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Permutation of Sparse Matrices to a Specific Lower BTF using Graph Decompositions

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Abstract

A new partitioning algorithm that permutes sparse matrices to a specific block lower-triangular form (BlTF) complying with special features required for instrumentation problems is presented. The proposal consists in the decomposition of the occurrence matrix in two stages, using methodologies based on graph theory. First of all, Hopcroft-Karp´s algorithm is employed to match the vertices, this classification being carried out by means of a modification of Dulmage-Mendelsohn´s technique, which was devised by the authors. The second step is the application of Tarjan´s algorithm to the square blocks obtained as a result of the first stage.

Keywords: *graph theory, directed graphs, bipartite graphs, sparse matrices, block lower-triangular forms, assignment algorithms, partitioning algorithms.*

INTRODUCTION

Solving systems of non-linear equations efficiently has been one of the most widely studied topics during the last few decades (Rabinowitz, 1970; Björk, 1996). A useful approach to handle this problem is to try to decompose the original system **S** into a sequence of subsystems $\mathbf{S_1}$, $\mathbf{S_2}$, ... $\mathbf{S_n}$, so that the solution can be reached by solving each of them separately in the proper order. The first step to determine $\{\mathbf{S_i}\}$ is to build the *occurrence matrix* **M**, whose rows and columns correspond to the system's equations and variables respectively. Then, **M** is permuted to a block triangular form (BTF), where each diagonal block corresponds to an $\mathbf{S_i}$ from **S**. The technique was first used for the analysis of the structure of large systems of equations (linear or non-linear) by Stewart (1962). Romagnoli and Stephanopoulos (1980) introduced the philosophy for the treatment of engineering problems connected with instrumentation design.

The methods employed to get a BTF are known as ***partitioning algorithms***. These strategies lead to savings in execution time and memory storage. In his book, Duff (1997) describes all the usual graph-oriented partitioning methodologies for square structurally non-singular matrices. Whenever structurally singular matrices might arise, the most efficient procedures available are also based on graph theory, specifically on Dulmage-Mendelsohn´s decomposition for bipartite graphs (1963). The resulting pattern is **upper**-triangular in blocks (BuTF), with the structure shown in **Fig. 1.**

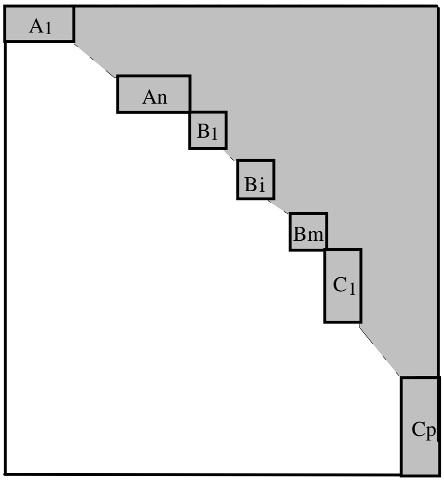

Fig. 1: *Classical BTF*

In the most general case, some of its diagonal blocks are horizontal (with more columns than rows), like $\mathbf{A_i}$; others are square (with the same amount of rows and columns), like $\mathbf{B_i}$; and the rest are vertical (with more rows than columns), like $\mathbf{C_i}$. The shaded area indicates the sections that can contain non-zero elements.

Unfortunately, the above mentioned BTF is inadequate for some specific applications to chemical engineering issues. The classification of unmeasured variables performed to analyse the instrumentation of industrial plants, in particular, requires permutation to a block **lower-**

triangular form (BlTF) like the one shown in **Fig. 2**. This BTF contains a square submatrix of order **p**, whose columns correspond to the *determinable variables*, **all** its diagonal blocks $\mathbf{A_i}$ being **square** and **structurally non-singular**. The block of dimension **rxp** is related to the system's *redundant equations*, whereas the equations in the block of dimension **q**x(**p**+**i**) are associated with the *indeterminable variables*. It is important to note that the pattern shown in **Fig. 2 cannot** be obtained just by transposing the classical BuTF.

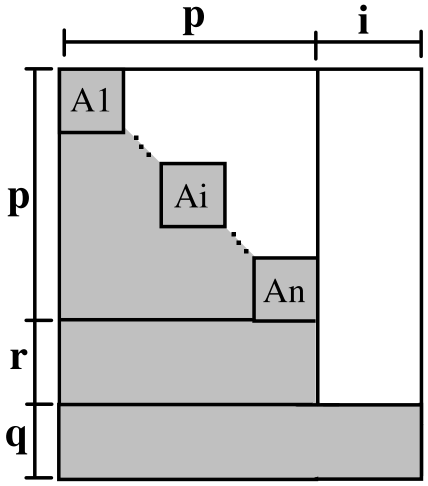

Fig. 2: *BlTF required for the Classification of Unmeasured Variables employed in Process Plant Instrumentation.*

The specific aim of this work is the development of a new partitioning algorithm to yield the above mentioned BlTF. The long-term objective of our research is to obtain a software package for the sensible and efficient choice of the most convenient configuration for plant instrumentation. Making improvements in the design of partitioning algorithms is the first step that should be taken in order to achieve this goal.

