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## A Comparison of Some Preconditioning Techniques for General Sparse Matrices

Michele Benzi<sup>2</sup> Miroslav Tůma<sup>3</sup>

Technical report No-Party and No-

### Abstract

We consider the solution of general sparse systems of linear equations  $Ax = b$  by means of the preconditioned conjugate gradient method (PCGNR) applied to the normal equations  $A^+Ax = A^-b$ . It is known that approaches based on the normal equations can be quite effective for solving problems which are unsymmetric and strongly indefinite. Also the PCGNR method is an attractive technique for solving large sparse linear least squares problems.

We obtain robust algebraic preconditioners for the normal equations by means of incomplete orthogonalization schemes applied to A- We focus on schemes based on the GramSchmidt process combined with various sparsitypreserving and stabilization strategies: in methods based on a present new methods based on an inperfection that in the inverse of the Unolesky factor of  $A^*A$  directly. The results of numerical experiments are discussed.

### Keywords

Sparse systems of linear equations sparse matrices normal equations preconditioned conjugate gradient contra problems problems problems problems problems and the problems problems problems of approximate inverse preconditioning-

<sup>-</sup>AMS subject classifications. Obtub, Obt IU, Obt 29, Obt 39, Obt 90  $^\circ$ 

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#### $\mathbf 1$ Introduction

In this paper we consider the solution of systems of linear equations

$$
(1.1)\t\t\t Ax = b
$$

where  $A$  is a general sparse matrix  $\mathcal{A}$  is a simplicity of the rectangular-simplicity of the simplicity of assume that the full column rank-that the full column rank-that is not supported in solving that the solving t - in the least squares sense- An important technique for solving problem - is the preconditioned conjugate gradient method applied to the normal equations

$$
(1.2)\t\t\t A^T A x = A^T b
$$

hereafter referred to as  $P(\alpha)$  as  $P(\alpha)$ algebra have been skeptical about the normal equations due to the fact that the spectral condition number of  $A^+A$  is the square of that of the original matrix  $A.$  Also, explicitly computing  $A<sup>T</sup>A$  usually entails loss of sparsity and may lead to a severe loss of information (due to cancellation).

In recent times however several authors have demonstrated that the precondi tioned conjugate gradient method applied to - can be an eective way of solving  $p$  is a good problem in the problem is available-to-distribution is available-to-distribution is a good problem in the set of  $p$ possible to construct a preconditioner for  $A<sup>T</sup>A$  directly from the original matrix A.  $\mathbf{A}$  -coefficient matrix of matrix  $\min$  multiplications, there is no need to form the product  $A^\tau A$  explicitly. Numerical experiments have pointed to the fact that PCGNR often exhibits a remarkable degree of robustness making it a viable alternative to nonsymmetric iterative solvers directly applied to problem (rir), we particularly the mannoon shown that approaches based on the case the normal equations can be quite effective for solving problems which are strongly index sees - Furthermore see - Furthermore for the PCGNR method is an attractive technique for the PCGNR method solving large linear least sparse linear large large linear large large large large large large large large la

We are interested in the construction and testing of robust algebraic preconditioners for the normal equations- Several authors have studied approaches based on the following observation: if  $A = QR$  is the QR factorization of A, with R upper triangular with positive diagonal entries and  $Q$  orthogonal, the Cholesky factorization of  $A^\ast A$  is given by  $A^*A = R^*R$ , and  $R^*A^*A R^* = I$ . This suggests that a sparse approximation to R can be used to precondition the CGNR iteration- A sparse approximation to R may be obtained by explicit formation of  $B = A<sup>T</sup>A$  followed by an incomplete Cholesky factorization of B - As already mentioned however there exist more robust procedures which approximates at minimate in the ethnologic map. The contraction of the complete  $\mathcal{L}_\mathcal{A}$ on incomplete orthogonalizations obtained by means of Givens rotations whereas in  $\lceil 10 \rceil$  the preconditioner is constructed using a Gram-Schmidt process; both authors use drop tolerances to preserve sparsity-

