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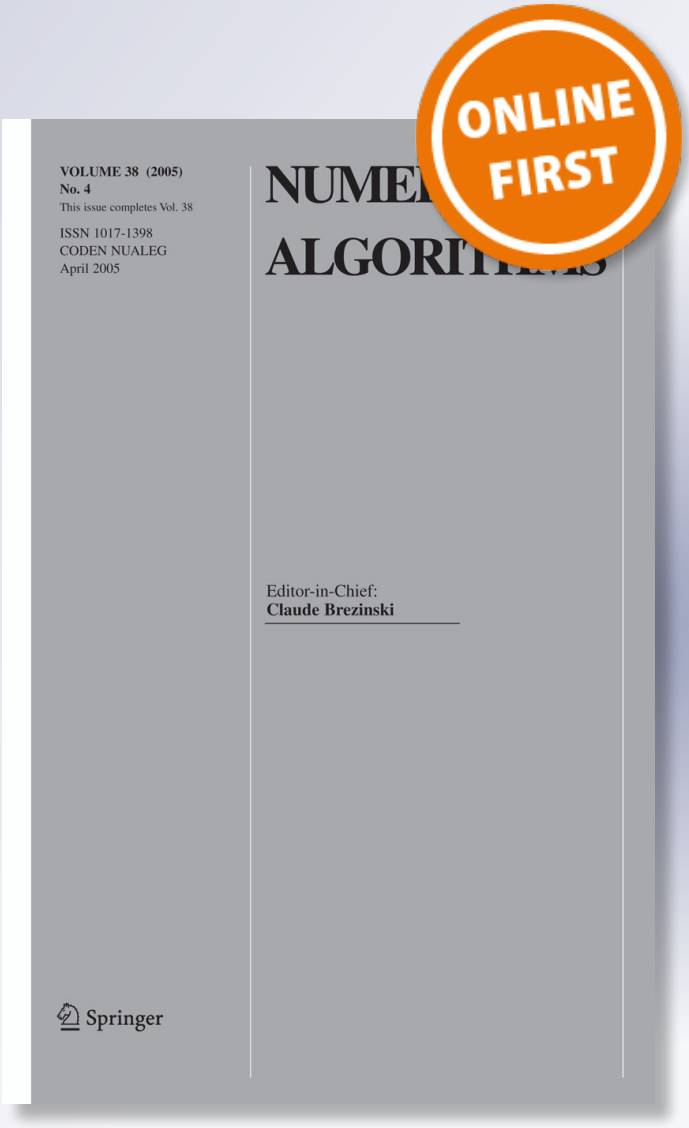
Numerical Algorithms

ISSN 1017-1398

Numer Algor
DOI 10.1007/s11075-018-0478-2



Springer

Numer Algor
https://doi.org/10.1007/s11075-018-0478-2

ORIGINAL PAPER

A Schur complement approach to preconditioning sparse linear least-squares problems with some dense rows

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Received: 11 April 2017 / Accepted: 10 January 2018

Abstract The effectiveness of sparse matrix techniques for directly solving large-scale linear least-squares problems is severely limited if the system matrix A has one or more nearly dense rows. In this paper, we partition the rows of A into sparse rows and dense rows (A_s and A_d) and apply the Schur complement approach. A potential difficulty is that the reduced normal matrix $A_s^T A_s$ is often rank-deficient, even if A is of full rank. To overcome this, we propose explicitly removing null columns of A_s and then employing a regularization parameter and using the resulting Cholesky factors as a preconditioner for an iterative solver applied to the symmetric indefinite reduced augmented system. We consider complete factorizations as well as incomplete Cholesky factorizations of the shifted reduced normal matrix. Numerical experiments are performed on a range of large least-squares problems arising from practical applications. These demonstrate the effectiveness of the proposed approach when combined with either a sparse parallel direct solver or a robust incomplete Cholesky factorization algorithm.

Jennifer Scott was supported by EPSRC grant EP/M025179/1.
Miroslav Tůma was supported by projects 17-04150J and 18-12719S of the Grant Agency of the Czech Republic.

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Published online: 31 January 2018

Keywords Large-scale linear least-squares problems · Dense rows · Augmented system · Schur complement · Iterative solvers · Preconditioning · Cholesky factorization · Incomplete factorizations

1 Introduction

We are interested in solving the linear least-squares (LS) problem

$$\min_x \|Ax - b\|_2, \tag{1.1}$$

where $A \in \Re^{m\times n}$ ($m \geq n$) and $b \in \Re^m$. The solution x satisfies the $n \times n$ *normal equations*

$$Cx = A^T b, \qquad C = A^T A, \tag{1.2}$$

where provided A has full column rank, the *normal matrix* C is symmetric and positive definite. Our focus is on the case where the system matrix A is large and sparse but has a number of "dense" rows (rows that contain significantly more entries than the other rows, although the number of entries in each such row may be less than n). Just a single dense row is sufficient to cause catastrophic fill in C and thus for the factors of a Cholesky or QR factorization to be dense. In practice, for large-scale problems, this means that it may not be possible to use a direct solver because the memory demands can be prohibitive. Moreover, if an incomplete factorization is used as a preconditioner for an iterative solver such as LSQR [37, 38] or LSMR [13] applied to (1.1), the error in the factorization can be so large as to prohibit its effectiveness as a preconditioner; this was recently observed in the study by Gould and Scott [20]. The effect of dense rows has long been recognised as a fundamental difficulty in the solution of sparse least-squares problems (see, for example, [2, 5, 8, 14, 17, 48–51]).

Let us assume that the rows of A are partitioned into two parts: rows that are sparse and those that are considered dense. We also assume conformal partitioning of the right-hand side vector b as follows:

$$A = \begin{pmatrix} A_s \\ A_d \end{pmatrix}, \ A_s \in R^{m_s\times n}, \ A_d \in R^{m_d\times n}, \ b = \begin{pmatrix} b_s \\ b_d \end{pmatrix}, \ b_s \in R^{m_s}, \ b_d \in R^{m_d}, \tag{1.3}$$

with $m = m_s + m_d$, $m_s \geq n$ and $m_d \geq 1$ (in general, $m_s \gg m_d$). Problem (1.1) then becomes

$$\min_x \left\| \begin{pmatrix} A_s \\ A_d \end{pmatrix} x - \begin{pmatrix} b_s \\ b_d \end{pmatrix} \right\|_2. \tag{1.4}$$

A number of approaches to tackling such systems have been proposed. For example, George and Heath [14] temporarily discard A_d to avoid severe fill-in in their Givens rotation-based orthogonal factorization of A_s. They then employ an updating scheme to allow for the effect of these rows. A completely general updating algorithm for the constrained least-squares problem based on QR decomposition and direct elimination is given by Björck [7], while Avron et al. [5] propose dropping dense rows before the QR factorization is performed and using the resulting R factor as a preconditioner for LSQR. Most recently, Scott and Tůma [48] process rows that are identified as

dense separately within a conjugate gradient method using an incomplete factorization preconditioner combined with the factorization of a dense matrix of size equal to the number of dense rows.