PARTITIONING ALGORITHM

We have designed a new method to yield the required BlTF. The procedure consists in partitioning the occurrence matrix by means of a decomposition carried out in two levels. In the first place, a bipartite graph (*bigraph*) is associated to the matrix. Then, a maximum matching for the bigraph is determined. As a result of this procedure, a preliminary partitioning of the matrix, whom we shall refer to as ***coarse decomposition,*** is obtained. The second stage, which will be called the ***fine decomposition,*** associates a directed graph (*digraph*) to each of the square blocks obtained through the coarse decomposition. Finally, the digraphs are explored by means of *depth-first searches* so as to determine all their strong components. Each strong component will correspond to a square diagonal block $\mathbf{A_i}$ from the BlTF given in **Fig. 2**.

At this point, it is interesting to mention that the idea of performing a decomposition in different levels had already been employed by Pothen and Fan (1990). Although they also used both a coarse and a fine decomposition, the procedures themselves are internally different, finally leading to a BTF like the one shown in **Fig. 1**.

The following algorithm shows the proposed partitioning procedure:

New Partitioning Algorithm

```
Given the occurrence matrix M

1. Coarse Decomposition
   1.1. Associate the bigraph G(M) = (R,C,E) to M.
   1.2. Obtain a maximum matching $P_m$.
   1.3. Classify the rows into VR, SR1, SR2, HR and the columns into SC1, SC2, HC based on $P_m$.

2. Fine Decomposition
   2.1. Associate a digraph G(M_1) = (V,E) to the submatrix M_1, made up of the block (SR1,SC1).
   2.2. Decompose G(M_1) into its strong components $M_{11}, M_{12}, ..., M_{1m}$.
        Each $M_{1i}$ corresponds to a diagonal block.
   2.3. Associate a digraph G(M_2) = (V,E) to the submatrix M_2, made up of the block (SR2,SC2).
   2.4. Decompose G(M_2) into its strong components $M_{21}, M_{22}, ..., M_{2k}$.
        Each $M_{2i}$ corresponds to a diagonal block.

3. Reordering
   Rearrange M´s blocks as follows: [$M_{11}, M_{12}, ..., M_{1m}, M_{21}, M_{22}, ..., M_{2k}$, (VR,SC1), (HR,HC)]
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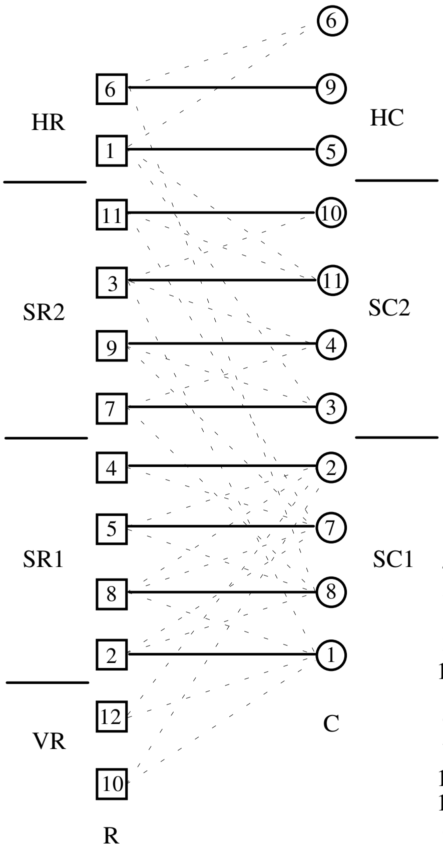
Coarse Decomposition

The **coarse decomposition** procedure is based on the classical algorithm devised by Dulmage and Mendelsohn. The technique associates the bigraph G(**M**) = (R,C,E) to a matrix **M,** where R and C are the vertex sets that correspond to **M**´s rows and columns respectively and E represents the set of G´s edges associated to **M**´s non-zero elements. In other words, if the component **M**(i,j) is not zero, then there is an edge $e_k \in E$ that joins vertices i and j, where $i \in R$ and $j \in C$.

Afterwards, a maximum matching P_m of the bigraph is searched for. P_m will determine **M**´s coarse decomposition. A *matching* P from G(**M**) is a subset of E, whose edges have no common endpoints. In terms of matrix **M**, this means that a matching corresponds to a set of non-zero elements, none of which belongs to the same row or column. This set of elements is also known as the matrix's *transversal.* A vertex is *matched* if it is the endpoint of an edge in a matching P; otherwise it is said to be *unmatched.* A matching of G(**M**)´s is called *maximum,* and noted P_m, if there are no other matchings P' among G(**M**)´s such that $|P'| > |P_m|$, where $|\ |$ indicates set cardinality. In the context of matrices, the methods employed to find a maximum matching in G(**M**), or a *maximum transversal* of **M**, are also known as ***assignment algorithms.*** **Fig. 3.a** shows a maximum matching for the bigraph associated with the matrix given in **Fig. 3.b**, where the matched edges are indicated with darker lines. The non-zero elements corresponding to the maximum transversal of the matrix are highlighted in bold in **Fig. 3.c.**



a) **M´**s Coarse Decomposition

$$\mathbf{M} = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

b) Occurrence Matrix

	2	7	8	1	10	11	4	3	6	9	5
4	**1**	1	0	0	0	0	0	0	0	0	0