In this contribution we restrict ourselves to methods based on the (incomplete) GramSchmidt process- We experiment with dierent sparsitypreserving and safe guarding strategies- in addition, we introduce new methods which approximate the strategies of the control of inverse matrix  $R^{-\tau}$  directly. Such incomplete inverse factorization techniques allow the

construction of sparse approximate inverses for  $A<sup>T</sup>A$  and are potentially advantageous on parallel architectures because they avoid the need for highly sequential back and forward solves in contrast with standard incomplete factorization preconditioners  Ch- see also -

An issue of paramount importance in incomplete factorization methods is the exis*tence* of the incomplete factorization itself. It is well known that if  $A^{\dagger}A$  is an H-matrix, then the incomplete Cholesky factorization of  $A<sup>T</sup>A$  based on a prescribed sparsity pattern always produces a nonsingular preconditioner in exact arithmetic- On the other hand a breakdown could take place during an incomplete QR factorization of A even if  $A^*A$  is an H-matrix (see  $\lvert \circ \rvert$ , where examples are given for an incomplete QR decomposition based on Givens rotations- In practice however incomplete orthogonal factorizations based on drop tolerances tend to be very stable and this is what makes them attractive- In our implementations we included safeguarding mechanisms in tended to prevent breakdown of the incomplete factorizations- Our codes always run to completion and produce a nonsingular approximation to R (or  $R^{-1}$ ).

Concerning sparsitypreserving strategies we tried a combination of drop toler ances and respectively. Computed they computed quantities whose mangitude falls below as  $\mathbf{r}$ preset positive drop tolerance is usually an effective way to preserve sparsity in the approximation to the triangular factor  $R$ , but there are some problems for which it is impossible to have both a sparse incomplete factor and rapid convergence of the . For such stringent problems it management problems it many minimum is the such that minimum contracts the minimum  $\mathcal{M}$  and  $\mathcal{M}$  requires information about the nonzeronly requires information about the nonzeronly requires in structure of A and is carried out before any oating point computation- After the column reordering to an incomplete orthogonal decomplete orthogonal decomplete orthogonal decomposition tion based on a drop to the drop to performed the performance problem with the strategy of the strategy of the is the fact that the rate of convergence of PCGNR could be adversely affected by the recrease is the modern computer of the risk of the matrix  $\alpha$  is the matrix problem. originates from the numerical solution of an elliptic PDE and the preconditioner is based on an incomplete factorization with the sparsity pattern of  $A^*A$ . In this case, reordering the unknowns i-e- the grid points according to the minimum degree algo rithm can lead to a severe deterioration of the convergence rate as compared with the original natural ordering see - However it appears from the experiments in that this deterioration is much less serious if the incomplete factorization is obtained with a drop tolerance- in our experience, with an analyzame degree does cause the use  $\sim$ convergence of PCGNR to somewhat slow down in many cases but it is useful in or der to obtained the more sparse precise more required that per iteration- per iteration-This remark applies to the preconditioners based on approximating  $R$  as well as to the preconditioners based on approximating  $R^{-1}$ .

The rest of this paper is organized as follows: in Sections 2 and 3 we describe the incomplete orthogonal and inverse orthogonal factorization schemes (respectively). and in Section 4 we present the results of numerical experiments on a variety of sparse matrix problems problems the relative extends of the various problems of the various preconditions of the various tioners- The results are compared with those obtained with a simple preconditioning technique based on the incomplete Cholesky factorization of ATA- Finally we draw some conclusions in Section 5.

### $\overline{2}$  Incomplete Orthogonal Factorization Precondi tioners

In this section we consider the problem of computing a sparse approximation to R the upper triangular factor in the QR decomposition of  $A$  (we assume that  $R$  has positive diagonal elements- To this end we can choose from a variety of available techniques since there are many algorithms to compute R and within each algorithm there are several ways of obtaining an incomplete factor- Of course incompleteness can inuence  $R$  in the various algorithms and implementations very differently.

We describe three versions of incomplete QR decompositions based on the sparse modies and a form of the complete orthogonal incomplete orthogonalization via the complete orthogonal incomplete  $\blacksquare$  see all  $\blacksquare$ 

The implementation of all schemes in this and the next section is based on the use of dynamic data structures similar to those adopted in submatrix formulations of sparse unsymmetric Gaussian elimination seeming the property of the coefficient matrix as a coefficient of the in the dynamics data structure by columns CCS for a natural choice formation  $\alpha$  formation  $\alpha$ carrying out the (incomplete) MGS process.

