| \leq \varepsilon < 1 \). Then \( M \) is nonsingular. Let \( M_d = M - F \). If

\[ \| F \| \leq \min \left\{ \frac{\varepsilon}{\| A \|}, \frac{1 - \varepsilon}{\| A \|} \right\}, \]

(3.6)

then \( M_d \) is nonsingular and

\[ \| AM_d - I \| \leq \min\{1, 2\varepsilon\}. \]

(3.7)

Specifically, if \( \varepsilon < 0.5 \), then

\[ \| F \| \leq \frac{\varepsilon}{\| A \|}. \]

(3.8)

and

\[ \| AM_d - I \| \leq 2\varepsilon. \]

(3.9)
The non-singularity of $M$ is already proved in Theorem 3.1. Since $F$ satisfying (3.6) must meet (3.2), the non-singularity of $M_d$ follows from Theorem 3.1 directly. From $\|AM - I\| \leq \varepsilon$ and (3.6), we obtain

\[
\|AM_d - I\| = \|AM - AF - I\| \leq \|AM - I\| + \|A\|\|F\| \leq \varepsilon + \min\{\varepsilon, 1 - \varepsilon\} = \min\{1, 2\varepsilon\}.
\]

(3.8) and (3.9) are direct from (3.6) and (3.7), respectively. \qed

In what follows we always assume that $\varepsilon < 0.5$, so that (3.8) is satisfied and the residual $\|AM_d - I\| \leq 2\varepsilon < 1$. This assumption is purely technical for the brevity and beauty of presentation. The case that $0.5 \leq \varepsilon < 1$ can be treated accordingly. The later theorems can be adapted for this case, but are not considered here.

It is known that $M$ is a good approximation to $A^{-1}$ for a small $\varepsilon$. This theorem tells us that if drop tolerances $tol_k$ make $F$ satisfy (3.8) then the $M_d$ and $M$ have comparable residuals and are approximate inverses of $A$ with comparable accuracy, provided that $\varepsilon$ is fairly small. In this case, we claim that they possess a similar preconditioning quality for a Krylov solver, and it is expected that the Krylov solver preconditioned by $M_d$ and $M$, respectively, use a comparable number of iterations to achieve convergence.

In the above results, the assumptions and bounds are determined by matrix norms, which are thus not directly applicable to our goals. To be more practical, we now present a theorem under the assumption that $\|Am_k - e_k\| \leq \varepsilon$ for $k = 1, 2, \ldots, n$, which is just the stopping criterion in Algorithms 1–2 and the SPAI algorithm [20], etc., where the norm is the 2-norm.

**Theorem 3.3** For a given vector norm $\| \cdot \|$, let $M = [m_1, m_2, \ldots, m_n]$ satisfy $\|Am_k - e_k\| \leq \varepsilon < 0.5$ for $k = 1, 2, \ldots, n$ and let $M_d = M - F = [m^d_1, m^d_2, \ldots, m^d_n]$ with $F = [f_1, f_2, \ldots, f_n]$. If

$$\|f_k\| \leq \frac{\varepsilon}{\|A\|}, \quad k = 1, 2, \ldots, n,$$

(3.10)

then

$$\|Am^d_k - e_k\| \leq 2\varepsilon.$$

(3.11)

**Proof** Let $r_k = Am_k - e_k$. Then from $m^d_k = m_k - f_k$ we get

$$\|Am^d_k - e_k\| = \|r_k - Af_k\| \leq \|r_k\| + \|Af_k\| \leq \varepsilon + \|Af_k\| \leq \varepsilon + \|A\|\|f_k\|,$$

from which, with the assumption of the theorem, (3.11) holds. \qed

Still, this theorem does not fit nicely for our use. For the later theoretical and practical background, we present a mixed norm result, which is a variant of Theorem 3.3.
Theorem 3.4 Let $M = [m_1, m_2, \ldots, m_n]$ satisfy $\|Am_k - e_k\|_2 \leq \varepsilon < 0.5$ for $k = 1, 2, \ldots, n$ and let $M_d = M - F = [m_1^d, m_2^d, \ldots, m_n^d]$ with $F = [f_1, f_2, \ldots, f_n]$. If

$$\|f_k\|_1 \leq \frac{\varepsilon}{\|A\|_1}, \quad k = 1, 2, \ldots, n,$$  \hspace{1cm} (3.12)

then

$$\|Am^d_k - e_k\|_2 \leq 2\varepsilon.$$  \hspace{1cm} (3.13)

Proof Let $r_k = Am_k - e_k$. Then from $m^d_k = m_k - f_k$ we get

$$\|Am^d_k - e_k\|_2 = \|r_k - Af_k\|_2 \leq \|r_k\|_2 + \|Af_k\|_2 \leq \|r_k\|_2 + \|Af_k\|_1 \\
\leq \varepsilon + \|Af_k\|_1 \leq \varepsilon + \|A\|_1\|f_k\|_1,$$

from which, with the assumption (3.12), (3.13) holds. \hfill \square

Theorem 3.4 cannot guarantee that $M$ and $M_d$ are nonsingular. In [20], Grote and Huckle have presented some theoretical properties of a sparse approximate inverse. Particularly, for the matrix 1-norm, Theorem 3.1 and Corollary 3.1 of [20] read as follows when applied to $M$ and $M_d$ defined by Theorem 3.4.

Theorem 3.5 Let $r_k = Am_k - e_k, r^d_k = Am^d_k - e_k$ and $p = \max_{1 \leq k \leq n} \{ \text{the number of nonzero entries of } r_k \}$, $p^d = \max_{1 \leq k \leq n} \{ \text{the number of nonzero entries of } r^d_k \}$. Then if $\|r_k\|_2 \leq \varepsilon$ and $\|r^d_k\|_2 \leq 2\varepsilon, k = 1, 2, \ldots, n$, we have

$$\|AM - I\|_1 \leq \sqrt{p}\varepsilon,$$  \hspace{1cm} (3.14)

$$\|AM_d - I\|_1 \leq 2\sqrt{p^d}\varepsilon.$$  \hspace{1cm} (3.15)

Furthermore, if $\sqrt{p}\varepsilon < 1$ and $2\sqrt{p^d}\varepsilon < 1$, respectively, $M$ and $M_d$ are nonsingular and

$$\frac{\|M - A^{-1}\|_1}{\|A^{-1}\|_1} \leq \sqrt{p}\varepsilon,$$  \hspace{1cm} (3.16)

$$\frac{\|M_d - A^{-1}\|_1}{\|A^{-1}\|_1} \leq 2\sqrt{p^d}\varepsilon.$$  \hspace{1cm} (3.17)

Theorem 3.4 indicates that given $\varepsilon < 0.5$ and $l_{\text{max}}$, if the while-loop in BPSAI terminates due to $\|r_k\| \leq \varepsilon$ for all $k$ and drop tolerance $tol_k$ is selected such that (3.12) holds, then the corresponding columns of $M_d$ and $M$ are of similar quality provided that $\varepsilon$ is fairly small. It is noted in [20] for the SPAI that $p$ is usually much smaller than $n$. This is also the case for BPSAI and PSAI($tol$). However, we should realize that such a sufficient condition is very conservative, as pointed out in [20]. In practice, for a rather mildly small $\varepsilon$, say $0.3$, $M$ is rarely singular.

Theorem 3.5 shows that $M_d$ and $M$ are approximate inverses of $A$ with similar accuracy and are expected to have a similar preconditioning quality. Besides, since
$m_k$ is generally denser than $m_k^d$. $r_k$ is heuristically denser than $r_k^d$, i.e., $p_d$ is more than likely to be smaller than $p$. Consequently, $2\sqrt{p_d}$ is comparable to $\sqrt{p}$. This means that the bounds for $M_d$ are close to and furthermore may not be bigger than the corresponding ones for $M$ in Theorem 3.5, so $M_d$ and $M$ are approximations to $A^{-1}$ with very similar accuracy or quality.