5	1	**1**	1	0	0	0	0	0	0	0	0
8	1	1	**1**	1	0	0	0	0	0	0	0
2	0	1	1	**1**	0	0	0	0	0	0	0
11	0	1	0	0	**1**	1	0	0	0	0	0
3	0	0	0	1	1	**1**	1	0	0	0	0
9	0	1	0	0	0	0	**1**	1	0	0	0
7	0	0	1	0	0	0	1	**1**	0	0	0
12	1	0	0	1	0	0	0	0	0	0	0
10	1	0	0	1	0	0	0	0	0	0	0
6	0	0	1	0	0	0	0	0	1	**1**	0
1	0	0	0	0	0	1	0	1	1	0	**1**

c) **M´**s Rearrangement after Coarse Decomposition.

Fig. 3: ***Example***

The problem of permuting **M** to BlTF is now reduced to the search for a maximum matching in G(**M**). The most efficient algorithm that performs this task was developed by Hopcroft and Karp (1973). It is based on searches along augmented paths. A *path* is a sequence of vertices v_0, v_1, ..., v_{n-1}, v_n, where (v_i,v_{i+1}) is an edge from G(**M**) and $v_i \neq v_j$ $\forall$ $i \neq j$. An *alternating path* in a matching P is a path in G(**M**) whose edges alternate in P. For example, if the first edge along the alternating path does not belong to P, then all the edges at even positions on the way do belong to P, while those in odd positions do not. Finally, an *augmented path* in a matching P is an alternating path in P that begins and ends at unmatched vertices. The *cardinality* of a matching is the number of edges that it contains. An augmented path A can be employed to increase the cardinality of a matching P by the removal from P of those edges that belong to both sets (A $\cap$ P) together with the addition to P of all the edges that are only present in A. It is easy to show that each augmented path A increases in one the cardinality of the matching. In this way, a maximum matching is achieved when there are no more augmented paths left.

Once a maximum matching has been found out, the vertices are categorized. This classification decomposes the matrix associated with the bigraph into several blocks, which lead to the desired BlTF after an appropriate rearrangement. The decomposition proposed in this paper partitions the sets of vertices, R and C, into the following disjoint subsets:

VR = {*unmatched row vertices* }

SR1 = { *matched row vertices*, reachable from some unmatched row vertex through an alternating path }

HR = { *matched row vertices*, reachable from some unmatched column vertex through an alternating path }

SR2 = R\(VR∪SR1∪HR)

SC1 = { *matched column vertices*, reachable from some unmatched row vertex through an alternating path }

HC = { *column vertices (either matched or unmatched)*, reachable from some unmatched column vertex through an alternating path }

SC2 = C\(SC1∪HC)

The main difference between this approach and Dulmage and Mendelsohn´s lies in the fact that the latter places the row vertices that belong to VR and SR1 in the same set, whereas our classification makes a distinction. **Fig. 3.a** illustrates our partitioning for the matrix in **Fig. 3.b**. **Fig. 3.c** shows the resulting matrix after being rearranged according to the coarse decomposition. It is evident that VR´s vertices are associated with the system's redundant equations, while HR´s correspond to the equations that contain indeterminable variables. As to the columns, SC1 and SC2 are related to the determinable variables and HC is connected with the indeterminable variables.

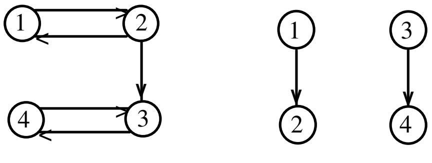
Fine Decomposition

The coarse decomposition yields two square blocks determined by the sets (SR1,SC1) and (SR2,SC2). The **fine decomposition** partitions these blocks into square irreducible subsystems by means of Tarjan´s algorithm for the decomposition of a directed graph into strong components (1972). This procedure associates a directed graph G(**N**) to each square block **N** obtained as a result of the first decomposition.

Given a square matrix **N** with full transversal (i.e., without zeroes in its diagonal), then it is possible to find an associated digraph G(**N**)=(V,E) where V and E are the sets of vertices and edges respectively. Then, |V| is equal to the order of **N** and there is an edge $(v_i,v_j)\in E$, directed from vertex i to vertex j, if and only if **N**(i,j)≠0, for i≠j. It is important to remark that the submatrices $\mathbf{M_1}$ and $\mathbf{M_2}$ have a full transversal because the square blocks yielded by the coarse decomposition correspond to matched rows and columns. The block (SR2,SC2) and its associated digraph are shown in **Fig. 4.a** and **Fig. 4.b** respectively.