A simple way to compute an incomplete QR decomposition is based on dropping elements of the reduced matrix  $A^{\vee\vee}$  obtained at step  $i$  of the orthogonalization process. We check for elements whose magnitude falls below a prescribed drop tolerance  $T<sub>d</sub>$  and remove these from the data structure- increase the diagonal control increase the diagonal complete the diagona element  $a_{ii}^{i,j}$  if the norm of the  $i-th$  column of  $A^{(i)}$  is less than the prescribed tolerance to the secretary and the proposition of the set to the continuation of the complete set to the set to the set  $\mathcal{W}$  in our tests-down-dimensional down-dimensional down-dimensional down-dimensional down-dimensional down-

The second algorithm in this Section Algorithm - is the one described in -Instead of removing "small" elements of updated  $A$  it removes "small" nondiagonal elements of the upper triangular factor-

It can be easily shown that Algorithm - cannot break down see -

Finally a third algorithm can be obtained by combining the dropping strategies of Algorithms - and - small elements are removed both from the factor R and from the set of vectors that remain to be (approximately) orthogonalized.

```
Algorithm -
 Incomplete QR decomposition by diagonally safeguarded MGS
      set A_1 = (a_1^{r_1}, \ldots, a_n^{r_n}) = A \in R^{m,n}for i  -
   -
n
        if ||a_i^{\vee}|| < T_d then
             set a_{ii}^{s}{}' = a_{ii}^{s}{}' + \mu || (a_{ii}^{s}{}' , \ldots, a_{mi}^{s}{}')^T ||end if
        set rii  jja
i jj
                              -
i
        set q_i = a_i^{\gamma \gamma}/r_{ii}for j  i  -
   -
n
             set \alpha = q_i^{\perp} a_i^{\vee}j
             . . . . .
                     the second contract of the second cont
                 for l  i-
    -
 m
                      if a_{i,j}^{(0)} \neq 0 \vee q_{ii} \neq 0 then
                           set \beta = a_{ij}^{\vee} - \alpha q_{li}if it is the contract to the set of \alphaa_{l,i}^{(1)} = 0else
                               a_{l,i}^{\cdots} = \betaend if
                      else
                           set a_i; \cdot =
                                    i,j = a_{i,j}l-
j
                      end if
                 end l
                 set a_i^{\vee} = a_i^{\vee}je poznata u predstavanje poznata u predstavanje poznata u predstavanje poznata u predstavanje poznata u preds
            end if
       end j
      end i
```
Algorithm -- Incomplete QR decomposition by MGS with incomplete updates of  $R$ 

$$
set\ A_1 = (a_1^{(1)}, \ldots, a_n^{(1)}) = A \in R^{m,n}
$$
\n
$$
for\ i = 1, \ldots, n
$$
\n
$$
set\ r_{ii} = ||a_i^{(i)}||
$$
\n
$$
set\ q_i = a_i^{(i)}/r_{ii}
$$
\n
$$
for\ j = i + 1, \ldots, n
$$
\n
$$
set\ \alpha = q_i^T a_j^{(i)}
$$
\n
$$
if \ |\alpha| < T_d\ then
$$
\n
$$
r_{ij} = 0
$$
\n
$$
a_j^{(i+1)} = a_j^{(i)}
$$
\n
$$
else
$$
\n
$$
r_{ij} = \alpha
$$
\n
$$
a_j^{(i+1)} = a_j^{(i)} - \alpha q_i
$$
\n
$$
end\ if
$$
\n
$$
end\ i
$$

### $\bf{3}$  Preconditioning by Incomplete Inverse QR Fac torization

In this section we describe some procedures that directly approximate the upper trian gular matrix  $Y$  such that  $(A^T A)^{-1} = Y^T Y$  . In the language of Statistics, we compute an incomplete *covariance pactorization*. This can be computed directly from A ap plying a procedure which orthogonalizes the columns as in the MGS algorithm and computes  $Y$  throughout these steps.

