

# Fast Stable Solver for Sequentially Semi-separable Linear Systems of Equations

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## 1 Introduction

In this paper we will present a fast backward stable algorithm for the solution of certain structured matrices which can be either sparse or dense. It essentially combines the fast solution techniques for banded plus semi-separable linear systems of equations of Chandrasekaran and Gu [4] with similar techniques of Dewilde and van der Veen for time-varying systems [12].

We will also use the proposed techniques to suggest fast direct solvers for a class of spectral methods for which there had been no known fast direct solvers (not even unstable ones). This will illustrate the usefulness of the algorithms presented in this paper. This is the spectral method by Kress [11] for solving the integral equations of classical exterior scattering theory in two dimensions.

To be more specific, let  $A$  be an  $N \times N$  (possibly complex) matrix satisfying the matrix structure. Then there exist  $n$  positive integers  $m_1, \dots, m_n$  with  $N = m_1 + \dots + m_n$  to block-partition  $A$  as  $A = (A_{i,j})$ , where  $A_{i,j} \in \mathbf{C}^{m_i \times m_j}$  satisfies

$$A_{ij} = \begin{cases} D_i, & \text{if } i = j, \\ U_i W_{i+1} \cdots W_{j-1} V_j^H, & \text{if } j > i, \\ P_i R_{i-1} \cdots R_{j+1} Q_j^H, & \text{if } j < i. \end{cases} \quad (1)$$

Here we use the superscript  $H$  to denote the Hermitian transpose. The sequences  $\{U_i\}_{i=1}^{n-1}$ ,  $\{V_i\}_{i=2}^n$ ,  $\{W_i\}_{i=2}^{n-1}$ ,  $\{P_i\}_{i=2}^n$ ,  $\{Q_i\}_{i=1}^{n-1}$ ,  $\{R_i\}_{i=2}^{n-1}$  and  $\{D_i\}_{i=1}^n$  are all matrices whose dimensions are defined in Table 1. While any matrix can be represented in this form for large enough  $k_i$ 's and  $l_i$ 's, our main focus will be on matrices of this special form that have relatively small values for the  $k_i$ 's and  $l_i$ 's (see Section 3). In the above equation, empty products are defined to

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**Table 1.** Dimensions of matrices in (1).  $k_i$  and  $l_i$  are column dimensions of  $U_i$  and  $P_i$ , respectively

Matrix	$U_i$	$V_i$	$W_i$	$P_i$	$Q_i$	$R_i$
Dimensions	$m_i \times k_i$	$m_i \times k_{i-1}$	$k_{i-1} \times k_i$	$m_i \times l_i$	$m_i \times l_{i+1}$	$l_{i+1} \times l_i$

be the identity matrix. For  $n = 4$ , the matrix  $A$  has the form

$$A = \begin{pmatrix} D_1 & U_1 V_2^H & U_1 W_2 V_3^H & U_1 W_2 W_3 V_4^H \\ P_2 Q_1^H & D_2 & U_2 V_3^H & U_2 W_3 V_4^H \\ P_3 R_2 Q_1^H & P_3 Q_2^H & D_3 & U_3 V_4^H \\ P_4 R_3 R_2 Q_1^H & P_4 R_3 Q_2^H & P_4 Q_3^H & D_4 \end{pmatrix}.$$

We say that the matrix  $A$  is **sequentially semi-separable** if it satisfies (1). In the case where all  $W_i$  and  $R_i$  are identities,  $A$  reduces to a block-diagonal plus semi-separable matrix, which can be handled directly using techniques in Chandrasekaran and Gu [4]. It is shown in [12] that this class of matrices is closed under inversion and includes banded matrices, semi-separable matrices as well as their inverses as special cases.

It should be noted that the sequentially semi-separable structure of a given matrix  $A$  depends on the sequence  $m_i$ . Different sequences will lead to different representations. Through out this paper we will assume that the  $D_i$ 's are square matrices. The methods in this paper can be generalized to non-square representations too, but that matter will not be pursued here.

