International Journal of Computer Mathematics
Vol. 00, No. 05, May 2007, 1–31

Frobenius Norm Minimization and Probing for Preconditioning

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(Received 00 Month 200x; In final form 00 Month 200x)

In this paper we introduce a new method for defining preconditioners for the iterative solution of a system of linear equations. By generalizing the class of modified preconditioners (e.g. MILU), the interface probing, and the class of preconditioners related to the Frobenius norm minimization (e.g. FSAI, SPAI) we develop a toolbox for computing preconditioners that are improved relative to a given small probing subspace. Furthermore, by this MSPAI (modified SPAI) probing approach we can improve any given preconditioner with respect to this probing subspace. All the computations are embarrassingly parallel. Additionally, for symmetric linear system we introduce new techniques for symmetrizing preconditioners. Many numerical examples, e.g. from PDE applications such as domain decomposition and Stokes problem, show that these new preconditioners often lead to faster convergence and smaller condition numbers.

Keywords: preconditioning, Schur complements, probing, sparse approximate inverses, modified incomplete factorization

AMS Subject Classification: 65F10, 65F50, 65F35

1 Introduction

For the iterative solution of sparse linear equations $Ax = b$, e.g. based on the conjugate gradient method, BiCGstab, GMRES, or QMR, the choice of preconditioner is very important (see [6]). Usually we differentiate between explicit preconditioners that are approximations on A itself like Jacobi, Gauss-Seidel, or ILU method, and approximations on A^{-1} such as polynomial preconditioners or Frobenius norm preconditioners like SPAI.

Here, we are interested in developing a new class of explicit and inverse preconditioners by improving three types of preconditioners:

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(i) approximate inverses by Frobenius norm minimization such as SPAI or FSAI
(ii) probing by choosing special subspaces where the preconditioner coincides with the action of the given matrix
(iii) modifying a given preconditioner in order to improve the behaviour of the preconditioner with respect to certain subspaces, like in modified ILU.

These three starting points lead to three modifications of well-known algorithms:

- Computing approximate inverses by Frobenius norm minimization can be generalized, e.g. by allowing weight matrices inside the Frobenius norm like described in [20], or by adding side conditions in the form of additional rows to the original matrix minimization problem. Here, the main task is to choose meaningful weight matrices that improve the behaviour of the preconditioner.
- Generalizing the probing approach by treating the probing ansatz as a regularized Least Squares (LS) problem. The regularization appears as an additional Frobenius norm matrix minimization problem. Then a wider choice of probing vectors can be used for any type of given matrices A.
- Modifying a given preconditioner by finding a nearby improved matrix with better approximation property on certain subspaces.

These new preconditioners can lead to better convergence in many examples and the involved computations are embarrassingly parallel. Surprisingly, these three tasks can be treated in the same way as special weighted Frobenius norm minimization problems. In the following we will call this approach *MSPAI probing.*

One drawback of preconditioners arising from Frobenius norm minimization is that certain properties like symmetry or positive definiteness are not maintained. Therefore, we develop techniques for symmetrizing sparse preconditioners in different ways. These methods deliver symmetric matrices that are often also symmetric and positive definite (spd) and allow the application of more efficient iterative solvers.

In the first section we give an overview of the well-known preconditioners, we are interested in. Then, we introduce a general minimization approach and apply this approach on explicit and inverse preconditioners combining the probing idea and the Least Squares minimization. This leads to new preconditioners for direct and inverse, resp. factorized and unfactorized approximations. Furthermore, symmetrization techniques for all cases are developed. In the last sections we present numerical examples and comparisons for PDE problems such as Laplace equation and Stokes problem.

1.1 *Frobenius Norm Minimization and SPAI*

The use of Frobenius norm minimization for constructing preconditioners for sparse matrices in a static way by

$$\min_M \|AM - I\|_F$$

for a prescribed allowed sparsity pattern for $M \approx A^{-1}$ goes back to [5]. The computation of M can be split into n independent subproblems $\min_{M_k} \|AM_k - e_k\|_2$, $k = 1, ..., n$ with M_k the columns of M and e_k the columns of the identity matrix. In view of the sparsity of these Least Squares (LS) problems, each subproblem is related to a small matrix $\hat{A}_k := A(I_k, J_k)$ with index set J_k given by the allowed pattern for M_k and I_k the so-called shadow of J_k, that is the indices of nonzero rows in $A(:, J_k)$. These n small LS problems can be solved independently, e.g. based on QR-decompositions of the matrices $\hat{A}_k$ by using the Householder method or the modified Gram Schmidt algorithm.

This approach has been improved and modified in different ways. Cosgrove, Díaz, Griewank, as well as Grote, Huckle and Gould, Scott introduced dynamic methods for capturing an efficient sparsity for M automatically (see [10, 13, 15]). Chow showed in [8] ways to prescribe an efficient static pattern a priori.

Holland, Shaw, and Wathen have generalized this ansatz allowing a target matrix on the right side in the form $\min_M \|AM - B\|_F$ in connection with some kind of two-level preconditioning: First compute preconditioner B for A and then improve this preconditioner by a Frobenius norm minimization (see [16]). From the algorithmic point of view the minimization with target matrix B instead of I introduces no additional difficulties. Only the pattern of M should be chosen more carefully with respect to A and B.

Kolotilina and Yeremin [20] generalized the method to compute factorized approximations and also allowing weight matrices inside the Frobenius norm,

$$\min_M \|AM - I\|_W^2 = \min_M \|W^{1/2}(AM - I)\|_F^2 = \min_M tr((AM - I)W(AM - I)^T)$$

(see also [19]). Huckle introduced in [17] dynamic versions of these factorized approximations. The factorized approximation in the spd case again can be computed as the solution of a Frobenius norm minimization problem: For $A = L_A^T L_A$ solve $\min_L \|L_A L - I\|_F$ with normal equations $A(J_k, J_k)L_k(J_k) = L_{A,kk}e_k(J_k)$ for computing the columns of L. Here, in a first step the unknown main diagonal entry $L_{A,kk}$ is replaced by 1; this allows the computation of a factor L by solving n small linear systems. In a second step L can be optimized by a diagonal scaling with $diag(D(L^T AL)D) = I$. The approximate Cholesky factor for A^{-1} is then given by $L_D := LD$.

An advantage of all these methods is that they can be used as black box methods and they are easy parallelizable. But often the approximation quality is not sufficient. Furthermore, the symmetry is only preserved in the factorized approach.

1.2 *Probing*

The probing technique was introduced for preconditioning interface matrices in domain decomposition methods (see Chan in [7] or Axelsson [3] or more recently Siefert and Sturler in [22]). Here, the interface matrix is a Schur complement S. As preconditioner for S one defines e.g. a band matrix M that shows the right behaviour on certain subspaces or probing vectors e_j, thus $Me_j = Se_j$, $j = 1, ..., k$. As probing vectors one has to choose very special vectors, e.g. $e_1 = (1, 0, 0, 1, 0, 0, 1, ...)^T$, $e_2 = (0, 1, 0, 0, 1, 0, 0, 1, ...)^T$, and $e_3 = (0, 0, 1, 0, 0, 1, ...)^T$. This choice results in simple equations for computing the preconditioner M:

$$\begin{pmatrix} m_{11} & m_{12} & & & \\ m_{21} & m_{22} & m_{23} & & \\ & m_{32} & m_{33} & m_{34} & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} & 0 \\ m_{21} & m_{22} & m_{23} \\ m_{34} & m_{32} & m_{33} \\ m_{44} & m_{45} & m_{43} \\ \vdots & \vdots & \vdots \end{pmatrix} \quad (1)$$

From this equation one can read off the entries of M by comparison with the prescribed vectors $Me_j = Se_j$. Note, that the resulting M will be not symmetric and that the probing equation $Me_j = Se_j$ will not be satisfied in view of the band structure of M, e.g. the first component in Se_3 may be not zero. In the special case of only one probing vector and M a diagonal matrix it holds $M = diag(Se)$.

Axelsson and Polman have improved this approach by introducing the method of action in [3] which in some cases leads to a spd preconditioner. The advantage of these methods is that without explicit knowledge of the problem it is possible to obtain a preconditioner that imitates the behaviour of the original problem on certain subspaces. The disadvantages are, that one has to choose special probing vectors that lead to an easy to solve system for M; furthermore it is not easy to include special properties like symmetry.

1.3 *Modified Incomplete Factorizations*

The modified incomplete factorizations were introduced by Gustafsson (see [14]) and by Axelsson [1] as an improvement of the ILU algorithm. In the ILU method the Gaussian elimination process is restricted to a certain sparsity pattern. Therefore, new entries that appear on certain not allowed positions in U are deleted. The result is an approximate factorization $A = LU + R$, where R contains the neglected entries. The aim of the modified approach is again to imitate the action of the given matrix on a certain subspace. In this case the subspace is generated by the vector of all ones. In PDE examples this vector plays an important role in the sense that the discretized problem leads to a matrix where $A \cdot (1, 1, ..., 1)^T$ is zero upto the boundary conditions. Hence, this vector can be used as an approximation of the subspace to small eigenvalues. If we force the preconditioner to coincide with the given problem on this subspace we expect to improve the condition number of the preconditioned system.