Solving (1.4) is equivalent to solving the larger $(m+n) \times (m+n)$ *augmented system*

$$\begin{pmatrix} I_{m_s} & & A_s \\ & I_{m_d} & A_d \\ A_s^T & A_d^T & 0 \end{pmatrix} \begin{pmatrix} r_s \\ r_d \\ x \end{pmatrix} = \begin{pmatrix} b_s \\ b_d \\ 0 \end{pmatrix}, \tag{1.5}$$

where

$$r = \begin{pmatrix} r_s \\ r_d \end{pmatrix} = \begin{pmatrix} b_s \\ b_d \end{pmatrix} - \begin{pmatrix} A_s \\ A_d \end{pmatrix} x$$

is the residual vector. Here and elsewhere, I_k denotes the $k \times k$ identity matrix. System (1.5) is symmetric indefinite and so, if there is sufficient memory available, a sparse direct solver that incorporates numerical pivoting for stability can be used (well-known examples include `MA57` [12] and `HSL_MA97` [23] from the HSL mathematical software library [24], MUMPS [31] and WSMP [53]). Employing a general-purpose sparse solver ignores the block structure, although its use of a sparsity-preserving ordering (such as a variant of minimum degree or nested dissection) will tend to lead to the dense rows being eliminated last [11].

An alternative approach is to eliminate r_s to reduce the problem from a 3-block saddle-point system to a 2-block system of order $(n+m_d) \times (n+m_d)$ that can be written in the form

$$K \begin{pmatrix} x \\ r_d \end{pmatrix} = \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix}, \qquad K = \begin{pmatrix} -C_s & A_d^T \\ A_d & I_{m_d} \end{pmatrix}, \tag{1.6}$$

where the $n \times n$ matrix $C_s = A_s^T A_s$ is termed the *reduced normal matrix*. We refer to (1.6) as the *reduced augmented system*. The reduced augmented matrix K can be factorized using a sparse indefinite solver, but this would again ignore the block structure. Instead, we use the so-called Schur complement method (see, for example, [15, 30, 42] and Section 2 below) that exploits the structure by performing a sparse Cholesky factorization of $A_s^T A_s$, forming an $m_d \times m_d$ dense Schur complement matrix and factorizing it using a dense Cholesky factorization; using the sparse and dense factors to solve a number of triangular systems completes the solution process. This has the advantage of using Cholesky factorizations that, because they do not involve numerical pivoting, are more efficient (especially in parallel) than an indefinite factorization. Moreover, it can be easily incorporated into the normal equations approach.

We observe that the reduced augmented matrix K is symmetric quasi-definite (SQD). Vanderbei [52] shows that SQD matrices are strongly factorisable and this allows general permutations to be used [35]. Recent work has shown that some classes of permutations can be beneficial and underlying theory has been developed that helps to find such permutations for deriving incomplete factorization preconditioners [21, 34, 47]. An interesting stability analysis of the factorization of SQD matrices that connects the stability with the effective condition number is given in [16] (see also [18]). Furthermore, analysis of a symmetric indefinite factorization based on the related generalized QR factorization in [33] points out that conditioning

of the principal leading submatrices may be determined by other factors such as the number of sign changes in the diagonal of the signed factorization. In this paper, we maintain the block structure and this means that the stability is predetermined by the splitting into sparse and dense rows. Note that the results in [48] show that iterative methods are very sensitive to keeping all the dense rows separate and not mixing any of them with the other rows.

Another possibility is to use an iterative solver such as LSQR [37, 38] that has the advantage of avoiding the construction of the dense matrices that are involved in the Schur complement approach (see (2.2) and (2.3) below). However, in many cases, the LS problems are hard to solve and a preconditioner is required to achieve acceptable convergence.

In practice, even if A is of full rank, A_s is often rank-deficient (indeed, it may have null columns). In this case, a Cholesky factorization of $A_s^T A_s$ will break down. To overcome this, we propose removing null columns and employing a regularization parameter and using the resulting Cholesky factors as a preconditioner for an iterative solver applied to the reduced augmented system. For large problems, even if A_s is sparse, memory limitations can mean that it is not possible to use a sparse direct solver. Thus, we consider using incomplete Cholesky factorizations combined with an iterative solver.

The outline of the rest of the paper is as follows. In Section 2, we recall the Schur complement approach and, in particular, we look at regularization and propose using the factors of the reduced regularized matrix $A_s^T A_s + \alpha I$ to obtain a block preconditioner. Use of a limited memory incomplete Cholesky factorization is also discussed. Section 3 introduces our numerical experiments. Computational results for complete and incomplete Cholesky factorizations are given in Sections 4 and 5, respectively. Concluding remarks are made in Section 6.

2 Schur complement method

2.1 Schur complement method with direct solvers

As already observed, an alternative to applying a direct solver to either the (dense) normal equations or the augmented system (1.5) is to solve the reduced augmented system (1.6). Provided A_s has full column rank, C_s is symmetric positive definite and, if the partitioning (1.3) is such that all the rows of A_s are sparse, C_s is generally significantly sparser than the original normal matrix C. Let $C_s = L_s L_s^T$ be the Cholesky factorization of C_s. Using this yields a block factorization

$$K = \begin{pmatrix} L_s & \\ B_d & I_{m_d} \end{pmatrix} \begin{pmatrix} -I_n & \\ & S_d \end{pmatrix} \begin{pmatrix} L_s^T & B_d^T \\ & I_{m_d} \end{pmatrix}, \tag{2.1}$$

where B_d and the Schur complement matrix S_d are given by

$$L_s B_d^T = -A_d^T \tag{2.2}$$

$$S_d = I_{m_d} + B_d B_d^T. \tag{2.3}$$

Since L_s is lower triangular, solving (2.2) for B_d^T is straightforward. B_d will normally be dense and hence S_d will be dense and symmetric positive definite. Once we have L_s, B_d and S_d, we can solve (1.6) by solving

$$\begin{pmatrix} -L_s & \\ -B_d & S_d \end{pmatrix} \begin{pmatrix} y_s \\ y_d \end{pmatrix} = \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix}, \tag{2.4}$$

followed by

$$\begin{pmatrix} L_s^T & B_d^T \\ & I_{m_d} \end{pmatrix} \begin{pmatrix} x \\ r_d \end{pmatrix} = \begin{pmatrix} y_s \\ y_d \end{pmatrix}. \tag{2.5}$$

With $r_d = y_d$, this requires us to solve

$$L_s y_s = A_s^T b_s, \tag{2.6}$$
$$S_d r_d = b_d + B_d y_s, \tag{2.7}$$
$$L_s^T x = y_s - B_d^T r_d. \tag{2.8}$$

Again, (2.6) and (2.8) are triangular systems and hence straightforward to solve. Solving (2.7) requires Cholesky factorization of the $m_d \times m_d$ dense matrix S_d. Observe that in the case of a single dense row ($m_d = 1$) this is trivial. In general, the LAPACK routine `_potrf` can be used to factorize S_d and then routine `_potrs` employed to solve (2.7). Note also that B_d need not be computed explicitly. Rather, S_d may be computed implicitly as $I_{m_d} + A_d L_s^{-T} L_s^{-1} A_d^T$, while $z = B_d y_s$ may be computed by solving $L_s w = y_s$ and then $z = -A_d w$ and $z = -B_d^T r_d$ may be obtained by solving $L_s z = A_d^T r_d$.

2.2 Scaling and stability

Poorly scaled entries in A_s may result in block elimination of the first m_s rows and columns of (1.5) being unstable. To overcome this, we prescale A so that the entries of the scaled A are small relative to 1. Thus, we scale A by normalising each column by its 2-norm. That is, we replace A by AD, where D is the diagonal matrix with entries $D_{jj} = 1/\|Ae_j\|_2$ (e_j denotes the j-th unit vector). The entries of AD are all less than one in absolute value. Elimination of the first m_s rows and columns is thus stable (the pivots can be chosen in order from the main diagonal and they satisfy the criteria for complete pivoting). However, this does not guarantee stability of the next step. The diagonal entries of the factor L_s of the positive definite C_s can be small, leading to large entries in B_d and hence large entries in S_d.