## 2 Fast Backward Stable Solver

In this section we describe a recursive and fast backward stable solver for the linear system of equations  $Ax = b$ , where  $A$  satisfies (1) and  $b$  itself is an unstructured matrix

We assume that the sequentially semi-separable matrix  $A$  is represented by the seven sequences  $\{U_i\}_{i=1}^{n-1}$ ,  $\{V_i\}_{i=2}^n$ ,  $\{W_i\}_{i=2}^{n-1}$ ,  $\{P_i\}_{i=2}^n$ ,  $\{Q_i\}_{i=1}^{n-1}$ ,  $\{R_i\}_{i=2}^{n-1}$  and  $\{D_i\}_{i=1}^n$  as in (1). We also partition  $x = (x_i)$  and  $b = (b_j)$  such that  $x_i$  and  $b_i$  have  $m_i$  rows. As in the  $4 \times 4$  example, there are two cases at each step of the recursion.

**Case of  $n > 1$  and  $k_1 < m_1$ : Elimination.** Our goal is to do orthogonal eliminations on both sides of  $A$  to create an  $(m_1 - k_1) \times (m_1 - k_1)$  lower triangular submatrix at the top left corner of  $A$ .

We perform orthogonal eliminations by computing  $QL$  and  $LQ$  factorizations

$$U_1 = q_1 \begin{pmatrix} 0 \\ \hat{U}_1 \end{pmatrix} \begin{matrix} m_1 - k_1 \\ k_1 \end{matrix} \quad \text{and} \quad (q_1^H D_1) = \begin{matrix} m_1 - k_1 \\ k_1 \end{matrix} \begin{pmatrix} m_1 - k_1 & k_1 \\ D_{11} & 0 \\ D_{21} & D_{22} \end{pmatrix} w_1,$$

where  $q_1$  and  $w_1$  are unitary matrices. To complete the eliminations, we also need to apply  $q_1^H$  to  $b_1$  and  $w_1$  to  $Q_1$  to obtain

$$q_1^H b_1 = \frac{m_1 - k_1}{k_1} \begin{pmatrix} \beta_1 \\ \gamma_1 \end{pmatrix} \quad \text{and} \quad w_1 Q_1 = \frac{m_1 - k_1}{k_1} \begin{pmatrix} Q_{11} \\ \hat{Q}_1 \end{pmatrix}.$$

Equations (1) have now become

$$\begin{pmatrix} q_1^H & 0 \\ 0 & I \end{pmatrix} A \begin{pmatrix} w_1^H & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} w_1 & 0 \\ 0 & I \end{pmatrix} x = \begin{pmatrix} q_1^H & 0 \\ 0 & I \end{pmatrix} b - \begin{pmatrix} 0 \\ P_2 \\ P_3 R_2 \\ P_4 R_3 R_2 \\ \vdots \\ P_n R_{n-1} \cdots R_2 \end{pmatrix} \tau, \quad (2)$$

We now orthogonally transform the unknowns  $x_1$  and solve the  $(m_1 - k_1) \times$

$(m_1 - k_1)$  lower triangular system of equations. Let  $\frac{m_1 - k_1}{k_1} \begin{pmatrix} z_1 \\ \hat{x}_1 \end{pmatrix} = w_1 x_1$ . Then the first  $m_1 - k_1$  equations of (2) has been simplified to  $D_{11} z_1 = \beta_1$ . Hence we compute  $z_1 = D_{11}^{-1} \beta_1$  by forward substitution.

We further compute  $\hat{b}_1 = \gamma_1 - D_{21} z_1$ . This in effect subtracts the  $D_{21}$  portion of the columns from the right-hand side. Finally we compute  $\hat{\tau} = \tau + Q_{11}^H z_1$ . This simple operation merges the previous pending subtraction at the right-hand side and the subtraction of the first  $m_1 - k_1$  columns (those corresponding to  $z_1$ ) from the new right-hand side.