	1	2	3	4
1	1	1	0	0
2	1	1	1	0
3	0	0	1	1
4	0	0	1	1

a) $\mathbf{M_2}$ = (SR2,SC2)



b) $\mathbf{M_2}$´s Digraph

c) Strong Components

	3	4	1	2
3	1	1	0	0
4	1	1	0	0
1	0	0	1	1
2	1	0	1	1

d) $\mathbf{M_2}$ after Rearrangement

Fig. 4: ***Fine Decomposition for Block*** $\mathbf{M_2}$ ***= (SR2, SC2)***

A digraph G=(V,E) is *strongly connected* if there is a path from *u* to *v* as well as another one from *v* to *u* for each different pair of vertices *u* and *v*, where $u,v \in$ V. If a digraph is ***not*** connected strongly, then it can be partitioned into strongly connected subgraphs, called G´s strongly connected components or just G´s *strong components*. **Fig. 4.c** represents the strong components for the digraph associated to block (SR2,SC2). **Fig. 4.d** corresponds to the same block after rearrangement. Tarjan´s algorithm determines the strong components by means of *depth-first searches*. A detailed description can be found in Tarjan´s paper (1972).

The third step of the new partitioning algorithm aims at rearranging the blocks resulting from the previous stages to yield the structure shown in **Fig. 2**. The blocks $\mathbf{M_{11}}$, ..., $\mathbf{M_{1m}}$, $\mathbf{M_{21}}$, ..., $\mathbf{M_{2k}}$ mentioned in the algorithm correspond to the blocks $\mathbf{A_1}$, ..., $\mathbf{A_n}$ in **Fig. 2**. The blocks (VR,SC1) and (HR,HC) correspond to the submatrices of dimension **rxp** and **q**x(**p+i**) respectively.

Efficiency and Correctness

The order of the proposed algorithm as regards execution time can be estimated from the order of each decomposition procedure. The coarse decomposition in particular employs Hopcroft-Karp´s algorithm, whose execution time is $O(n^{3/2}\tau)$ in the worst cases, where n is the number of vertices in G(**M**) and τ is the number of non-zero elements in **M**. Since $\tau \leq n^2$ it can be stated that Hopcroft-Karp´s algorithm has execution times of $O(n^{5/2})$. As to the fine decomposition, Tarjan´s method is of ($O(n)+O(\tau)$). Taking into account that both methods are applied sequentially, it is immediate that the proposed algorithm has $O(n^{3/2}\tau)$. Finally, it is important to remark that the correctness of our procedure can be assessed from the correctness of Hopcroft-Karp and Tarjan´s algorithms. The methodology is both robust and trustworthy, preserving the high quality of the partitions yielded by those two individual techniques.

CONCLUSIONS

A new partitioning algorithm for the search of a specific BlTF specially adapted to solve process plant instrumentation problems is presented in this paper. In this context, the method performs a structural rearrangement of the occurrence matrix associated to the mathematical model of industrial processes. To perform this task, already existing algorithms (Hopcroft-Karp and Tarjan) were combined on the basis of a new vertex classification proposed by the authors. This classification leads to a structure which is different from the typical one employed for other applications, yielding a BlTF specially adapted to fulfil our requirements.

In practice, some of the diagonal blocks in a BlTF may correspond to subsystems which are unsolvable due to physical considerations associated with the meaning or scope of the model equations. Since these limitations go beyond a mere structural analysis, the incorporation of block constraints that avoid inadequate assignments becomes indispensable. We are currently working on this issue.

A lot of work remains to be done in order to accomplish our long-term objective: an efficient and reliable software package for plant instrumentation design. The next step is to incorporate the analysis of constraints. The final stages are the implementation of the program and its testing on real plants of huge size, typically systems involving 10.000 equations.

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