In order to maintain the action of the preconditioner relative to the vector of all ones, we try to preserve the row sum of the triangular factors in the ILU method. Therefore, in the MILU algorithm we do not delete the entries on not-allowed positions but we add them to the related main diagonal entry, therefore maintaining the row sum. For PDE problems such as the 2D Laplacian this MILU improves the condition number significantly. As a disadvantage, this approach is restricted to the vector of all ones, and the method is not very robust for more general problems.

2 Generalized Form of Frobenius Norm Minimization and Probing

As we have seen in the previous sections it seems to be desirable to introduce a probing or modified approach for more general problems. With this aim, we consider a SPAI-like Frobenius norm minimization in the most general form. This new form allows the approximation of an arbitrary rectangular matrix B replacing the identity matrix I in SPAI form $\|AM - I\|_F$ (compare the target matrix SPAI form in [16]). Furthermore we replace A by any rectangular matrix C. Here, B and C should be sparse matrices, but we allow also a small number of dense rows in C and B. The matrix M that we want to compute has a prescribed sparsity pattern (it is also possible to update the sparsity pattern dynamically, e.g. by a SPAI-like approach, but we do not consider this dynamic method here). Technically, this causes no difference in the implementation compared with the original SPAI algorithm. Thus, for given matrices $C, B \in \mathbb{R}^{m \times n}$ we want to find a matrix $M \in \mathbb{R}^{n \times n}$ by solving the MSPAI minimization

$$\min_M \|CM - B\|_F^2 . \tag{2}$$

Analoguously to SPAI-type algorithms, we can solve the minimization (2) completely in parallel, because we can still compute M column-wise. Another property inherited from SPAI is the ability to prescribe an almost arbitrary sparsity pattern for M. Note, that a meaningful pattern for M should take into account the sparsity structure of C and of B as well. This new approach also allows one to consider lower/upper triangular matrices for M, C, and B.

As the main advantage of this general formulation we can add further conditions to a given Frobenius norm minimization. This allows the inclusion of probing constraints in the general computation of a preconditioner. Consider the given minimization problem

$$\min_M \|C_0 M - B_0\|_F^2$$

e.g. with $C_0 = A$ and $B_0 = I$ for approximating A^{-1}, or $C_0 = I$ and $B_0 = A$ for approximating A. Then for any given set of probing vectors collected in the rectangular matrix e^T we can add probing conditions $\min_M \|e^T(C_0 M - B_0)\|_2 = \min_M \|g^T M - h^T\|_2$ with $g^T := e^T C_0$ and $h^T := e^T B_0$ in the form

$$\min_M \left\| \begin{pmatrix} C_0 \\ \rho g^T \end{pmatrix} M - \begin{pmatrix} B_0 \\ \rho h^T \end{pmatrix} \right\|_F^2, \qquad 0 \leq \rho \in \mathbb{R} \tag{3}$$

with a weight ρ. The number ρ determines whether we want to give more weight to the original norm minimization or the additional probing condition. The k probing vectors which are stored in $e \in \mathbb{R}^{n \times k}$ are added row-wise to the corresponding matrices C_0 and B_0 in form of the matrices $g, h \in \mathbb{R}^{n \times k}$. This can be seen as a generalization of a Frobenius norm approximation which tries to improve the preconditioner on a certain subspace given by e.

Just as well this can be seen as a regularization technique for a general probing approach. In standard probing we can only consider probing vectors and sparsity patterns of M that lead to easy to solve linear systems for computing the entries of M from the probing conditions. In this new approach we can choose any probing vectors e and sparsity pattern of M that also lead to under- or overdetermined linear systems because of the imbedding of the probing method into the general matrix approximation setting.

In the given original problem $\min_M \|C_0 M - B_0\|_F$ we could also replace the Frobenius norm by any other norm, e.g. by adding a weight matrix (as considered in [20]) $\min_M \|W(C_0 M - B_0)\|_F$. By choosing as weight the rectangular matrix

$$W := \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \tag{4}$$

we end up with the same generalized MSPAI norm minimization (3).

2.1 *Sparse Approximate Inverses and Probing*

As a first application, we can use the method described above to add some probing information to a SPAI, i.e. unfactorized approximation of the inverse A^{-1} of a given matrix $A \in \mathbb{R}^{n\times n}$: We choose $C_0 = A$ in (3), and for B_0 we take the n-dimensional identity matrix I. Here, h becomes the given probing vector e, and $g = e^T A$. With that, we obtain the MSPAI Frobenius norm minimization

$$\min_M \left\| \begin{pmatrix} A \\ \rho e^T A \end{pmatrix} M - \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \right\|_F^2 = \min_M \|W(AM - I)\|_F^2 \tag{5}$$

with weight matrix (4). The result of this method is an approximation M to the inverse A^{-1}, which fulfills

$$g^T = e^T A \quad \overset{M\approx A^{-1}}{\Longrightarrow} \quad g^T M \approx e^T.$$

In many applications the matrix A is not given explicitly but only via a sparse approximation $\tilde{A}$. Nevertheless, we assume that we are able to compute $g^T = e^T A$ exactly. In this situation, we modify the above minimization to

$$\min_M \left\| \begin{pmatrix} \tilde{A} \\ \rho e^T A \end{pmatrix} M - \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \right\|_F^2 . \tag{6}$$

Then probing is used to derive a sparse approximate inverse M for $\tilde{A} \approx A$ with respect to the exact probing conditions $e^T AM = e^T$, where $\tilde{A}$ is an approximation of the original matrix A.

2.2 *Explicit Approximation and Probing*

With our approach, we can not only add constraints to the approximation of the inverse A^{-1} of a given matrix, but also to explicit approximations of A. This can be used if A is (nearly) dense in order to get a sparse approximation on A. In contrast to the last section, we choose $C_0 = I$ and $B_0 = A$ with probing vector $g = e$. Consequently, we choose $h^T = e^T A$. Altogether, this yields

$$\min_M \left\| \begin{pmatrix} I \\ \rho e^T \end{pmatrix} M - \begin{pmatrix} A \\ \rho e^T A \end{pmatrix} \right\|_F^2 = \min_M \|W(M - A)\|_F^2 \tag{7}$$

with the above weight matrix W (4). Now, we get a sparse approximation M of A which also tries to reflect the properties of A on certain vectors:

$$h^T = e^T A \approx e^T M.$$

In many cases, A is again only given implicitly or (nearly) dense, and we have to use a sparse approximation $\tilde{A}$. This leads to the MSPAI problem

$$\min_M \left\| \begin{pmatrix} I \\ \rho e^T \end{pmatrix} M - \begin{pmatrix} \tilde{A} \\ \rho e^T A \end{pmatrix} \right\|_F^2 . \tag{8}$$

Note, that this explicit approach makes sense only if linear equations in M can be solved easily, as the inverse of M has to be used for preconditioning.

2.3 *Symmetrization in the Unfactorized Case*

For the SPAI algorithm as well as the generalized problem (2) the solution matrices M are usually nonsymmetric. Nevertheless, for (positive definite) symmetric matrices A we would like to have a (positive definite) symmetric preconditioner, so it is still possible to use e.g. the preconditioned conjugate gradient method (pcg). Otherwise, one has to rely on iterative methods for nonsymmetric problems, such as BiCGstab, GMRES, or QMR which have higher computational costs. To overcome this problem, we present two symmetrization techniques, e.g. for the preconditioner M of the previous two sections. The first approach is based on MSPAI Frobenius norm minimization. In the second approach we combine two iteration steps writing the resulting iteration as one step with a symmetric preconditioner.

2.3.1 ***Symmetrization by Frobenius Norm Minimization.*** First, we consider M derived by the MSPAI minimization relative to symmetric matrices C_0 and B_0, and a set of general probing vectors in e. We want to derive a symmetrization of M with a similar sparsity pattern. We start with the trivial symmetrization

$$\bar{M} := M + M^T .$$

We can improve this matrix by returning to the initial minimization problem allowing additional changes on the main diagonal entries. Hence we define

$$\hat{M} := \alpha \left(M + M^T \right) + D = \alpha \bar{M} + D \tag{9}$$

with a scaling factor $\alpha \in \mathbb{R}$ and a diagonal correction $D \in \mathbb{R}^{n\times n}$. Obviously, $\hat{M}$ is symmetric by construction. We determine α and D in two steps. In order to find an optimal value for α, we insert $\alpha\bar{M}$ into the basic problem (3):

$$\min_{\alpha} \left\| \underbrace{\begin{pmatrix} C_0 \\ \rho g^T \end{pmatrix}}_{:=C} \alpha\bar{M} - \underbrace{\begin{pmatrix} B_0 \\ \rho h^T \end{pmatrix}}_{:=B} \right\|_F^2 = \min_{\alpha} \left\|\alpha C\bar{M} - B\right\|_F^2 . \tag{10}$$

For the analytic solution, we consider the inner product (denoted as $\langle .,.\rangle_F$), which for general A and B is defined by the Frobenius norm:

$$\langle A, B\rangle_F = \|AB\|_F^2 = tr\left(A^T B\right). \tag{11}$$

In these minimizations, the trace of the product of two matrices can be evaluated by sparse dot products and only a few possibly dense dot products:

$$tr\,(AB) = \sum_{j=1}^{N} a_j^T b_j \tag{12}$$

with the j-th *row* a_j of A and b_j the j-th *column* of the matrix B.