Theorems 3.2–3.5 are fundamental and relate the quality of $M_d$ to that of $M$ in terms of $\varepsilon$ quantitatively and explicitly. They provide necessary ingredients for reasonably selecting relative drop tolerance $\mu_k$ in (3.1) to get a possibly much sparser preconditioner $M_d$ that has a similar preconditioning quality to $M$. In what follows we present a detailed analysis and propose robust selection criteria for drop tolerance $tol_k$.

For given $l_{\max}$, suppose that $M$ obtained by BPSAI is nonsingular and satisfies $\|Am_k - e_k\| \leq \varepsilon < 0.5$ for $k = 1, 2, \ldots, n$. To achieve our goal, the crucial point is how to combine (3.1) with condition (3.12) in Theorem 3.4 in an organic and reasonable way. For the 1-norm in (3.1), a unification of (3.1) and (3.12) means that

$$\|f_k\|_1 \leq \mu_k \|m_k\|_1 \quad \text{and} \quad \|f_k\|_1 \leq \frac{\varepsilon}{\|A\|_1}$$

at every while-loop in PSAI($tol$), where the bound in the first relation is to be determined and the bound in the second relation is given explicitly. This is the starting point for the analysis determining how to drop the small entries $m_{jk}$ in $m_k$.

Before proceeding, supposing that $\mu_k$ is given in a disguise, we investigate how to choose $f_k$ to make (3.18) hold. Obviously, it suffices to drop nonzero $m_{jk}$, $1 \leq j \leq n$ in $m_k$ as long as its size is no more than the bounds in (3.18) divided by $\text{nnz}(f_k)$. Since $\text{nnz}(f_k)$ is not known a-priori, in practice we replace it by the currently available $\text{nnz}(m_k)$ before dropping, which is an upper bound for $\text{nnz}(f_k)$. Therefore, we should drop an $m_{jk}$ when it satisfies

$$|m_{jk}| \leq \frac{\mu_k \|m_k\|_1}{\text{nnz}(m_k)} \quad \text{and} \quad |m_{jk}| \leq \frac{\varepsilon}{\text{nnz}(m_k) \|A\|_1}, \quad k = 1, 2, \ldots, n. \quad (3.19)$$

Given (3.18), we comment that each of the above bounds may be correspondingly conservative as $\text{nnz}(m_k) > \text{nnz}(f_k)$. But it seems hard, if not impossible, to replace the unknown $\text{nnz}(f_k)$ by any other better computable estimate than $\text{nnz}(m_k)$.

Next we go to our central concern and discuss how to relate $\mu_k$ to $\varepsilon$ so as to establish a robust selection criterion $tol_k$ for drop tolerances. Precisely, as (3.19) has indicated, we aim at selecting suitable relative tolerance $\mu_k$ and then drop entries of small magnitude in $m_k$ below $\frac{\mu_k \|m_k\|_1}{\text{nnz}(m_k)}$. By Theorems 3.4–3.5, the second bound in (3.18) and its induced bound in (3.19) serve to guarantee that $M_d$ has comparable preconditioning quality to $M$. Therefore, if an $m_{jk}$ satisfies the second relation in (3.19), it should be dropped. Otherwise, if $\mu_k$ satisfies

$$\mu_k \|m_k\|_1 > \frac{\varepsilon}{\|A\|_1}$$

and we use the dropping criterion

$$tol_k = \frac{\mu_k \|m_k\|_1}{\text{nnz}(m_k)} > \frac{\varepsilon}{\text{nnz}(m_k) \|A\|_1}$$
for some $k$, we would possibly drop an excessive number of nonzero entries and $M_d$ would be too sparse. The resulting $M_d$ may mean that (3.12) is not satisfied and that $M_d$ is a poor quality preconditioner, possibly also numerically singular, which could lead to a complete failure of the Krylov solver. Thus larger $t_{ol_k}$ should not be selected.

On the other hand, if we chose $\mu_k$ such that

$$\mu_k \|m_k\|_1 < \frac{\varepsilon}{\|A\|_1}$$

and took the dropping criterion

$$t_{ol_k} = \frac{\mu_k \|m_k\|_1}{\text{nnz}(m_k)} < \frac{\varepsilon}{\text{nnz}(m_k) \|A\|_1},$$

Theorem 3.4 would hold and the preconditioning quality of $M_d$ would be guaranteed and comparable to that of $M$. However, Theorems 3.4–3.5 show that the accuracy of such $M_d$ cannot be improved as approximate inverses of $A$ as $\mu_k$ and $t_{ol_k}$ become smaller. Computationally, it is crucial to realize that the smaller $t_{ol_k}$, generally the denser $M_d$, leading to an increased setup cost for $M_d$ and more expensive application of $M_d$ in a Krylov iteration. As a consequence, such smaller $t_{ol_k}$ are not desirable and may lower the efficiency of constructing $M_d$. Consequently such smaller values for $t_{ol_k}$ should be abandoned.

In view of the above analysis, it is imperative that we find an optimal balance point. Our above arguments have suggested an optimal and most effective choice for $\mu_k$: we should select $\mu_k$ to make two bounds in (3.18) equal:

$$\mu_k \|m_k\|_1 = \frac{\varepsilon}{\|A\|_1}. \quad (3.20)$$

From (3.19), this selection leads to our ultimate dropping criterion

$$t_{ol_k} = \frac{\varepsilon}{\text{nnz}(m_k) \|A\|_1}. \quad (3.21)$$

We point out that since (3.12) is a sufficient but not necessary condition for (3.13), $t_{ol_k}$ defined above is also sufficient but not necessary for (3.13). Also, it may be conservative since we replace the smaller true value $\text{nnz}(f_k)$ by its upper bound $\text{nnz}(m_k)$ in the denominator. As a result, $t_{ol_k}$ may be considerably smaller than it should be in an ideal case. We should note that $\mu_k$ and $t_{ol_k}$ are varying parameters during the while-loop in Algorithm 2 as $\text{nnz}(m_k)$ changes when the while-loop $l$ increases from 0 to $l_{\text{max}}$.

In the literature one commonly uses fixed drop tolerance $t_{ol}$ when constructing a SAI preconditioner $M$, which is, empirically and heuristically, taken as some seemingly small quantity, say $10^{-2}$, $10^{-3}$ or $10^{-4}$, without taking $\varepsilon$ into consideration; see, e.g., [16, 27, 37, 38]. Our theory has indicated that the non-singularity and preconditioning quality of $M_d$ is critically dependent and possibly sensitive to the choice of the drop tolerance. For fixed tolerances that are larger than that defined by (3.21) for some $k$ during the construction of $M_d$, we report numerical experiments that indicate that the resulting $M_d$ obtained by PSAI($t_{ol}$) can be exactly singular in finite
precision arithmetic. We also report experiments that show decreasing such large tolerances by one order of magnitude, can provide high quality and nonsingular $M_d$. Thus, the robustness and effectiveness of $M_d$ depends directly on the tolerance.

We stress that Theorems 3.1–3.5 hold for a generally given approximate inverse $M$ of $A$ and do not depend on a specific F-norm minimization based SAI preconditioning procedure. Note that, for all the static F-norm minimization based SAI preconditioning procedures, the high quality $M$ constructed from $A$ itself are often quite dense and their applications in Krylov solvers can be time consuming. To improve the overall performance of solving $Ax=b$, one often sparsifies $M$ after its computation, by using postfiltration on $M$ to obtain a new sparser approximate inverse $M_d$ [13, 37]. However, as already stated in the introduction, postfiltration itself cannot reduce the cost of constructing $M$ but can reduce the cost of applying $M$ in Krylov iterations.

