

Multigroup LSQ method and its generalization

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Abstract:

Multigroup least squares method (also known as a sequential LSQ method) was generalized into the cases of 1) two level parameter partition; 2) normal matrices with bordered tridiagonal structure. The latter case occurs when some parameters are modeled by linear splines. Algorithms for obtaining the adjustments and their covariance matrices are derived. The number of arithmetic operations is estimated as well. The number of arithmetic operations asymptotically depends on the third degree of the number of groups of parameters for a straightforward LSQ solution. It was shown that the number of operations for the proposed algorithms depends linearly on the number of groups of parameters, which allows a dramatic decrease in computation time.

Keywords: least squares method; sparse matrix; fast algorithms

1 Introduction

Problems of estimation of hundreds thousands parameters using millions observations arise frequently during analysis of modern experimental data such as GPS measurements, VLBI observations and some other space geodetic techniques. Straightforward solution of the system of 10^6 equations with 10^5 unknowns is a hopeless venture at the present time even using the most powerful supercomputers. Therefore it is necessary to take advantage of any particularities of the matrices of the equations which may allow us to construct more efficient algorithms. One such property is the fact that matrices of equations of conditions usually contain large fraction of zeroes. Indeed, each observation depends not on the entire set of parameters (their amount may exceed 10^5), but only on a small subset — tens or hundreds of parameters. Those parameters on which the observations are not dependent yield zeroes in the equations of conditions. A matrix which contains many zeroes is called "sparse matrix". Solving the system of linear equations results in executing arithmetic operations on the matrix elements. In treating sparse matrix a considerable fraction of operations will be executed on zeroes and although the result of such operations is known beforehand, these operations take the same resources as the operations on non-zero elements.

When we treat sparse matrices it is possible to implement special algorithms which take into account the presence of zeroes in the matrices and don't operate on the zero elements. General methods for solving systems of linear algebraic equations with sparse matrices were developed

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during the last 30 years and such approaches are called "sparse matrix technology" (Pissanetzky, 1984). The essence of the approaches is in finding some matrix reordering (e.g. permutation of rows and columns) to preserve the sparsity of the matrix for the maximum number of steps. In the general case this problem is difficult and requires rather sophisticated methods.

However for the case of parametric estimation of results of the measurements by LSQ method the problem is substantially facilitated for two reasons. We frequently can easily and without overhead reorder equations during the step of constructing the conditional system. Moreover, the distribution of the zeroes in the matrix (so-called "matrix portrait") for the typical cases is regular, what allows us to construct efficient algorithms for a number of important applications. Four partial cases of LSQ problem for sparse matrices will be considered. Algorithms for obtaining the adjustments and their covariance matrices will be derived. The number of arithmetic operations will be estimated as well.

2 Particular cases

The first case which we shall consider is the following. The parameters are partitioned into a global set and K blocks of local sets. Each observation depends on global parameters and only one block of local parameters. No one observation depends on parameters entering more than one block of local parameters. After reordering the system of conditional equations will have a form presented in fig. 1a. The corresponding normal matrix will be double bordered block diagonal as seen in fig. 1b. We denote this case as B_1D . Such a case was considered in Kaula (1963), Ma et al. (1990) and sometimes is called sequential least squares method.

Let's complicate this example by adding the next level of partitioning. We partition each group of observations which depends on one group of local parameters on k subsets of equations. Each such subset depends on one group of parameters which we shall call segmented parameters. As a result the parameters are partitioned into a set of global parameters, K groups of local parameters and k groups of segmented parameters. Each observation depends on a set of global parameters, a set of only one group of local parameters of i -th block and a set of only one group of segmented parameters of j -th block which corresponds to the i -th block of local parameters. The portrait of matrix of equations of conditions is shown in fig. 2a. The corresponding normal matrix is a double bordered block diagonal, but each large diagonal block is in turn a double bordered block diagonal matrix (fig. 2b). We call this case as B_1B_1D . This case was first used in Aksnes et al. (1988).

In the third case, which we denote as B_3D , a whole set of parameters is partitioned in the same manner as in case B_1D . But each observation depends on global parameters and on two adjacent groups of local parameters (fig. 3a). The normal matrix which corresponds to this case is double bordered block tridiagonal as it seen in fig. 3b.

And in the last case which we denote as B_1B_3D we modify case B_1B_1D in the same way as we transformed case B_1D into B_3D . Two level partitioning is used. The whole set of observations is divided into a global block, K blocks of local parameters and m blocks of segmented parameters. Each observation depends on a block of global parameters, i -th block of local parameters, j -th and $j+1$ -th blocks of segmented parameters which correspond to the i -th block of local ones. Matrices of equations of conditions and the normal matrix for this case are shown in figures 4a, 4b, respectively. Note that using linear spline parametrization results in the cases B_3D and B_1B_3D .

Now we shall derive algorithms for solving systems of normal equations for these cases. We

shall use a special scheme of Gauss with the operations performed on blocks rather than on numbers. This is legitimate if it is kept in mind that in general $AB \neq BA$ if A and B are matrices.

3 Algorithm B_1D

Let's consider for the first the simplest case. To produce a solution from the normal equations, decompose the normal matrix on the product of lower triangular matrices, find the estimates of global parameters, having substituted them to decomposed system consecutively obtain the estimates of local parameters. Finally find blocks of covariance matrices of the estimates. The technique used for solving problem for this case further will be generalized.

Step 1. Form blocks of the matrices of normal equations.

Cycle for $i = 1, 2, \dots, K$

1.1 For each i-th block we calculate the following quantities:

$$\begin{aligned} N_i^{gg} &= A_i^{g\top} A_i^g \\ N_i^{lg} &= A_i^{l\top} A_i^g \\ N_i^{ll} &= A_i^{l\top} A_i^l \end{aligned} \quad (1)$$

$$\begin{aligned} v_i^g &= A_i^{g\top} y_i \\ v_i^l &= A_i^{l\top} y_i \end{aligned} \quad (2)$$

1.2 And form blocks of normal system:

$$\begin{aligned} B_o &= \sum_i^K N_i^{gg} & z_o &= \sum_i^K v_i^g \\ B_i &= N_i^{lg} & C_i &= N_i^{ll} & z_i &= v_i^l \end{aligned} \quad (3)$$

End of cycle

Step 2. Transform the matrix to lower triangular form by eliminating upper o-th row. We multiply $B_i^\top C_i^{-1}$ by the i-th row and subtract result from the o-th row:

Cycle for $i = 1, 2, \dots, K$

$$\begin{aligned} B_o &:= B_o - \sum_i^K B_i^\top C_i^{-1} B_i \\ z_o &:= z_o - \sum_i^K B_i^\top C_i^{-1} z_i \end{aligned} \quad (4)$$

End of cycle

Decomposition completed. The matrix of the normal equations now has lower block triangular form with the block of global parameters at the left upper corner.