With formula (11), we can solve (10) for α using standard properties of the inner product. In a following step we can determine the optimal diagonal matrix D by standard Frobenius norm minimization. Note that these computations are fast because of the sparsity of the underlying matrices and the low rank of the possibly dense submatrices g and h. But in general, this symmetrization technique does not necessarily yield a positive definite preconditioner.

2.3.2 ***Symmetrization by Combining two Basic Iteration Steps.*** A second approach for a symmetrization of M considers two basic iterative steps one with preconditioner M, the other with M^T. Here, we consider M as approximation of the inverse of A, so the first method is related to the iteration matrix $I - AM$, the second to $I - AM^T$. The two consecutive steps are described by the iteration matrix

$$\begin{aligned}(I - AM^T)\cdot(I - AM) &= I - AM^T - AM + AM^T AM \\ &= I - A(\bar{M} - M^T AM).\end{aligned}$$

Hence, the resulting symmetric preconditioner is given by $\bar{M} - M^T AM$. To add an additional degree of freedom we consider the damped iteration with preconditioner αM. This leads to

$$\begin{aligned}(I - \alpha AM^T) \cdot (I - \alpha AM) &= I - \alpha AM^T - \alpha AM + \alpha^2 AM^T AM \\ &= I - \alpha A(\bar{M} - \alpha M^T AM)\end{aligned}$$

and the symmetrized preconditioner

$$\hat{M}_\alpha := \bar{M} - \alpha M^T AM. \tag{13}$$

This preconditioner is denser than M, but may lead to a reduction of the error comparable with two steps based on αM. To be sure that the two iteration steps lead to an improved approximate solution we need $\|I - \alpha AM\| < 1$:

THEOREM 2.1 *Let us assume that $\lambda(AM) > 0$ holds for all eigenvalues of AM. Then for*

$$0 \le \alpha < \frac{2}{\lambda_{max}(AM)}$$

we get $\|I - \alpha AM\| < 1$ in the spectral norm. The optimal choice of α that leads to a minimum norm of $I - \alpha AM$ is given by

$$\alpha = \frac{2}{\lambda_{max}(AM) + \lambda_{min}(AM)}$$

with

$$\|I - \alpha AM\| \approx \left| \frac{\lambda_{max}(AM) - \lambda_{min}(AM)}{\lambda_{max}(AM) + \lambda_{min}(AM)} \right| < 1.$$

Remark 1 To derive this optimal α, one needs approximations for the extreme eigenvalues of AM.

This symmetrization with $\bar{M}$ and $\hat{M}_\alpha$ does not include an additional probing condition. Fortunately, we can show, that this symmetrization process preserves the probing property for slightly modified preconditioners:

THEOREM 2.2 *Assume that M is a preconditioner that satisfies the probing condition $e^T AM = e^T$ exactly. For $\tilde{M} := M + M^T - \alpha MAM^T$ with $\alpha < 2$ (e.g. $\alpha = 0$ and $\bar{M}$) the Rayleigh quotient for vector Ae is given by*

$$(e^T A)\tilde{M}(Ae) = (2 - \alpha)(e^T A)A^{-1}(Ae) = (2 - \alpha)(e^T A)M(Ae) \ ,$$

and therefore the range of values of the preconditioned matrix with $\tilde{M}$ is nearly unchanged relative to the probing space.

Proof It holds

$$\begin{aligned}(e^T A)\tilde{M}(Ae) &= (e^T A)(M + M^T - \alpha M A M^T)(Ae) \\ &= e^T Ae + e^T Ae - \alpha e^T Ae = (2-\alpha)e^T Ae \ , \\ (2-\alpha)e^T Ae &= (2-\alpha)(e^T A)A^{-1}(Ae) \ , \\ (2-\alpha)e^T Ae &= (2-\alpha)(e^T AM)Ae \ = \ (2-\alpha)(e^T A)M(Ae) \ .\end{aligned}$$

□

Remark 2 For $\alpha = 1$, $\tilde{M}$ satisfies the probing condition exactly:

$$e^T A\tilde{M} = e^T A(M + M^T - \alpha MAM^T) = e^T + e^T AM^T - \alpha e^T AM^T = e^T .$$

2.3.3 ***The Case of Symmetric Positive Definite Matrices.*** Until now we only derived symmetric preconditioners. But often for spd A we need a spd preconditioner. So now we consider only spd matrices A. If $\bar{M}$ is symmetric indefinite the above methods will not lead to a spd preconditioner. So let us assume that $\bar{M} = M + M^T$ is positive definite. If this is not true we could replace $\bar{M}$ by $\bar{M} + \beta I$ with small β. Note, that for a good approximation M it should hold that $\bar{M}$ is nearly positive definite, and therefore we can hope to find such a small $\beta > 0$.

PROPOSITION 2.3 *Let A and $\bar{M}$ be symmetric positive definite. Then $\hat{M}_\alpha = \bar{M} - \alpha M^T AM$ will also be positive definite as long as $\alpha < \lambda_{min}(\bar{M}, M^T AM)$, the minimum eigenvalue of the generalized positive definite eigenvalue problem $\bar{M} = \lambda M^T AM$.*

Remark 3 Therefore, we have to choose α such that it satisfies the inequalities

$$\alpha \leq \min\left\{\frac{2}{\lambda_{max}(AM) + \lambda_{min}(AM)}, \lambda_{min}(\bar{M}, M^T AM)\right\} =: \alpha_{opt}.$$

We can derive a deeper analysis by considering the preconditioner $\bar{M} - \alpha\bar{M}A\bar{M}/4$ that is the result of applying the above symmetrizing construction on $\bar{M}/2$.

THEOREM 2.4 *Let A and $\bar{M}$ be spd. Then, for $\bar{M} - \alpha\bar{M}A\bar{M}/4$ the optimal α is given by $\alpha = 2/(\lambda_{max}(A\bar{M}/2) + \lambda_{min}(A\bar{M}/2))$. With this choice we get a new improved condition number of the preconditioned system. The condition* *is improved by a factor*

$$\frac{\lambda + 2\mu}{4\lambda} \approx \frac{1}{4}.$$

Proof The minimum eigenvalue of the preconditioned system is given by $\frac{2\lambda\mu}{\lambda+\mu}$ and the maximum eigenvalue by $\frac{\lambda(\lambda+2\mu)}{2(\lambda+\mu)}$ with λ and μ the maximum, resp. minimum eigenvalues of $\bar{M}A/2$. □

Note, that we can also sparsify $\bar{M} - \alpha M^T AM$ carefully in order to avoid a preconditioner that would be too dense. Furthermore, we can sometimes save costs in computing $\hat{M}_\alpha$ or $A\hat{M}_\alpha$. In SPAI for example we have already computed $R = I - AM$ and can use this information, e.g. in the form

$$M + M^T - \alpha M^T AM = M + M^T(I - \alpha AM) = M + M^T(1 - \alpha + \alpha R)\ .$$

In case we want to symmetrize a preconditioner M that is an approximation of A itself based on AM^{-1}, we can apply the same method on M^{-1} and get

$$M^{-1} + M^{-T} - \alpha M^{-T} AM^{-1} \tag{14}$$

as a symmetric approximation for A. When M is the upper or lower triangular part of A – the Gauss-Seidel-preconditioner – this symmetrization approach is closely related to SSOR-preconditioners.

In general, we can apply this symmetrizing method if AM has only positive eigenvalues, and for spd A we can derive a spd preconditioner if $\bar{M}$ is spd.