As a byproduct, our theory can be very easily adapted to a static F-norm minimization based SAI preconditioning procedure. The difference and simplification is that, for a static SAI procedure, $\mu_k$ in (3.21) and $tol_k$ are fixed for each $k$ as $m_k$ and $nnz(m_k)$ are already determined a-priori before dropping is performed on $M$. Practically, after computing $M$ by a static SAI procedure, we record $\|Am_k - e_k\| = \varepsilon_k$, $k = 1, 2, \ldots, n$ and compute the constants $nnz(m_k)$ for $k = 1, 2, \ldots, n$. Assume that $\varepsilon_k < 0.5$, $k = 1, 2, \ldots, n$. Then by (3.19) and (3.21) we drop $m_{jk}$ whenever

$$|m_{jk}| \leq tol_k = \frac{\varepsilon_k}{nnz(m_k)\|A\|_1}, \quad j = 1, 2, \ldots, n.$$  

(3.22)

In such a way, based on Theorem 3.4 we get a new sparser approximate inverse $M_d$ whose $k$th column $m_d^k$ satisfies $\|Am_d^k - e_k\| \leq 2\varepsilon_k$. Define $\varepsilon = \max_{k=1,2,\ldots,n} \varepsilon_k$. Then Theorem 3.5 holds. So $M_d$ has a similar preconditioning quality to the generally denser $M$ obtained by the static SAI procedure without dropping. We reiterate, however, that in contrast to adaptive PSAI($tol$) where small entries below a tolerance are dropped immediately when they are generated during the while loop of Algorithm 2, the static SAI procedure does not reduce the setup cost of $M_d$ since it performs sparsification only after computation of $M$. There is relatively greater benefit in dropping in adaptive SAI preconditioning.

4 Numerical experiments

In this section we test a number of real world problems coming from scientific and engineering applications, which are described in Table 1.\textsuperscript{1} We shall demonstrate the robustness and effectiveness of our selection criteria for drop tolerances applied to PSAI($tol$) and, as a byproduct, three F-norm minimization based static SAI preconditioning procedures.

The numerical experiments are performed on an Intel(R) Core (TM)2Duo Quad CPU E8400 @ 3.00 GHz processor with main memory 2 GB using Matlab 7.8.0

\textsuperscript{1} All of these matrices are from the Matrix Market of the National Institute of Standards and Technology at \url{http://math.nist.gov/MatrixMarket} or from the University of Florida Sparse Matrix Collection at \url{http://www.cise.ufl.edu/research/sparse/matrices/}.
Table 1 The description of test matrices ($n$ is the order of a matrix; nnz is the number of nonzero entries)

| Matrix     | $n$  | nnz  | Description                           |
|------------|------|------|---------------------------------------|
| epb1       | 14734| 95053| Plate-fin heat exchanger              |
| fidap024   | 2283 | 48733| Computational fluid dynamics problem   |
| fidap028   | 2603 | 77653| Computational fluid dynamics problem   |
| fidap031   | 3909 | 115299| Computational fluid dynamics problem  |
| fidap036   | 3079 | 53851| Computational fluid dynamics problem  |
| nos3       | 960  | 8402 | Biharmonic equation                   |
| nos6       | 675  | 1965 | Poisson equation                      |
| orsreg_1   | 2205 | 14133| Oil reservoir simulation. Jacobian Matrix |
| orsirr_1   | 1030 | 6858 | As ORSREG1, but unnecessary cells coalesced |
| orsirr_2   | 886  | 5970 | As ORSIRR1, with further coarsening of grid |
| pores_2    | 1224 | 9613 | Reservoir simulation                  |
| sherman1   | 1000 | 3750 | Oil reservoir simulation $10 \times 10 \times 10$ grid |
| sherman2   | 1080 | 23094| Oil reservoir simulation $6 \times 6 \times 5$ grid |
| sherman3   | 5005 | 20033| Oil reservoir simulation $35 \times 11 \times 13$ grid |
| sherman4   | 1104 | 3786 | Oil reservoir simulation $16 \times 23 \times 3$ grid |
| sherman5   | 3312 | 20793| Oil reservoir simulation $16 \times 23 \times 3$ grid |

with the machine precision $\varepsilon_{\text{mach}} = 2.22 \times 10^{-16}$ under the Linux operating system. Preconditioning is from the right except pores_2, for which we found that left preconditioning outperforms right preconditioning very considerably. It appears that the rows of pores_2’s inverse can be approximated more effectively than its columns by PSAI($\varepsilon$). Krylov solvers employed are BiCGStab and the restarted GMRES(50) algorithms [1], and we use the codes from Matlab 7.8.0. We comment that if the output of iterations for the code BiCGStab.m is $k$, the dimension of the Krylov subspace is $2^k$ and BiCGStab performs $2^k$ matrix-vector products. The initial guess is always $x_0 = 0$, and the right-hand side $b$ is formed by choosing the solution $x = [1, 1, \ldots, 1]^T$. The stopping criterion is

$$\frac{\|b - Ax_m\|_2}{\|b\|_2} < 10^{-8}, \quad x_m = M y_m,$$

where $y_m$ is the approximate solution obtained by BiCGStab or GMRES(50) applied to the preconditioned linear system $AMy = b$. We run all the algorithms in a sequential environment. We will observe that the setup cost for $M$ dominates the entire cost of solving $Ax = b$. As stressed in the introduction, this is a distinctive feature of SAI preconditioning procedures even in a distributed parallel environment.

In the experiments, we take different $\varepsilon$ and suitably small integer $l_{\text{max}}$ so as to control the quality of $M$ in Algorithms 1–2, i.e., the BPSAI and PSAI($\varepsilon$) algorithms, in which the while-loop terminates when $\|Am_k - e_k\|_2 \leq \varepsilon$ or $l > l_{\text{max}}$. In all the tables, we use the following notations:

- $\varepsilon$: the accuracy requirements in Algorithms 1–2;
- $l_{\text{max}}$: the maximum while-loops that Algorithms 1–2 allow;
– \textit{iter\_b} and \textit{iter\_g}: the iteration numbers of BiCGStab and GMRES(50), respectively;
– \textit{spar} = \frac{\text{nz}(M)}{\text{nz}(A)}: the sparsity of \( M \) relative to \( A \);
– \textit{mintol} and \textit{maxtol}: the minimum and maximum of \( tol_k \) defined by (3.21) for \( k = 1, 2, \ldots, n \) and \( l = 0, 1, \ldots, l_{\max} \);
– \textit{ptime}: the setup time (in second) of \( M \);
– \( r_{\max} = \max_{k=1,\ldots,n} \| A m_k - e_k \| \);
– \textit{coln}: the number of columns of \( M \) that fail to meet the accuracy requirement \( \epsilon \); 
– \( \dagger \): flags convergence not attained within 1000 iterations.

We report the results in Tables 2–8. Our aims are four fold: (i) our selection criterion (3.21) for \( tol_k \) works very robustly and effectively since Krylov solvers preconditioned by PSAI(\( tol \)) and BPSAI use almost the same iterations, the \( tol_k \) smaller than those defined by (3.21) are not necessary, rather they increase the total cost of solving linear systems since they do not improve the preconditioning quality of \( M_d \), increase the setup time of \( M_d \) and make \( M_d \) become denser. (ii) the quality of \( M_d \) depends on the choice of \( tol_k \) critically and an empirically chosen fixed small \( tol_k \) may produce a numerically singular \( M_d \). (iii) \( tol_k \) of one order smaller than those in case (ii) may dramatically improve the preconditioning effectiveness of \( M_d \). This means that an empirically chosen \( tol \) may fail to produce a good preconditioner. (iv) As a byproduct, we show that the selection criterion (3.22) for \( tol_k \) works well for static F-norm minimization SAI preconditioning procedures with three common prescribed patterns. We present the results on (i)–(iii) in Sect. 4.1 and the results on (iv) in Sect. 4.2, respectively.

