

Pattern Graphs for Sparse Matrices¹

Shahadat Hossain

Department of Mathematics and Computer Science,
University of Lethbridge, Canada

and

Trond Steihaug

Department of Informatics
University of Bergen
Bergen, Norway

The excellent research in the area of sparse derivative matrix determination over the last three decades culminated into some highly innovative and efficient determination techniques. Graph theory has been employed as an important tool to study the complexity of the problems and to design “good” heuristics for solving them. Consequently, different graph models that have been proposed are rather dependent on specific properties e.g., symmetry, that the methods try to exploit. We introduce a new graph model that is a natural representation of the zero-nonzero structure of a sparse matrix [5]. This new representation is also economical with respect to the storage space compared with the “Element Isolation (EI)” graph [6]. Furthermore, the unidirectional (see [2]) and the bidirectional determination problems (see [1, 4]) can now be stated using a single graph in a natural way and the connection between the two problems can be clearly stated as compared with the bipartite graph [3].

Let $A \in R^{m \times n}$ be a given matrix with known sparsity pattern. Then $a_{i'j'} \neq 0$ is a *lateral neighbor* of $a_{ij} \neq 0$ if $i = i'$ and, $j' > j$ minimizes $j' - j$ or $j' < j$ minimizes $j - j'$. Similarly, $a_{i'j'} \neq 0$ is a *vertical neighbor* of $a_{ij} \neq 0$ if $j = j'$ and, $i' > i$ minimizes $i' - i$ or $i' < i$ minimizes $i - i'$.

Informally, a lateral neighbor of $a_{ij} \neq 0$ is a nonzero $a_{i'j'} \neq 0$ in row i of A such that $j' - j$ is the smallest if $j' > j$ or such that $j - j'$ is the smallest if $j > j'$ among all such indices j' in row i . Vertical neighbors can be interpreted in an analogous way with the roles of i and j interchanged.

Given $A \in R^{m \times n}$ we define the *sparsity-pattern graph* (or simply the pattern graph) associated with A , $G_p(A) = (V, E)$, where

$$V = \{v_{ij} : a_{ij} \neq 0, i = 1, 2, \dots, m, j = 1, 2, \dots, n\}$$

and

$$\{v_{ij}, v_{i'j'}\} \in E \text{ if } a_{ij} \text{ and } a_{i'j'} \text{ are lateral or vertical neighbors.}$$

Figure 1 displays the sparsity structure of the Eisenstat example matrix on 6 columns on the left and its associated sparsity graph on the right.

We have a *path* connecting vertices $v_{ij} \neq v_{i'j'}$ denoted $v_{ij} \stackrel{\ell}{\sim} v_{i'j'}$ if $v_{ij} \equiv v_{i_0j_0}, v_{i_1j_1}, \dots, v_{i_\ell j_\ell} \equiv v_{i'j'}$ is a sequence of vertices such that $\{v_{i_{k-1}j_{k-1}}, v_{i_kj_k}\} \in E, k = 1, 2, \dots, \ell$. We also use the notation $v_{ij} \stackrel{\geq \ell}{\sim} v_{i'j'}$ to denote that the path in question is of length at least ℓ .

Let $\Phi : V \mapsto \{1, 2, \dots, p\}$ be a mapping such that for $v_{ij} \in V$, $v_{ij} \stackrel{1}{\sim} v_{i'j'}, j \neq j'$ implies $\Phi(v_{ij}) \neq \Phi(v_{i'j'})$ and $v_{ij} \stackrel{\geq 1}{\sim} v_{i'j'} \stackrel{\geq 1}{\sim} v_{i''j''}, i \neq i', j \neq j'$ implies $\Phi(v_{ij}) \neq \Phi(v_{i''j''})$. Then the mapping Φ is said to yield a *column induced direct cover* for the vertices of $G_p(A)$. The first of the above conditions implies that the vertices in the same row (i.e. reachable by a path) are differently covered so that the corresponding columns belong to

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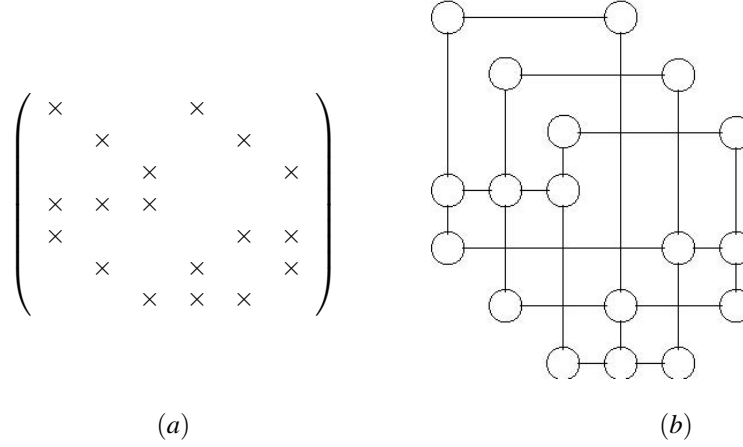


Figure 1: The Eisenstat (6×7) matrix and its associated sparsity-pattern graph

different groups. The second condition requires that for each nonzero a_{ij} to be directly determined, columns j and j' of A must belong to different groups whenever $a_{ij'} \neq 0$. It can be shown that a column induced direct cover of $G_{\mathcal{P}}(A)$ is equivalent to a coloring of the vertices of EI graph $G_I(A)$. The novelty of the pattern graph lies in its ability to express a host of coloring problems associated with the determination of sparse derivative matrices (unidirectional, bidirectional, symmetric etc.) with the same graph [5].

References

- [1] T. F. Coleman and A. Verma. The efficient computation of sparse Jacobian matrices using automatic differentiation. *SIAM J. Sci. Comput.*, 19(4):1210–1233, 1998.
- [2] A. R. Curtis, M. J. D. Powell, and J. K. Reid. On the estimation of sparse Jacobian matrices. *J. Inst. Math. Appl.*, 13:117–119, 1974.
- [3] A. H. Gebremedhin, F. Manne, and A. Pothen. What color is your Jacobian? Graph Coloring for Computing Derivatives. *SIAM Rev.*, 47(4):629–705, 2005.
- [4] A. S. Hossain and T. Steihaug. Computing a sparse Jacobian matrix by rows and columns. *Optimization Methods and Software*, 10:33–48, 1998.
- [5] Shahadat Hossain and Trond Steihaug. The CPR Method and Beyond – A Unified Approach. To be submitted to *IMA Journal of Numerical Analysis*.
- [6] G. N. Newsam and J. D. Ramsdell. Estimation of sparse Jacobian matrices. *SIAM J. Alg. Disc. Meth.*, 4(3):404–417, 1983.