2.3.4 ***Numerical Examples.*** The effectiveness of these simple symmetrization techniques emerges in the following small examples. For the case of explicit

Table 1. Condition numbers for no preconditioning I, unsymmetrized preconditioner M, $\bar{M}$, $\hat{M}$ and $\hat{M}_\alpha$ employed as explicit approximative preconditioners AM^{-1}.

n	I	M	$\bar{M}$	$\hat{M}$	$\hat{M}_\alpha$
100	12.061	8.288	8.255	8.155	2.604
400	13.849	7.085	7.055	7.017	2.302
1600	14.436	5.759	5.759	5.759	1.984

approximations of A, we choose an $A := LL^T$, where L comes from an IC(0) factorization of the 5-point discretization of the 2D Laplacian, and therefore is of block tridiagonal structure. This example is completely artificial and its only purpose is to demonstrate the result of a symmetrization step. We probe it with $e = (1, \ldots, 1)^T$ and $\rho = 20$ with a tridiagonal prescribed sparsity pattern and obtain an M. This M is then symmetrized both to $\hat{M}$ using the $\alpha\bar{M} + D$ approach (9) and to $\hat{M}_\alpha$ from (13). As shown in table 1 this ansatz yields symmetric preconditioners with nearly unchanged condition numbers which can then be employed in iterative solvers for spd matrices, e.g. the pcg method. Furthermore, in this example $\hat{M}_\alpha$ leads to a condition number improved by nearly a factor 1/4 – as expected. Note, that in the explicit approximation we use M^{-1} in the symmetrization via $\hat{M}_\alpha$ (14). In all examples the simple and cheap symmetrization $(M + M^T)/2$ is sufficient to obtain a symmetric preconditioner of the same quality as the original nonsymmetric M. Hence, the costly computation of an optimal α and D in $\hat{M}$ is often unnecessary. For

Table 2. Condition numbers for no preconditioning I, unsymmetrized preconditioner M, $\bar{M}$, $\hat{M}$ and $\hat{M}_\alpha$ employed as approximative inverse preconditioners AM.

n	I	M	$\bar{M}$	$\hat{M}$	$\hat{M}_\alpha$
100	48.374	8.448	8.459	8.463	2.638
400	178.064	30.706	30.713	30.720	8.194
1600	680.617	117.031	117.035	117.050	29.773

the symmetrization of an approximate inverse preconditioner, we compute M by SPAI applied on the 2D Laplacian with the static pattern of A^2. The condition numbers of the symmetrized versions are shown in table 2. Note, that in this second example, we do not apply probing. We only want to display the symmetrization aspect. Again the cheap symmetrization $\bar{M}$ is sufficient, and $\hat{M}_\alpha$ leads to a reduction of nearly 1/4.

2.4 *Explicit Factorized Approximation and Probing*

The MSPAI probing approach does not only allow one to improve unfactorized methods, but also preconditioners which are computed in a factorized form such as ILU or incomplete Cholesky. Here, we assume an already computed factored approximation $A \approx LU$, e.g. given by ILU or the Gauss-Seidel method. The aim is to improve the factors with respect to the given probing conditions. Thereby, we keep one factor (L or U) fixed, and recompute the other factor. That means, we set in (3) $B_0 = A$, $C_0 = L$ and for the probing constraints $g^T = e^T L$, $h^T = e^T A$. In order to get an upper (respectively lower) triangular factor, we restrict the pattern for M, e.g. to upper triangular $\tilde{U}$. Altogether, we solve

$$\min_{\tilde{U}} \left\| \begin{pmatrix} L \\ \rho e^T L \end{pmatrix} \tilde{U} - \begin{pmatrix} A \\ \rho e^T A \end{pmatrix} \right\|_F^2 = \min_{\tilde{U}} \left\| W(L\tilde{U} - A) \right\|_F^2 . \quad (15)$$

Having computed this improved version $\tilde{U}$ of U, we consider $A \approx L\tilde{U}$ with $\tilde{U}$ fixed. We obtain the ansatz for the improved lower triangular factor $\tilde{L}$ through transposition:

$$\min_{\tilde{L}} \left\| \begin{pmatrix} \tilde{U}^T \\ \rho e^T \tilde{U}^T \end{pmatrix} \tilde{L}^T - \begin{pmatrix} A^T \\ \rho e^T A^T \end{pmatrix} \right\|_F^2 = \min_{\tilde{L}} \left\| W(\tilde{U}^T \tilde{L}^T - A^T) \right\|_F^2 .$$

The probing constraints have to be modified as well to $g^T = e^T \tilde{U}$ and $h^T = e^T A^T$. The result of these probing steps are the improved factorization

$$A \approx L\tilde{U} \ , \text{ and } \ A \approx \tilde{L}\tilde{U}.$$

Note, that the initial factorization $A \approx LU$ can be produced by any preconditioning technique, which yields factorized approximations of A.

As an important special case, we have to deal with the problem that A may not be given explicitly, but only via an approximation $\tilde{A}$. We assume that we can compute the exact values for $e^T A$ and $e^T A^T$. Then we have to modify the minimization to the form

$$\min_{\tilde{U}} \left\| \begin{pmatrix} L \\ \rho e^T L \end{pmatrix} \tilde{U} - \begin{pmatrix} \tilde{A} \\ \rho e^T A \end{pmatrix} \right\|_F^2 , \tag{16}$$

resp.

$$\min_{\tilde{L}} \left\| \begin{pmatrix} \tilde{U}^T \\ \rho e^T \tilde{U}^T \end{pmatrix} \tilde{L}^T - \begin{pmatrix} \tilde{A}^T \\ \rho e^T A^T \end{pmatrix} \right\|_F^2 . \tag{17}$$

2.5 *Approximating a Factorization of A^{-1}*

In contrast to the section above, we start with a given sparse factorized approximation of the inverse $A^{-1} \approx UL$ or $UAL \approx I$. U and L may be the result of some algorithm like AINV or FSPAI. Again, we add the probing conditions and set in formula (3) from above $B = I$, $C = UA$, $g^T = e^T UA$ and $h^T = e^T$. This gives the following MSPAI probing problem:

$$\min_{\tilde{L}} \left\| \begin{pmatrix} UA \\ \rho e^T UA \end{pmatrix} \tilde{L} - \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \right\|_F^2 = \min_{\tilde{L}} \left\| W(UA\tilde{L} - I) \right\|_F^2 . \tag{18}$$

To ensure, that $\tilde{L}$ has lower triangular sparsity pattern, we restrict the pattern to that form. Again, the result is an improved new factor $\tilde{L}$. As in the explicit factorized case before, we can apply the same method once again on the transposed problem, in order to obtain an improved $\tilde{U}$, too.

For unknown A we again have to use an approximation $\tilde{A}$ and arrive at

$$\min_{\tilde{L}} \left\| \begin{pmatrix} U\tilde{A} \\ \rho e^T UA \end{pmatrix} \tilde{L} - \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \right\|_F^2 . \tag{19}$$

2.6 *Symmetrization for Factorized Approximations*

If the given A is symmetric positive definite, we can compute a symmetric factorization based on e.g. incomplete Cholesky or FSPAI, resulting in a triangular matrix L and preconditioned system $A \approx LL^T$ or $L^T AL \approx I$. Then with the methods of the previous two sections we can add probing conditions and replace, e.g. L^T by another factor, e.g. $\tilde{U} =: \tilde{L}^T$ for fixed L . But then we lose symmetry because we have two different factors L and $\tilde{U}$ for the preconditioner $L\tilde{U}$. To regain symmetry we can set

$$L_\alpha := L_\alpha(L, \tilde{L}) := L + \alpha(\tilde{L} - L) \tag{20}$$

as convex combination of both factors, $\alpha \in [0, 1]$. An optimal α can be computed by substituting L_α into the original MSPAI minimization problem

$$\min_\alpha \|W(L_\alpha L_\alpha^T - A)\|_F , \tag{21}$$

resp.

$$\min_\alpha \|W(L_\alpha^T AL_\alpha - I)\|_F \tag{22}$$

in the approximative inverse case. This leads to a polynomial of degree 4 in α of the form

$$\begin{aligned} \|WR + \alpha WH + \alpha^2 WK\|_F^2 = {} & tr(RW^T WR) + 2\alpha tr(HW^T WR) + \\ & + \alpha^2 tr(HW^T WH + 2KW^T WR) + \\ & + 2\alpha^3 tr(KW^T WH) + \alpha^4 tr(KW^T WK) . \end{aligned} \tag{23}$$

For (21) the matrices H, K, and R are given by

$$R := LL^T - A \ , \ \ K := (\tilde{L} - L)(\tilde{L} - L)^T \ , \ \ H := (\tilde{L} - L)L^T + L(\tilde{L} - L)^T ,$$

and for (22) by

$$R := L^T AL - I \ , \ \ K := (\tilde{L}-L)^T A(\tilde{L}-L) \ , \ \ H := (\tilde{L}-L)^T AL + L^T A(\tilde{L}-L) \ .$$

We can compute the minima of these polynomials and choose for α the solution with minimum norm. Therefore we only have to compute the trace of products of sparse matrices. Note, that if in L_α both L and $\tilde{L}$ satisfy the probing condition, then also L_α satisfies the probing condition.