If instability is detected, then a general-purpose symmetric indefinite sparse solver that incorporates numerical pivoting can be applied to solve the reduced augmented system (1.6). Whilst this offers a robust approach, it has the disadvantage that the block structure within (1.6) is not exploited. Furthermore, if A_s is fixed and the interest lies in adding new rows A_d, the factorization must be redone in its entirety for each A_d. Thus, in Section 2.4, we propose an alternative approach to maintain stability.

We assume throughout the remainder of our discussion and in all our numerical experiments that A has been prescaled, but we omit D to simplify the notation.

2.3 Removal of null columns

In practice, when A is partitioned, the sparse part A_s often contains a (small) number of null columns. It is possible to remove these columns explicitly, as we now show. Let A have full column rank and assume A_s has n_2 null columns with $n_2 \ll n$. Assuming these columns are permuted to the end, we can split A into the form

$$A = \begin{pmatrix} A_1 & A_2 \end{pmatrix} \equiv \begin{pmatrix} A_{s_1} & 0 \\ A_{d_1} & A_{d_2} \end{pmatrix} \tag{2.9}$$

with $A_1 \in R^{m \times n_1}$ and $A_2 \in R^{m \times n_2}$ ($n = n_1 + n_2$). The following result from [48] shows that the solution of the least-squares problem can be expressed as a combination of partial solutions.

Lemma 2.1 *Let the columns of A be split as in (2.9) and let $z \in R^{n_1}$ and $W \in R^{n_1 \times n_2}$ be the solutions to the problems*

$$\min_z \|A_1 z - b\|_2 \quad \text{and} \quad \min_W \|A_1 W - A_2\|_F \,, \tag{2.10}$$

respectively. Assuming A_1 is of rank n_1, the solution $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ of the least-squares problem (1.1) with its splitting consistent with (2.9) (that is, $x_1 \in R^{n_1}$, $x_2 \in R^{n_2}$) is given by

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} z - W x_2 \\ x_2 \end{pmatrix} \tag{2.11}$$

with

$$x_2 = (A_2^T (A_2 - A_1 W))^{-1} A_2^T (b - A_1 z). \tag{2.12}$$

The least-squares problems (2.10) again have m_d dense rows and thus can be solved using the Schur complement method as described in (2.1) – (2.8). In this case, we use the subscripts s_1 and d_1 for C_{s_1}, L_{s_1}, S_{d_1} and B_{d_1} to emphasize we are working with A_1, which has fewer columns than A. The factorizations of the reduced normal matrix $C_{s_1} = A_{s_1}^T A_{s_1}$ and the Schur complement matrix S_{d_1} needed to compute z can be used to solve for W. For the latter, if A_{2j} denotes a column j of A_{d_2} ($1 \le j \le n_2$), the right-hand side in (2.4) based on A_1 becomes $\begin{pmatrix} 0 \\ A_{2j} \end{pmatrix}$ and thus (2.6) – (2.8) reduce to solving systems of the form $S_{d_1} R_{dj} = A_{2j}$ and $L_{s_1}^T W_j = -B_{d_1}^T R_{dj}$. If we are using direct solvers that allow for solves with multiple right-hand sides, we can perform these solves for all the R_{dj} and W_j simultaneously with solving (2.7) and (2.8). Thus, as solving for multiple right-hand sides is generally significantly less expensive than repeatedly solving for a single right-hand side (since multiple right-hand sides allow the use of level 3 BLAS), the extra solves add only a small overhead. Furthermore, using (2.9), (2.12) reduces to

$$x_2 = (A_{d_2}^T (A_{d_2} - A_{d_1} W))^{-1} A_{d_2}^T (b_d - A_{d_1} z). \tag{2.13}$$

Forming and then solving with $A_{d_2}^T (A_{d_2} - A_{d_1} W)$ is inexpensive provided $n_2 \ll n$.

2.4 Regularization and preconditioning

While Lemma 2.1 provides a way of removing null columns, it is possible that even if A has full column rank, A_s (or A_{s_1} after the removal of null columns) is rank-deficient (or is close to rank-deficient). To simplify notation, in our discussion, we use A_s but this may be replaced by A_{s_1} if A_s contains null columns. If A_s is rank-deficient, the reduced normal matrix C_s is positive semidefinite and a Cholesky factorization breaks down (that is, a very small or a non-positive pivot is encountered). If breakdown occurs, we employ a shift $\alpha > 0$ and compute a Cholesky factorization of the shifted matrix

$$C_s(\alpha) = A_s^T A_s + \alpha I_n. \tag{2.14}$$

The shift α is also referred to as a *Tikhonov regularization* parameter. The choice of α should be related to the smallest eigenvalue of $A_s^T A_s$, but this information is not readily available. Clearly, it is always possible to find an $\alpha > 0$ so that the factorization does not breakdown; if the initial choice α is too small, it may be necessary to restart the factorization more than once, increasing α on each restart until breakdown is avoided. Use of a shift was discussed by Lustig et al. [28] (see also [1, 2]). It was observed that careful and often substantial use of iterative refinement to compute each column of B_d^T was required. However, we adopt a different approach in which we use the factorization of (2.14) to obtain a preconditioner for the system (1.6). Note that this regularization that shifts all the diagonal entries could be considered as an over-regularization of the system since we could regularize only those entries that cause the factorization to break down. Our strategy is based on experimental evidence that shows that for incomplete Cholesky (IC) factorizations, it is better to use a global shift as introduced by Manteuffel [29] rather than a local shifting strategy [6, 45]. Contemporary incomplete factorizations such as that described in [45] increase and decrease the shift automatically (see also [27]).

With $\alpha > 0$ in (2.14), we approximate the solution of (1.6) by changing K to

$$K(\alpha) = \begin{pmatrix} -C_s(\alpha) & A_d^T \\ A_d & I_{m_d} \end{pmatrix}.$$

Thus, the computed value of the least-squares objective may differ from the optimum for the original problem. Having solved the regularized problem, we want to recover the solution of the original problem. Following Scott [44], we propose doing this by using the factors of $K(\alpha)$ as a preconditioner for an iterative method applied to (1.6).

Let the Cholesky factorization of $C_s(\alpha)$ be $L_s(\alpha)L_s(\alpha)^T$. For $\alpha > 0$, this is an approximate factorization of C_s, that is, $C_s \approx L_s(\alpha)L_s(\alpha)^T$. More generally, let

$$C_s \approx \tilde{L}_s \tilde{L}_s^T, \tag{2.15}$$

where $\tilde{L}_s$ is lower triangular. We are interested in the case $\tilde{L}_s = L_s(\alpha)$ but our main focus is where $\tilde{L}_s$ is an incomplete Cholesky (IC) factor, that is, one that contains fewer entries than occur in a complete factorization. For very large systems, computing and factorizing C_s (or $C_s(\alpha)$) is prohibitively expensive in terms of memory

and/or computational time. Over the last 50 or more years, IC factorizations have been an important tool in the armoury of preconditioners for the numerical solution of large sparse symmetric positive-definite linear systems of equations; for an introduction and overview see, for example, [6, 40, 46] and the long lists of references therein. Here, we consider preconditioning the symmetric indefinite system (1.6) using a factorization of the form (2.15) and exploiting the block structure of (1.6).