4.1 Results for PSAI(\( tol \))

We shall illustrate that our dropping criterion (3.21) for \( tol_k \) works very robustly for various parameters \( \epsilon \) and \( l_{\max} \). We will show that for a smaller \( \epsilon \) we need more while loops, and resulting \( M_d \) are denser and cost more to construct, but are more effective for accelerating BiCGStab and GMRES(50), that is, the Krylov solvers use fewer iterations to achieve convergence. We also show that for fairly small \( \epsilon = 0.2, 0.3, 0.4 \), Algorithms 1–2 can compute a good sparse approximation \( M \) of \( A^{-1} \) with accuracy \( \epsilon \) for small integer \( l_{\max} \), and the maximum \( l_{\max} = 11 \) is needed for \( \epsilon = 0.2 \).

We summarize the results obtained by the two Krylov solvers with and without PSAI(\( tol \)) preconditioning in Table 2. We see that the two Krylov solvers without preconditioning failed to solve most test problems within 1000 iterations while two Krylov solvers are accelerated by PSAI(\( tol \)) preconditioning substantially and they solved all the problems quite successfully except for \( \epsilon = 0.4 \) and \( l_{\max} = 5, 8 \), where GMRES(50) did not converge for fidap024, fidap036 and sherman3. Particularly, the Krylov solvers preconditioned by PSAI(\( tol \)) solved sherman2 very quickly and converged within 10 iterations for three given \( \epsilon = 0.2, 0.3, 0.4 \), but they failed to solve the problem when no preconditioning is used.

Now we take a closer look at PSAI(\( tol \)). The table shows that for \( \epsilon = 0.2, 0.3, 0.4 \), Algorithm 2 used \( l_{\max} = 11, 10, 8 \) to attain the accuracy requirements, respectively. If we reduced \( l_{\max} \) to 8, 6, 5, there are only very few columns of \( M \) for only a few matrices which do not satisfy the accuracy requirements, but the corresponding \( r_{\max} \) are...
Table 2  Convergence results for all the test problems: unpreconditioned ($M = I$) and PSAI($tol$) procedure with different $\varepsilon$ and $l_{max}$. Note: when the iterations for BiCGStab are $k$, the dimension of the Krylov subspace is $2k$.

| Matrix | $M = I$ | PSAI($tol$), $\varepsilon = 0.2$, $l_{max} = 8$ | PSAI($tol$), $\varepsilon = 0.2$, $l_{max} = 11$ |
|--------|---------|--------------------------------------------------|--------------------------------------------------|
|        | iter, $\varepsilon$ | $b_{spar}$ iter, $\varepsilon$ | coln | iter, $\varepsilon$ | $b_{spar}$ iter, $\varepsilon$ | coln |
| epbl1  | 433, $\dagger$ | 3.20 112.36 120, 272 | 0.20 0.20 | 3.20 111.36 120, 272 | 0.20 0.20 |
| fidap024 $\dagger$, $\dagger$ | 8.80 121.52 27, 40 | 0.20 0.20 | 8.80 121.52 27, 40 | 0.20 0.20 |
| fidap028 $\dagger$, $\dagger$ | 9.7 423.75 31, 42 | 0.26 0.29 | 10.11 437.36 31, 41 | 0.20 0.20 |
| fidap031 $\dagger$, $\dagger$ | 6.40 267.74 58, 103 | 0.35 1 | 6.41 269.70 58, 102 | 0.20 0.20 |
| fidap036 $\dagger$, $\dagger$ | 5.78 63.88 34, 48 | 0.20 0 | 5.78 63.88 34, 48 | 0.20 0.20 |
| nos3   | 213, $\dagger$ | 3.89 3.72 49, 98 | 0.20 0.20 | 3.89 3.72 49, 98 | 0.20 0.20 |
| nos6   | $\dagger$, $\dagger$ | 2.73 0.48 19, 24 | 0.20 0.20 | 2.73 0.48 19, 24 | 0.20 0.20 |
| orsirr_1 $\dagger$, $\dagger$ | 10.15 7.41 15, 26 | 0.20 0.20 | 10.15 7.41 15, 26 | 0.20 0.20 |
| orsirr_2 $\dagger$, $\dagger$ | 10.71 6.53 16, 25 | 0.20 0.20 | 10.71 6.53 16, 25 | 0.20 0.20 |
| orsreg_1 687, 346 | 9.16 19.49 18, 29 | 0.20 0.20 | 9.16 19.49 18, 29 | 0.20 0.20 |
| pores_2 $\dagger$, $\dagger$ | 17.41 26.38 19, 26 | 0.27 0.27 | 17.66 27.53 19, 27 | 0.20 0.20 |
| sherman1 356, $\dagger$ | 6.54 1.37 18, 28 | 0.27 0.27 | 6.58 1.38 18, 28 | 0.20 0.20 |
| sherman2 $\dagger$, $\dagger$ | 3.40 6.58 4, 6 | 0.20 0.20 | 3.40 6.58 4, 6 | 0.20 0.20 |
| sherman3 $\dagger$, $\dagger$ | 4.86 10.52 81, 229 | 0.32 0.32 | 4.90 10.71 81, 228 | 0.20 0.20 |
| sherman4 101, 377 | 3.36 0.76 24, 34 | 0.20 0.20 | 3.36 0.76 24, 34 | 0.20 0.20 |
| sherman5 $\dagger$, $\dagger$ | 3.34 4.89 21, 30 | 0.20 0.20 | 3.34 4.89 21, 30 | 0.20 0.20 |

| Matrix | $M = I$ | PSAI($tol$), $\varepsilon = 0.3$, $l_{max} = 6$ | PSAI($tol$), $\varepsilon = 0.3$, $l_{max} = 10$ |
|--------|---------|--------------------------------------------------|--------------------------------------------------|
|        | iter, $\varepsilon$ | $b_{spar}$ iter, $\varepsilon$ | coln | iter, $\varepsilon$ | $b_{spar}$ iter, $\varepsilon$ | coln |
| epbl1  | 433, $\dagger$ | 1.17 36.71 170, 408 | 0.30 0.30 | 1.17 36.71 170, 408 | 0.30 0.30 |
| fidap024 $\dagger$, $\dagger$ | 5.22 34.52 46, 98 | 0.38 0.38 | 5.27 34.91 46, 97 | 0.30 0.30 |
| fidap028 $\dagger$, $\dagger$ | 5.48 113.09 64, 168 | 0.33 0.33 | 5.50 117.28 64, 159 | 0.30 0.30 |
| fidap031 $\dagger$, $\dagger$ | 3.08 58.39 104, 387 | 0.56 0.56 | 3.09 59.18 104, 444 | 0.30 0.30 |
| fidap036 $\dagger$, $\dagger$ | 2.51 12.73 69, 119 | 0.30 0.30 | 2.51 12.73 69, 119 | 0.30 0.30 |
| nos3   | 213, $\dagger$ | 1.65 1.29 69, 144 | 0.30 0.30 | 1.65 1.29 69, 144 | 0.30 0.30 |
| nos6   | $\dagger$, $\dagger$ | 0.94 0.20 35, 37 | 0.30 0.30 | 0.94 0.20 35, 37 | 0.30 0.30 |
| orsirr_1 $\dagger$, $\dagger$ | 5.36 3.46 25, 37 | 0.30 0.30 | 5.36 3.46 25, 37 | 0.30 0.30 |
| orsirr_2 $\dagger$, $\dagger$ | 5.66 3.05 23, 36 | 0.30 0.30 | 5.66 3.05 23, 36 | 0.30 0.30 |
| orsreg_1 687, 346 | 4.02 7.31 27, 47 | 0.30 0.30 | 4.02 7.31 27, 47 | 0.30 0.30 |
| pores_2 $\dagger$, $\dagger$ | 8.67 6.84 37, 51 | 0.51 0.51 | 8.78 7.31 37, 50 | 0.30 0.30 |
| sherman1 356, $\dagger$ | 2.86 0.70 27, 40 | 0.38 0.38 | 2.89 0.74 27, 40 | 0.30 0.30 |
| sherman2 $\dagger$, $\dagger$ | 2.74 4.54 4, 7 | 0.30 0.30 | 2.74 4.54 4, 7 | 0.30 0.30 |
| sherman3 $\dagger$, $\dagger$ | 1.93 4.89 145, 627 | 0.35 0.35 | 1.96 5.07 143, 900 | 0.30 0.30 |
| sherman4 101, 377 | 1.25 0.35 34, 49 | 0.30 0.30 | 1.25 0.35 34, 49 | 0.30 0.30 |
| sherman5 $\dagger$, $\dagger$ | 1.57 2.05 29, 43 | 0.30 0.30 | 1.57 2.05 29, 43 | 0.30 0.30 |
Table 2  (Continued)