The substitute matrix K contains the difference $\tilde{L}-L$ in second order. This difference is supposed to be quite small by construction. So, we can simplify (23) by dropping the coefficients which contain K. The result is a polynomial in α of second order:

$$\begin{aligned} \|WR + \alpha WH + \alpha^2 WK\|_F^2 \approx tr(RW^T WR) + 2\alpha tr(HW^T WR) + \\ + \alpha^2 tr(HW^T WH). \end{aligned} \tag{24}$$

Equation (24) has one unique minimum which can be computed directly by the derivative with respect to α and evaluation of one trace and one Frobenius norm. Due to the structure of W, the evaluation of the traces is quite cheap. For instance, $tr(HW^T WR)$ can be computed exploiting $W^T W = I + \rho^2 ee^T$ and properties of the trace:

$$tr(HW^T WR) = tr(HR + \rho^2 Hee^T R) = tr(HR) + \rho^2 tr((e^T R)(He)).$$

We compute both summands without evaluating the matrix-matrix products using (12).

Note that it is not advisable to add an additional diagonal correction in L because this would result in the minimization of a function of degree 4 in the diagonal entries $d_1, ..., d_n$. But it is possible to add a diagonal correction by neglecting the probing part and choosing the diagonal correction only with respect to the matrix approximation problem, in order to generate all ones on the main diagonal positions. So after having computed L like above, we can choose a diagonal D by

$$diag(DL^T ALD) = (1, \ldots, 1) \tag{25}$$

and replace L by $L_D := LD$.

For unknown A we again have to replace the weight matrix W and consider the minimization

$$\min_\alpha \left\| \begin{pmatrix} L_\alpha L_\alpha^T - \tilde{A} \\ \rho e^T L_\alpha L_\alpha^T - e^T A \end{pmatrix} \right\|_F^2 \quad \text{or} \quad \min_\alpha \left\| \begin{pmatrix} L_\alpha^T \tilde{A} L_\alpha - I \\ \rho e^T L_\alpha^T A L_\alpha - e^T \end{pmatrix} \right\|_F^2$$

in order to determine the optimal value for α.

So, let us assume, that starting with a factor L we have generated an approximation $\tilde{U}$ by probing. With fixed $\tilde{U}$ we can compute a new factor $\tilde{L}$ by the transposed minimization. Then basically we have the following choices for symmetrizing one or two approximate factors:

- take factors $\tilde{U}$ and $\tilde{U}^T$, e.g. $A \approx \tilde{U}^T\tilde{U}$ or $\tilde{U}A\tilde{U}^T \approx I$.
- take the symmetrization relative to L and $\tilde{U}$, either by exact minimization based on the polynomial of degree 4, denoted by $L_{\alpha,4}(L,\tilde{U}^T)$, or by approximate minimization denoted by $L_{\alpha,2}(L,\tilde{U}^T)$
- use $\tilde{L}$ and $\tilde{L}^T$ as factorization
- use $L_{\alpha,m}(\tilde{L},\tilde{U}^T)$ with exact ($m = 4$) or approximate ($m = 2$) minimization.

2.6.1 ***Numerical Examples.*** The MSPAI symmetrization techniques described in the previous section yield factorized preconditioners, where symmetry is regained. The following examples demonstrate that the symmetrization does not deteriorate the condition number of the system. As an example, we

Table 3. Condition numbers for no preconditioning I, L from IC(0), $\tilde{U}$ by probing L, $\tilde{U}$ employed together with L, for $L_\alpha = L + \alpha(\tilde{U}^T - L)$ with approximated and exact polynomial as explicit factorized preconditioners.

n	I	L	$L,\tilde{U}$	$L_{\alpha,2}(L,\tilde{U}^T)$	$L_{\alpha,4}(L,\tilde{U}^T)$
100	48.374	5.120	3.462	3.177	3.050
400	178.064	16.593	7.650	8.716	7.899
1600	680.617	61.020	41.922	38.475	39.045

take again a 2D Laplacian for different dimensions n. Then, we compute an incomplete Cholesky factor for the explicit case and a static FSPAI with the pattern of A for inverse preconditioning. Then we apply probing and use the different symmetrization approaches in order to have a preconditioner, which we can use for iterative solvers for symmetric problems. For the explicit ap-

Table 4. Condition numbers for no preconditioning I, FSPAI L, probed FSPAI $\tilde{L}$ employed together with L, for $L_\alpha = L + \alpha(\tilde{L} - L)$ as inverse approximative preconditioners.

n	I	L^TAL	$L^TA\tilde{L}$	$L_{\alpha,4}^TAL_{\alpha,4}$
100	48.374	13.827	13.729	13.722
400	178.064	50.223	50.862	50.400
1600	680.617	191.529	194.574	192.433

proximation, we choose $\rho = 50$ and $e = (1, \ldots, 1)^T$ as probing parameters and combine the incomplete Cholesky factor with the one obtained from probing. To do so, we apply convex symmetrization (20) using the exact and the approximative polynomials. Table 3 shows that the condition numbers are preserved throughout symmetrizing. To save costs we should use only one step of probing and possibly one additional step of approximate minimization $L_{\alpha,2}$.

For the inverse case with the FSPAI, we set $\rho = 7$ and the eigenvector which corresponds to the smallest eigenvalue as probing vector. Because even quite rough approximations are sufficient here, the computation of this probing vector is not too costly. The resulting condition numbers are shown in table 4. In other computations not reported, condition numbers remained essentially unchanged when symmetrized versions were used.

2.7 *Application to Schur Complements*

The MSPAI probing approach is especially interesting for preconditioning Schur complements. Therefore, we consider the Frobenius norm minimization method in this case more deeply. Given a matrix

$$H = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

we consider preconditioning the Schur complement $S_D = D - CA^{-1}B$. In a first step, we need approximations of S_D which avoid the explicit computation of this matrix. To this aim we can use different methods, e.g. factorized SPAI or SPAI for approximation A^{-1} by some $\tilde{M}$ and computing the sparse approximation $\tilde{S}_D = D - C\tilde{M}B$, or using SPAI with target matrix for a sparse approximation of $A^{-1}B$ by $\min_M \|AM - B\|_F$ which again leads to a sparse approximation for the Schur complement. Based on $\tilde{S}_D$ we can use the probing approach to define a sparse approximation on $\tilde{S}_D$ or $\tilde{S}_D^{-1}$ which is improved with respect to a collection of probing vectors relative to the exact Schur complement.

A second approach can de derived by observing that the left lower block in the inverse of the given matrix H is the inverse of the Schur complement S_D. It holds

$$H^{-1} = \begin{pmatrix} S_A^{-1} & -A^{-1}BS_D^{-1} \\ -D^{-1}CS_A^{-1} & S_D^{-1} \end{pmatrix} .$$

Therefore, we can modify the general probing approach to

$$\min_{M_B,M_D} \left\| \begin{pmatrix} A & B \\ C & D \\ 0 & \rho e^T S_D \end{pmatrix} \cdot \begin{pmatrix} M_B \\ M_D \end{pmatrix} - \begin{pmatrix} 0 \\ I \\ \rho e^T \end{pmatrix} \right\|_F^2 . \tag{26}$$

Then the computed M_D gives an approximation to S_D^{-1}, because the last columns of H^{-1} are approximated by M_B and M_D.

We can formulate another method for computing M_D based on the weight matrix W. By using the equation

$$(\,\rho u^T \quad \rho e^T\,) \cdot \begin{pmatrix} A & B \\ C & D \end{pmatrix} \cdot \begin{pmatrix} -A^{-1}BS_D^{-1} \\ S_D^{-1} \end{pmatrix} = -\rho e^T CA^{-1}BS_D^{-1} + \rho e^T DS_D^{-1} = \rho e^T ,$$

we arrive at the probing minimization

$$\min_{M_B,M_D} \left\| \begin{pmatrix} I & \\ \rho u^T & \rho e^T \end{pmatrix} \cdot \left[\begin{pmatrix} A & B \\ C & D \end{pmatrix} \cdot \begin{pmatrix} M_B \\ M_D \end{pmatrix} - \begin{pmatrix} 0 \\ I \end{pmatrix} \right] \right\|_F^2 , \tag{27}$$

again with M_D as approximate inverse for the Schur complement. Note, that for $u^T = -e^T CA^{-1}$ (26) and (27) are identical. Hence, problem (27) is more general, but in the following we will only consider (26).