At this stage, we discard the first  $m_1 - k_1$  equations and are left with a new linear system of equations

$$\hat{A} \hat{x} = \hat{b} - \begin{pmatrix} 0 \\ P_2 \\ P_3 R_2 \\ P_4 R_3 R_2 \\ \vdots \\ P_n R_{n-1} \cdots R_2 \end{pmatrix} \hat{\tau}$$

with exactly the same form as (1). To see this, we note that among the seven sequences  $\{U_i\}_{i=1}^{n-1}$ ,  $\{V_i\}_{i=2}^n$ ,  $\{W_i\}_{i=2}^{n-1}$ ,  $\{P_i\}_{i=2}^n$ ,  $\{Q_i\}_{i=1}^{n-1}$ ,  $\{R_i\}_{i=2}^{n-1}$  and  $\{D_i\}_{i=1}^n$ , everything remains the same except that  $U_1$ ,  $Q_1$ , and  $D_1$  have been replaced by  $\hat{U}_1$ ,  $\hat{Q}_1$ , and  $D_{22}$ . Among the partitioned unknown subvectors  $x_i$ 's and right hand side subvectors  $b_i$ 's, the only changes are that  $x_1$  and  $b_1$  have been replaced by  $\hat{x}_1$  and  $\hat{b}_1$ , respectively. Of course, the new linear system of equations has a strictly smaller dimension, hence we can indeed proceed with this recursion. After we

have computed the unknowns  $x_2$  to  $x_n$  and the transformed unknowns  $\hat{x}_1$ , we can recover  $x_1$  using the formula

$$x_1 = w_1^H \begin{pmatrix} z_1 \\ \hat{x}_1 \end{pmatrix}.$$

**Case of  $k_1 \geq m_1$ : Merge.** We perform merging in this case. In the case  $n > 1$  and  $m_1 \leq k_1$ , we cannot perform eliminations. Instead we merge the first two block rows and columns of  $A$  while still maintaining the sequentially semi-separable structure.

We merge the first two blocks by computing

$$\hat{D}_1 = \begin{pmatrix} D_1 & U_1 V_2^H \\ P_2 Q_1^H & D_2 \end{pmatrix}, \quad \hat{U}_1 = \begin{pmatrix} U_1 W_2 \\ U_2 \end{pmatrix}, \quad \text{and} \quad \hat{Q}_1 = \begin{pmatrix} Q_1 R_2^H \\ Q_2 \end{pmatrix}.$$

We merge  $x_1$  and  $x_2$  into  $\hat{x}_1$ , and we merge the right hand sides by computing

$$\hat{b}_1 = \begin{pmatrix} b_1 \\ b_2 - P_2 \tau \end{pmatrix} \quad \text{and} \quad \hat{\tau} = R_2 \tau.$$

Let  $\hat{A}$  and  $\hat{b}$  denote the matrix  $A$  and the vector  $b$  after this merge. We can rewrite (1) equivalently as

$$\hat{A} \hat{x} = \hat{b} - \begin{pmatrix} 0 \\ P_2 \\ P_3 R_2 \\ P_4 R_3 R_2 \\ \vdots \\ P_{n-1} R_{n-2} \cdots R_2 \end{pmatrix} \hat{\tau}.$$

Clearly  $\hat{A}$  is again a sequentially semi-separable matrix associated with the seven hatted sequences except that we have reduced the number of blocks from  $n$  to  $n - 1$ .

To complete the recursion, we observe that if  $n = 1$ , the equations (1) become the standard linear system of equations and can therefore be solved by standard solution techniques.