| Matrix  | Matrix M  | \( \text{PSAI(tol), } \varepsilon = 0.4, l_{\text{max}} = 5 \) | \( \text{PSAI(tol), } \varepsilon = 0.4, l_{\text{max}} = 8 \) |
|---------|-----------|-------------------------------------------------|-------------------------------------------------|
|         | \( \text{iter}_b, \text{iter}_g \) | \( \text{spar} \) \( \text{ptime} \) \( \text{iter}_b, \text{iter}_g \) \( \text{r}_{\text{max}} \) \( \text{coln} \) | \( \text{spar} \) \( \text{ptime} \) \( \text{iter}_b, \text{iter}_g \) \( \text{r}_{\text{max}} \) \( \text{coln} \) |
| epb1    | 433, †    | 0.60 22.23 237, 474 | 0.40 0 | 0.60 22.23 237, 474 | 0.40 0 |
| fidap024| †, †      | 3.26 12.77 95, †   | 0.42 6 | 3.28 11.54 91, †   | 0.40 0 |
| fidap028| †, †      | 3.33 37.70 99, 299 | 0.40 0 | 3.33 37.70 99, 299 | 0.40 0 |
| fidap031| †, †      | 1.66 18.70 137, †  | 0.65 2 | 1.68 20.71 141, 801 | 0.40 0 |
| fidap036| †, †      | 1.76 5.99 85, 250  | 0.40 0 | 1.76 5.99 85, 250  | 0.40 0 |
| nos3    | 213, †    | 0.50 0.40 106, 536 | 0.38 0 | 0.50 0.40 106, 536 | 0.38 0 |
| nos6    | †, †      | 0.56 0.14 38, 44  | 0.40 0 | 0.56 0.14 38, 44  | 0.40 0 |
| orsirr_1| †, †      | 3.19 1.79 37, 59  | 0.39 0 | 3.19 1.79 37, 59  | 0.39 0 |
| orsirr_2| †, †      | 3.26 1.49 38, 60  | 0.39 0 | 3.26 1.49 38, 60  | 0.39 0 |
| orsreg_1| 687, 346  | 2.13 4.02 40, 67  | 0.38 0 | 2.13 4.02 40, 67  | 0.38 0 |
| pores_2 | †, †      | 3.53 1.97 53, 146 | 0.68 3 | 3.58 2.04 59, 147 | 0.40 0 |
| sherman1| 356, †    | 1.62 0.49 37, 60  | 0.43 1 | 1.63 0.49 36, 60  | 0.40 0 |
| sherman2| †, †      | 2.42 3.59 5, 8   | 0.40 0 | 2.42 3.59 5, 8   | 0.40 0 |
| sherman3| †, †      | 1.15 3.33 201, †  | 0.40 0 | 1.15 3.33 201, †  | 0.40 0 |
| sherman4| 101, 377  | 0.88 0.25 41, 59  | 0.40 0 | 0.88 0.25 41, 59  | 0.40 0 |
| sherman5| †, †      | 1.18 1.64 35, 53  | 0.40 0 | 1.18 1.64 35, 53  | 0.40 0 |

still reasonably small and exceed \( \varepsilon \) no more than twice. This indicates that the corresponding \( M \) are still effective preconditioners, as confirmed by the iterations used, but they are generally less effective than the corresponding ones obtained by the bigger \( l_{\text{max}} \) which guarantee that \( M \) computed by \( \text{PSAI(tol)} \) succeeds for very small \( l_{\text{max}} \). Table 2 clearly tells us that for a smaller \( \varepsilon \), \( \text{PSAI(tol)} \) needs larger \( l_{\text{max}} \) for the while loop. But a remarkable finding is that \( \text{PSAI(tol)} \) succeeds for very small \( l_{\text{max}} \). Given a rather mildly small \( \varepsilon \) like 0.3 and the generality of test problems, these experiments suggest that we may well set \( l_{\text{max}} = 10 \) as a default value in Algorithm 2.

We observe from Table 2 that for each problem the smaller \( \varepsilon \) the fewer iterations the two Krylov solvers use. However, in the experiments, we notice that, for all problems except fidap024, fidap031 and sherman3, for which GMRES(50) failed when \( \varepsilon = 0.4 \), and given \( \varepsilon \) and \( l_{\text{max}} \), setup time of \( \text{ptime} \) of \( M \) and Krylov iterations only occupy a very small percent. As we have addressed in the introduction, this is a typical feature of an effective SAI preconditioning procedure and has been recognized widely in the literature, e.g., [5]. This is true even in a parallel computing environment. Moreover, our Matlab codes have not been optimized, and thus may give rise to lower performance. Thus, we do not list the time for the Krylov iterations in Table 2. With this in mind, we find from Table 2 that for the first five matrices, orsreg_1 and pores_2, the sparsity and construction cost of \( M \) increases considerably as \( \varepsilon \) decreases. Overall, to tradeoff effectiveness and general application, \( \varepsilon = 0.3 \) is a good choice for accuracy and the maximum number of while loops in \( \text{PSAI(tol)} \) should be 10.

Regarding Table 2, we finally point out a very important fact: for each of the test problems and given three choices for \( \varepsilon \), BPSAI and \( \text{PSAI(tol)} \) with our dropping crite-
rion use exactly the same value for $l_{\text{max}}$ to yield preconditioners attaining accuracy $\epsilon$. This fact is important because it illustrates that the latter behaves like the former with the same choice for $l_{\text{max}}$, while obtaining an equally effective preconditioner at less computational cost for setup.

The next results illustrate three considerations. First, choosing a smaller $tol_k$ is not required because the resulting $M_d$ is denser and costs more to set up but is not necessarily a better preconditioner. Second, for an improperly chosen fixed small $tol$, that is, $tol > \frac{\epsilon}{\text{nnz}(m_k)\|A\|_1}$ at some while-loops of Algorithm 2, PSAI($tol$) may produce a numerically singular $M_d$ which will cause the complete failure of the preconditioning. Third, for a $tol$ that produces a singular $M_d$, reducing $tol$ by one order of magnitude, will yield an $M_d$ which is a good preconditioner but is less effective than the $M_d$ obtained with $tol_k$ defined by (3.21). This illustrates that choosing a fixed $tol$ empirically is at risk for generating an ineffective $M_d$.