The right-preconditioned reduced augmented system is

$$K M^{-1} \begin{pmatrix} w_s \\ w_d \end{pmatrix} = \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix}, \qquad M \begin{pmatrix} x \\ r_d \end{pmatrix} = \begin{pmatrix} w_s \\ w_d \end{pmatrix}, \tag{2.16}$$

where M is the chosen preconditioner. Using (2.15), we obtain an indefinite preconditioner M given by

$$M = \begin{pmatrix} \tilde{L}_s & \\ \tilde{B}_d & I_{m_d} \end{pmatrix} \begin{pmatrix} -I_n & \\ & \tilde{S}_d \end{pmatrix} \begin{pmatrix} \tilde{L}_s^T & \tilde{B}_d^T \\ & I_{m_d} \end{pmatrix}, \tag{2.17}$$

where $\tilde{B}_d$ and $\tilde{S}_d$ are given by (2.2) and (2.3) with the complete factor L_s replaced by the incomplete one $\tilde{L}_s$, that is,

$$\tilde{L}_s \tilde{B}_d^T = -A_d^T \tag{2.18}$$

$$\tilde{S}_d = I_{m_d} + \tilde{B}_d \tilde{B}_d^T. \tag{2.19}$$

Applying this preconditioner requires a number of steps that are analogous to (2.6)–(2.8). In particular, a dense $m_d \times m_d$ symmetric positive-definite system of the form $\tilde{S}_d y_d = u_d$ must be solved. We again assume that LAPACK may be used. If m_d is so large that this is too expensive, an incomplete factorization of $\tilde{S}_d$ could be used. Algorithm 1 outlines the steps required for each application of the preconditioner. We see that it involves a triangular solve with $\tilde{L}_s$ and with $\tilde{L}_s^T$, calls to the BLAS routine `_gemv` for steps 2 and 4, and triangular solves using the factors of $\tilde{S}_d$. As before, $\tilde{B}_d$ need not be held explicitly but can be applied implicitly using $\tilde{B}_d^T = -\tilde{L}_s^{-1} A_d^T$.

Algorithm 1 Application of the block factorization preconditioner, that is, compute $y = M^{-1} z$.

Input: $\tilde{L}_s$, $\tilde{B}_d$, the Cholesky factors of $\tilde{S}_d$, and the vector $z = \begin{pmatrix} z_s \\ z_d \end{pmatrix}$.

Output: $y = \begin{pmatrix} y_s \\ y_d \end{pmatrix} = M^{-1} z$.

1: Solve $\tilde{L}_s u_s = -z_s$.
2: Compute $u_d = z_d + \tilde{B}_d u_s$.
3: Use the Cholesky factors of $\tilde{S}_d$ to solve $\tilde{S}_d y_d = u_d$.
4: Form $u_s = u_s - \tilde{B}_d^T y_d$.
5: Solve $\tilde{L}_s^T y_s = u_s$.

As the preconditioner (2.17) is indefinite, it needs to be used with a general non-symmetric iterative method such as GMRES [41]. We can obtain a positive-definite preconditioner for use with MINRES [36] by replacing M by

$$|M| = \begin{pmatrix} \tilde{L}_s & \\ \tilde{B}_d & I_{m_d} \end{pmatrix} \begin{pmatrix} I_n & \\ & \tilde{S}_d \end{pmatrix} \begin{pmatrix} \tilde{L}_s^T & \tilde{B}_d^T \\ & I_{m_d} \end{pmatrix}, \tag{2.20}$$

In Algorithm 1, steps 1 and 2 are then replaced by 1. Solve $\tilde{L}_s u_s = z_s$ and 2. Compute $u_d = z_d - \tilde{B}_d u_s$. MINRES has the advantage over GMRES of using short recurrences that limit the storage requirements.

Many different IC factorizations have been proposed. Although they may be considered to be general-purpose, most are best-suited to solving particular classes of problems. For example, level-based methods are often appropriate for systems with underlying structure, such as from finite element or finite difference applications. Here, we use the limited memory approach of Scott and Tůma [45, 46] that has been shown in [20] to result in effective preconditioners for a wide range of least-squares problems. The basic scheme employs a matrix factorization of the form

$$C_s \approx (\tilde{L}_s + \tilde{R}_s)(\tilde{L}_s + \tilde{R}_s)^T, \tag{2.21}$$

where $\tilde{L}_s$ is the lower triangular matrix with positive diagonal entries that is used for preconditioning and $\tilde{R}_s$ is a strictly lower triangular matrix with small entries that is used to stabilize the factorization process but is then discarded (it is not used as part of the preconditioner). The user specifies the maximum number of entries in each column of $\tilde{L}_s$ and $\tilde{R}_s$. At each step j of the incomplete factorization process, the largest entries are kept in column j of $\tilde{L}_s$, the next largest are kept in column j of $\tilde{R}_s$, and the remainder (the smallest entries) are dropped. In practice, C_s is optionally pre-ordered and scaled and, if necessary, shifted to avoid breakdown of the factorization (which occurs if a non-positive pivot is encountered) [29].

3 Numerical experiments

In this section, we present numerical results to illustrate potential of the Schur complement approach and, in particular, demonstrate that it allows us to solve some problems that are intractable if dense rows are ignored. Results are included for direct solvers and for iterative solvers that can be used to solve very large problems.

3.1 Test environment

The characteristics of the machine used to perform our tests are given in Table 1.

All software is written in Fortran and all reported timings are elapsed times in seconds. In our experiments, we employ the Cholesky sparse direct solver `HSL_MA87` [22] for positive-definite systems and `HSL_MA97` [23] for general sparse symmetric indefinite systems; both employ OpenMP and are run in parallel, using four processors. Both solvers are run with a nested dissection ordering [26]. Sparse matrix-vector products required by the iterative solvers are performed in parallel using the Intel Mathematics Kernel Library (MKL) routines; no attempt is made to parallelize the

Table 1 Test machine characteristics

CPU	Two Intel Xeon E5620 quadcore processors
Memory	24 GB
Compiler	gfortran version 4.8.4 with options -O3 -fopenmp
BLAS	Intel MKL

iterative methods themselves. In each test, we impose a time limit of 600 s per problem and for the iterative methods, the number of iterations is limited to 100,000.

Following Gould and Scott [20], we want the computed residual r to satisfy either $\|r_k\|_2 < \delta_1$ or

$$ratio(r) < \delta_2 \quad \text{with} \quad ratio(r) = \frac{\|A^T r\|_2/\|r\|_2}{\|A^T b\|_2/\|b\|_2}. \tag{3.1}$$

We set the tolerances δ_1 and δ_2 to 10^{-8} and 10^{-6}, respectively, and in our experiments, the right-hand side b is taken to be the vector of 1's. We use right-preconditioned restarted GMRES with the restart parameter set to 500, and in some experiments, we also report on using preconditioned MINRES. Since the iterative solver is applied to the reduced augmented system matrix K, the stopping criterion is applied to K. With the available implementations of GMRES and MINRES, it is not possible during the computation to check whether (3.1) is satisfied; this can only be checked once the solver has terminated. Instead, we use the scaled backward error

$$\frac{\left\| K \begin{pmatrix} x^{(k)} \\ r_d^{(k)} \end{pmatrix} - \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix} \right\|_2}{\left\| \begin{pmatrix} -A_s^T b_s \\ b_d \end{pmatrix} \right\|_2} < \tilde{\delta}, \tag{3.2}$$

where $\begin{pmatrix} x^{(k)} \\ r_d^{(k)} \end{pmatrix}$ is the computed solution of (1.6) on the kth step. In our experiments, we set $\tilde{\delta} = 10^{-7}$. With this choice, in most of our experiments, (3.1) is satisfied with $\delta_2 = 10^{-6}$.