### 2.1 Flop Count

The total flop count for this algorithm can be estimated as follows. For simplicity we assume that compression and merging steps always alternate. We also assume without loss of generality that  $b$  has only one column. Then we can show that the leading terms of the flop count are given by

$$2 \sum_{i=1}^n (m_i + k_{i-1}) k_i^2 + (m_i + k_{i-1})^3 + (m_i + k_{i-1})^2 l_{i+1} + k_i^2 m_{i+1} + k_i l_{i+1} (m_{i+1} + l_i + l_{i+2}).$$

To get a better feel for the operation count we look at the important case when  $m_i = m$ ,  $k_i = k$  and  $l_i = l$ . Then the count simplifies to

$$2n(m^3 + m^2(3k + l) + m(3k + l) + m(3kl + 5k^2) + 2k^3 + k^2l + 2kl^2).$$

We observe that the count is not symmetric in  $k_i$  and  $l_i$ . Therefore sometimes it is cheaper to compute a  $URV^T$  factorization instead. This matter is also covered in [4]. When  $k = l$ , the count simplifies further to

$$2n(m^3 + 4m^2k + 8mk^2 + 5k^3).$$

If we make the further assumption that  $m = k$  then we get the flop count  $36nk^3$ . Note that the constant in front of the leading term is not large.

## 2.2 Experimental Run-Times

We now report the run-times of this algorithm on a PowerBook G4 running at 400 MHz with 768 MB of RAM. We used the ATLAS BLAS version 3.3.14 and LAPACK version 3 libraries. For comparison we also report the run-times of the standard dense solvers from LAPACK and ATLAS BLAS. All timings are reported in Table 2. The columns are indexed by the actual size of the matrix, which range from 256 to 8192. The horizontal rows are indexed by the value of  $m_i$  which is set equal to  $k_i$  and  $l_i$  for all  $i$  and ranges from 16 to 128. These are representative for many classes of problems (see [9]). In the last row we report the run-times in seconds of a standard dense (Gaussian elimination) solver from the LAPACK version 3 library running on top of the ATLAS BLAS version 3.3.14. These are highly-tuned routines which essentially run at peak flop rates.

From the table we can see the expected linear dependence on the size of the matrix. The non-quadratic dependence on  $m_i$  (and  $k_i$  and  $l_i$ ) seems to be due to the dominance of the low-order complexity terms. For example we observe a *decrease* in run-time when we increase  $m_i$  from 64 to 128 for a matrix of size 256! This is because at this size and rank the matrix has no structure and essentially a dense solver (without any of the overhead associated with a fast solver) is being used. There is also a non-linear increase in the run-time when we increase the size from 256 to 512 for  $m_i = k_i = l_i = 128$ . This is due to the lower over-heads associated with standard solver.

Restricting our attention to the last two rows in Table 2 where  $m_i = k_i = l_i = 128$  for all  $i$ , we observe that the fast algorithm breaks even with the dense solver for matrices of size between 512 and 1024. (The estimated flop count actually predicts a break-even around matrices of size 940.) For matrices of size 4096 we have speed-ups in excess of 17.2401. Since the standard solver becomes unusually slower for matrices of size 8192 (possibly due to a shortage of RAM) we get a speed-up of 130 at this size. The speed-ups are even better for smaller values of  $m_i$ 's.

We could further speed up the fast algorithm by using Gaussian elimination with partial pivoting instead of orthogonal transforms. This approach would still be completely stable as long as the dimensions of the diagonal blocks remain small.

**Table 2.** Run-times in seconds for both the fast stable algorithm and standard solver for random sequentially semi-separable matrices with  $m_i = k_i = l_i$  for all  $i$

$m_i = l_i = k_i$ for all $i$	size					
	256	512	1024	2048	4096	8192
16	0.04	0.08	0.16	0.36	0.67	1.34
32	0.08	0.19	0.42	0.83	1.66	3.44
64	0.18	0.48	1.12	2.36	4.8	9.87
128	0.15	1.01	2.73	6.09	12.91	26.9
Standard Solver (GEPP)	0.15	0.72	4.57	30.46	222.57	3499.46

### 3 Constructing Sequentially Semi-separable Matrices

In this section we consider the problem of computing the sequentially semi-separable structure of a matrix given the sequence  $\{m_i\}_{i=1}^n$  and a low-rank representation of some off-diagonal blocks. The second assumption is to allow for the efficient computation of the sequentially semi-separable representation of matrices possessing some other structure. The method presented can be applied to any unstructured matrix, thus proving that any matrix has a sequentially semi-separable structure (of course,  $k_i$  and  $l_i$  will usually be large in this case, precluding any speed-ups).