Step 3. Invert modified block B_o and find the estimates of the global parameters:

$$\begin{aligned} V_o &= B_o^{-1} \\ \hat{x}_o &= V_o z_o \end{aligned} \quad (5)$$

Step 4. Substituting the obtained estimates of global parameters we find local unknowns:

Cycle for $i = 1, 2, \dots, K$

$$\hat{x}_i = C_i^{-1}(z_i - B_i \hat{x}_o) \quad (6)$$

End of cycle

Let's find covariance matrices of the estimates under condition $\text{Cov}(y, y^\top) = I\sigma_o$. To derive them we prove the following lemma.

Lemma: Assume $\text{Cov}(y, y^\top) = I\sigma_o$. Let z be a transformed vector of right part of the normal equations after their triangular decomposition. Then $\text{Cov}(z, z^\top) = T\sigma_o$, where T is a block diagonal matrix with diagonal blocks of the decomposed normal matrix.

Proof: For a symmetric matrix N decomposition means a representation in form $L^\top TL$ where T is a block diagonal matrix and L is a lower triangular matrix with a unity main diagonal. The procedure of decomposition that was considered above transforms N to LT . Let us designate the matrix of that transformation as M . So we can write: $MN = LT$. Having multiplied all parts of the equality by N^{-1} and taking into account that matrix multiplication where one of the constituents is a diagonal matrix is a transitive operation we obtain:

$$M = L T (L^\top T L)^{-1} = (L^{-1})^\top$$

The right and left parts of the normal system have undergone the same transformation. Therefore, $z = MA^\top y$. Now we can easily calculate the covariance matrix of the vector z :

$$\text{Cov}(z, z^\top) = M A^\top \text{Cov}(y, y^\top) A M^\top = M N M^\top \sigma_o = (L^{-1})^\top (L^\top T L) L^{-1} \sigma_o = T \sigma_o$$

The lemma has been proven.

Consequently, we can write the blocks of the covariance matrix of the transformed vector z in the form:

$$\begin{aligned} \text{Cov}(z_o, z_o^\top) &= B_o \sigma_o \\ \text{Cov}(z_o, z_i^\top) &= 0 \\ \text{Cov}(z_i, z_j^\top) &= \begin{cases} C_i \sigma_o & i = j \\ 0 & i \neq j \end{cases} \end{aligned} \quad (7)$$

Taking into account (7) we find the covariance matrices of the blocks of the estimates:

1. Covariance between global parameters:

$$\text{Cov}(\hat{x}_o, \hat{x}_o^\top) = \text{Cov}(V_o z_o, z_o^\top V_o) = V_o B_o V_o \sigma_o = V_o \sigma_o \quad (8)$$

2. Covariance between local and global parameters:

$$\begin{aligned} \text{Cov}(\hat{x}_i, \hat{x}_o^\top) &= \text{Cov}(C_i^{-1} z_i - C_i^{-1} B_i \hat{x}_o, \hat{x}_o^\top) = \\ &= C_i^{-1} \text{Cov}(z_i, \hat{x}_o^\top) V_o - C_i^{-1} B_i \text{Cov}(\hat{x}_o, \hat{x}_o^\top) = -C_i^{-1} B_i V_o \sigma_o \end{aligned} \quad (9)$$

3. Covariance between local parameters:

$$\begin{aligned}
\text{Cov}(\hat{x}_i, \hat{x}_i^\top) &= \text{Cov}(\hat{x}_i, z_i^\top C_i^{-1} - \hat{x}_o^\top B_i^\top C_i^{-1}) = \\
&\quad \text{Cov}(\hat{x}_i, z_i^\top) C_i^{-1} - \text{Cov}(\hat{x}_i, \hat{x}_o^\top) B_i^\top C_i^{-1} = \\
&\quad \text{Cov}(C_i^{-1} z_i - C_i^{-1} B_i \hat{x}_o, z_i^\top C_i^{-1}) - \text{Cov}(\hat{x}_i, \hat{x}_o^\top) B_i^\top C_i^{-1} = \\
&\quad C_i^{-1} \sigma_o - \text{Cov}(\hat{x}_i, \hat{x}_o^\top) B_i^\top C_i^{-1} \\
\text{Cov}(\hat{x}_i, \hat{x}_j^\top) &= \text{Cov}(\hat{x}_i, z_j^\top C_j^{-1} - \hat{x}_o^\top B_j^\top C_j^{-1}) = \\
&\quad \text{Cov}(\hat{x}_i, z_j^\top) C_j^{-1} - \text{Cov}(\hat{x}_i, \hat{x}_o^\top) B_j^\top C_j^{-1} = \\
&\quad \text{Cov}(C_i^{-1} z_i - C_i^{-1} B_i \hat{x}_o, z_j^\top C_j^{-1}) - \text{Cov}(\hat{x}_i, \hat{x}_o^\top) B_j^\top C_j^{-1} = \\
&\quad - \text{Cov}(\hat{x}_i, \hat{x}_o^\top) B_j^\top C_j^{-1}
\end{aligned} \tag{10}$$

Comments.

1. The algorithm consists of three runs: decomposition, obtaining global parameters, and obtaining local parameters using calculated global ones. It is important that operations for each i-th steps of the 1-st and 3-rd run are independent and therefore may be accomplished in parallel. It is a consequence of the fact that different blocks of local parameters have no common parameters.
2. In general we need to know the values of dispersion of the unknowns (which are diagonal elements of covariance matrix), so usually it is necessary to calculate diagonal blocks of the covariance matrix, although knowledge of the full covariance matrix is seldom required. The cost of calculation diagonal covariance blocks is comparable to the cost for the full solution. Calculation of the full covariance matrix requires significantly more resources than obtaining estimates for the reason that in general the result of inversion of the sparse matrix is not a sparse matrix.

4 Algorithm $B_1 B_1 D$

Generalize the approach used for deriving previous solution to the case of two level partitioning. Let the matrix of normal equations be partitioned into K blocks of local parameters and each i-th block of local parameters be partitioned into k_i blocks of segmented parameters.

I. Form particular matrices of normal equations.

CYCLE FOR $i = 1, 2, \dots, K$

cycle for $j = 1, 2, \dots, k_i$

1.1 For each block of segmented parameters calculate the following quantities:

$$\begin{aligned}
N_{ij}^{ss} &= A_{ij}^{s,\top} A_{ij}^s \\
N_{ij}^{sl} &= A_{ij}^{s,\top} A_{ij}^l \\
N_{ij}^{sg} &= A_{ij}^{s,\top} A_{ij}^g \\
N_{ij}^{ll} &= A_{ij}^{l,\top} A_{ij}^l \\
N_{ij}^{lg} &= A_{ij}^{l,\top} A_{ij}^g \\
N_{ij}^{gg} &= A_{ij}^{g,\top} A_{ij}^g
\end{aligned} \tag{11}$$

$$\begin{aligned}
v_{ij}^s &= A_{ij}^{s \top} y_{ij} \\
v_{ij}^l &= A_{ij}^{l \top} y_{ij} \\
v_{ij}^g &= A_{ij}^{g \top} y_{ij}
\end{aligned} \tag{12}$$