When applied without dropping this decomposition computes the matrix Y which is equal (up to a diagonal matrix factor) to the transposed inverse of the Cholesky factor of ATA which is usually a dense triangular matrix- A sparse approximation may be obtained by removing suitably small fill-in occurring in the course of the computation, or else by a dropping position strategy- electronic we use position to the day of the strategy of the strategy previous section-

The algorithms to compute an incomplete Y that is an approximate inverse of R in the QR factorization of  $A$ ) update the values of Y in such a way that dynamic data structures must be used- We store Y in this data structure by rows- Elements in these rows are kept in partial order throughout the algorithm- Pointers to elements of the actual column of Y or behind it are kept and updated by a mechanism similar to the one adopted in the numerical factorization procedure in  $SPARSPAK$  (see  $[6]$ ).

The computation of the preconditioner is based on the matrix decomposition  $ADY =$  $Q$ , where  $Q$  is a matrix with orthonormal columns,  $D$  is a positive diagonal matrix,  $Y$ is unit upper triangular and  $Y = D Y$  -is the inverse of the upper triangular factor in the QR decomposition of  $A$ .

We give first the pseudocode for the algorithm with incomplete updates of  $Y$  based on the complete sparse MGS and then for the algorithm with complete updates of  $Y$ .

Algorithm  $\delta$ , I  $ADI = Q$  decomposition with incomplete updates of *I* 

$$
set\ A_1 = (a_1^{(1)}, \dots, a_n^{(1)}) = A \in R^{m,n}
$$
\n
$$
for\ i = 1, \dots, n
$$
\n
$$
set\ d_{ii} = \frac{1}{||a_i^{(i)}||}
$$
\n
$$
set\ q_i = a_i^{(i)}d_{ii}
$$
\n
$$
for\ j = i + 1, \dots, n
$$
\n
$$
set\ \alpha = q_i^T a_j^{(i)}
$$
\n
$$
if\ |\alpha| \ge T_d\ then
$$
\n
$$
a_j^{(i+1)} = a_j^{(i)} - \alpha q_i
$$
\n
$$
for\ k = 1, \dots, i
$$
\n
$$
if\ y_{kj}' \neq 0 \lor y_{ki}' \neq 0\ then
$$
\n
$$
y_{kj}' = y_{kj}' - y_{ki}'\alpha
$$
\n
$$
end\ if
$$
\n
$$
end\ if
$$
\n
$$
end\ if
$$
\n
$$
if\ y_{ji}' \neq 0\ then
$$
\n
$$
y_{ji}' = d_{ii}y_{ji}'
$$
\n
$$
end\ if
$$

Algorithm 5.2 incomplete  $A\bar{D}Y^{\dagger}=Q$  decomposition diagonally safeguarded set  $A_1 = (a_1^{(1)}, \ldots, a_n^{(1)}) = \binom{A}{0} \in R$  $\in R$  matrix  $\sim$  $\cdots$  is a set in  $\cdots$  $\left|u_i^{(r)}\right| \le T_d$  then set  $a_{ii}^{y'} = a_{ii}^{y'} + \mu ||(a_{ii}^{y'}, \ldots, a_{mi}^{y'})^T||$ end if $\textit{set a}_{ii} = \frac{1}{\|a_i^{(i)}\|}$ set  $q_i = a_i^{\vee} d_{ii}$ <sup>i</sup> dii  $\mathbf{y}$  is a set of  $\mathbf{y}$  . It is a set of  $\mathbf{y}$  is a set of  $\mathbf{y}$  is a set of  $\mathbf{y}$ set  $\alpha = q_i^{\mu} a_i^{\nu}$ je poznata u predstavanje postavanje postavanje postavanje postavanje postavanje postavanje postavanje postava if then for l i - - - m if  $a_{li}^{\vee\vee} \neq 0 \vee q_{li} \neq 0$  then set  $\beta = a_{li}^{\cdots} - \alpha q_{li}$ if jj Td then  $a_{ij}^{\ldots} = 0$  $a_{l}^{\dots} = \beta$ end ifelseset  $a_i$ ;  $\cdot$  =  $i, i'' = a_{i, i}^{\gamma}$ l-<sup>j</sup> end ifend l elseset  $a_i^{(1)} = a_i^{(1)}$ je poznata u predstavanje poznata u predstavanje poznata u predstavanje poznata u predstavanje poznata u preds end iffor k -- $y_{ki} \neq 0$  v  $y_{ki} \neq 0$  then  $y_{ki} = y_{ki} - y_{ki}\alpha$ end if end ke end j  $\mathbf{r}$  is a set of  $\mathbf{r}$  . The set of  $\mathbf{r}$  $y_{ii} = a_{ii}y_{ii}$ end j

