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Kamer Kaya, Bora Uçar

## - To cite this version:

Kamer Kaya, Bora Uçar. Constructing elimination trees for sparse unsymmetric matrices. SIAM Journal on Matrix Analysis and Applications, 2013, 34 (2), pp.345-354. 10.1137/110825443 . inria00567970v4

## HAL Id: inria-00567970 https://inria.hal.science/inria-00567970v4

Submitted on 4 Oct 2012

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# Constructing elimination trees for sparse unsymmetric matrices 

Kamer Kaya, Bora Uçar

## RESEARCH

# Constructing elimination trees for sparse unsymmetric matrices 

Kamer Kaya, Bora Uçar<br>Project-Team ROMA<br>Research Report n ${ }^{\circ} 7549$ — February 2011 - 13 pages


#### Abstract

Eisenstat and Liu, SIAM J. Matrix Anal. Appl., 26 (2005) and 29 (2008)]. The construction algorithm has a worst-case time complexity of $\Theta(m n)$ for an $n \times n$ unsymmetric matrix having $m$ off-diagonal nonzeros. We propose another algorithm that has a worst-case time complexity of $\mathcal{O}(m \log n)$. We compare the two algorithms experimentally and show that both algorithms are efficient in general. The algorithm of Eisenstat and Liu is faster in many practical cases, yet there are instances in which there is a significant difference between the running time of the two algorithms in favor of the proposed one.


Key-words: Elimination tree, sparse matrix factorization

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\text { Revised: October } 2012
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RESEARCH CENTRE
GRENOBLE - RHÔNE-ALPES
Inovallée
6 5 5 \text { avenue de l'Europe Montbonnot}
3 8 3 3 4 \text { Saint Ismier Cedex}
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## Construire les arbes d'élimination pour des matrices creuses non symétriques

Résumé : Eisenstat et Liu ont récemment décrit l'arbre d'élimination pour des matrices creuses non symétriques et ont proposé un algorithme pour le construire en temps $\mathcal{O}(m n)$ pour une matrice de taille $n$ ayant $m$ éléments non nuls hors diagonaux [Eisenstat and Liu, SIAM J. Matrix Anal. Appl., 26 (2005) and 29 (2008)]. Nous décrivons un algorithme dont la complexité en temps est $\mathcal{O}(m \log n)$. Nous comparons les deux algorithmes expérimentalement et montrent que les deux sont efficaces en général. L'algorithme de Eisenstat et Liu est plus rapide dans de nombreux cas pratiques, mais il y a des cas dans lesquels la différence entre le temps d'exécution de deux algorithmes est significative en faveur de le nôtre.
Mots-clés : Arbre d'élimination, factorisation des matrices creuses

## 1 Introduction

Arguably, the elimination tree is the single most important data structure in sparse matrix factorization methods. It is used to estimate and optimize the storage and computational requirements during symbolic and numerical factorizations [10]. The elimination tree for symmetric (positive definite) systems dates from 80s [11] and even before (see [4, Section 3.3] and [10]), whereas the elimination tree for unsymmetric matrices is a recent development. Eisenstat and Liu [6] define the elimination tree for unsymmetric matrices and discuss its properties. In a follow up paper [7], they describe algorithms to construct those trees and discuss the use of the elimination trees to improve the performance of a symbolic factorization algorithm. The algorithm of Eisenstat and Liu [7] for constructing the elimination tree of an $n \times n$ unsymmetric matrix with $m$ off-diagonal nonzeros has a worst-case time complexity of $\Theta(m n)$. We present an $\mathcal{O}(m \log n)$ time algorithm for the same purpose.

A directed graph (digraph) $G=(V, E)$ consists of a finite set of vertices $V$ and a set of edges $E$, where each edge $(u, v) \in E$ is an ordered pair in $V$. The directed graph $G(\mathbf{A})=(V, E)$ of an $n \times n$ matrix $\mathbf{A}$ with $m$ off-diagonal nonzeros contains $n$ vertices, $V=\left\{v_{1}, v_{2}, \ldots, v_{n}\right\}$, and $m$ edges, $E=\left\{\left(v_{i}, v_{j}\right)\right.$ : $a_{i j} \neq 0$, for $\left.1 \leq i \neq j \leq n\right\}$. We assume that $\mathbf{A}$ has a zero-free diagonal. However, as the definition of $G(\mathbf{A})$ shows, we will omit the self loops implied by the diagonal entries. We also assume that $m \geq n$ to simplify some definitions and complexity analysis.