1.2 Calculate the blocks of the normal equations:

$$\begin{aligned}
W_{oo} &= \sum_i^K \sum_j^{k_i} N_{ij}^{gg} & z_{oo} &= \sum_i^K \sum_j^{k_i} v_{ij}^{gg} \\
W_{io} &= \sum_j^{k_i} N_{ij}^{lg} & z_{io} &= \sum_j^{k_i} v_{ij}^l \\
W_{ij} &= N_{ij}^{sg} & z_{ij} &= v_{ij}^s \\
B_{io} &= \sum_j^{k_i} N_{ij}^{ll} \\
B_{ij} &= N_{ij}^{sl} \\
C_{ij} &= N^{ss}
\end{aligned} \tag{13}$$

end of cycle

END OF CYCLE

II. Matrix decomposition.

CYCLE FOR $i = 1, 2, \dots, K$

cycle for $j = 1, 2, \dots, k_i$

2.1 To exclude block W_{ij}^\top on the upper global row we multiply $W_{ij}^\top C_{ij}^{-1}$ by the ij-th row and subtract the result from the oo-th global row:

$$\begin{aligned}
W_{oo} &:= W_{oo} - W_{ij}^\top C_{ij}^{-1} W_{ij} \\
z_{oo} &:= z_{oo} - W_{ij}^\top C_{ij}^{-1} z_{ij}
\end{aligned} \tag{14}$$

2.2 To exclude block B_{ij}^\top on the upper i-th local row we multiply $B_{ij}^\top C_{ij}^{-1}$ by the ij-th row and subtract the result from the io-th row:

$$\begin{aligned}
B_{io} &:= B_{io} - B_{ij}^\top C_{ij}^{-1} B_{ij} \\
W_{io} &:= W_{io} - B_{ij}^\top C_{ij}^{-1} W_{ij} \\
z_{io} &:= z_{io} - B_{ij}^\top C_{ij}^{-1} z_{ij}
\end{aligned} \tag{15}$$

end of cycle

2.3 To exclude block W_{io}^\top on the upper global row we multiply $W_{io}^\top B_{io}^{-1}$ by the io-th row and subtract the result from the oo-th row:

$$\begin{aligned}
W_{oo} &:= W_{oo} - W_{io}^\top B_{io}^{-1} W_{io} \\
z_{oo} &:= z_{oo} - W_{io}^\top B_{io}^{-1} z_{io}
\end{aligned} \tag{16}$$

END OF CYCLE.

Decomposition completed.

III. Invert modified block B_{oo} and find the estimates of the global parameters:

$$\begin{aligned} V_{oo} &= W_{oo}^{-1} \\ \hat{x}_{oo} &= V_{oo} z_{oo} \end{aligned} \quad (17)$$

IV. Substituting the obtained estimates of global and local parameters we find local and segmented unknowns:

CYCLE FOR $i = 1, 2, \dots, K$

4.1 Obtain local parameters.

$$\hat{x}_{io} = B_{io}^{-1}(z_{io} - W_{io} \hat{x}_{oo}) \quad (18)$$

4.2 Obtain segmented parameters.

cycle for $j = 1, 2, \dots, k_i$

$$\hat{x}_{ij} = C_{ij}^{-1}(z_{ij} - W_{ij} \hat{x}_{oo} - B_{ij} \hat{x}_{io}) \quad (19)$$

end of cycle

END OF CYCLE

Now we find the covariance matrices for the blocks of the estimates.

1. Covariance between global parameters. Since the expression for the global parameters is the same as for the case $B_1 D$ we can rewrite the formula for the covariance matrix (8):

$$\text{Cov}(\hat{x}_{oo}, \hat{x}_{oo}^\top) = V_{oo} \sigma_o \quad (20)$$

2. Covariance between local and global parameters. Since the expression for the estimates of local parameters (18) is identical to the expression for the case $B_1 D$ (6), the formula for covariance matrix coincides with (9):

$$\text{Cov}(\hat{x}_{io}, \hat{x}_{oo}^\top) = -B_{io}^{-1} W_{io} V_{oo} \sigma_o \quad (21)$$

3. Covariance between segmented and global parameters.

$$\begin{aligned} \text{Cov}(\hat{x}_{ij}, \hat{x}_{oo}^\top) &= \text{Cov}(C_{ij}^{-1} z_{ij} - C_{ij}^{-1} W_{ij} \hat{x}_{oo} - C_{ij}^{-1} B_{ij} \hat{x}_{io}, \hat{x}_{oo}^\top) = \\ &= \text{Cov}(C_{ij}^{-1} z_{ij}, \hat{x}_{oo}^\top) - \text{Cov}(C_{ij}^{-1} W_{ij} \hat{x}_{oo}, \hat{x}_{oo}^\top) - \text{Cov}(C_{ij}^{-1} B_{ij} \hat{x}_{io}, \hat{x}_{oo}^\top) = \\ &= -\left(C_{ij}^{-1} W_{ij} \text{Cov}(\hat{x}_{oo}, \hat{x}_{oo}^\top) + C_{ij}^{-1} B_{ij} \text{Cov}(\hat{x}_{io}, \hat{x}_{oo}^\top) \right) \end{aligned} \quad (22)$$

4. Covariance between local parameters. Since the expression for the local parameters is the same as for the case $B_1 D$ we can rewrite the formula for the covariance matrix (10):

$$\text{Cov}(\hat{x}_{io}, \hat{x}_{io}^\top) = B_{io}^{-1} \sigma_o - \text{Cov}(\hat{x}_{io}, \hat{x}_{oo}^\top) W_{io}^\top B_{io}^{-1} \quad (23)$$

5. Covariance between segmented and local parameters $\text{Cov}(\hat{x}_{ij}, \hat{x}_{io}^\top)$:

$$\begin{aligned} \text{Cov}(\hat{x}_{ij}, \hat{x}_{io}^\top) &= \text{Cov}(C_{ij}^{-1}z_{ij} - C_{ij}^{-1}W_{ij}\hat{x}_{oo} - C_{ij}^{-1}B_{ij}\hat{x}_{io}, \hat{x}_{io}^\top) = \\ &- \left(C_{ij}^{-1}W_{ij}\text{Cov}^\top(\hat{x}_{io}, \hat{x}_{oo}^\top) + C_{ij}^{-1}B_{ij}\text{Cov}(\hat{x}_{io}, \hat{x}_{io}^\top) \right) \end{aligned} \quad (24)$$

6. Covariance matrix $\text{Cov}(\hat{x}_{ij}, \hat{x}_{ij}^\top)$:

$$\begin{aligned} \text{Cov}(\hat{x}_{ij}, \hat{x}_{ij}^\top) &= \\ \text{Cov}(C_{ij}^{-1}z_{ij} - C_{ij}^{-1}W_{ij}\hat{x}_{oo} - C_{ij}^{-1}B_{ij}\hat{x}_{io}, \hat{x}_{ij}^\top) &= \\ C_{ij}^{-1}\sigma_o - \left(C_{ij}^{-1}W_{ij}\text{Cov}(\hat{x}_{oo}, \hat{x}_{ij}^\top) + C_{ij}^{-1}B_{ij}\text{Cov}(\hat{x}_{io}, \hat{x}_{ij}^\top) \right) & \end{aligned} \quad (25)$$

5 Algorithm B_3D

Now we apply technique which we developed for the case B_1D to solve the system of equations with the double bordered block-tridiagonal matrix.