Finally a third incomplete inverse factorization scheme may be obtained combining the drop strategies adopted in Algorithm -  $\lambda$  and Algorithm -  $\lambda$ lgorithm -  $\lambda$ 

end i

#### $\boldsymbol{4}$ Experimental Results

In this Section we present the results of experiments with the preconditioned CGNR schemes- Most test matrices are from the HarwellBoeing collection - Matrices WATSONx are from Y- Saads collection of sparse problems- The test matrices used are representative or problems arising in a variety or applications, a value of a various constant kinetics computer system simulation uid ow chemical engineering and others-

The goal of our experiments is to explore the relation between the amount of fillin allowed in the incomplete factor (or inverse factor) and the rate of convergence of PCGNR- Furthermore we want to compare the approximate inverse preconditioners described in Section with the more standard implicit preconditioners of Section - For completeness we have also included the results for an incomplete Cholesky factorization (with a drop tolerance) of  $A^\ast A$ . This is the only preconditioner which does not require a dynamic data structure.

Concerning the differences in the computation of the preconditioners themselves. it should be mentioned that in most cases (though not always) it is more expensive to construct an explicit preconditioner than an implicit one- This dierence however becomes negligible if many linear systems with the same coefficient matrix (or a slightly modification and discussed sides to the side one in this case the side of the solved this case the solve cost of the iterative part dominates the cost of the overall computation- Furthermore on parallel architectures the approximate inverse preconditioners can take advantage of explicitness-

We present the results of experiments with variants of the incomplete MGS (IMGS) and incomplete in the instrument process  $\alpha$  is a complete international processes that the income plete choicher, it all preconditioners which we have not not an one case in the second state of the seconditio we adopted the column ordering of A induced by the minimum degree ordering on the structure of  $A^*A$ , for the reasons discussed in the Introduction. The first column in the the contains the matrix names the number  $\alpha$  of  $\alpha$  of  $\alpha$  of  $\alpha$  of  $\alpha$  of  $\alpha$  of  $\alpha$  $NADJ$  of nonzeros in the triangular part of  $A^*A$  (after reordering). In case of rectanguesse executed and not show the number matrix rows in the second case and the table since a since  $\sim$ incomplete algorithms are only affected by the structure of  $A<sup>T</sup>A$ .

For both groups of Gram-Schmidt algorithms we tried different options for drop- $\mathbf{M}$  and  $\mathbf{M}$  and IMGS2 combines removing elements from the factor  $R$  and from the set of vectors to be approximately orthogonalized in these algorithms- It uses the same drop tolerance is a first types of dropping. If the same was interested in the algorithm -  $\mathcal{A}$  $\mathbf{A}$  and  $\mathbf{A}$  and

All the computations were performed in double precision on a SGI Crimson com puter- Convergence of the PCGNR iteration was considered achieved when the eu choean norm of the residual was less than TU  $^{\circ}$ ; for all matrices we allowed a maximum number of iterations equal to the number N of unknowns- Notice that without any preconditioning, converge in N or less iterations for the second test in N or less iterations for  $\sim$ problems-

The key role in the comparison is played by the size of fill-in in the approximate factor which is controlled by the value of the drop tolerance Td- Note that dierent matrices and different preconditioners often require totally different values of  $T<sub>d</sub>$  and it is the drop to have a good guess for the drop to have a good guess for the drop to  $\mathbb{R}$ general principle is that severely ill-conditioned problems force the use of small drop to a causing high  $\mathcal{U}$  is the iteration will converge very slowly-definition will converge very slowly-definition will converge very slowly-definition will converge very slowly-definition will converge very slowly-def  $[11]$  for a discussion of this important issue.