A path of length $k$ in a directed graph $G=(V, E)$ is a sequence of vertices $u_{0}, u_{1}, \ldots, u_{k}$ such that $\left(u_{i}, u_{i+1}\right) \in E$ for $i=0, \ldots, k-1$. For two vertices $u, v \in V$, we say that $u$ is connected to $v$ in $G$, denoted $u \xrightarrow{G} v$, if there is path $u=u_{0}, u_{1}, \ldots, u_{k}=v$ from $u$ to $v$. A cycle is a path which starts and ends at the same vertex. A simple cycle is a path $u_{0}, u_{1}, \ldots, u_{k}, u_{0}$ where $k \geq 1$ and $u_{i} \neq u_{j}$ for $0 \leq i<j \leq k$.

A directed graph $G^{\prime}=\left(V^{\prime}, E^{\prime}\right)$ is a subgraph of a larger digraph $G=(V, E)$ if $V^{\prime} \subseteq V$ and $E^{\prime} \subseteq E \cap\left(V^{\prime} \times V^{\prime}\right)$. A subgraph is said to be a induced subgraph if $E^{\prime}=E \cap\left(V^{\prime} \times V^{\prime}\right)$. Let $V=\left\{v_{1}, v_{2}, \ldots, v_{n}\right\}$ and we have a total order on the vertices. Then, $G_{k}$ denotes a special induced subgraph containing the first $k$ vertices in $V$. That is,

$$
G_{k}=\left(\left\{v_{1}, \ldots, v_{k}\right\}, E \cap\left\{v_{1}, \ldots, v_{k}\right\} \times\left\{v_{1}, \ldots, v_{k}\right\}\right) .
$$

If $u \xrightarrow{G} v$ for all $u, v \in V$, the digraph $G$ is called strongly connected. A maximal, strongly connected, induced subgraph $C$ of $G$ is called a strong component of $G$. A directed graph without simple cycles is called a directed acyclic graph (dag). The strong components of a dag are its vertices, i.e., each vertex forms a trivial strong component.

We say that a matrix $\mathbf{A}$ with a zero-free diagonal is irreducible if $G(\mathbf{A})$ is strongly connected, i.e., it only has one strong component.

Let $\Pi=\left\{V_{1}, V_{2}, \ldots, V_{\ell}\right\}$ be a partition of the vertex set $V$ of a directed graph $G=(V, E)$. The quotient graph $G^{\Pi}=\left(V^{\Pi}, E^{\Pi}\right)$ induced by $\Pi$ has $\ell$ super-vertices $V_{1}, \ldots, V_{\ell}$ and a directed edge $\left(V_{i}, V_{j}\right) \in E^{\Pi}$ iff $(u, v) \in E$ for some $u \in V_{i}$ and $v \in V_{j}$.

Let $\mathbf{A}$ be a nonsingular, sparse, unsymmetric $n \times n$ matrix with a nonzero diagonal, and assume that the LU-factorization $\mathbf{A}=\mathbf{L U}$ with unit lower trian-
gular $\mathbf{L}$ and upper triangular $\mathbf{U}$ exists. Then, the elimination tree $T(\mathbf{A})$ of an unsymmetric $\mathbf{A}$ is defined by Eisenstat and Liu [6, 7] as follows.

$$
\begin{equation*}
\operatorname{PARENT}(i)=\min \{j: j>i \text { and } j \xrightarrow{G(\mathbf{L})} i \xrightarrow{G(\mathbf{U})} j\} \tag{1}
\end{equation*}
$$

where $\operatorname{Parent}(i)$ denotes the parent of vertex $i$ in the elimination tree if $i$ is not a root. Otherwise, $\operatorname{Parent}(i)=\infty$. Eisenstat and Liu prove the following theorem in order to develop an algorithm for constructing $T(\mathbf{A})$ without knowing $G(\mathbf{L})$ and $G(\mathbf{U})$.

Theorem 1 (see Theorem 3.3 of [6]). Vertex $k$ is the parent of vertex $i$ in the elimination tree $T(\mathbf{A})$ if and only if $k$ is the first vertex after $i$ such that $k$ and $i$ belong to the same strong component of the subgraph $G_{k}(\mathbf{A})$ of $G(\mathbf{A})$.

Given this theorem, Eisenstat and Liu [7] propose Algorithm 1 to compute the parent pointers (1) and hence to construct the elimination tree.

```
for vertex \(k=1\) to \(n\) do
    Find the strong component \(C\) of \(G_{k}(\mathbf{A})\) that contains \(k\)
    for each vertex \(i \in C \backslash\{k\}\) do
        if \(\operatorname{Parent}(i)=\infty\) then
            \(\operatorname{Parent}(i)=k\)
    \(\operatorname{Parent}(k)=\infty\)
```

Algorithm 1: ETREE

The strong components of a digraph with $m$ edges and $n$ vertices can be found in $\Theta(n+m)$ time [12]. Hence, the worst-case time complexity of the algorithm eTree is $\Theta(m n)$ for a graph containing $n$ vertices and $m$ edges. Eisenstat and Liu reduce the practical running time of the algorithm by using quotient graphs [7] and specialized algorithms to find the strong component containing a given vertex, but report that the worst-case time complexity of the improved algorithm is still $\Theta(m n)$.