#### 3.1 General Construction Algorithm

Let  $A$  represent the matrix for which we wish to construct a sequentially semi-separable representation corresponding to the sequence  $\{m_i\}_{i=1}^n$ , where  $\sum m_i = N$ , the order of the matrix. Our procedure is similar to that of Dewilde and van der Veen [12]. Since the upper triangular part and lower triangular parts are so similar, we will only describe how to construct the sequentially semi-separable representation of the strictly block upper triangular part of  $A$ . The basic idea is to recursively compress off-diagonal blocks into low-rank representations.

Let  $H_i$  denote the off-diagonal block

$$H_i = \begin{pmatrix} U_1 W_2 \cdots W_i V_{i+1}^H & \cdots & U_1 W_2 \cdots W_{n-1} V_n^H \\ \vdots & \vdots & \vdots \\ U_i V_{i+1}^H & \cdots & U_i W_{i+1} \cdots W_{n-1} V_n^H \end{pmatrix}, \tag{3}$$

and let  $H_i \approx E_i \Sigma_i F_i^H$  denote a low-rank (also called economy) SVD of  $H_i$ . That is, we assume that the matrix of singular values  $\Sigma_i$ , is a square invertible matrix, all of whose singular values below a certain threshold have been set to zero. Therefore,  $E_i$  and  $F_i$  have an orthonormal set of columns, but they may not be unitary. Following Dewilde and van der Veen [12] we will call  $H_i$  the  $i$ th Hankel block. Each  $H_i$  is a  $\mu_i \times \nu_i$  matrix with  $\mu_i = m_1 + \cdots + m_i$  and  $\nu_i = m_{i+1} + \cdots + m_n$ .

Observe that we can obtain  $H_{i+1}$  from  $H_i$  by dropping the first  $m_{i+1}$  columns of  $H_i$  and then appending to the resulting matrix the last  $m_{i+1}$  rows of  $H_{i+1}$ . We will discuss the details of computing the SVD of  $H_{i+1}$  from that of  $H_i$  shortly.

For now, we want to compute the representation of  $H_i$  in (3) using the SVDs. Partition the SVD of  $H_i \approx E_i \Sigma_i F_i^H$  as:

$$E_i = \begin{matrix} \mu_{i-1} \\ m_i \end{matrix} \begin{pmatrix} E_{i,1} \\ E_{i,2} \end{pmatrix} \quad \text{and} \quad F_i = \begin{matrix} m_{i+1} \\ \nu_{i+1} \end{matrix} \begin{pmatrix} F_{i,1} \\ F_{i,2} \end{pmatrix}. \quad (4)$$

Observe that we can pick  $U_i = E_{i,2}$  and  $V_{i+1} = F_{i,1} \Sigma_i^H$  (of course  $\Sigma_i^H = \Sigma_i$ ).

How do we pick  $W_i$ ? Observe that  $H_{i+1}$  and  $H_i$  share a large block of the matrix. It follows from the sequentially semi-separable representation that we should pick  $W_{i+1}$  such that  $E_i W_{i+1}$  will give a column basis for the upper portion of  $H_{i+1}$ . It follows that we should pick  $W_{i+1}$  to satisfy the following requirement,  $E_i W_{i+1} = E_{i+1,1}$ . We can solve this easily to obtain  $W_{i+1} = E_i^H E_{i+1,1}$ .

The proof that these formulas work can be seen by substituting them back into the sequentially semi-separable representation beginning with  $H_1$ .