3.2 Test set 1

Our test problems are taken from the CUTEst linear programme set [19] and the University of Florida Sparse Matrix Collection [9]. In each case, the matrix is "cleaned" (duplicates are summed, out-of-range entries and explicit zeros are removed along with any null rows or columns). In our experiments, we use the following definition for a dense row of A: given ρ ($0 < \rho \leq 1$), row i of A is defined to be dense if the percentage of entries in row i is at least ρ.

Our first test set is given in Table 2. The problems were chosen because they have at least one row that is more than 10% dense. They are also difficult problems to solve (see [20]); at least three of the problems are rank-deficient. An estimate of the rank was computed by running the sparse symmetric indefinite solver `HSL_MA97` on the

Table 2 Statistics for test set 1

Problem	m	n	$nnz(A)$	nullity	rdensity(A)	m_{10}	m_{20}	m_{30}	m_{40}	m_{50}	density(C)
`Trec14`	15,904	3159	2,872,265	14	0.791	2664	1232	649	346	150	9.32×10^{-1}
`Maragal_6`	21,251	10,144	537,694	516	0.586	68	68	30	21	0	7.49×10^{-1}
`Maragal_7`	46,845	26,525	1,200,537	2046	0.360	85	43	21	0	0	3.10×10^{-1}
`scsd8-2r`	60,550	8650	190,210	0	0.100	40	0	0	0	0	5.22×10^{-2}
`PDE1`	271,792	270,595	990,587	–	0.670	1	1	1	1	1	–
`12month1`	872,622	12,471	22,624,727	–	0.274	284	4	0	0	0	6.87×10^{-1}

m, n and $nnz(A)$ are the number of rows and columns and nonzeros in A. nullity is the estimated deficiency in the rank of A, rdensity(A) is the largest ratio of number of nonzeros in a row of A to n over all rows, m_j ($j = 10, 20, 30, 40, 50$) is the number of rows of A with at least $j\%$ entries, and $density(C)$ is the ratio of the number of entries in C to n^2. – denotes insufficient memory to compute the statistic

augmented system (1.5) (with the pivot threshold parameter set to 0.5); for problems `12month1` and `PDE1`, there was insufficient memory to do this.

In Table 3, we report the effects of varying the parameter ρ that controls which rows are classified as dense. Increasing ρ reduces the number m_d of dense rows and the number n_2 of null columns in A_s but increases the density of the reduced normal matrix C_s. Problem `PDE1` has only one row that is classified as dense for

Table 3 The effects of varying the row density parameter ρ on the number m_d of rows that are classed as dense, the number n_2 of null columns in A_s, and the density of C_s (the ratio of the number of entries in C_s to n^2)

Identifier	m	n	ρ	m_d	n_2	density(C_s)
`Trec14`	15,904	3159	0.005	12,643	0	2.38×10^{-2}
			0.010	9676	0	8.52×10^{-2}
			0.050	4467	0	6.17×10^{-1}
			0.100	2664	0	8.31×10^{-1}
`Maragal_6`	21,251	10,144	0.005	2923	759	6.22×10^{-4}
			0.010	823	3	1.93×10^{-2}
			0.100	68	2	5.49×10^{-2}
`Maragal_7`	46,845	26,525	0.001	4668	2352	2.15×10^{-4}
			0.005	687	6	9.02×10^{-3}
			0.010	108	6	1.70×10^{-2}
			0.100	85	6	1.78×10^{-2}
`scsd8-2r`	60,550	8650	0.050	50	5	1.44×10^{-3}
			0.100	40	0	1.39×10^{-2}
`PDE1`	271,792	270,595	0.660	1	0	4.52×10^{-5}
`12month1`	872,622	12,471	0.010	43,951	387	1.10×10^{-1}
			0.050	3641	17	5.66×10^{-1}
			0.100	284	3	6.56×10^{-1}

$\rho \in [0.001, 0.66]$. We see that for `12month1` and `Trec14`, ρ has to be very small for C_s to be sparse but, in this case, m_d is large compared to m. For the `Maragal` problems, C_s is highly sparse if approximately 10% of the rows are classified as dense.

3.3 Test set 2

For our second test set, we take some of the CUTEst and UFL examples that do not initially contain dense rows and append some rows. This allows us to explore the effect of varying the number of dense rows as well as the density of these rows. The problems are listed in Table 4; these problems are all of full rank. The pattern of each appended row is generated randomly with the requested density and the values of the entries are random numbers in $[-1, 1]$.

For our solvers, the number of entries $nnz(C)$ in the normal matrix C can be at most `huge(1)` ($\approx 2\times 10^9$), where `huge` is the Fortran intrinsic function. If we add a single row with density $\rho \geq 0.1$ to each of the matrices A_s in the lower part of Table 4 then $nnz(C)$ exceeds this limit. Thus for these examples and our current software, we cannot use any approach that requires the normal matrix to be computed.

4 Direct solver results

Our first experiments look at the effectiveness of the Schur complement approach using the Cholesky direct solver `HSL_MA87` to factorize the reduced normal matrix C_s. We compare this with using `HSL_MA87` to solve the original normal matrix C (1.2) without partitioning A into sparse and dense parts. If the Cholesky factorization of C breaks down because of a non-positive pivot, we factorize the shifted normal

Table 4 Statistics for test set 2

Problem	m_s	n	$nnz(A_s)$	rdensity(A_s)	density(C_s)
`IG5-15`	11,369	6146	323,509	1.95×10^{-2}	1.52×10^{-1}
`psse0`	26,722	11,028	102,432	3.63×10^{-4}	5.88×10^{-4}
`graphics`	29,493	11,822	117,954	3.38×10^{-4}	5.91×10^{-4}
`WORLD`	67,147	34,506	198,883	4.64×10^{-4}	4.89×10^{-4}
`STAT96V3`	1,113,780	33,841	3,317,736	3.55×10^{-4}	3.58×10^{-4}
`STORMG21K`	1,377,306	526,185	3,459,881	1.93×10^{-3}	3.00×10^{-4}
`GL7d20`	1,911,124	1,437,546	29,893,084	2.99×10^{-5}	2.23×10^{-4}
`CONT11_L`	1,961,394	1,468,599	5,382,999	4.77×10^{-6}	8.38×10^{-6}
`LargeRegFile`	2,111,154	801,374	4,944,201	4.99×10^{-6}	9.93×10^{-6}
`relat9`	9,746,232	274,667	38,955,420	1.46×10^{-5}	5.09×10^{-4}

m_s, n and $nnz(A_s)$ are the number of row and column and nonzeros in A_s. rdensity(A_s) is the largest ratio of number of nonzeros in a row of A_s to n over all rows, and density(C_s) is the ratio of the number of entries in C_s to n^2

Table 5 Results for test set 1 of running the Cholesky direct solver `HSL_MA87` on the normal equations (without exploiting dense rows), using LSMR for refinement

Identifier	m	n	$nnz(L)$	*Its*	T_f	T_s	T_{total}
`Trec14`	15,904	3159	4.85×10^6	1	4.79	0.03	4.82
`Maragal_6`	21,251	10,144	4.96×10^7	3	13.1	0.12	13.2
`Maragal_7`	46,845	26,525	1.43×10^8	4	37.8	0.40	38.2
`scsd8-2r`	60,550	8650	1.20×10^7	0	0.88	0.00	0.88
`PDE1`	271,792	270,595	–	–	–	–	–
`12month1`	872,622	12,471	7.27×10^7	1	42.5	0.35	42.9

$nnz(L)$ denotes the number of entries in the Cholesky factor L of C and *Its*Its is the number of LSMR iterations. T_f, T_s and T_{total} denote the times (in seconds) to compute the normal matrix and factorize it, to run LSMR and the total time. – denotes unable to form normal matrix C

matrix $C+\alpha I_n = L(\alpha)L(\alpha)^T$ and use the factors as a preconditioner for the iterative method LSMR [13] (see [44]). In our tests, we set $\alpha = 10^{-12}$.