To illustrate the first consideration, we use the three matrices orsirr_1, orsirr_2 and orsreg_1 and use PSAI($tol$) with $\epsilon = 0.2$, $l_{\text{max}} = 8$ and with $tol_k$ ranging from a little smaller to considerably smaller than that indicated by (3.21). Specifically, denote the right hand side in (3.21) by RHS, then we use RHS, RHS/2, RHS/10 and RHS/100, and investigate the impact of the choice for the tolerance on the quality, sparsity and computational cost of setup of $M_d$. We report the results in Table 3, where the tolerance $tol_k = 0$ corresponds to the BPSAI procedure. For the three matrices, as $\text{coln}$ in Table 2 and $r_{\text{max}}$ in Table 3 indicate, the approximate inverses $M$ obtained by PSAI($tol$) with these different tolerances $tol_k$ and BPSAI have attained the accuracy $\epsilon$. For each of these three problems, we can easily observe that $M$ becomes increasingly denser as $tol_k$ decreases and $M$ is the densest for $tol_k = 0$. However, the preconditioning quality of denser $M$ is not improved, since the corresponding numbers of Krylov iterations are almost the same, as shown by $\text{iter}_b$ and $\text{iter}_g$. Moreover, we can see that the setup time $\text{ptime}$ of $M$ increases as $tol_k$ decreases. For all the other test problems in Table 1, we have also made numerical experiments in the above way. We find that the sparsity and preconditioning quality of $M$ obtained by PSAI($tol$) with the five $tol_k$ changes very little. This means that our dropping criterion (3.21) enables us to drop entries of small magnitude in $M$ and smaller $tol_k$ does not help any. Together with Table 3, we conclude that our dropping criterion is effective and robust and it is not necessary to take smaller $tol_k$ in PSAI($tol$).

To illustrate the second and third consideration, we investigate the behavior of $M$ obtained by PSAI($tol$) for improperly chosen drop tolerance $tol$ that seems small intuitively. We attempt to show that a choice of fixed $tol$ that is apparently small, but bigger than that defined by (3.21) for some $k$ may produce a numerically singular $M$. Specifically, we take

$$tol > \frac{\epsilon}{\text{nnz}(m_k)\|A\|_1},$$

in the while-loop of Algorithm 2, where the right-hand side is just our drop tolerance (3.21). We drop the entries whose sizes are below such improper $tol$. Table 4(a) lists the matrices, each with the drop tolerance $tol$ that leads to a numerically singular $M$ for $\epsilon = 0.2$, $l_{\text{max}} = 8$. The $\text{mintol}$ and $\text{maxtol}$ in Table 4(a) denote the minimum and maximum of $tol_k$ defined by (3.21). However, if we decrease the tolerance $tol$ by one order of magnitude, we will obtain good preconditioners; see Table 4(b) for
Table 3  Effects of smaller tolerant $\text{tol}_k$ for PSAI($\text{tol}$) with $\varepsilon = 0.2$ and $l_{\text{max}} = 8$. Note: when the iterations for BICGSTab are $k$, the dimension of the Krylov subspace is $2k$

|       | $\text{tol}_k = \text{RHS}$ | $\text{tol}_k = \text{RHS} \div 2$ | $\text{tol}_k = \text{RHS} \div 10$ | $\text{tol}_k = \text{RHS} \div 100$ | $\text{tol}_k = 0$ |
|-------|-----------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------|
| orsirr_1 | $\text{spar}$              | 10.15                             | 10.81                             | 12.02                             | 13.13           | 16.77           |
|        | $\text{ptime}$              | 7.41                              | 7.60                              | 8.34                              | 8.56            | 9.05            |
|        | $\text{iter}_b, \text{iter}_g$ | 15, 26                            | 15, 26                            | 15, 26                            | 15, 26           | 15, 26          |
|        | $\text{r}_\text{max}$      | 0.199974                          | 0.199971                          | 0.199970                          | 0.199970         | 0.199970        |
| orsirr_2 | $\text{spar}$              | 10.71                             | 11.29                             | 12.42                             | 13.52           | 16.70           |
|        | $\text{ptime}$              | 6.53                              | 6.58                              | 6.68                              | 7.45            | 8.11            |
|        | $\text{iter}_b, \text{iter}_g$ | 16, 25                            | 16, 25                            | 14, 25                            | 14, 25           | 14, 25          |
|        | $\text{r}_\text{max}$      | 0.199974                          | 0.199970                          | 0.199970                          | 0.199970         | 0.199970        |
| orsreg_1 | $\text{spar}$              | 9.16                              | 9.63                              | 11.27                             | 12.97           | 16.82           |
|        | $\text{ptime}$              | 19.49                             | 20.42                             | 23.35                             | 25.84           | 35.47           |
|        | $\text{iter}_b, \text{iter}_g$ | 18, 29                            | 18, 29                            | 18, 29                            | 18, 29           | 18, 29          |
|        | $\text{r}_\text{max}$      | 0.199853                          | 0.199841                          | 0.199840                          | 0.199839         | 0.199839        |

Table 4  Sensitivity of the quality of $M$ to fixed drop tolerance $\text{tol}$

(a): Bad $\text{tol}$ resulting in numerically singular $M$ for $\varepsilon = 0.2$, $l_{\text{max}} = 8$

|       | nos3 | nos6 | orsirr_1 | orsirr_2 | orsreg_1 | sherman5  |
|-------|------|------|----------|----------|----------|----------|
| $\text{tol}$ | $10^{-2}$ | $10^{-6}$ | $10^{-3}$ | $10^{-3}$ | $10^{-3}$ | $10^{-2}$ |
| $\text{r}_\text{max}$ | 3.00    | 1.93  | 285.17   | 71.34    | 23.12    | 24.71    |
| $\text{mintol}$ | $1.61 \times 10^{-6}$ | $3.97 \times 10^{-10}$ | $8.48 \times 10^{-10}$ | $8.48 \times 10^{-10}$ | $1.44 \times 10^{-8}$ | $2.10 \times 10^{-7}$ |
| $\text{maxtol}$ | $4.34 \times 10^{-5}$ | $6.25 \times 10^{-9}$ | $8.80 \times 10^{-8}$ | $1.17 \times 10^{-7}$ | $1.39 \times 10^{-6}$ | $7.91 \times 10^{-6}$ |

(b): Good $\text{tol}$ leading to effective $M$ for $\varepsilon = 0.2$, $l_{\text{max}} = 8$

|       | nos3 | nos6 | orsirr_1 | orsirr_2 | orsreg_1 | sherman5  |
|-------|------|------|----------|----------|----------|----------|
| $\text{tol}$ | $10^{-3}$ | $10^{-7}$ | $10^{-4}$ | $10^{-4}$ | $10^{-4}$ | $10^{-3}$ |
| $\text{ptime}$ | 3.53  | 0.47  | 7.09     | 6.32     | 17.86    | 4.64     |
| $\text{spar}$ | 0.67  | 1.78  | 2.31     | 2.62     | 3.05     | 1.72     |
| $\text{iter}_b$ | 162   | 79    | 21       | 41       | 25       | 22       |
| $\text{iter}_g$ | †     | 72    | 34       | 50       | 39       | 32       |
| $\text{r}_\text{max}$ | 0.68  | 0.73  | 14.11    | 14.11    | 2.33     | 4.14     |

details. We emphasize that for the given $\varepsilon$ and $l_{\text{max}}$ and all the matrices in Table 4(b), PSAI($\text{tol}$) with dropping criterion (3.21) has computed the sparse approximations $M$ of $A^{-1}$ with the desired accuracy $\varepsilon$, as shown in Table 2.

We see from Table 4(a) that the maximum residual $r_{\text{max}}$ for each problem is not small at all for the chosen bad fixed drop tolerance $\text{tol}$. On the other hand, Table 4(b) indicates that the one order reduction of $\text{tol}$ results in essential improvements on the effectiveness of preconditioners, not only delivering nonsingular $M$ but also acceler-
Fig. 1  Column residual norms of $M$ for orsirr_2 obtained by PSAI(tol) with bad and good fixed tol and adaptive tol$_k$ defined by (3.21)

Evaluating the convergence considerably. These tests indicate that the non-singularity and quality of $M_d$ obtained by PSAI(tol) can be very sensitive to the choice of drop tolerance $tol$. However, compared with the corresponding results for $\varepsilon = 0.2$, $l_{\text{max}} = 8$ on the same test problems in Table 4(b) and Table 2, we find that the preconditioner obtained by PSAI(tol) with the good fixed tolerance $tol$ is not so effective as that with $tol_k$ defined by (3.21), as shown by values of $\text{iter}_b$ and $\text{iter}_g$. Indeed, the preconditioners obtained by fixed tolerance $tol$ do not satisfy the accuracy $\varepsilon$, as $r_{\text{max}}$ indicate.