## 2 An $\mathcal{O}(m \log n)$ time algorithm

The essence of the proposed algorithm lies in the following theorem of Eisenstat and Liu [7, Theorem 3.2].

Theorem 2. (see [7, Theorem 3.2]) Let $C=\left(V_{c}, E_{c}\right)$ be a strong component of $G_{k}(\mathbf{A})$ and let $i_{t}$ be the highest numbered vertex in $V_{c}$. Then the vertex set $V_{c}$ corresponds to the vertex set of the subtree of the elimination tree $T(\mathbf{A})$ rooted at $i_{t}$.

Eisenstat and Liu make use of this theorem in a bottom-up approach in the improved version of Algorithm 1. Each time $k$ is incremented, the newly formed connected component (a union of a set of strong components) is detected using quotient graphs and the vertex $k$ is set to be the root of the new component whose children are the roots of the strong components that form the component of $k$. The algorithm that we propose makes use of Theorem 2 in a top-down
approach. Assume we have detected the strong components of $G_{k}$. Then, we can build the subtrees of $T(\mathbf{A})$ rooted at the highest numbered vertex in each component recursively. Furthermore, we can build the quotient graph induced by the partition formed by the components of $G_{k}$ and the vertices of $G$ that are not in $G_{k}$ (each as a single vertex) and compute the elimination tree associated with this quotient graph recursively. Once this is done, the whole tree $T(\mathbf{A})$ can be obtained by replacing each super-vertex with the associated subtree. The algorithm that we propose below implements this recursion. The proposed algorithm is based on an algorithm of Tarjan [13]. Tarjan's original algorithm constructs a tree whose leaves correspond to the vertices of a given graph and applies a recursion to the edge set, whereas the proposed elimination tree algorithm constructs a tree whose vertices correspond to the vertices of the given graph by applying a recursion to the vertex set.

### 2.1 The algorithm

Let $\mathbf{A}$ be an irreducible, unsymmetric, $n \times n$ matrix. Algorithm 2 displays the proposed algorithm UET which finds the elimination tree $T(\mathbf{A})$. There are two inputs for the algorithm: a strongly connected digraph $G$ with $\eta$ vertices and an integer $s<\eta$ such that $G_{s}$ is acyclic. That is, all the strong components of $G_{s}$ are trivial. The initial call is $\operatorname{UET}(G(\mathbf{A})=(\{1,2, \ldots, n\}, E), 0)$. We assume that the parent pointers are initialized to $\infty$ before the execution of the algorithm.

Since $G$ is strongly connected and $G_{s}$ is known to be acyclic, if $s=\eta-1$, the vertex $i_{\eta}$ must be the vertex that makes $G$ strongly connected. If this is the case, we set the parent pointers appropriately; vertex $i_{\eta}$ becomes the parent of all vertices $i_{1}, \ldots, i_{\eta-1}$. If this is not the case, the algorithm examines $G_{k}$ where $k=\lceil(s+\eta) / 2\rceil$. Assume that $G_{k}$ has $p$ strong components $C_{\ell}=\left(V_{\ell}, E_{\ell}\right)$ for $\ell=1, \ldots, p$. By Theorem 2 , the vertex set of each strong component $V_{\ell}$ corresponds to the vertices of the subtree of the elimination tree rooted at the highest numbered vertex in $V_{\ell}$. In this case, each recursive call at line 11 is responsible for setting the parent pointers of the vertices in these subtrees where the root of each subtree is the highest numbered vertex in the associated component. When we have computed the subtrees associated with each strong component of $G$, UET is called on the quotient graph with partition $\Pi=\left\{V_{1}, \ldots, V_{p}, i_{k+1}, i_{k+2}, \ldots, i_{\eta}\right\}$, where $V_{1}, \ldots, V_{p}$ correspond to the $p$ strong components of $G_{k}$, to set the parents of the roots of these subtrees. As we need a vertex to represent $V_{\ell}$ for $\ell=1, \ldots, p$, we find it convenient to use the root, i.e., the highest numbered vertex in $V_{\ell}$.