Results are given in Tables 5 and 6 for the normal equations and Schur complement approaches, respectively. For problem `PDE1`, the number of entries in the normal matrix C exceeds `huge(1)` so we cannot form C and use the direct solver `HSL_MA87`. The reported times T_f and T_p for computing the Cholesky factorization of C (Table 5) and the block factorization preconditioner (Table 6) include the time to form C and C_s, respectively. For problem `12month1`, forming C (or C_s)

Table 6 Results for test set 1 of solving the reduced augmented system (1.6) using the Schur complement approach and the Cholesky direct solver `HSL_MA87`. Results are also given for the indefinite solver `HSL_MA97`

Identifier	ρ	m_d	density(C_s)	$nnz(L)$	*Its*	T_p	T_s	T_{total}	$nnz(L_K)$	T_K
`Trec14`	0.050	4467	6.17×10^{-1}	1.48×10^7	1	4.09	0.06	4.14	7.97×10^6	7.18
	0.100	2664	8.31×10^{-1}	8.50×10^6	1	2.48	0.04	2.52	7.13×10^6	6.59
	0.200	1234	9.09×10^{-1}	5.73×10^6	1	2.41	0.02	2.43	6.76×10^6	5.63
`Maragal_6`	0.001	2923	6.22×10^{-4}	4.39×10^6	3	1.78	0.16	1.94	1.78×10^7	2.54
	0.010	823	1.93×10^{-2}	2.46×10^7	3	2.77	0.12	2.88	2.95×10^7	5.58
	0.100	68	5.49×10^{-2}	4.30×10^7	3	4.61	0.15	4.76	4.15×10^7	18.3
`Maragal_7`	0.001	4668	2.15×10^{-4}	1.12×10^7	4	9.51	0.69	10.2	6.15×10^7	12.9
	0.005	687	9.02×10^{-3}	9.04×10^7	3	11.7	0.36	12.1	1.10×10^8	26.5
`scsd8-2r`	0.050	50	1.44×10^{-3}	9.20×10^4	3	0.03	0.00	0.03	5.77×10^5	0.03
	0.100	40	1.39×10^{-2}	5.40×10^6	3	0.30	0.04	0.34	5.25×10^6	0.29
`PDE1`	0.100	1	4.52×10^{-5}	2.04×10^7	0	1.24	0.03	1.27	2.07×10^7	5.02
`12month1`	0.050	3641	5.66×10^{-1}	7.74×10^7	3	49.3	0.70	50.0	8.91×10^7	61.4
	0.100	284	6.56×10^{-1}	7.23×10^7	3	42.1	0.54	42.7	7.53×10^7	70.0

ρ is the row density parameter. density(C_s) is the ratio of the number of entries in the reduced normal matrix C_s to n^2, $nnz(L)$ is total number of entries in the factors (that is, $nnz(L_s) + m_d(m_d+1)/2$), *Its* is the number of GMRES iterations. T_p, T_s and T_{total} denote the times (in seconds) to compute the preconditioner, to run GMRES and the total time. T_K is the time to form the reduced augmented matrix and solve using the sparse symmetric indefinite direct solver `HSL_MA97` and $nnz(L_K)$ is the number of entries in `HSL_MA97` factors

accounts for approximately half the total time. Note we could try to employ a solver that avoids storing C in main memory. The out-of-core solver HSL_MA77 [39] only requires one column of C at a time and both matrix and factor data are written to files on disk, thus minimizing memory requirements. However, HSL_MA77 is for sparse matrices and when n is large and C is dense the amount of in-core memory available is still exceeded.

The results reported in Table 6 illustrate that the Schur complement approach is successful but to achieve savings compared to using the normal equations in terms of the size of the factors and/or the computation time, m_d must be small compared to n and the reduced normal matrix C_s must be sparse. For the Maragal problems, we are able to choose the density ρ to achieve this. In Table 6, we include the time T_K to form the reduced normal matrix K and then factorize and solve (1.6) using the symmetric indefinite solver HSL_MA97; we also report the number $nnz(L_K)$ of entries in the HSL_MA97 factors of K. A comparison of the times in the T_{total} and T_K columns illustrates the savings offered by the Schur complement approach that result from being able to exploit a Cholesky solver. Observe that although the symmetric indefinite solver HSL_MA97 ignores the block structure of K, as already noted, the sparsity-preserving nested dissection ordering it computes prior to the numerical factorization orders the dense rows last and thus the difference between $nnz(L)$ and $nnz(L_K)$ is generally relatively small. Furthermore, HSL_MA97 is able to take advantage of any zeros in the "dense" rows. If the number m_d of dense rows is not small, $nnz(L)$ is dominated by the storage needed for the dense factors of S_d (2.3) and $nnz(L)$ can then exceed $nnz(L_K)$; this is illustrated by problem Trec14.

5 Iterative method results

A software package HSL_MI35 that implements the limited memory IC algorithm outlined in Section 2.4 for computing a preconditioner for the normal equations has been developed for the HSL library. We employ this package in our experiments. Note that it handles ordering for sparsity and scaling and also automatically selects the shift α. We use the default settings and set the parameters $lsize$ and $rsize$ that control the maximum number of entries in each column of the factors to 20 (see [45] for more details of the parameters).

Before we present results for our two test sets, we illustrate that, for an iterative solver, handling null columns using the approach from Lemma 2.1 can be less efficient than using a global shift when constructing the preconditioner. Results are given in Table 7 for problem scagr7-2b from the University of Florida Collection ($m = 13,247$, $n = 9,743$). This example has a single row with a density greater than 10% (this row has a density of 18.4%). It was chosen because it illustrates how the number n_2 of null columns can increase as the number m_d of rows that are classified as dense increases. With $\rho > 0$, no shift is needed when computing the IC factorization but for $\rho = 0$, the shift that is automatically selected by HSL_MI35 is $\alpha = 4.1$ and preconditioned GMRES requires 370 iterations. With $\rho = 0.001$, $m_d = 263$ rows are classified as dense and there are $n_2 = 257$ null columns in A_s. For each solve, only 2 GMRES iterations are required but as there are 257 solves to

Table 7 Results for problem `scagr7-2b` of solving the reduced augmented system (1.6) using the Schur complement approach and restarted GMRES with the block IC factorization preconditioner

ρ	0	0.1	0.01	0.001
m_d	0	1	7	263
n_2	0	1	1	257
density(C_s)	4.15×10^{-2}	1.45×10^{-2}	7.13×10^{-4}	5.74×10^{-4}
T_p	0.48	0.50	0.03	0.10
T_s (*Its*) for z	0.33 (370)	0.09 (99)	0.004 (3)	0.007 (2)
T_s (*Its*) for W		0.06 (73)	0.002 (2)	1.65 (514)
T_{total}	0.81	0.65	0.04	1.75

ρ is the row density parameter. For $\rho > 0$, null columns are handled using (2.10) and (2.13); z and W refer to (2.10). m_d and n_2 are, respectively, the number of dense rows and the number of null columns in A_s. T_p, T_s and T_{total} denote the times (in seconds) to compute the preconditioner, to run GMRES and the total time. *Its* denotes the number of iterations

compute the solution W of (2.10), there is a total of 514 iterations, which dominate the total cost. If we ignore the null columns, then for $\rho = 0.001$, `HSL_MI35` selects a global shift of 9.67×10^{-7}, GMRES then requires two iterations and the total time reduces from 1.75 to 0.12 s. Based on this and experiments with other matrices, in the remainder of this section, we handle null columns in A_s using a global shift.