I. Form particular matrices of normal equations.

Cycle for $i = 1, 2, \dots, K$

1.1 Calculate the following quantities:

$$\begin{aligned} N_i^{gg} &= A_i^{g\top} A_i^g \\ N_i^{l1g} &= A_i^{l1\top} A_i^g \\ N_i^{l2g} &= A_i^{l2\top} A_i^g \\ N_i^{l1l1} &= A_i^{l1\top} A_i^{l1} \\ N_i^{l2l1} &= A_i^{l2\top} A_i^{l1} \\ N_i^{l2l2} &= A_i^{l2\top} A_i^{l2} \end{aligned} \quad (26)$$

$$\begin{aligned} v_i^g &= A_i^{g\top} y_i \\ v_i^{l1} &= A_i^{l1\top} y_i \\ v_i^{l2} &= A_i^{l2\top} y_i \end{aligned} \quad (27)$$

1.2 Calculate the blocks of the normal system:

$$\begin{array}{llllll} \forall i & B_o = \sum_i^K N_i^{gg} & & & z_o = \sum_i^K v_i^g & \\ i = 1 & B_1 = N_1^{l1g} & C_1 = N_1^{l1l1} & & z_1 = v_1^{l1} & \\ i \neq 1 \\ i \neq n & B_i = N_i^{l1g} + N_{i-1}^{l2g} & C_i = N_i^{l1l1} + N_{i-1}^{l2l2} & D_i = N_i^{l2l1} & z_i = v_i^{l1} + v_{i-1}^{l2} & \\ i = n & B_n = N_n^{l2g} & C_n = N_n^{l2l2} & D_n = N_n^{l2l1} & z_n = v_n^{l2} & \end{array} \quad (28)$$

End of cycle

II. Matrix decomposition:

Cycle for $i = K, K-1, \dots, 1$ (in back direction)

- 2.1 To exclude block B_i^\top on the upper row we multiply $B_i^\top C_i^{-1}$ by the i-th row and subtract the result from the o-th row:

$$\begin{aligned} B_o &:= B_o - B_i^\top C_i^{-1} B_i \\ z_o &:= z_o - B_i^\top C_i^{-1} z_i \end{aligned} \quad (29)$$

- 2.2 (only if $i > 1$) To exclude upper diagonal block D_i^\top we multiply $D_i^\top C_i^{-1}$ by the i-th row and subtract the result from the $i-1$ -th row:

$$\begin{aligned} B_{i-1} &:= B_{i-1} - D_i^\top C_i^{-1} B_i \\ C_{i-1} &:= C_{i-1} - D_i^\top C_i^{-1} D_i \\ z_{i-1} &:= z_{i-1} - D_i^\top C_i^{-1} z_i \end{aligned} \quad (30)$$

End of cycle.

Decomposition completed. As a result the matrix became lower triangular.

III. Invert modified block B_o and find the estimates of the global parameters:

$$\begin{aligned} V_o &= B_o^{-1} \\ \hat{x}_o &= V_o z_o \end{aligned} \quad (31)$$

IV. Determination local parameters. Subsequently substituting estimates of global parameters and estimates of antecedent block of local parameters we obtain the values of the estimates of local parameters of the i-th block.

Cycle for $i = 1, 2, \dots, K$ (in forward direction)

$$\begin{aligned} i = 1 &\quad \hat{x}_1 = C_1^{-1}(z_1 - B_1 \hat{x}_o) \\ \forall i > 1 &\quad \hat{x}_i = C_i^{-1}(z_i - B_i \hat{x}_o - D_i \hat{x}_{i-1}) \end{aligned} \quad (32)$$

End of cycle.

Let's find covariance matrices of the estimates. The covariance matrix of the transformed vectors of the right part will be the same as for the case $B_1 D$ (7) but now the letters B and C will denote the results of decomposition for the considered case.

1. Covariance between global parameters. Since the expression for the global parameters is the same as for the case $B_1 D$ we can rewrite the formula for the covariance matrix (8):

$$\text{Cov}(\hat{x}_o, \hat{x}_o^\top) = V_o \sigma_o \quad (33)$$

2. Covariance between global and local parameters of the 1-st block. Since the expression for the estimates of local parameters of the 1-st block (32) is identical to the expression for the estimates of local parameters for the case $B_1 D$ (6), the formula for covariance matrix coincides with (9):

$$\text{Cov}(\hat{x}_1, \hat{x}_o^\top) = -C_1^{-1} B_1 V_o \sigma_o \quad (34)$$

3. Covariance between local parameters of the 1-st block. For the same reason the expression for the covariance matrix coincides with (10):

$$\text{Cov}(\hat{x}_1, \hat{x}_1^\top) = C_1^{-1} \sigma_o - \text{Cov}(\hat{x}_1, \hat{x}_o^\top) B_1^\top C_1^{-1} \quad (35)$$

4. Covariance between local and global parameters of the i-st block ($i > 1$):

$$\begin{aligned} \text{Cov}(\hat{x}_i, \hat{x}_o^\top) = & \text{Cov}(C_i^{-1} z_i - C_i^{-1} B_i \hat{x}_o - C_i^{-1} D_i \hat{x}_{i-1}, \hat{x}_o^\top) = \\ & \text{Cov}(C_i^{-1} z_i, \hat{x}_o^\top) - \text{Cov}(C_i^{-1} B_i \hat{x}_o, \hat{x}_o^\top) - \text{Cov}(C_i^{-1} D_i \hat{x}_{i-1}, \hat{x}_o^\top) = \\ & - \left(C_i^{-1} B_i V_o \sigma_o + C_i^{-1} D_i \text{Cov}(\hat{x}_{i-1}, \hat{x}_o^\top) \right) \end{aligned} \quad (36)$$

5. Covariance between the same blocks of local parameters ($i > 1$):

$$\begin{aligned} \text{Cov}(\hat{x}_i, \hat{x}_i^\top) = & \text{Cov}(\hat{x}_i, z_i^\top C_i^{-1} - \hat{x}_o^\top B_i^\top C_i^{-1} - \hat{x}_{i-1}^\top D_i^\top C_i^{-1}) = \\ & \text{Cov}(\hat{x}_i, z_i^\top C_i^{-1}) - \text{Cov}(\hat{x}_i, \hat{x}_o^\top B_i^\top C_i^{-1}) - \text{Cov}(\hat{x}_i, \hat{x}_{i-1}^\top D_i^\top C_i^{-1}) = \\ & C_i^{-1} - \left(\text{Cov}(\hat{x}_i, \hat{x}_o^\top) B_i^\top C_i^{-1} + \text{Cov}(\hat{x}_i, \hat{x}_{i-1}^\top) D_i^\top C_i^{-1} \right) \end{aligned} \quad (37)$$