In a recursive call with a strong component $C_{\ell}, s_{\ell}$ is equal to the number of vertices in $V_{\ell}$ at an index smaller than or equal to $s$. Hence, the subgraph of $C_{\ell}$ containing the first $s_{\ell}$ vertices is acyclic (has only trivial strong components). On the other hand, for the graph $G^{\Pi}$, we know that the first $p$ vertices form a directed acyclic graph since they correspond to the strong components of $G_{k}$. These two observations show that at an invocation of UET each vertex $i_{j} \in V$ such that $j \leq s$ represents a subtree in $T(\mathbf{A})$ with root $i_{j}$ (may also be a leaf node).

Consider the sample matrix from [7] shown in Fig. 1(a) whose graph is shown in Fig. 1(b). The first call with the whole graph finds $k=5, p=3$ with $V_{1}=\{1\}, V_{2}=\{4\}, V_{3}=\{2,3,5\}$, and then recursively calls the algorithm in $V_{3}$; then the algorithm reaches line 14, yielding the subtree shown in Fig. 1(c)

Input A graph $G=\left(\left\{i_{1}, i_{2}, \ldots, i_{\eta}\right\}, E\right)$ and a nonnegative integer $s<\eta$ such that
(i) $G$ is strongly connected,
(ii) $G_{s}$ is acyclic,
(iii) the remaining vertices satisfy $i_{s+1}<i_{s+2}<\cdots<i_{\eta}$ whenever $s<\eta-1$.

Output Parent pointers are set.
if $s=\eta-1$ then
for $j=1$ to $\eta-1$ do
$\operatorname{Parent}\left(i_{j}\right)=i_{\eta}$
else
$k=\lceil(s+\eta) / 2\rceil$
Let $p$ be the number of strong components of $G_{k}$
for $\ell=1$ to $p$ do
Let $C_{\ell}=\left(V_{\ell}, E_{\ell}\right)$ be the $\ell$ th strong component of $G_{k}$
if $\left|V_{\ell}\right|>1$ then
$s_{\ell}=\left|\left\{i_{j}: i_{j} \in V_{\ell}, j \leq s\right\}\right|>$ the first $s$ vertices form a dag
$\operatorname{UET}\left(C_{\ell}, s_{\ell}\right)$ Set parents for the vertices in each str
comp.
Let $\Pi=\left\{V_{1}, \ldots, V_{p}, i_{k+1}, i_{k+2}, \ldots, i_{\eta}\right\}$ be a partition of $V$
Let $G^{\Pi}=\left(V^{\Pi}=\left\{r_{1}, \ldots, r_{p}, i_{k+1}, i_{k+2}, \ldots, i_{\eta}\right\}, E^{\Pi}\right)$ be the quotient graph induced by $\Pi$ where $V_{\ell}$ is represented by the highest numbered vertex $r_{\ell} \in V_{\ell}$ for $\ell=1, \ldots, p$
$\operatorname{UET}\left(G^{\Pi}=\left(V^{\Pi}, E^{\Pi}\right), p\right) \quad G^{\Pi}$ is strongly connected, $G_{p}^{\Pi}$ is acyclic
Algorithm 2: $\mathrm{UET}\left(G=\left(\left\{i_{1}, i_{2}, \ldots, i_{\eta}\right\}, E\right), s\right)$

(a) The matrix $\mathbf{A}$

(c) Initial call reaches line 14
(e) Final pass at line 14

(f) Constructed tree
(b) The directed graph of $\mathbf{A}$


Figure 1: Tracing the algorithm on the sample matrix.
with $V^{\Pi}=\left\{r_{1}=1 ; r_{2}=4 ; r_{3}=5 ; 6 ; 7 ; 8 ; 9 ; 10\right\}$. The recursive call is made with $s=3$ and then finds $k=6$ (pointing to vertex 8 ). Three strong components $V_{1}=\{1,4,6,7\}, V_{2}=\{2,3,5\}$, and $V_{3}=\{8\}$ are found; 7 becomes the root of $V_{1}$, and 5 becomes the root of $V_{1}$ after the recursive calls at line 11, yielding the subtrees shown in Fig. 1(d). Then the algorithm reaches again to line 14 with $V^{\Pi}=\left\{r_{1}=7 ; r_{2}=5 ; r_{3}=8 ; 9 ; 10\right\}$ and $s=3$. This time $k=4$ (points at vertex 9). Again, three strong components are found and 9 becomes the root of the component containing 5, yielding the tree shown in Fig. 1(e). The last call results in the elimination tree shown in Fig. 1(f).