5.1 Results for test set 1

Table 8 presents results for running LSMR on (1.1) using the IC preconditioner. Here, the density of the rows is ignored. In Table 9, results are given for running GMRES on the reduced augmented system using the block IC factorization preconditioner. The time T_p includes the time for forming the reduced normal matrix C_s and computing its IC factorization, for solving (2.18), and for forming and factorizing the Schur complement matrix (2.19). For problems `Trec14`, `scsd8-2r` and `12month1`, results are given for more than one value of the parameter ρ that controls which rows

Table 8 Results for test set 1 of running LMSR on (1.1) with the `HSL_MI35` IC preconditioner

Identifier	m	n	α	*Its*	T_p	T_s	T_{total}
`Trec14`	15,904	3159	1.638×10^{1}	1050	4.52	3.19	7.71
`Maragal_6`	21,251	10,144	5.120×10^{-1}	1130	6.41	1.59	8.00
`Maragal_7`	46,845	26,525	2.048	410	19.9	1.47	21.4
`scsd8-2r`	60,550	8650	3.277×10^{1}	140	0.46	0.19	0.64
`PDE1`	271,792	270,595	–	–	–	–	–
`12month1`	872,622	12,471	1.024	200	32.6	10.0	42.7

α denotes the global shift, *Its* is the number of LSMR iterations. T_p, T_s and T_{total} denote the times (in seconds) to compute the IC preconditioner, to run LSMR and the total time

Table 9 Results for test set 1 of solving the reduced augmented system (1.6) using the Schur complement approach and restarted GMRES with the block IC factorization preconditioner

Identifier	m	n	ρ	m_d	density(C_s)	α	*Its*	T_p	T_s	T_{total}
`Trec14`	15,904	3159	0.050	4467	6.17×10^{-1}	6.400×10^{-2}	163	2.72	4.17	6.89
			0.100	2664	8.31×10^{-1}	2.560×10^{-1}	245	1.41	3.49	4.90
			0.200	1234	9.09×10^{-1}	1.024	352	1.71	2.74	4.45
`Maragal_6`	21,251	10,144	0.001	2923	6.22×10^{-4}	1.562×10^{-5}	62	1.46	1.86	3.33
`Maragal_7`	46,845	26,525	0.001	4668	2.15×10^{-4}	2.500×10^{-4}	15	8.95	1.74	10.7
`scsd8-2r`	60,550	8650	0.050	50	1.44×10^{-3}	9.766×10^{-7}	2	0.03	0.00	0.03
			0.100	40	1.39×10^{-2}	3.227×10^{1}	68	0.32	0.13	0.44
`PDE1`	27,1792	270,595	0.100	1	4.52×10^{-5}	8.000×10^{-3}	174	1.25	4.19	5.44
`12month1`	872,622	12,471	0.050	3641	5.66×10^{-1}	1.024	127	32.8	13.0	45.8
			0.100	284	6.56×10^{-1}	1.024	151	36.1	10.3	46.4

density(C_s) is the ratio of the number of entries in the reduced normal matrix C_s to n^2, α denotes the global shift, *Its* is the number of GMRES iterations. T_p, T_s and T_{total} denote the times (in seconds) to compute the preconditioner, to run GMRES and the total time

are classified as dense. As the density of C_s increases, a larger shift α is needed to prevent breakdown of the IC factorization and this has the effect of decreasing the quality of the preconditioner. However, for small ρ, for examples `12month1` and `Trec14`, m_d is large and each application of the preconditioner is relatively expensive. Consequently, although the GMRES iteration count is much less than the LSMR count, for these two problems, the Schur complement approach offers no significant benefit in terms of total time. For the other problems, exploiting the dense rows is advantageous. In particular, `PDE1` could not be solved using preconditioned LSMR on (1.1) but the reduced augmented system approach performs well. We observe that for the rank-deficient `Maragal` problems, we found it was necessary to use a very small ρ to obtain a preconditioner that gave rapid convergence of GMRES (larger values of ρ led to unacceptably slow convergence). Finally, we remark that the size of the incomplete factors for the normal equations approach is approximately $lsize * n$ while for the Schur complement approach, it is $lsize * n + m_d(m_d + 1)/2$ (recall in our experiments the `HSL_MI35` memory parameter $lsize$ is set to 20).

5.2 Results for test set 2

We now look at adding rows to the examples in test set 2. We first append a single row ($m_d = 1$) of increasing density and solve using LMSR on (1.1) with the `HSL_MI35` IC preconditioner. In Table 10, we report results for $\rho = 0.01, 0.1, 0.5$. Problem `CONT11_L` is omitted because the time to compute the IC factorization exceeds 600 s. In Table 11, results are given for $\rho = 1$; results are also given for running GMRES on the reduced augmented system using the block IC factorization preconditioner. We see that, if the normal equations are used, as ρ and hence the density of C increases, so too do the shift α needed to prevent breakdown, the

Table 10 Results for test set 2 with a single dense row of density ρ appended

Problem	density(C)	α	*Its*	T_p	T_s	T_{total}
$\rho = 0.01$						
IG5-15	1.52×10^{-1}	5.120×10^{-1}	280	0.18	0.29	0.47
psse0	5.33×10^{-4}	2.500×10^{-4}	1030	0.09	0.92	1.00
graphics	6.56×10^{-4}	2.500×10^{-4}	6350	0.03	6.30	6.33
WORLD	5.88×10^{-4}	1.638×10^{1}	1340	0.28	3.57	3.85
STAT96V3	4.57×10^{-4}	1.024	560	0.27	12.1	12.4
STORMG21K	4.00×10^{-4}	1.311×10^{2}	1620	51.9	101	153
GL7d20	3.23×10^{-4}	5.243×10^{2}	40	166	19.1	185
LargeRegFile	1.10×10^{-4}	1.311×10^{2}	70	127	7.68	134
relat9	6.09×10^{-4}	1.311×10^{2}	90	19.8	29.1	48.9
$\rho = 0.1$						
IG5-15	1.61×10^{-1}	3.277×10^{1}	810	0.23	0.83	1.07
psse0	1.06×10^{-2}	3.277×10^{1}	38,200	0.22	40.2	40.4
graphics	1.06×10^{-2}	3.277×10^{1}	$>$ 100,000	0.23	–	–
WORLD	1.05×10^{-2}	1.311×10^{2}	1840	0.88	4.91	5.79
STAT96V3	1.04×10^{-2}	1.311×10^{2}	880	1.19	19.86	21.0
STORMG21K	1.03×10^{-2}	1.049×10^{3}	1470	192	97.8	290
GL7d20	–	–	–	$>$ 600	–	$>$ 600
LargeRegFile	–	–	–	$>$ 600	–	$>$ 600
relat9	1.05×10^{-2}	5.243×10^{2}	90	63.7	28.6	92.3
$\rho = 0.5$						
IG5-15	3.64×10^{-1}	6.554×10^{1}	880	0.50	0.91	1.41
psse0	2.50×10^{-1}	2.621×10^{2}	34,570	1.31	40.64	41.96
graphics	2.50×10^{-1}	2.621×10^{2}	$>$ 100,000	1.38	–	–
WORLD	2.50×10^{-1}	5.243×10^{2}	2020	13.10	6.42	19.52
STAT96V3	2.50×10^{-1}	5.243×10^{2}	760	10.91	17.03	27.94
STORMG21K	–	–	–	$>$ 600	–	$>$ 600
GL7d20	–	–	–	$>$ 600	–	$>$ 600
LargeRegFile	–	–	–	$>$ 600	–	$>$ 600
relat9	–	–	–	$>$ 600	–	$>$ 600