6. Covariance between the adjacent blocks of local parameters ($i < n$):

$$\begin{aligned} \text{Cov}(\hat{x}_{i+1}, \hat{x}_i^\top) = & \text{Cov}(C_{i+1}^{-1} z_{i+1} - C_{i+1}^{-1} B_{i+1} \hat{x}_o - C_{i+1}^{-1} D_{i+1} \hat{x}_i, \hat{x}_i^\top) = \\ & \text{Cov}(C_{i+1}^{-1} z_{i+1}, \hat{x}_i^\top) - \text{Cov}(C_{i+1}^{-1} B_{i+1} \hat{x}_o, \hat{x}_i^\top) - \text{Cov}(C_{i+1}^{-1} D_{i+1} \hat{x}_i, \hat{x}_i^\top) = \\ & - \left(C_{i+1}^{-1} B_{i+1} \text{Cov}^\top(\hat{x}_i, \hat{x}_o^\top) + C_{i+1}^{-1} D_{i+1} \text{Cov}(\hat{x}_i, \hat{x}_i^\top) \right) \end{aligned} \quad (38)$$

Comment: This algorithm doesn't permit to make operations on blocks in arbitrary order in contrast to the algorithm $B_1 D$; it is substantially sequential. This property stems from the presence of off-diagonal blocks in the normal matrix.

6 Algorithm $B_1 B_3 D$

Using the approaches developed for deriving previous solutions we find a solution for the case $B_1 B_3 D$. Let the matrix of normal equations be partitioned on into blocks of local parameters and each i-th block of local parameters be partitioned into k_i blocks of segmented parameters.

I. Form particular matrices of normal equations.

CYCLE FOR $i = 1, 2 \dots K$

cycle for $j = 1, 2 \dots k_i$

1.1 Calculate the following quantities:

$$\begin{aligned} N_{ij}^{s1s1} &= A_{ij}^{s1\top} A_{ij}^{s1} \\ N_{ij}^{s1l} &= A_{ij}^{s1\top} A_{ij}^l \\ N_{ij}^{s1g} &= A_{ij}^{s1\top} A_{ij}^g \\ N_{ij}^{s2l} &= A_{ij}^{s2\top} A_{ij}^l \\ N_{ij}^{s2g} &= A_{ij}^{s2\top} A_{ij}^g \\ N_{ij}^{s2s1} &= A_{ij}^{s2\top} A_{ij}^{s1} \\ N_{ij}^{ll} &= A_{ij}^{l\top} A_{ij}^l \\ N_{ij}^{lg} &= A_{ij}^{l\top} A_{ij}^g \\ N_{ij}^{gg} &= A_{ij}^{g\top} A_{ij}^g \end{aligned} \quad (39)$$

$$\begin{aligned}
v_{ij}^{s1} &= A_{ij}^{s1\top} y_{ij} \\
v_{ij}^{s2} &= A_{ij}^{s2\top} y_{ij} \\
v_{ij}^l &= A_{ij}^{l\top} y_{ij} \\
v_{ij}^g &= A_{ij}^{g\top} y_{ij}
\end{aligned} \tag{40}$$

1.2 Calculate the blocks of the normal equations:

$$\begin{aligned}
W_{oo} &= \sum_i^K \sum_j^{k_i} N_{ij}^{gg} & z_{oo} &= \sum_i^K \sum_j^{k_i} v_{ij}^{gg} \\
W_{io} &= \sum_j^{k_i} N_{ij}^{lg} & z_{io} &= \sum_j^{k_i} v_{ij}^l \\
W_{ij} &= \begin{cases} j=1 & N_{i1}^{s1g} \\ j \neq 1, k_i & N_{ij}^{s1g} + N_{ij-1}^{s2g} \\ j=k_i & N_{ik-1}^{s2g} \end{cases} & z_{ij} &= \begin{cases} j=1 & v_{i1}^{s1} \\ j \neq 1, k_i & v_{ij}^{s1} + v_{ij-1}^{s2} \\ j=k_i & v_{ik-1}^{s2} \end{cases} \\
B_{io} &= \sum_j^{k_i} N_{ij}^{ll} & & \\
B_{ij} &= \begin{cases} j=1 & N_{i1}^{s1l} \\ j \neq 1, k_i & N_{ij}^{s1l} + N_{ij-1}^{s2l} \\ j=k_i & N_{ik-1}^{s2l} \end{cases} & & \\
C_{ij} &= \begin{cases} j=1 & N_{i1}^{s1s1} \\ j \neq 1, k_i & N_{ij}^{s1s1} + N_{ij-1}^{s2s2} \\ j=k_i & N_{ik-1}^{s2s2} \end{cases} & & \\
D_{ij} &= N_{ij}^{s2s1} & &
\end{aligned} \tag{41}$$

end of cycle

END OF CYCLE

II. Matrix decomposition.

CYCLE FOR $i = 1 \dots K$

cycle for $j = k_i, k_i - 1 \dots 1$ (in back direction)

2.1 To exclude block W_{ij}^\top on the upper global row we multiply $W_{ij}^\top C_{ij}^{-1}$ by the ij-th row and subtract the result from the oo-th global row:

$$\begin{aligned}
W_{oo} &:= W_{oo} - W_{ij}^\top C_{ij}^{-1} W_{ij} \\
z_{oo} &:= z_{oo} - W_{ij}^\top C_{ij}^{-1} z_{ij}
\end{aligned} \tag{42}$$

2.2 To exclude block B_{ij}^\top on the upper i-th local row we multiply $B_{ij}^\top C_{ij}^{-1}$ by

the ij-th row and subtract the result from the io-th row:

$$\begin{aligned} B_{io} &:= B_{io} - B_{ij}^T C_{ij}^{-1} B_{ij} \\ W_{io} &:= W_{io} - B_{ij}^T C_{ij}^{-1} W_{ij} \\ z_{io} &:= z_{io} - B_{ij}^T C_{ij}^{-1} z_{ij} \end{aligned} \quad (43)$$

2.3 (only if $j > 1$) To exclude the upper diagonal block D_{ij}^T we multiply $D_{ij}^T C_{ij}^{-1}$ by the ij-th row and subtract the result from the ij-1-th row:

$$\begin{aligned} C_{ij-1} &:= C_{ij-1} - D_{ij}^T C_{ij}^{-1} D_{ij} \\ B_{ij-1} &:= B_{ij-1} - D_{ij}^T C_{ij}^{-1} B_{ij} \\ W_{ij-1} &:= W_{ij-1} - D_{ij}^T C_{ij}^{-1} W_{ij} \\ z_{ij-1} &:= z_{ij-1} - D_{ij}^T C_{ij}^{-1} z_{ij} \end{aligned} \quad (44)$$

end of cycle

2.4 To exclude block W_{io}^T on the upper global row we multiply $W_{io}^T B_{io}^{-1}$ by the io-th row and subtract the result from the oo-th row:

$$\begin{aligned} W_{oo} &:= W_{oo} - W_{io}^T B_{io}^{-1} W_{io} \\ z_{oo} &:= z_{oo} - W_{io}^T B_{io}^{-1} z_{io} \end{aligned} \quad (45)$$

END OF CYCLE.