### 2.2 Complexity analysis

We now analyze the worst-case running time complexity of Algorithm 2. Consider the call tree for UET where the root node is the initial call and the children of a node are the recursive calls it makes. The complexity of the body of the algorithm without the recursive calls is $\mathcal{O}(|E|)$, as the running time of the body is dominated by the computation of the strong components (in $\mathcal{O}(|E|)$ time) of a graph and the construction of the associated quotient graph (which is done in $\mathcal{O}(|E|)$ time as we also discuss in the next subsection). That is, at each node of the call tree, the complexity is $\mathcal{O}(|E|)$. We now proceed in two steps to bound the running time for an $n \times n$ matrix with $m$ off-diagonal nonzero etnries. In the first step, we obtain the bound $\mathcal{O}(m)$ on the sum of the nonrecursive work of all nodes of the call tree at a given depth. In the second step, we obtain the bound $\mathcal{O}(\log n)$ on the height of the call tree.

Consider the algorithm UET making the recursive calls for a given graph with $|E|$ edges and $p$ strong components. Each edge in $E$ is included either in one recursive call at line 11 , or in the call at line 14 on the quotient graph, or discarded while building the quotient graph. This implies that $\sum_{\ell=1}^{p}\left|E_{\ell}\right|+$ $\left|E^{\Pi}\right| \leq|E|$. Therefore the total number of edges in all calls at a given depth is no larger than the number of edges $m$ in the initial call, and hence the complexity of nonrecursive work at a given depth is $\mathcal{O}(m)$. Let $\eta-s$ be the rank of the problem, i.e., the number of vertices to be examined for strong connectivity in $G$. Among the vertices of $C_{\ell}$, there are $s_{\ell}$ of them in the acyclic graph $G_{s}$. The remaining vertices all should be between $s$ and $k$. Therefore, for a strong component $C_{\ell}$, we have $\left|V_{\ell}\right|-s_{\ell} \leq k-s$. The problem containing the quotient graph has rank $\eta-k$, as among a total of $\eta-k+p$ vertices, the first $p$ of them form a dag. By the definition $k=\lceil(n+s) / 2\rceil$, we have $\max \{k-s, \eta-k\} \leq 2(\eta-k) / 3$; notice that the inequality is tight only when $n-s=3$. Therefore, the rank of a node of the call tree is at most $2 / 3$ as large as its parent. Since the rank of the initial problem is $n$, the height of the call tree is $\mathcal{O}(\log n)$, and the worst-case time complexity of the algorithm is $\mathcal{O}(m \log n)$.

### 2.3 Implementation details

Our implementation of UET allocates $10 n+m$ space for a strongly connected graph before calling the recursive function (this does not include the parent pointers), and overwrites the input matrix, essentially requiring $11 n+2 m$ space. The recursive function itself allocates $2 n+p$ extra space before the recursive calls on the $p$ strong components (at line 11) and frees up this space just before the recursive call on $G^{\Pi}$. By following an analysis similar to the one in the previous subsection, we can see that the recursive calls allocate and free a total of $\mathcal{O}(n \log n)$ space throughout the whole process. Notice that this is not the peak memory requirement at a given time. In comparison, EL uses $9 n+2 m$ space (this does not include the parent pointers).

The most involved part of the proposed UET algorithm is the construction of the subgraphs $C_{\ell}$ and the graph quotient $G^{\Pi}$ while discarding the duplicate edges. In short, we do this operation as follows: we visit the edges of $G$ once and construct the graphs of $C_{\ell}$ for $\ell=1, \ldots, p$ and the graph $G^{\Pi}$ during this visit. We implemented this operation in two different for-loops. In the first for-loop, we visit the vertices that are not in $G_{k}$ to add some edges to $G^{\Pi}$. For each such vertex $v$, we visit its neighbors in order. If a neighbor $u$ of $v$ is not in $G_{k}$, then the edge is copied into $G^{\Pi}$. Otherwise, we put an edge from $v$ to the vertex representing $u$ 's strong component, if such an edge was not put before (an array of markers is used to do this without searching). In the second for-loop, we visit the vertices of a strong component before visiting the vertices of another one. When we visit a vertex $v$ in a strong component $C_{\ell}$, the neighbors of $v$ that are in $C_{\ell}$ are copied into the graph of $C_{\ell}$. For a neighbor $u$ of $v$ which is either in another strong component $C_{q}$ or not in $G_{k}$, we add an edge from the vertex representing $C_{\ell}$ to the vertex representing $C_{q}$ (or to $u$ itself if $u$ is not in $G_{k}$ ) if such an edge was not added before (we again use an array of markers to avoid searches). Note that the vertices representing the strong components are the roots, and their ids along with the ids of vertices not in $G_{k}$ are passed to the recursive call on $G^{\Pi}$ to set their parent pointers.