2.8 *Choice of the Probing Vectors*

The choice of meaningful probing vectors is essential. This question is closely related to the origin of the given problem and further a priori knowledge may be very helpful. Possible choices considered in this paper are:

- $kp = 0$: For given k we define

  $$e_m(j) = 1 \text{ for } j = m, k+m, 2k+m, ..., \text{ and } m = 1, ..., k.$$

  Then, we normalize the vectors e_m to be of length 1. For $k = 1$ this leads to the probing vector $e = (1, 1, ..., 1)^T/\sqrt{n}$, and for $k = 2$ to $e = (e_1, e_2)/\sqrt{n/2}$ with $e_1 = (1, 0, 1, 0, 1, 0, ...)^T$ and $e_2 = (0, 1, 0, 1, 0, 1, ...)^T$. This choice is motivated by PDE examples and MILU, and by the usual probing vector approach.
- $kp = 1$: k vectors from a set of orthogonal basis vectors, e.g.

  $$\sqrt{\frac{2}{n+1}} \left(\sin\left(\frac{\pi j m}{(n+1)} \right) \right)_{j=1,...,n} \quad \text{for } m = 1, ..., k. \tag{28}$$

This is motivated by the close relation between the Sine Transform and many examples from PDE or image restoration. Similarly, for 2D problems we can define the Kronecker product of these 1D vectors.

- $kp = 2$: computing k eigenvector approximations relative to the largest and/or smallest eigenvalues (or singular vectors). This is some kind of black box approach when there is no a priori knowledge at hand. In this case, we have additional costs for computing eigenvector approximations. But usually very rough and cheap approximations are sufficient. In the following we choose eigenvectors to the smallest eigenvalues only.

The weight ρ used in the probing Frobenius norm minimization is usually chosen $\rho > 1$. In cases where it is well known that the standard probing approach works well, large values for ρ lead to good preconditioners. So the choice of ρ indicates whether we consider the given problem as a regularized Least Squares problem related to given probing vectors (large ρ) or whether the minimization is used for a slight modification of a given preconditioner (ρ close to 1).

Sometimes it is impossible to satisfy the probing condition sufficiently. For the unfactorized or factorized approximate inverse approach, the probing vector $e^T = (1, 1, ..., 1)^T$ leads to a sparse vector $g^T = e^T A$, e.g. for the discretization of the Laplace operator or other elliptic PDE problems. Therefore, for sparse pattern of M, the vector $g^T M$ will be also sparse and cannot be a good approximation to the given dense vector e. In such cases the above approach is only efficient for approximating A itself. For A^{-1} one has to choose ρ carefully. Otherwise a slight improvement in the probing condition by choosing a much larger ρ will spoil the matrix approximation and result in a bad preconditioner.

3 Numerical Examples for MSPAI Probing

Now, we want to demonstrate our methods in several applications. All the following numerical examples were computed in MATLAB. If iteration counts are given, we used the MATLAB pcg with zero starting vector, random right-hand sides and a relative residual reduction of 10^{-6} as stopping criterion.

3.1 *MSPAI Probing for Domain Decomposition Methods*

Here, we consider the 5-point discretization of the 2D elliptic problem $u_{xx} + \epsilon u_{yy}$ on a rectangular grid; usually we consider the isotropic problem with $\epsilon = 1$. We partition the matrix such that it has the "dissection" form

Table 5. Condition numbers for domain decomposition Laplace with explicit approximate probing for $k = 3$ and $kp = 0$.

m	$dim(A)$	$dim(S)$	$cond(SM^{-1})$	$cond(SM^{-1}_{\rho=0})$	ρ	$cond(SM^{-1}_{\rho})$
5	2916	216	83.99	18.2	25	6.34
6	4225	325	118.6	25.7	25	8.83
7	5776	456	159.6	34.6	30	11.4
8	7569	609	206.9	44.8	30	15.8
9	9604	784	260.5	56.4	30	19.3
10	11881	981	320.4	69.4	30	25.4

$$\begin{pmatrix} A_1 & & & & F_1 \\ & A_2 & & & F_2 \\ & & \ddots & & \vdots \\ & & & A_m & F_m \\ G_1 & G_2 & \cdots & G_m & A_{m+1} \end{pmatrix}$$

e.g. by a domain decomposition method with m domains. To reduce the linear system in A to the smaller problems A_1, ... A_m, we need the Schur complement

$$S = A_{m+1} - G_1 A_1^{-1} F_1 - ... - F_m A_m^{-1} G_m \ .$$

Here, S will in general be a dense matrix. To avoid the explicit computation of S we seek sparse approximations $\tilde{S}$. In a first step we can determine $\tilde{A}_{i,inv}$ approximations for A_i^{-1}, e.g. by SPAI, and then compute $\tilde{S} = A_{m+1} - F_1 A_{1,inv} G_1 - ... - F_m A_{m,inv} G_m$. Now we try to modify this approximation with respect to some probing vectors in order to improve the condition of $\tilde{S}^{-1} \cdot S$. First we use the explicit approximation from section 2.2.

In tables 5 and 6 we compare the resulting explicit preconditioners for different choices of ρ and the probing vectors. Again, we denote with $kp = 0, 1, 2$ the method of probing vector as stated in section 2.8. In a first step we approximate the matrices A_i^{-1} by sparse approximate inverses M_i with the pattern of A_i. Then, we probe the resulting $\tilde{S}$ keeping the sparsity pattern unchanged which leads to a tridiagonal pattern in the preconditioner. In a second group of examples we allow more entries in M_i and $\tilde{S}$, which leads to a pentadiagonal pattern. In table 7 we compare different iteration numbers for pcg with symmetrized preconditioner $M + M^T$. All tables 5–7 show that the prconditioner is improved by probing for a wide range of choices for probing vectors and ρ. For these examples the best results were achieved for $kp = 0$, $k = 3$, and $\rho \approx 30$. Unfortunately, for the probing with approximate inverse (table 8) the probing vectors transform into a nearly sparse $e^T S$. Hence, also for large ρ the difference $e^T(M - S)$ cannot be reduced significantly; furthermore, for

Table 6. Condition numbers for domain decomposition Laplace with explicit approximate probing, for $n = 10$, $m = 8$, different anisotropy, and different sparsity pattern.

sparsity	kp	k	ρ	ϵ	$cond(SM_\rho^{-1})$
tri	1	3	30	1	15.14
tri	2	3	30	1	16.21
tri	0	3	30	1	15.75
tri	0	1	30	1	15.79
tri	0	2	30	1	16.68
tri	0	4	30	1	22.24
tri	0	3	100	1	23.70
tri	0	3	30	0.1	23.60
penta	0	3	25	1	14.08
penta	0	3	30	1	14.80
penta	0	5	30	1	14.00

Table 7. Iteration count for domain decomposition Laplace ($\epsilon = 1$) with explicit approximate probing for $kp = 0$, $k = 3$, $\rho = 0$ or $\rho = 30$.

m	2	3	4	5	6	7	8	9	10	11
#it, $\rho = 0$	19	32	39	44	49	56	62	68	74	81
#it, $\rho = 30$	7	10	12	13	13	15	17	19	22	24

large ρ the Frobenius norm of the matrix approximation $SM - I$ will get large, and for large ρ the preconditioner gets worse. Nevertheless, we can observe a slight improvement of the condition number also for approximate inverse preconditioner by choosing k, kp, and especially ρ very carefully. The next three

Table 8. Condition numbers for domain decomposition Laplace with approximate inverse probing, three probing vectors $kp = 0$, minimization relative to the weighted Frobenius norm.

m	$cond(S)$	$cond(SM_{\rho=0})$	ρ	$cond(SM_\rho)$
5	83.99	32.90	200	27.07
6	118.6	46.47	200	38.26
7	159.6	62.53	200	51.48
8	206.9	81.04	200	66.76
9	260.5	102.0	250	84.03
10	320.4	125.5	250	103.4

tables 9, 10, and 11 display the same behaviour for the explicit factorized approximations and different symmetrizations. This shows that e.g. the probing vectors to $kp = 1$ and $kp = 2$ are not so efficient for this problem. Nevertheless, probing and MSPAI symmetrization leads to improved condition numbers and faster convergence also in the factorized form.