Decomposition completed.

III. Invert modified block B_{oo} and find the estimates of the global parameters:

$$\begin{aligned} V_{oo} &= W_{oo}^{-1} \\ \hat{x}_{oo} &= V_{oo} z_{oo} \end{aligned} \quad (46)$$

IV. Substituting the obtained estimates of global, local and segmented parameters we consequently find local and segmented unknowns:

CYCLE FOR $i = 1, 2, \dots, K$

4.1 Obtain local parameters.

$$\hat{x}_{io} = B_{io}^{-1} (z_{io} - W_{io} \hat{x}_{oo}) \quad (47)$$

4.2 Obtain segmented parameters.

cycle for $j = 1, 2, \dots, k_i$ (in forward direction)

$$\begin{aligned} j = 1 &\quad \hat{x}_{i1} = C_{i1}^{-1} (z_{i1} - W_{i1} \hat{x}_{oo} - B_{i1} \hat{x}_{io}) \\ j > 1 &\quad \hat{x}_{ij} = C_{ij}^{-1} (z_{ij} - W_{ij} \hat{x}_{oo} - B_{ij} \hat{x}_{io} - D_{ij} \hat{x}_{ij-1}) \end{aligned} \quad (48)$$

end of cycle

END OF CYCLE

Find the covariance matrices for the blocks of the estimates using the same technique as for the previous cases.

1. Covariance matrices $\text{Cov}(\hat{x}_{oo}, \hat{x}_{oo}^\top)$, $\text{Cov}(\hat{x}_{io}, \hat{x}_{oo}^\top)$, $\text{Cov}(\hat{x}_{io}, \hat{x}_{io}^\top)$ are the same as for the case $B_1 B_1 D$ since the expressions for the estimates are the same:

$$\begin{aligned}\text{Cov}(\hat{x}_{oo}, \hat{x}_{oo}^\top) &= V_{oo} \sigma_o \\ \text{Cov}(\hat{x}_{io}, \hat{x}_{oo}^\top) &= -B_{io}^{-1} W_{io} V_{oo} \sigma_o \\ \text{Cov}(\hat{x}_{io}, \hat{x}_{io}^\top) &= B_{io}^{-1} \sigma_o - \text{Cov}(\hat{x}_{io}, \hat{x}_{oo}^\top) W_{io}^\top B_{io}^{-1}\end{aligned}\quad (49)$$

For the same reason covariance matrices with the first block of segmented parameters are exactly the same as for $B_1 B_1 D$ case:

$$\begin{aligned}\text{Cov}(\hat{x}_{i1}, \hat{x}_{oo}^\top) &= -\left(C_{i1}^{-1} W_{i1} \text{Cov}(\hat{x}_{oo}, \hat{x}_{oo}^\top) + C_{i1}^{-1} B_{i1} \text{Cov}(\hat{x}_{io}, \hat{x}_{oo}^\top)\right) \\ \text{Cov}(\hat{x}_{i1}, \hat{x}_{io}^\top) &= -\left(C_{i1}^{-1} W_{i1} \text{Cov}^\top(\hat{x}_{io}, \hat{x}_{oo}^\top) + C_{i1}^{-1} B_{i1} \text{Cov}(\hat{x}_{io}, \hat{x}_{io}^\top)\right) \\ \text{Cov}(\hat{x}_{i1}, \hat{x}_{i1}^\top) &= C_{i1}^{-1} \sigma_o - \left(C_{i1}^{-1} W_{i1} \text{Cov}^\top(\hat{x}_{i1}, \hat{x}_{oo}^\top) + C_{i1}^{-1} B_{i1} \text{Cov}^\top(\hat{x}_{i1}, \hat{x}_{io}^\top)\right)\end{aligned}\quad (50)$$

2. Covariance matrix $\text{Cov}(\hat{x}_{ij}, \hat{x}_{io}^\top)$:

$$\begin{aligned}\text{Cov}(\hat{x}_{ij}, \hat{x}_{io}^\top) &= \text{Cov}(C_{ij}^{-1} z_{ij} - C_{ij}^{-1} W_{ij} \hat{x}_{oo} - C_{ij}^{-1} B_{ij} \hat{x}_{io} - C_{ij}^{-1} D_{ij} \hat{x}_{ij-1}, \hat{x}_{io}^\top) = \\ &- \left(C_{ij}^{-1} W_{ij} \text{Cov}^\top(\hat{x}_{io}, \hat{x}_{oo}^\top) + C_{ij}^{-1} B_{ij} \text{Cov}(\hat{x}_{io}, \hat{x}_{io}^\top) + C_{ij}^{-1} D_{ij} \text{Cov}(\hat{x}_{ij-1}, \hat{x}_{io}^\top)\right)\end{aligned}\quad (51)$$

3. Covariance matrix $\text{Cov}(\hat{x}_{ij}, \hat{x}_{ij}^\top)$:

$$\begin{aligned}\text{Cov}(\hat{x}_{ij}, \hat{x}_{ij}^\top) &= \text{Cov}(C_{ij}^{-1} z_{ij} - C_{ij}^{-1} W_{ij} \hat{x}_{oo} - C_{ij}^{-1} B_{ij} \hat{x}_{io} - C_{ij}^{-1} D_{ij} \hat{x}_{ij-1}, \hat{x}_{ij}^\top) = \\ &C_{ij}^{-1} - \left(C_{ij}^{-1} W_{ij} \text{Cov}^\top(\hat{x}_{ij}, \hat{x}_{oo}^\top) + C_{ij}^{-1} B_{ij} \text{Cov}^\top(\hat{x}_{ij}, \hat{x}_{io}^\top) + C_{ij}^{-1} D_{ij} \text{Cov}^\top(\hat{x}_{ij}, \hat{x}_{ij-1}^\top)\right)\end{aligned}\quad (52)$$

4. Covariance matrix $\text{Cov}(\hat{x}_{ij+1}, \hat{x}_{ij}^\top)$:

$$\begin{aligned}\text{Cov}(\hat{x}_{ij+1}, \hat{x}_{ij}^\top) &= \\ \text{Cov}(C_{ij+1}^{-1} z_{ij+1} - C_{ij+1}^{-1} W_{ij+1} \hat{x}_{oo} - C_{ij+1}^{-1} B_{ij+1} \hat{x}_{io} - C_{ij+1}^{-1} D_{ij+1} \hat{x}_{ij}, \hat{x}_{ij}^\top) &= \\ - \left(C_{ij+1}^{-1} W_{ij+1} \text{Cov}^\top(\hat{x}_{ij}, \hat{x}_{oo}^\top) + C_{ij+1}^{-1} B_{ij+1} \text{Cov}^\top(\hat{x}_{ij}, \hat{x}_{io}^\top) + C_{ij+1}^{-1} D_{ij+1} \text{Cov}(\hat{x}_{ij}, \hat{x}_{ij}^\top)\right) &\end{aligned}\quad (53)$$

7 Cost of the algorithms

Let's estimate asymptotic complexity of the algorithms taking into account the fact that multiplying matrix with dimension $n \times l$ by matrix $l \times m$ requires $n \cdot l \cdot m$ pairs of additions and multiplications (in the case when $n = m$ and the result is a symmetric matrix — $l \cdot n^2/2$ operations), and inversion of square symmetric matrix with dimension $n \times n$ requires approximately $n^3/2$ pairs of operations.