To be more illustrative, for orsirr_2 we depict the residual norms $\|Am_k - e_k\|$, $k = 1, 2, \ldots, n$ of three such $M$ obtained by PSAI(tol) with the adaptive $tol_k$ defined by (3.21), bad and good fixed $tol = 10^{-3}, 10^{-4}$; see Fig. 1, where the solid line $y = \varepsilon = 0.2$ parallel to the $x$-axis denotes our accuracy requirement, the circle ‘o’, the plus ‘+’ and the triangle ‘△’ are $\|Am_k - e_k\|$, $k = 1, 2, \ldots, n$ of each $M$. We find from the figure that all the circles ‘o’ fall below the solid line, meaning that PSAI(tol) with $tol_k$ defined by (3.21) computes all the columns of $M$ with desired accuracy; many ‘+’ reside above the solid line and some of them are far away from $\varepsilon = 0.2$ and can be up to 10~100, indicating that $M$ obtained by PSAI(tol) is very bad and of poor quality for preconditioning; most of the triangles ‘△’ are below $\varepsilon = 0.2$, and a small part of them is above it, revealing that $M$ is improved very substantially but is not so good like $M$ computed by PSAI(tol) with $tol_k$ defined by (3.21).
Table 5  Sensitivity of the quality of $M_d$ to some fixed $tol$ for the static SAI procedure with the pattern of $(I + A)^3$. Note: when the iterations for BiCGStab are $k$, the dimension of the Krylov subspace is $2k$

(a): Bad $tol$ resulting in numerically singular $M_d$

|  | orsirr_1 | orsirr_2 | orsreg_1 | pores_2 | sherman5 |
|---|---|---|---|---|---|
| $tol$  | $10^{-5}$ | $10^{-5}$ | $10^{-3}$ | $10^{-6}$ | $10^{-2}$ |
| $r_{\text{max}}$  | 1.32 | 1.00 | 15.2 | 18.0 | 24.7 |
| mintol  | $1.37 \times 10^{-9}$ | $1.37 \times 10^{-9}$ | $4.93 \times 10^{-8}$ | $6.53 \times 10^{-12}$ | $1.63 \times 10^{-7}$ |
| maxtol  | $2.64 \times 10^{-8}$ | $2.23 \times 10^{-8}$ | $3.52 \times 10^{-7}$ | $1.55 \times 10^{-10}$ | $2.37 \times 10^{-5}$ |

(b): Good $tol$ leading to effective $M_d$

| Matrix | $tol$ | $p_{\text{time}}$ | spar | iter$_b$ | iter$_g$ | $r_{\text{max}}$ |
|---|---|---|---|---|---|---|
| orsirr_1 | $10^{-6}$ | 1.63 | 1.82 | 33 | 50 | 0.42 |
| orsirr_2 | $10^{-6}$ | 1.31 | 2.69 | 32 | 48 | 0.42 |
| orsreg_1 | $10^{-4}$ | 4.09 | 0.91 | 45 | 74 | 1.32 |
| pores_2 | $10^{-7}$ | 3.10 | 2.47 | 124 | 158 | 1.74 |
| sherman5 | $10^{-3}$ | 11.79 | 1.55 | 24 | 34 | 3.76 |

Table 4 and Fig. 1 tell us that empirically chosen tolerances are problematic and susceptible to failure. In contrast, Tables 2–4 demonstrate that our selection criterion (3.21) is very robust for PSAI($tol$).

4.2 Results for three static SAI procedures

As an application of our theory, in this subsection, we test the static F-norm minimization based SAI preconditioning procedures with the three popular patterns of $(I + A)^3$, $(I + |A| + |A^T|)^3A^T$ and $(AA^T)^2A^T$, respectively; see [23] for the effectiveness of these patterns. We attempt to show the effectiveness of dropping criterion (3.22) and exhibit the sensitiveness of the preconditioning quality of $M$ to drop tolerances $tol_k$. We first compute $M$ by predetermining its pattern and solving $n$ independent LS problems, and then get a sparser $M_d$ by dropping the entries of small magnitude in $M$ below the tolerance defined by (3.22) or some empirically chosen ones.

We summarize the results in Tables 5–8, where $p_{\text{time}}$ includes the time for predetermination of the pattern of $M$, the computation of $M$ and the sparsification of $M$, and $stime_b$ and $stime_g$ denote the CPU time in second of BiCGStab and GMRES(50) applied to solve the preconditioned linear systems. We observed that there are some columns whose residual norms $\|Am_k - e_k\| = \varepsilon_k$ are very small (some are at the level of $\varepsilon_{\text{mach}}$). Therefore, to drop entries of small magnitude as many as possible, we replace those $\varepsilon_k$ below 0.1 by 0.1 in (3.22).

We test the static SAI procedure with the pattern of $(I + A)^3$. Table 5(a) lists the matrices, each with the fixed tolerance $tol$ leading to a numerically singular $M$ and Table 5(b) exhibits the good performance of $M_d$ generated from the static SAI by decreasing the corresponding $tol$ in Table 5(a) by one order of magnitude. Tables 6, 7,
Table 6  Static SAI procedure with the pattern of \((I + A)^3\). Note: when the iterations for BiCGStab are \(k\), the dimension of the Krylov subspace is \(2k\)

|       | \(p\)time | spar | iter\(_b\) | iter\(_g\) | stime\(_b\) | stime\(_g\) | \(r\)max |
|-------|-------|------|--------|--------|--------|--------|--------|
| orsirr\(_1\) | \(M\) | 1.65 | 8.36   | 29     | 45     | 0.03   | 0.08   | 0.42   |
|       | \(M_d\) | 1.78 | 4.54   | 29     | 45     | 0.01   | 0.06   | 0.42   |
| orsirr\(_2\) | \(M\) | 1.48 | 8.62   | 30     | 44     | 0.02   | 0.04   | 0.42   |
|       | \(M_d\) | 1.56 | 5.24   | 30     | 44     | 0.02   | 0.03   | 0.42   |
| orsreg\(_1\) | \(M\) | 4.39 | 7.53   | 28     | 51     | 0.04   | 0.09   | 0.42   |
|       | \(M_d\) | 4.69 | 2.95   | 33     | 51     | 0.01   | 0.08   | 0.42   |
| pores\(_2\)   | \(M\) | 2.74 | 9.25   | 52     | 118    | 0.09   | 0.14   | 0.94   |
|       | \(M_d\) | 3.00 | 4.98   | 52     | 118    | 0.06   | 0.13   | 0.94   |
| sherman\(_5\) | \(M\) | 13.26 | 8.39  | 22     | 31     | 0.04   | 0.05   | 0.32   |
|       | \(M_d\) | 14.07 | 3.54  | 22     | 31     | 0.02   | 0.04   | 0.32   |

Table 7  Static SAI procedure with the pattern of \((I + |A| + |A^T|)^3 A^T\). Note: when the iterations for BiCGStab are \(k\), the dimension of the Krylov subspace is \(2k\)

|       | \(p\)time | spar | iter\(_b\) | iter\(_g\) | stime\(_b\) | stime\(_g\) | \(r\)max |
|-------|-------|------|--------|--------|--------|--------|--------|
| orsirr\(_1\) | \(M\) | 5.45 | 16.41  | 18     | 28     | 0.03   | 0.04   | 0.32   |
|       | \(M_d\) | 6.00 | 10.06  | 18     | 28     | 0.01   | 0.03   | 0.32   |
| orsirr\(_2\) | \(M\) | 4.64 | 17.03  | 18     | 28     | 0.02   | 0.05   | 0.32   |
|       | \(M_d\) | 5.19 | 11.23  | 16     | 28     | 0.01   | 0.02   | 0.32   |
| orsreg\(_1\) | \(M\) | 14.86 | 14.03 | 19     | 34     | 0.05   | 0.06   | 0.34   |
|       | \(M_d\) | 16.82 | 6.83  | 19     | 34     | 0.02   | 0.05   | 0.34   |
| pores\(_2\)   | \(M\) | 11.02 | 18.42 | 26     | 38     | 0.05   | 0.07   | 0.86   |
|       | \(M_d\) | 13.25 | 11.91 | 26     | 38     | 0.05   | 0.06   | 0.86   |
| sherman\(_5\) | \(M\) | 52.36 | 14.94 | 16     | 23     | 0.06   | 0.06   | 0.25   |
|       | \(M_d\) | 56.50 | 6.41  | 16     | 23     | 0.02   | 0.04   | 0.25   |

8 show the results obtained by the three static SAI procedures with dropping criterion (3.22).