The proposed algorithm requires an irreducible matrix $\mathbf{A}$ (or a strongly con-
nected graph) at the initial call. One can therefore detect the irreducible blocks of a general $\mathbf{A}$ and call the proposed algorithm to construct the elimination tree of each block separately and build the elimination tree (forest in this case) of the initial matrix A. Alternatively, one can append a zero-free row and column to any input matrix, and create an irreducible matrix, say B. The new row/column will be the root of the elimination tree of $\mathbf{B}$. By removing the newly added vertex from the elimination tree of $\mathbf{B}$, one can obtain the elimination tree of $\mathbf{A}$. We found it convenient to not to add those edges, but assume their presence and handle them by the if check at line 1 of Algorithm 2.

One further detail we need to mention is that the body of the else statement at line 4 handles the case where $p=k$ differently. If we have $p=k$, then $G_{k}$ is acyclic and the strong components of the graph $G_{k}$ are all trivial. Therefore, instead of doing recursive calls on the components of $G_{k}$, the variable $s$ is modified and another $k$ between the new $s$ and $\eta$ is searched in a while loop, where at each iteration the strong components of $G_{k}$ are found. If during this search we find a $G_{k}$ with a non-trivial strong component, then the algorithm continues with the body of the else statement as displayed in Algorithm 2. If $s$ is found to be $\eta-1$, then the parent pointers of all vertices are set to the last vertex of $G$ and the control returns to the caller. This technique does not affect the theoretical complexity of the algorithm, as it is equivalent to calling the algorithm recursively with $s=k$.

## 3 Experimental results

We have implemented the proposed elimination tree construction algorithm in C and compared it with a Fortran implementation of the algorithm of Eisenstat and Liu [7]. In the sequel, UET refers to the proposed algorithm with the modification discussed in the last paragraph of Section 2.3, and EL refers to the algorithm of Eisenstat and Liu. We compiled the C and Fortran codes with mex of Matlab which uses gcc and gfortran versions 4.4 .2 with the optimization flag -0 . We run the compiled codes on a machine with a 2.4 Ghz AMD Opteron 250 processor and 8Gbytes of RAM.

### 3.1 Constructed examples

There are matrices on which the algorithm EL runs in time $\Theta(m n)$. For a given positive integer $k$, let $A$ be a matrix of size $n=2 k$ whose nonzero set is the following:

$$
\begin{array}{r}
\left\{a_{i i} \mid i=1, \ldots, n\right\} \cup\left\{a_{i+1, i} \mid i=k, \ldots, n-2\right\} \cup\left\{a_{i-k, i} \mid i=k+1, \ldots, n\right\} \\
\cup\left\{a_{n i} \mid i=1, \ldots, n\right\} \cup\left\{a_{i n} \mid i=k+1, \ldots, n-1\right\} . \tag{2}
\end{array}
$$

A sample matrix of size $10 \times 10$ (with $k=5$ ) from this family is shown in Fig. 2(a).

The matrices as described above are irreducible and have zero fill-in when the natural order is used during the elimination process. For these matrices, using the quotient graphs does not have any effect (each component is of size one until the $n$th vertex) and therefore EL runs in $\Theta(m n)=\Theta\left(n^{2}\right)$ time. The proposed algorithm, without the modification presented at the last paragraph

(a) Sample $10 \times 10$ matrix

(b) Elimination tree

Figure 2: A matrix on which EL runs in quadratic time and the corresponding elimination tree.

| $n$ | $m$ | etree | EL | UET |
| ---: | ---: | ---: | ---: | ---: |
| 100000 | 249997 | 0.005 | 27.509 | 0.073 |
| 200000 | 499997 | 0.010 | 125.064 | 0.147 |
| 300000 | 749997 | 0.014 | 269.573 | 0.223 |

Table 1: Running time of the algorithms on instances on which EL runs in quadratic time.
of Section 2.3, starts with the initial call with $s=0$ and all of the 10 vertices. Then, the graph $G_{5}$ is found to be acyclic, and a recursive call is made with $s=5$ and again with 10 vertices. The graph $G_{8}$ is found to be acyclic, and a recursive call is made with $s=8$ and again with 10 vertices. The graph $G_{9}$ is found to be acyclic, and a recursive call is made with $s=9$ and all the 10 vertices. This last call finds $s=9$ and $\eta=10$ (the condition holds at the first if statement) and sets all parent pointers to 10 resulting in the elimination tree shown in Fig 2(b). Note that UET, the implementation with the modification presented at the last paragraph of Section 2.3, sets the parent pointers without any recursive call (but computes the strong components of $G_{5}, G_{8}$ and $G_{9}$ ).