It is not difficult to find asymptotic estimates for the number of pairs of arithmetic operations under the assumption that the number of local and segmented parameters is equal for each block.

The number of operations for constructing normal matrix for the considered cases and for the case when sparseness of the matrix is ignored (F) is:

$$\begin{aligned}
\text{Op}^n(F) &\approx \frac{M}{2} \left(K(ks + l) + g \right)^2 \\
\text{Op}^n(B_1 D) &\approx \frac{M}{2} (l + g)^2 \\
\text{Op}^n(B_3 D) &\approx \frac{M}{2} (2l + g)^2 \\
\text{Op}^n(B_1 B_1 D) &\approx \frac{M}{2} (s + l + g)^2 \\
\text{Op}^n(B_1 B_3 D) &\approx \frac{M}{2} (2s + l + g)^2
\end{aligned} \tag{54}$$

where M — the number of equations, l — the number of local parameters in one group, K — the number of groups of local parameters, k — the number of groups of segmented parameters in one block of local ones, g — the number of global parameters.

The number of operations for solving normal system of equations is:

$$\begin{aligned}
\text{Op}^s(F) &\approx \frac{(K(ks + l) + g)^3}{6} \\
\text{Op}^s(B_1 D) &\approx \frac{Kl(l + g)^2}{2} + \frac{g^3}{2} \\
\text{Op}^s(B_3 D) &\approx \frac{Kl(2l + g)^2}{2} + \frac{g^3}{2} \\
\text{Op}^s(B_1 B_1 D) &\approx \frac{Kks(s + l + g)^2}{2} + \frac{Kl(l + g)^2}{2} + \frac{g^3}{2} \\
\text{Op}^s(B_1 B_3 D) &\approx \frac{Kks(2s + l + g)^2}{2} + \frac{Kl(l + g)^2}{2} + \frac{g^3}{2}
\end{aligned} \tag{55}$$

It is worth noticing that if we make operation to be reciprocal to decomposition: multiply the decomposed matrix by transposed matrix and avoid all operations on zero blocks, it will asymptotically require exactly the same number of operations. That means that the matrix sparseness was fully exploited in decomposition process.

The number of additional pairs of operations needed for calculation of the covariance matrices for the blocks which correspond to non-zero blocks of normal matrix is:

$$\begin{aligned}
\text{Op}^c(F) &\approx \frac{1}{3}(K(ks + l) + g)^3 \\
\text{Op}^c(B_1 D) &\approx Klg \left(\frac{1}{2}l + g \right) \\
\text{Op}^c(B_3 D) &\approx Kl(l + g) \left(\frac{3}{2}l + g \right) \\
\text{Op}^c(B_1 B_1 D) &\approx Kks(s + l + g) \left(\frac{1}{2}s + l + g \right) + Kl(l + g) \left(\frac{1}{2}l + g \right) \\
\text{Op}^c(B_1 B_3 D) &\approx Kks(s + l + g) \left(\frac{3}{2}s + l + g \right) + Kl(l + g) \left(\frac{1}{2}l + g \right)
\end{aligned} \tag{56}$$

As it seen from expressions (54)–(56) the number of operations for multigroup algorithms depends linearly on the number of groups of parameters whereas it depends asymptotically on the third degree of the number of groups of parameters for the straightforward solution if we neglect sparseness of the normal matrix.

8 Hints at further improvement of performance

When we calculated the estimates of the number of operations during constructing normal matrix we assumed that each observation depends on the entire set of global parameters, entire set of local and segmented parameters of its group and subgroup. In general this is not always true. In the case when there are global, local and segmented parameters on which an equation does not depend we can exclude them from computation. As a result we should substitute in expression (54) not the actual number of parameters in their blocks but the average number of parameters on which an equation depends. For this reason time required to form the normal matrix is usually less than time of decomposition.

In using two-level partitioning algorithms (B_1B_1D and B_1B_3D) we can exploit the fact that a local subgroup of equations can depend on only a subset of global parameters. In that case we should construct the reduced matrices W_{oo}^r , W_{io}^r and W_{ij}^r for the subset of global parameters on which equations of considered local subgroup depend (W_{oo}^r should be initialized by zeroes). These matrices will have smaller dimensions. Operations (14, 15) or (42, 43) will be executed on the W^r matrices. After completing the cycle, the matrices W^r should be rearranged by adding zero columns and rows for augmenting their dimensions. In using this trick we should substitute in (55) not the number of all global parameters but the average number of global parameters on which equations of one local subgroup depend.

9 Acknowledgments.

The author is grateful to J. Ryan for help in implementation developed algorithms in SOLVE software system for data analysis of very long baseline interferometric observations.

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A_1^g	A_1^ℓ					y_1
A_2^g		A_2^ℓ				y_2
A_3^g			A_3^ℓ			y_3
A_4^g				A_4^ℓ		y_4
A_5^g					A_5^ℓ	y_5

fig. 1a

\mathbf{B}_o	B_1^T	B_2^T	B_3^T	B_4^T	B_5^T	\mathbf{z}_o
B_1	C_1					z_1
B_2		C_2				z_2
B_3			C_3			z_3
B_4				C_4		z_4
B_5					C_5	z_5