However, we are still not done. To compute the sequentially semi-separable representation efficiently it is important to compute the SVD of  $H_{i+1}$  quickly. To do that we need to use the SVD of  $H_i$ . As we mentioned earlier,  $H_{i+1}$  is obtained from  $H_i$  by dropping the first  $m_{i+1}$  columns of  $H_i$  and then appending to the resulting matrix the last  $m_{i+1}$  rows of  $H_{i+1}$ , which we will call  $Z$ . Hence we can rewrite  $H_{i+1}$  in the notation of (4) as

$$H_{i+1} \approx \begin{pmatrix} E_i \Sigma_i F_{i,2} \\ Z \end{pmatrix} = \begin{pmatrix} E_i & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} \Sigma_i F_{i,2} \\ Z \end{pmatrix}.$$

Hence we compute the low-rank SVD  $\begin{pmatrix} \Sigma_i F_{i,2} \\ Z \end{pmatrix} \approx \tilde{E} \tilde{\Sigma} \tilde{F}^H$  and obtain the low-rank SVD of  $H_{i+1}$  as follows:

$$H_{i+1} \approx \left( \begin{pmatrix} E_i & 0 \\ 0 & I \end{pmatrix} \tilde{E} \right) \tilde{\Sigma} \tilde{F}^H.$$

Finally, we note that the sequentially semi-separable representation for the lower triangular part of  $A$  can be computed by applying exactly the same procedure above to  $A^H$ . The computational costs are similar as well.

This algorithm takes  $O(N^2)$  flops, where the hidden constants depend on  $m_i$ ,  $k_i$  and  $l_i$ . The algorithm can be implemented to require only  $O(N)$  memory locations. This is particularly important in those applications where a large dense structured matrix can be generated (or read from a file) on the fly. Many computational electromagnetics problems involving integral equations fall in this class.

We can replace the use of singular value decompositions with rank-revealing  $QR$  factorizations ( $QR$  factorizations with column pivoting) quite easily. This

may result in some speed ups with little loss of compression. The only difficulty might be the lack of easily available software.

A totally different alternative is to use the recursively semi-separable (RSS) representation presented in the paper by Chandrasekaran and Gu [4]. This is usually easier to compute efficiently, but may be less flexible.

In many important applications the sequentially semi-separable representation needs to be computed only once for a fixed problem size and stored in a file. In such cases the cost of the exact algorithm is not important. Such cases include computing the sequentially semi-separable structure of spectral discretization methods of Greengard and Rokhlin [23, 29] for two-point boundary value problems and that of Kress [11] for integral equations of classical potential theory in two dimensions.

## 4 Two-Dimensional Scattering

For two-dimensional exterior scattering problems on analytic curves for acoustic and electro-magnetic waves, Kress' method of discretization of order  $2n$  will lead to a  $2n \times 2n$  matrix of the form

$$A = I + R \odot K_1 + K_2,$$

where  $K_1$  and  $K_2$  are low-rank matrices and

$$R_{ij} = -\frac{2\pi}{n} \sum_{m=1}^{n-1} \frac{1}{m} \cos \frac{m|i-j|\pi}{n} - \frac{(-1)^{|i-j|\pi}}{n^2}.$$

From the results in [9] we see that it is sufficient to verify that  $R$  is a sequentially semi-separable matrix of low Hankel-block ranks. It would then follow that  $A$  is a sequentially semi-separable matrix of low Hankel-block ranks. In Table 3 we exhibit the peak Hankel block ranks of  $R$ . The rows are indexed by the (absolute) tolerance we used to determine the numerical ranks of the Hankel blocks. In particular we used tolerances of  $10^{-8}$  and  $10^{-12}$  that are useful in practice. The columns are indexed by the size of  $R$ .

As can be seen the ranks seem to depend logarithmically on the size  $N$ , of  $R$ . This implies that the fast algorithm will take  $O(N \log^2 N)$  flops to solve linear systems involving  $A$ . We observe that the sequentially semi-separable representations of  $R$  for different sizes and tolerances need to be computed once and stored off-line. Then using the results in [9] we can compute the sequentially semi-separable representation of  $A$  rapidly on the fly.

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**Table 3.** Peak Hankel block ranks for the spectral method of Kress, Martensen and Kussmaul for the exterior Helmholtz problem.

tolerance	size					
	256	512	1024	2048	4096	8192
1E-8	28	32	34	37	38	40
1E-12	40	46	52	58	62	66

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