For each preconditioning strategy we report the size of fill-in (FILL) and the corresponding number of PCGNR iterations (NIT) for two different values of the drop to the  $\Gamma$ incomplete factor becomes sensibly smaller than the fill in the complete factor and it still takes only a few PCGNR iterations to ful ll the stopping criterion- The second larger value corresponds to the point after which the number of iterative steps becomes promission that in some cases there is not much dierence between the two some the two two two dierence between results-that it may well happen that a larger value of Td produces more contract that the contract more complete a smaller value nevertheless incomplete factor corresponding to the smaller value of the smaller value of the s of the sense it is more in the sense that it is gone in less iterations see the second convergence in less iter results for IMGS1 and IMGS2 on matrix FS6801).

For some ill-conditioned matrices we report the results for only one value of  $T<sub>d</sub>$ . This means that larger values of  $T_d$  cause the PCGNR iteration to fail to converge in less than the maximum allowed number  $N$  of iterations.

For some extremely ill-conditioned matrices (such as FS5413) we observed convergence only for very small values of  $T<sub>d</sub>$ , which were ineffective at producing incomplete factors with reduced very slow convergence-dimensional convergence-dimensional convergence-dimensional convergencefore we did not include those results-



Table Comparison of iteration counts and ll-in in preconditioners in thePCGNR procedure (CGNR preconditioned by incomplete MGS, incomplete inverse  $m$  and  $m$  algorithms).

#### $\overline{5}$ Conclusions

The first conclusion drawn from the experiments concerns the comparison of methods with each of the groups IMGS and IIMGS  $\mathbf{M}$ and  $\mathbf{f}$  the option is often worse that  $\mathbf{f}$  is often worse that  $\mathbf{f}$  is often worse that  $\mathbf{f}$ incomplete factor is especial methods-is especially true for the IIMGS class of methods-is

, and in the correction of robustiness, which is the incomplete factor and  $\alpha$ eectiveness at reducing the number of PCGNR iterations the overall winner is pre conditioner IMGS3.

An observation which applies to all the preconditioning schemes studied in this paper is that it is difficult to predict in advance what kind of fill-in and convergence behavior will correspond to a given value of the drop tolerance Td- However matrices from the same type of application such as the FS matrices which arise from the solu tion of systems of ODEs in chemical kinetics studies) tend to have a similar behavior. ences it may be worthwhile to spend some times that to make a good value of the species these matrices and then use it also for other matrices in the same class-clas stratagem will not work on extremely ill-conditioned problems.

An interesting and perhaps surprising result of the experiments is the existence of some matrices for which the preconditioners based on the incomplete inverse factor ization behave very well- In fact for some of these matrices the size of the incomplete inverse factor Y (in terms of fill-in) can even be less than the size of the incomplete factor R and yet produce the same or a similar number of PCGNR iterations- For most test matrices however the approximate inverse preconditioners require substan tially fuller incomplete factors in order to produce convergence rates comparable with those for the implicit precision in other words and inverse words in the proximate  $\alpha$  presented in the space preconditioners are usually not as effective at reducing the number of PCGNR iterations as the implicite ones. Expliciting this price is whether this whether this price whether this price is paying it will depend on the particular problem and problem and computer architecture at hand-

Finally it should be observed that in many cases the simple approach based on computing an incomplete Cholesky decomposition of  $A<sup>T</sup>A$  gives very satisfactory resurvey to be contract density that well a converged that in practice and in practice  $\mu$  well as the contract incomplete Cholesky approach is more prone to suffer from instability problems than the approach based on incomplete orthogonalization-incomplete orthogonalization-incomplete orthogonalization-i vation which led researchers to consider the use of incomplete orthogonal factorizations in the seen from the last place-last place-last column in Table  $\mathcal{N}$ with comparatively large drop tolerances failed to produce a stable preconditioner in six cases- The most robust of all preconditioners on the basis of our experiments is IMGS ALGORITHM - ALGORITHM

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