fig. 1b

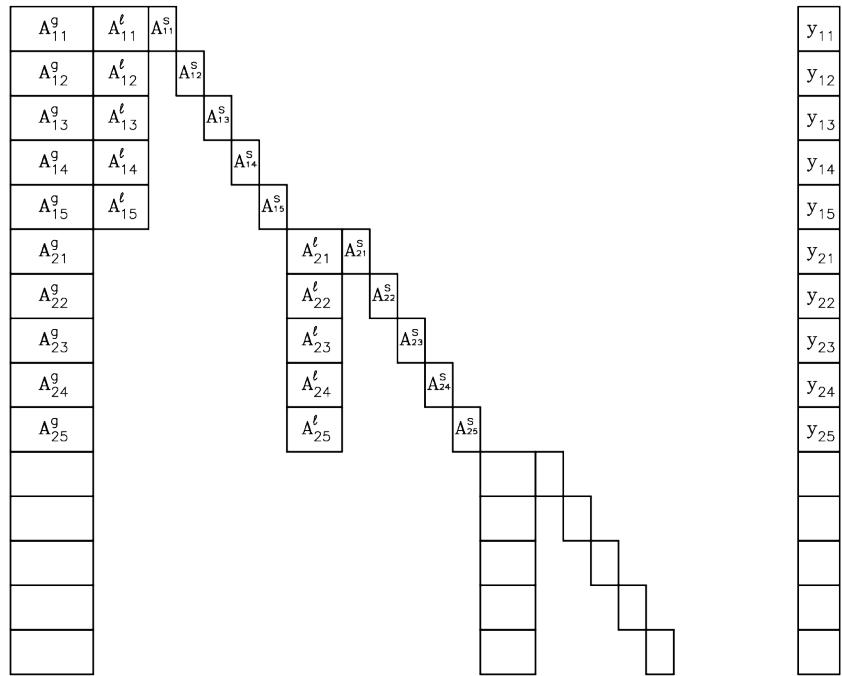


fig. 2a

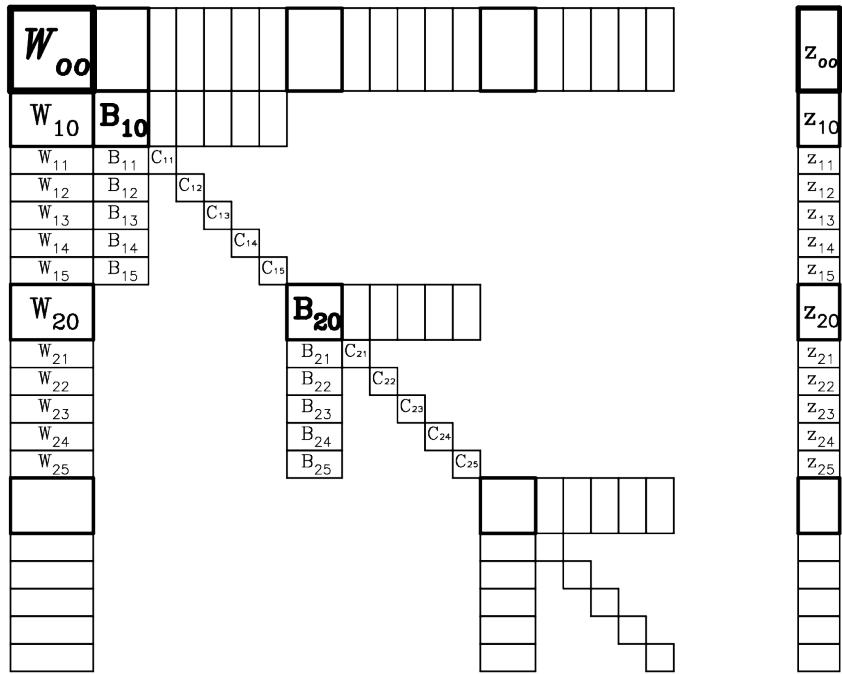


fig. 2b

A_1^g	$A_1^{\ell 1}$	$A_1^{\ell 2}$			y_1
A_2^g		$A_2^{\ell 1}$	$A_2^{\ell 2}$		y_2
A_3^g		$A_3^{\ell 1}$	$A_3^{\ell 2}$		y_3
A_4^g		$A_4^{\ell 1}$	$A_4^{\ell 2}$		y_4
A_5^g		$A_5^{\ell 1}$	$A_5^{\ell 2}$		y_5

fig. 3a

\mathbf{B}_o	B_1^T	B_2^T	B_3^T	B_4^T	B_5^T	\mathbf{z}_o
B_1	C_1	D_2^T				z_1
B_2	D_2	C_2	D_3^T			z_2
B_3		D_3	C_3	D_4^T		z_3
B_4			D_4	C_4	D_5^T	z_4
B_5				D_5	C_5	z_5

fig. 3b

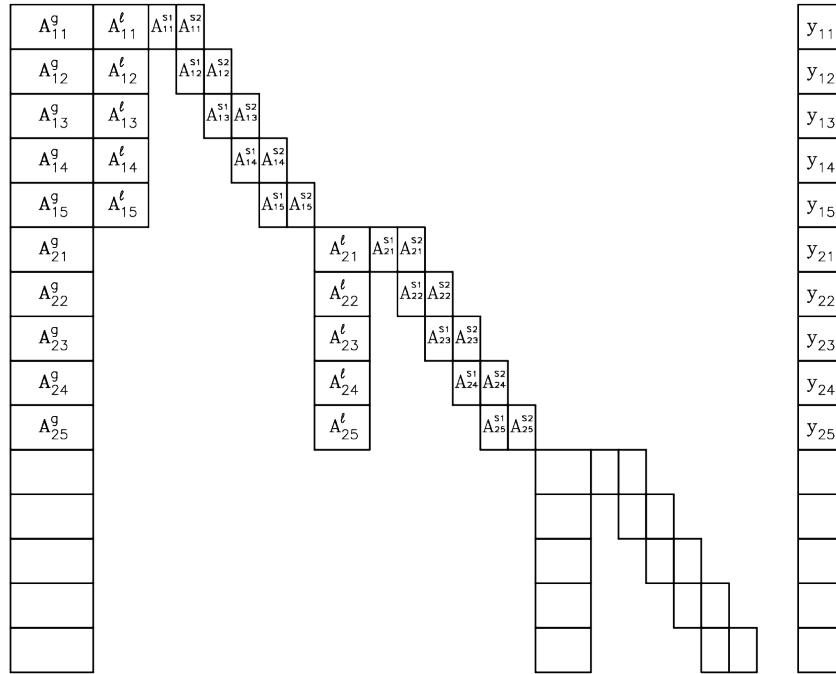


fig. 4a

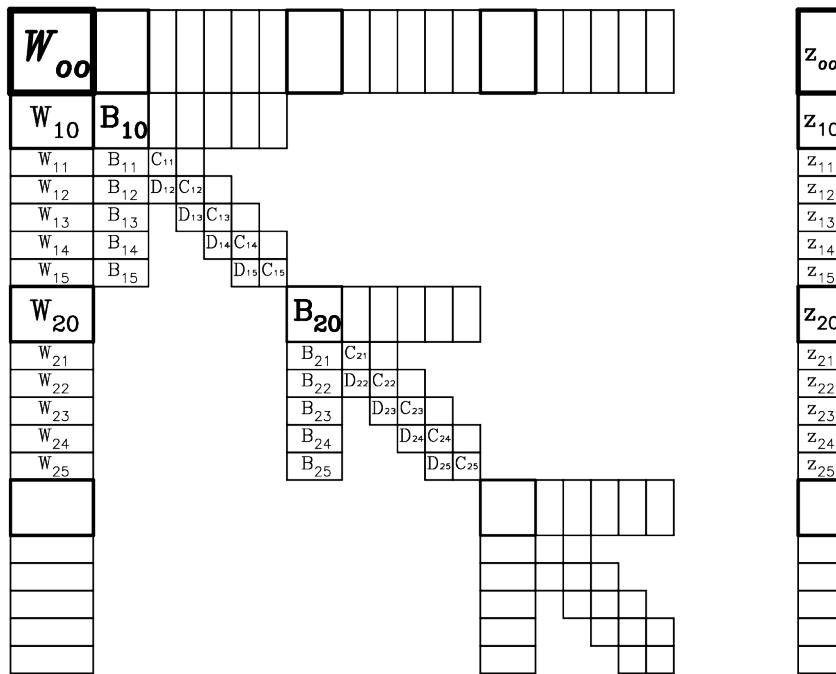


fig. 4b