Table 9. Condition numbers for domain decomposition Laplace with explicit approximate factorized probing,one probing vector $kp = 0$ and different symmetrizations.

m	S	M_{ILU}	ρ	$L, \tilde{U}$	$\tilde{U}^T, \tilde{U}$	$\tilde{L}, \tilde{U}$	$\tilde{L}, \tilde{L}^T$	$L_{\alpha,4}(\tilde{L}, \tilde{U}^T)$
5	83.99	18.2	22	7.47	5.74	5.95	6.30	5.97
6	118.6	25.7	28	9.84	8.00	8.13	8.39	8.15
7	159.6	34.6	32	13.5	10.5	10.6	10.9	10.7
8	206.9	44.8	36	17.8	13.4	13.6	13.9	13.6
9	260.5	56.4	42	20.5	16.9	17.1	17.3	17.1
10	320.4	69.4	46	25.8	20.7	20.8	21.0	20.8

Table 10. Condition numbers for domain decomposition Laplace with approximate factorized probing for $m = 8$, for different choices.

kp	k	ρ	$L, \tilde{U}$	$\tilde{U}^T, \tilde{U}$	$L_{\alpha,4}(L, \tilde{U}^T)$	$\tilde{L}, \tilde{U}$	$\tilde{L}, \tilde{L}^T$	$L_{\alpha,4}(\tilde{L}, \tilde{U}^T)$
0	1	20	29.6	22.2	15.0	21.8	21.4	21.8
0	1	30	21.5	14.9	13.7	15.2	15.5	15.2
0	1	40	15.8	13.6	17.4	13.8	14.0	13.8
0	1	50	13.3	14.5	29.8	14.9	15.5	14.9
0	1	60	13.4	17.7	43.3	17.5	19.2	17.1
0	1	70	13.7	25.7	53.7	23.9	27.6	22.0
0	2	38	16.8	13.5	16.0	13.7	14.1	13.9
0	3	80	32.2	25.2	23.5	22.3	20.0	16.2
1	3	20	20.3	19.5	36.1	17.6	16.9	17.6
1	3	40	14.7	44.4	52.0	25.2	18.1	25.1
2	3	20	17.6	24.3	63.8	20.5	18.1	20.1
2	1	20	28.3	36.6	67.7	32.3	29.0	32.1

Table 11. Condition numbers for domain decomposition Laplace with explicit approximate factorized probing with optimal symmetrization.

m	2	3	4	5	6	7	8	9	10
ρ	5	9	12	15	18	21	23	26	29
$cond$	1.69	2.36	3.71	5.48	7.66	10.3	13.3	16.7	20.5

As a last example we consider the approximation of the Schur complement described by (26) in section 2.7. Following table 12 the condition number is strongly deteriorated in the case $\rho = 0$, when we do not include probing. Only the choice $kp = 0$ and large $\rho \approx 100$ leads to a reduction of the condition number. Hence, this approach is only applicable when combined with probing.

Table 12. Condition numbers ($cond(S_D M_D)$) for Schur complement preconditioning with probing vectors based on (26) from section 2.7, $cond(S_D) = 12.67$.

ρ	0	1	10	20	50	100	200
$kp = 0,\ k = 2$	376.04	364.51	131.61	64.32	20.87	10.43	28.64
$kp = 2,\ k = 3$	376.04	359.10	173.54	82.37	24.93	17.42	28.99

3.2 *MSPAI Probing for Stokes Problems*

We consider the four Stokes examples from IFISS [18] by Silvester, Elman and Ramage [11]. The stabilized matrices are of the form

$$\begin{pmatrix} Ast & Bst \\ Bst^T & -\beta C \end{pmatrix}$$

with Schur complement $S_s := -\beta C - Bst \cdot Ast^{-1} Bst^T$; we also consider the unstabilized problems

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}$$

with Schur complement $S_u = -B \cdot A^{-1} B^T = -B \cdot (A \backslash B^T)$. In a first step we again approximate A^{-1} by a sparse matrix with the same pattern as A; then by MSPAI probing with this pattern we get the preconditioner for the Schur complement. In the unfactorized case we consider the trivial symmetrization via $\bar{M}$. For factored preconditioners we apply also the symmetrization $L_{\alpha,4}$, possibly with an additional diagonal scaling D to obtain diagonal elements equal to 1 in the preconditioned system (25).

- Example 1: Channel domain with natural boundary on a 16×16 grid, Q1-P0, stabilization parameter $\beta = 1/4$, and uniform pattern. The condition number of S_s is 12.67.
- Example 2: Flow over backward facing step with natural outflow boundary, Q1-P0, $\beta = 1/4$, $cond(S_s) = 78.13$.
- Example 3: Lid driven cavity, regularized on stretched 16×16 grid, Q1-P0, $\beta = 1/4$, exponential streamlines with singular S, but essential condition number $\lambda_{max}(S_s)/\lambda_2(S_s) = 129.6$.
- Example 4: Colliding flow on uniform 16×16 grid, Q1-P0, $\beta = 1/4$, uniform streamlines, with singular S, but essential condition number $\lambda_{max}(S_s)/\lambda_2(S_s) = 6.92$.

For the stabilized and unstabilized case we display the iteration count for pcg with factorized and unfactorized preconditioner and simple symmetrizations in tables 13 resp. 14. Obviously, the MSPAI probing with different probing

Table 13. Iteration count for unstabilized Stokes examples, unfactorized (with $kp = 0$, $k = 1$, $\rho = 5$) and factorized (with $kp = 1$, $k = 2$, $\rho = 3$). L_D denotes the preconditioner L_α diagonally transformed as described in (25).

	unfactorized			factorized			
Problem	1	2	3	1	2	3	symmetrization
unprec	39	65	78	39	65	78	
explicit $\rho = 0$	20	34	26	20	34	26	
explicit $\rho = 5$	12	17	19				$\rho = 3$
				18	28	26	$\tilde{L}, \tilde{L}^T$
				18	17	26	$L_\alpha(L, \tilde{L}^T)$
				16	24	15	L_D
inverse $\rho = 0$	25	43	33	28	39	36	
inverse $\rho = 5$	15	24	25				$\rho = 3$
				20	25	31	$\tilde{L}, \tilde{L}^T$
				17	28	17	$L_\alpha(L, \tilde{L}^T)$
				16	27	16	L_D

Table 14. Iteration count for stabilized Stokes examples, unfactorized (with $kp = 1$, $k = 3$, $\rho = 3$) and factorized (with $kp = 1$, $k = 3$, $\rho = 3$). Problem 4 with $\rho = 1.5$) in the unfactorized case.

	unfactorized				factorized				
Problem	1	2	3	4	1	2	3	4	symmetrization
unprec	24	33	74	23	24	33	74	23	
explicit $\rho = 0$	23	34	20	19	23	34	20	19	
explicit ρ	16	22	16	17					
					18	24	19	18	$\tilde{L}, \tilde{L}^T$
					18	24	19	18	$L_\alpha(L, \tilde{L}^T)$
					16	22	19	18	L_D
inverse $\rho = 0$	18	24	17	16	20	27	23	19	
inverse ρ	15	21	21	15					
					18	23	18	15	$\tilde{L}, \tilde{L}^T$
					16	22	19	16	$L_\alpha(L, \tilde{L}^T)$
					16	22	18	16	L_D

vectors and appropriate ρ always gives better results. Following [11] for the above examples one can choose a diagonal preconditioner Q that is given by the underlying Finite Element method. In nearly all examples presented here this preconditioner is only a multiple of the identity matrix and therefore does not lead to a comparable improvement of the iteration count.

3.3 *MSPAI Probing for Dense Matrices*

In many applications we have to deal with dense or nearly dense matrices A. To apply a preconditioner it is helpful to derive a sparse approximation $\tilde{A}$ of A. In a first step we can sparsify the dense matrix by deleting all entries outside a allowed pattern or with small entries. This gives a first approximation $\tilde{A}$. Here, we consider two examples. In a first setting we choose a discretization of the 2D Laplacian with a quite thick bandwidth that should be approximated by a sparser matrix A_p such that $A_p^{-1}A$ has bounded condition. In figure 1 we display the given thick pattern and the sparse pattern that should be used for the approximation in $\tilde{A}$ and A_p. Again, we compute A_p by explicit probing on $\tilde{A}$ and A. In table 15 we display the resulting condition numbers. For large ρ we see that the approximation based on probing is much better than the matrix $\tilde{A}$ that is obtained by reducing A to the allowed pattern by simply deleting nonzero entries.

Figure 1. Sparsity pattern of original matrix A (left) and sparse approximation A_p (right).

Table 15. Condition numbers for sparse 2D Laplacian approximations AA_p^{-1} for different ρ, $kp = 0$, $k = 1$.

n	A	$\tilde{A}$, $\rho = 0$	10	50	100	500	1000
100	127.95	799.85	3.15	2.86	2.88	2.90	2.90
225	286.45	372.68	68.40	4.25	3.59	3.50	3.50
400	506.06	1204.35	596.67	41.06	4.72	4.17	4.16
625	786.57	6962.76	20016.42	53.35	9.06	4.84	4.81
900	1127.94	3405.30	4251.85	60.03	14.66	5.54	5.47

In a second example we consider a dense Toeplitz matrix with first row given by $a(1,1) = \pi/2$, $a(1,2j) = 2/(\pi(2j-1)^2)$, $j = 1, 2, ...$ This matrix is related to the generating function $f(x) = |x - \pi|$, $x \in [0, 2\pi]$ (see [21]). First we replace A by a tridiagonal matrix $\tilde{A}$ by deleting all entries outside the bandwidth. In a second step by explicit probing we compute the improved tridiagonal approximation A_p. For $n = 1000$ the condition number of A is $1.36 \cdot 10^3$, and the preconditioned system $\tilde{A}^{-1}A$ has condition 150.9. As probing vector we additionally allow the vector $e_\pm := (1, -1, 1, -1, ...)$. Table 16 shows that probing with $e_\pm$ and $kp = 2$ leads to a significantly improved condition number. The choices $kp = 1$ and $kp = 0, k = 1$ fail, while $kp = 0, k = 2$ again gives a better preconditioner. This is caused by the fact that $e_\pm$ is contained in the probing subspace related to $kp = 0, k = 2$. Note, that this example is dense, not related to a PDE problem, and allows a new probing vector.