Singular \(M_d\) as in Table 5(a) lead to complete failure of preconditioning. We also see from the table that all the maximum residuals \(r_{max}\) of \(M_d\) for the five matrices are not small, meaning that the \(M_d\) are definitely ineffective for preconditioning. But Table 5(b) shows that the situation is improved drastically when the corresponding tolerances \(tol\) are decreased only by one order of magnitude.

Similar to PSAI(\(tol\)), the quality of static SAI preconditioners depends on, and can be very sensitive to, the drop tolerances. Figure 2 depicts the residual norms of three \(M_d\) obtained by the static SAI procedure with the pattern of \((I + A)^3\) using the
Table 8 Static SAI procedure with the pattern of $(A^T A)^2 A^T$. Note: when the iterations for BiCGStab are $k$, the dimension of the Krylov subspace is $2k$

|                  | $p_{time}$ | $spar$ | $iter_b$ | $iter_g$ | $s_{time_b}$ | $s_{time_g}$ | $r_{max}$ |
|------------------|-----------|--------|----------|----------|--------------|--------------|----------|
| orsirr_1 M      | 15.37     | 27.79  | 13       | 20       | 0.02         | 0.02         | 0.24     |
| $M_d$           | 18.26     | 18.39  | 13       | 20       | 0.01         | 0.02         | 0.24     |
| orsirr_2 M      | 12.11     | 28.84  | 14       | 19       | 0.02         | 0.03         | 0.24     |
| $M_d$           | 14.20     | 20.26  | 14       | 19       | 0.02         | 0.02         | 0.24     |
| orsreg_1 M      | 49.42     | 22.77  | 14       | 24       | 0.05         | 0.04         | 0.31     |
| $M_d$           | 57.22     | 12.75  | 14       | 24       | 0.02         | 0.04         | 0.31     |
| pores_2 M       | 41.83     | 30.84  | 16       | 26       | 0.06         | 0.05         | 0.68     |
| $M_d$           | 49.71     | 19.46  | 16       | 26       | 0.05         | 0.04         | 0.68     |
| sherman5 M      | 129.25    | 22.53  | 14       | 19       | 0.06         | 0.06         | 0.20     |
| $M_d$           | 138.41    | 9.09   | 14       | 19       | 0.02         | 0.03         | 0.20     |

Fig. 2 Column residual norms of $M_d$ for orsirr_2 obtained by the static SAI with bad and good fixed tol and $tol_k$ defined by (3.22)

bad $tol = 10^{-5}$, the good $tol = 10^{-6}$ and our criterion (3.22), which are denoted by the plus ‘+’, the triangle ‘△’ and circle ‘◦’, respectively, and the solid line $y = r_{max}$ parallel to the x-axis is the maximum column residual norm of $M_d$ obtained with

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We see from the figure that $M_d$ constructed with (3.22) and the good fixed tolerance $tol = 10^{-6}$ are fairly good but the former one is more effective than the latter one, since the triangles ‘Δ’ are either indistinguishable with or a little bit higher than the corresponding circles ‘○’. Such effectiveness is also reflected in the values of $iter_b$ and $iter_g$ in Table 5 and Table 6. In contrast, $M_d$ obtained with the tolerance $tol = 10^{-5}$ has many columns, which are poorer than those of $M_d$ obtained with (3.22), since the ‘+’ are above the corresponding ‘○’, and it has some columns whose residual norms reside above the solid line $y = r_{\text{max}}$.

For Tables 6–8, we see that each $M_d$ is sparser than the corresponding $M$ and it is cheaper to apply $M_d$ than $M$ in Krylov solvers, as $\text{stime}_b$ and $\text{stime}_g$ indicate. Furthermore, for each matrix, since we use (3.22) to only drop the entries of small magnitude, two $r_{\text{max}}$ corresponding to each pair $M$ and $M_d$ are approximately the same and they are fairly small. So it is expected that each $M_d$ and the corresponding $M$ have very similar accelerating quality. This is indeed the case, because for all the problems but orsreg_2, each Krylov solver preconditioned by $M_d$ and the corresponding $M$ uses exactly the same number of iterations to achieve convergence. For orsreg_2 in Table 6, BiCGSTab preconditioned by $M_d$ uses only three more iterations than it preconditioned by $M$. These results demonstrate that our selection criterion (3.22) is effective and robust. Compared with Table 5, we see from Table 6 that the SAI preconditioning with our criterion (3.22) is more effective than that with the good fixed tolerance $tol = 10^{-6}$, since the maximum residual norms $r_{\text{max}}$ for the former are always not bigger than those for the latter and the Krylov solvers preconditioned by the former used fewer iterations to achieve convergence. In addition, we notice from Table 8 that the pattern of $(A^T A)^2 A^T$ leads to considerably denser $M$ and $M_d$ that are good approximate inverses but are much more expensive to compute, compared with the other two patterns. Therefore, as far as the overall performance is concerned, this static SAI procedure is less effective than the other two.

5 Conclusions

Selection criteria for drop tolerances are vital to SAI preconditioning. However, this important problem has received little attention and never been studied rigorously and systematically. For F-norm minimization based SAI preconditioning, such criteria affect the non-singularity, the quality and effectiveness of a preconditioner $M$. An improper choice of drop tolerance may produce a numerically singular $M$, causing the complete failure in preconditioning, or may produce a good but denser $M$ possibly at more cost for setup and application. To develop a robust PSAI($tol$) preconditioning procedure, we have analyzed the effects of drop tolerances on the non-singularity, quality and effectiveness of preconditioners. We have established some important and intimate relationships between them. Based on them, we have proposed adaptive robust selection criteria for drop tolerances that can make $M$ as sparse as possible and of comparable quality to those obtained by BPSAI, so that it is possible to lower the cost of setup and application. The theory on selection criteria has been adapted to static F-norm minimization based SAI preconditioning procedures. Numerical experiments have shown that our criteria work very well. However, we point out that it is more
important and beneficial to perform dropping in the adaptive PSAI preconditioning procedure than a static SAI one.

For general purposes and effectiveness, robust selection criteria for drop tolerances also play a key role in other adaptive F-norm minimization based SAI preconditioning procedures whenever dropping is used. Just like for PSAI(tol), dropping criteria serve two purposes, one of which is to make an approximate inverse $M$ as sparse as possible and the other is to guarantee its comparable preconditioning quality to that obtained from SAI procedure without dropping. For adaptive factorized sparse approximate inverse preconditioning, such as AINV type algorithms [3, 5], dropping is equally important. Different from F-norm minimization based SAI preconditioning, the non-singularity of the factorized $M$ is guaranteed naturally. Nonetheless, how to drop entries of small magnitude is nontrivial and has not yet been well studied. All of these are significant and are topics for further consideration.

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