Results are for LMSR on (1.1) using the IC factorization preconditioner. α denotes the global shift, *Its* is the number of iterations. T_p, T_s and T_{total} denote the times (in seconds) to compute the IC preconditioner, to run the iterative solver and the total time. – indicates statistic unavailable

time to compute the IC factorization, and the iterations for convergence. Indeed, for the large examples, the time exceeds our limit of 600 s. By contrast, for preconditioned GMRES on the reduced augmented system, the shift and the times to compute the incomplete factorization and achieve convergence are essentially independent of ρ (and for this reason only results for $\rho = 1.0$ are included in Table 11). Furthermore, this approach uses a smaller shift than for the normal equations and

Table 11 Results for test set 2 with a single dense row ($\rho = 1.0$) appended

Problem	Preconditioned LSMR					Reduced augmented system with GMRES				
	α	*Its*	T_p	T_s	T_{total}	α	*Its*	T_p	T_s	T_{total}
IG5-15	6.5536×10^{1}	810	0.92	0.82	1.73	1.024	337	0.47	1.08	1.55
psse0	2.6214×10^{2}	33,690	2.06	39.8	41.9	0.0	81	0.01	0.05	0.06
graphics	2.6214×10^{2}	>100,000	3.56	> 134	> 138	9.766×10^{-7}	900	0.02	1.49	1.51
WORLD	5.2429×10^{2}	2040	39.9	7.16	47.1	1.280×10^{-1}	294	1.32	1.31	2.63
STAT96V3	5.2429×10^{2}	750	23.9	16.8	40.7	0.0	20	0.20	0.04	0.23
STORMG21K	–	–	> 600	–	> 600	2.621×10^{2}	1320	19.5	211	230
GL7d20	–	–	> 600	–	> 600	5.120×10^{-1}	32	187	39.0	226
CONT11_L	–	–	> 600	–	> 600	8.000×10^{-3}	142	9.23	22.8	32.0
LargeRegFile	–	–	> 600	–	> 600	0.0	11	1.61	0.53	2.14
relat9	–	–	> 600	–	> 600	9.766×10^{-7}	41	32.3	3.18	35.5

Results are for LMSR on (1.1) using the IC factorization preconditioner and for solving the reduced augmented system (1.6) using the Schur complement approach and restarted GMRES with the block IC factorization preconditioner. α denotes the global shift, *Its* is the number of iterations. T_p, T_s and T_{total} denote the times (in seconds) to compute the IC preconditioner, to run the iterative solver and the total time. – indicates statistic unavailable

produces a much higher quality preconditioner, leading to significantly faster times. With more than one added row, the density of C often increases further, making the normal equation approach even less feasible. For the augmented approach, adding

Table 12 Results for test set 2 when m_d =1, 50 and 100 rows are appended

Problem	GMRES						MINRES					
	$m_d = 1$		$m_d = 50$		$m_d = 100$		$m_d = 1$		$m_d = 50$		$m_d = 100$	
	Its	T_{total}	*Its*	T_{total}	*Its*	T_{total}	*Its*	T_{total}	*Its*	T_{total}	*Its*	T_{total}
IG5-15	337	1.55	151	0.95	129	0.91	427	1.06	554	1.48	480	1.21
psse0	81	0.06	40	0.05	30	0.07	117	0.16	202	0.25	210	0.31
graphics	900	1.51	107	0.12	68	0.11	841	0.66	517	0.45	389	0.46
WORLD	294	2.63	158	2.13	116	2.21	348	2.35	563	3.77	463	4.48
STAT96V3	20	0.23	7	0.25	7	0.32	31	0.52	50	0.81	55	1.04
STORMG21K	1320	230	906	194	959	228	6197	335	–	> 600	–	> 600
GL7d20	32	226	22	222	22	231	36	207	60	232	60	241
CONT11_L	142	32.0	12	13.0	13	15.9	173	26.6	1556	290	1455	395
LargeRegFile	11	2.14	9	3.28	9	4.83	16	2.71	23	4.86	22	6.58
relat9	41	35.5	160	33.3	279	65.1	54	56.7	726	379	–	> 600

The reduced augmented system (1.6) is solved using the Schur complement approach and restarted GMRES and MINRES with the block IC factorization preconditioner. *Its* is the number of iterations and T_{total} is the total time

more than one row does not affect C_s or the time to compute the incomplete factorization but does result in the dense factorization of the Schur complement matrix becoming more expensive. For most of our test problems, the number of GMRES iterations decreases as the number of added rows increases (for example, `psse0` and `graphics`) but for others (including `relat9`), the converse is true (see Table 12). In these tests, MINRES was uncompetitive compared to GMRES in terms of iteration counts and times but has the advantage of requiring less storage. We remark that for problem `STORMG21K`, the iteration counts are high. For this example, the shift α that is needed by the IC factorization is large, which negatively effects the quality of the resulting preconditioner.

6 Concluding remarks

In this paper, we have focused on using the Schur complement approach to solve large-scale linear least-squares problems in which the system matrix A contains a number of nearly dense rows. Our proposed approach involves using a regularization parameter and then applying a Cholesky solver to the shifted reduced normal equations. A small number of steps of the iterative solver GMRES applied to the reduced augmented system are then employed to recover the solution of the original (unshifted) problem. We have considered some hard-to-solve problems (including some rank-deficient examples) from practical applications and shown that this approach offers savings (in terms of time and the size of the factors) compared to using a general sparse symmetric indefinite solver. The approach can be used with an incomplete Cholesky factorization preconditioner. In this case, a larger shift is required to prevent breakdown of the factorization, and this increases with the density of the reduced normal matrix and leads to a greater number of iterations being needed for convergence.

In addition to problems in which A contains some dense rows, we have considered examples where we added a number of dense rows to A. We found that, if the appended dense rows were not explicitly exploited, in some cases we were unable to achieve acceptable convergence using IC preconditioned LMSR. However, the use of the reduced normal matrix reduces the size of the shift that is needed, resulting in a higher quality preconditioner that successfully solved these examples.

We note that this paper complements the recent work in [48] in which preconditioned conjugate gradients (CGLS) is the main iterative method. It is shown there that once the dense rows are clearly defined and detected, the preconditioned iterative method is able to solve the problem extremely efficiently. In this study, we have gone beyond preconditioned conjugate gradients and use the power of direct methods to extend the solution of mixed sparse-dense problems to tough problems such as `WORLD` and the `Maragal` matrices that have so many null columns that further research is needed to be able to treat them as in [48].

Finally, we remark that although our main motivation for partitioning A is the presence of one or more dense rows, there are other possible reasons for employing a partitioning of the form (1.3). For example, a set of additional rows, that are not necessarily dense, is obtained by repeatedly adding new data into the least-squares

estimation of parameters in a linear model (see, for example, [3, 4]). Nowadays, there exist important applications based on this motivation related to Kalman filtering or solving recursive least-squares problems, see the seminal paper [25] or for a comprehensive introduction [10, 43]. Furthermore, additional constraints for the least-squares problem represented by A_d and b_d naturally arise with rank-deficient least-squares problems (for instance, [5, 7, 32]). If extra rows are added, the sparse (incomplete) Cholesky factorization within the Schur complement approach can be reused and so the only work needed to solve the updated system (or, in the incomplete case, to apply a preconditioner for the enlarged system) is the solution of triangular systems.

Acknowledgements We are very grateful to Michael Saunders and to an anonymous reviewer for their careful reading of our manuscript and for their constructive comments and suggestions that led to improvements in the presentation of this paper.

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