In order to assess the difference in the execution times of both algorithms, we run them on matrices described above with parameter $k=5 \times 10^{4}, 10 \times 10^{4}$, and $15 \times 10^{4}$. The execution times are reported in seconds in Table 1. In order to put the running times into perspective, we also report the running time of the standard symmetric elimination tree algorithm (etree in Matlab) in Table 1, where etree was run on the symmetrized matrices. As seen in the table, EL has a much higher execution time than UET on these instances. As expected, both algorithms are much slower than the linear time etree algorithm.

### 3.2 Real life matrices

We have compared the execution times of the algorithms EL and UET on a set of matrices from the UFL sparse matrix collection [2]. The matrices are listed with the properties: square, $50000<n \leq 5000000$, numerical symmetry is less than $1.0,2 \times n \leq m \leq 15000000$, real, and not of type Graph. There were a total of 102 matrices having these properties at the time of experimentation.

We preprocessed these matrices as follows. First, we ensured that the diagonal is zero-free. We have two alternatives for this purpose. The first one is to

|  | dmperm | MC64 |
| ---: | ---: | ---: |
| AMD | 84 | 84 |
| MeTiS | 89 | 90 |

Table 2: Number of instances on which EL had a smaller running time than UET. Each cell can be at most 102 .

| matrix | dmperm diagonal |  |  |  | MC64 diagonal |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | AMD |  | MeTiS |  | AMD |  | MeTiS |  |
|  | EL | UET | EL | UET | EL | UET | EL | UET |
| pre2 | 0.387 | 0.825 | 0.333 | 1.038 | 0.478 | 0.869 | 0.320 | 1.000 |
| Hamrle3 | 11.239 | 2.017 | 6.358 | 2.377 | 17.493 | 2.240 | 13.016 | 2.439 |
| largebasis | 0.212 | 0.991 | 0.222 | 1.051 | 0.191 | 1.010 | 0.237 | 1.047 |
| t2em | 0.232 | 1.094 | 0.249 | 1.406 | 0.232 | 1.090 | 0.251 | 1.396 |
| tmt_unsym | 0.244 | 1.130 | 0.255 | 1.383 | 0.244 | 1.139 | 0.251 | 1.398 |
| ch7-8-b5 | 80.421 | 0.297 | 3.173 | 0.238 | 90.689 | 0.310 | 2.852 | 0.247 |
| m133-b3 | 140.486 | 0.459 | 7.333 | 0.334 | 285.167 | 0.459 | 11.183 | 0.392 |
| shar te2-b3 | 134.650 | 0.450 | 19.268 | 0.391 | 297.392 | 0.462 | 4.953 | 0.324 |
| atmosmodd | 0.467 | 1.827 | 0.534 | 2.574 | 0.465 | 1.825 | 0.537 | 2.604 |
| atmosmodj | 0.465 | 1.839 | 0.534 | 2.593 | 0.464 | 1.832 | 0.534 | 2.590 |
| atmosmodl | 0.543 | 2.230 | 0.623 | 3.129 | 0.543 | 2.220 | 0.622 | 3.124 |
| atmosmodm | 0.543 | 2.237 | 0.622 | 3.062 | 0.543 | 2.255 | 0.623 | 3.157 |
| memchip | 0.804 | 3.627 | 0.818 | 4.198 | 0.805 | 3.559 | 0.814 | 4.241 |
| circuit5M_dc | 0.968 | 4.678 | 0.979 | 4.949 | 0.959 | 4.627 | 0.978 | 4.836 |

Table 3: Running time of EL and UET (in seconds) on real-life matrices where at least one of the algorithms run in more than one second.
use MC64 [3] to find a maximum product matching and to permute the entries in the matching to the diagonal. The second one is to use an arbitrary zerofree diagonal using a maximum cardinality matching algorithm (such as those resulting from dmperm of Matlab). Next, we obtained the Dulmage-Mendelsohn decomposition [5] and permuted the matrix accordingly (using the output of dmperm), and deleted all entries that are in the off-diagonal blocks. The reason in deleting those entries is that it is advisable to factor only the diagonal blocks of a reducible matrix. As the last step, we used AMD [1] (the command amd in Matlab) and MeTiS [9] (using MeshPart toolbox [8]) to reorder the matrices using their symmetrized versions. We use the term "instance"to refer to a matrix preprocessed in one of the four possible alternative ways. Therefore, we have $4 \times 102=408$ instances. We run EL and UET ten times for each instance resulting from this preprocessing step in order to be able to report reproducible running time results. We did not use randomization for AMD in Matlab, and we did not turn the randomization off in MeTiS. As we expect the same running time when AMD was used in ordering, we report the minimum of ten running times for each algorithm. On the other hand, we report the median of ten running times for each algorithm when MeTiS was used, since the expected behavior in this case is the median one.