Table 16. Condition numbers for tridiagonal approximations of the dense Toeplitz matrix to generating function $f(x) = |x - \pi|$ for $\rho = 1000$ and different probing vectors.

$e_\pm$	$kp = 2$: $k = 2$	$k = 1$	$kp = 0$: $k = 2$	$k = 1$	$kp = 1$: $k = 2$	$k = 1$
22.9	18.2	12.7	22.0	113.8	119.2	114.6

Figure 2. Resulting condition numbers for $\rho \in [0, 100]$ with symmetrizations $L_{\alpha,4}$ (solid dotted) and $L_{\alpha,2}$ (dash-dot) compared to modified incomplete Cholesky (solid) and incomplete Cholesky (dashed) preconditioner.

3.4 *Comparison of Probing, ILU, and MILU with MSPAI Probing*

In a first example we compare the direct factorized probing approach with the well-known modified ILU (MILU) resp. modified incomplete Cholesky (MIC) preconditioners. We will show that in cases where MILU is well behaved the more generel MSPAI approach leads to a similar improvement of the condition number. In a second part we compare the classical probing with MSPAI probing for the domain decomposition example from the previous section. Starting point of the first example is a 2D Laplacian A with $n = 225$ and a random right-hand side b. The condition number of A is 103.1 and for the solution of the corresponding system, we use a preconditioned conjugate gradient method (pcg). At first, we compute an incomplete Cholesky (IC(0)) preconditioner L with the lower triangular sparsity pattern of A. This reduces the condition number to $cond(L^{-1}AL^{-T}) = 9.961$. The solution to a relative residual of TOL= 10^{-6} takes 16 iterations (started with a initial vector of all zeros). Considering the modified incomplete Cholesky precon-

Table 17. Iteration count for 2D Laplacian with explicit factorized and symmetrized probing with $kp = 0$, $k = 1$, and different ρ.

ρ	0	20	40	60	80	100
$L_{\alpha,4}$	17	13	12	12	12	12
$L_{\alpha,2}$	17	13	13	12	12	12

Table 18. Iteration count for 2D Laplacian with explicit factorized and symmetrized probing with $kp = 0$, $k = 2$, and different ρ.

ρ	0	20	40	60	80	100
$L_{\alpha,4}$	17	14	13	13	12	12
$L_{\alpha,2}$	17	14	13	13	13	13

ditioner L_M (MIC(0)) which preserves the row sums of A, leads to a condition number $cond(L_M^{-1}AL_M^{-T}) = 4.463$ and 11 iterations until convergence.

Table 19. Iteration count for Laplace with explicit factorized and symmetrized probing using one sine basis vector from (28) ($kp = 1$, $k = 1$), and different ρ.

ρ	0	20	40	60	80	100
$L_{\alpha,4}$	17	14	13	13	14	15
$L_{\alpha,2}$	17	14	13	13	13	13

Table 20. Iteration count for Laplace with explicit factorized and symmetrized probing with $kp = 2$, $k = 1$, and different ρ.

ρ	0	20	40	60	80	100
$L_{\alpha,4}$	17	14	13	14	17	18
$L_{\alpha,2}$	17	14	13	13	14	14

In order to demonstrate the effect of our probing approach, we apply the direct factorized probing ansatz (15) to the incomplete Cholesky L for the normalized probing vector $e = \frac{1}{n}(1, \ldots, 1)^T$ and $\rho \in [0, 100]$. The result $\tilde{U}$ is then symmetrized to L_α using both (23) and (24). The former solves the resulting polynomial exactly, the latter yields an approximation to the optimal symmetrization parameter α. Figure 2 shows the resulting condition numbers $cond(L_\alpha^{-1} A L_\alpha^{-T})$. For increasing ρ the condition number tends to the condition number of the MIC, which meets our expectations as the error of the probing condition $e^T(L_\alpha L_\alpha^T - A)$ decreases. As a consequence, the iteration numbers also decrease as shown in tables 17–20. These examples also display, that the approximative symmetrization approach leads to reasonable values of α.

Albeit the iteration number is improved only slightly, one advantage over MIC is the inherent parallelism of the underlying Frobenius norm minimization which is inherited from SPAI. Furthermore, MIC is restricted to a single vector $(1, \ldots, 1)^T$, whereas we can probe with an arbitrary number of arbitrary probing constraints, see section 2.8.

Note, that for the Laplacian the probing approach for deriving an approximate inverse preconditioner cannot be very successful. This is caused by the fact that probing vectors like $e = (1, 1, ..., 1)^T$ will lead to a sparse vector $e^T A$. Hence, we try to approximate a dense vector e^T by a necessarily sparse vector $e^T AM$, which is impossible. Nevertheless, for small ρ a special choice of probing vectors can improve the condition number of the preconditioned system in comparison with standard Frobenius norm approximation with $\rho = 0$. We set $k = 1$ and use a rough approximation to the eigenvector to the smallest eigenvalue as probing vector which can be computed quite fast. Furthermore, we use the symmetrization $\hat{M}_\alpha$. The resulting condition numbers are shown in table 21. For very carefully chosen ρ we can achieve an improved preconditioner also in this case. Here, theorem 2.2 may give an explanation for the improved behaviour of this symmetrization. In the last example we compare

Table 21. Iteration count for 2D Laplacian with approximate inverse probing with $kp = 2$, $k = 1$, symmetrization $\hat{M}_\alpha$, and different ρ.

n	100			225			400			625			900		
ρ	0	9	12	0	18	22	0	32	36	0	48	52	0	52	56
#it	14	10	23	20	13	22	26	16	36	32	19	42	37	22	23

the classical interface probing approach based on three vectors with the explicit MSPAI probing to the same subspace $kp = 0$, $k = 3$ for the domain decomposition matrix with $m = 8$. It turns out that the new MSPAI probing gives much better condition numbers than the old approach (see table 22). We also would like to emphasize, that classic probing corresponds to the choice of three probing vectors ($k = 3$) whereas our new probing method yields much better results with only one probing vector ($k = 1$). For small m (number of subdomains) both preconditioners lead to similar results. But for large m MSPAI probing is significantly superior.

Table 22. Condition numbers for domain decomposition Laplace with preconditioned Schur complement S of size 609. The case $m = 8$, $k = 1$, $cond(S) = 206.89$ compared with classic tridiagonal $kp = 0$-style probing M_p (3 probing vectors) with $cond(M_p^{-1}S) = 151.26$.

$kp \mid \rho$	0	5	10	20	50	100
0	44.82	40.45	32.47	21.15	14.56	23.54
1	44.82	39.79	33.40	28.01	36.04	40.48
2	44.82	38.95	33.21	27.88	28.68	22.98

4 Conclusions

We have shown that the new MSPAI probing preconditioners often lead to faster convergence compared with algorithms like SPAI or classical probing. In many cases the choice of ρ or the set of probing vectors is not very crucial. Advantages of this approach are the versatility and the inherent parallelism. So for explicit probing one could start with a Gauss-Seidel approximation and improve the factors by probing. All these computations are easy to parallelize compared with MIC or MILU.

Unfortunately, it may happen that the probing condition cannot be satisfied approximately. So for approximate inverses with $e = (1, 1, ..., 1)^T$ and 1D Laplacian the probing condition is $(1, 0, ..., 0, 1)^T \cdot M = e^T AM = e^T$ with sparse $e^T A$ of small norm while e is dense with large norm. In such cases a large ρ could only lead to slightly improved probing condition but strongly deteriorated norm approximation; this spoils the preconditioner and gives bad condition numbers. Hence, the explicit probing is usually easier to set up. In the factorized form it is only possible to improve one factor with respect to the probing subspace. It is possible to obtain the second factor by a further probing step, and so on. So we could generate a sequence of factors that satisfy the probing condition. Unfortunately, again the Frobenius norm matrix approximation would be deteriorated by this procedure. Hence, one should use only one or two probing steps for improving or symmetrization of the factor L and U once. So, the explicit unfactorized probing seems to be the most stable form. Nevertheless, also the approximate inverse probing and the factorized probing are useful in view of better parallelism or easier inversion of the preconditioner. But then one has to choose ρ and the probing subspace more carefully.

An important application of MSPAI probing considered in this paper is the approximation of matrices that are known only implicitly or (nearly) dense, like the Schur complement. In the future it might be interesting to consider MSPAI probing also for regularization problems, e.g. in image restoration, or smoothing in Multigrid. Furthermore, the probing approach could be used in updating preconditioners after some minor changes, e.g. in the Newton method or in eigenvalue computations.

5 Acknowledgements

The first author is grateful to Peter Jimack for contributing a lot of suggestions and motivation during a sabbatical in Leeds.

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