We first give the number of instances on which EL had a smaller running time than UET in Table 2. As we have 102 matrices in total, the table shows that EL's
practical running time is faster than that of UET in a significant number of cases. We highlight that both of the algorithms are efficient; in only 14 matrices one of the algorithms had a running time larger than one second with any of the four preprocessing alternatives. In Table 3, we present the matrices (in increasing order of ids at the UFL collection) on which this latter case occurred. In this table, in only 16 out of 56 instances, running time of EL is larger than that of UET. These instances correspond to the matrices Hamrle3, ch7-8-b5, m133-b3, and shar_te2-b3. As seen in these instances, the difference in the running time can be significant in favor of UET. We note that the three matrices for which there are two orders of difference in the running times are from the same family in the UFL collection. Combined with the previous subsection results, we conclude that there are matrices for which the running time of EL can be significantly larger than that of UET.

## 4 Conclusion

We have proposed an algorithm to compute the elimination tree of an $n \times n$ unsymmetric matrix with a zero-free diagonal and $m$ off-diagonal nonzeros in $\mathcal{O}(m \log n)$ time. The previously known algorithm [7] has the worst-case time complexity of $\Theta(m n)$.

We have implemented the proposed algorithm and compared it with the algorithm of Eisenstat and Liu [7]. Both algorithms are found to be fast in general. On 88 among 102 real life matrices satisfying the properties $50000<$ $n \leq 5000000$ and $2 \times n \leq m \leq 15000000$, both of the algorithms run in less than one second on current desktop computers. The algorithm of Eisenstat and Liu is found, in a significantly large number of cases, to be faster than the proposed one. However, there are both real life and constructed matrices where the proposed algorithm is significantly faster.

## Acknowledgments

We thank an anonymous referee whose suggestions improved the paper. We also thank Stanley Eisenstat for his editorial and technical comments, for sharing the code of the algorithm EL, for a simplified analysis of the running time complexity, and for the worst-case examples presented in the experiments. We are appreciative of his help in designing the experimental set up as well. The proposed algorithm is available at authors' web pages.

## Bibliography

[1] P. R. Amestoy, T. A. Davis, and I. S. Duff. An approximate minimum degree ordering algorithm. SIAM Journal on Matrix Analysis and Applications, 17(4):886-905, 1996.
[2] T. A. Davis and Y. Hu. The University of Florida sparse matrix collection. ACM Trans. Math. Softw., 38(1):1:1-1:25, 2011.
[3] I. S. Duff and J. Koster. On algorithms for permuting large entries to the diagonal of a sparse matrix. SIAM Journal on Matrix Analysis and Applications, 22:973-996, 2001.
[4] I. S. Duff and B. Uçar. Combinatorial problems in solving linear systems. Technical Report TR/PA/09/60, CERFACS, Toulouse, France, 2009.
[5] A. L. Dulmage and N. S. Mendelsohn. Coverings of bipartite graphs. Canadian Journal of Mathematics, 10:517-534, 1958.
[6] S. C. Eisenstat and J. W. H. Liu. The theory of elimination trees for sparse unsymmetric matrices. SIAM J. Matrix Anal. Appl., 26:686-705, January 2005.
[7] S. C. Eisenstat and J. W. H. Liu. Algorithmic aspects of elimination trees for sparse unsymmetric matrices. SIAM J. Matrix Anal. Appl., 29:13631381, January 2008.
[8] J. R. Gilbert, G. L. Miller, and S.-H. Teng. Geometric mesh partitioning: Implementation and experiments. SIAM Journal on Scientific Computing, 19(6):2091-2110, 1998.
[9] G. Karypis and V. Kumar. MeTiS: A Software Package for Partitioning Unstructured Graphs, Partitioning Meshes, and Computing Fill-Reducing Orderings of Sparse Matrices Version 4.0. University of Minnesota, Department of Comp. Sci. and Eng., Army HPC Research Center, Minneapolis, 1998.
[10] J. W. H. Liu. The role of elimination trees in sparse factorization. SIAM J. Matrix Anal. Appl., 11(1):134-172, 1990.
[11] R. Schreiber. A new implementation of sparse Gaussian elimination. ACM T. Math. Software, 8(3):256-276, 1982.
[12] R. E. Tarjan. Depth-first search and linear graph algorithms. SIAM J. Comput., 1(2):146-160, 1972.
[13] R. E. Tarjan. An improved algorithm for hierarchical clustering using strong components. Inform. Process. Lett., 17(1):37-41, 1983.

RESEARCH CENTRE
GRENOBLE - RHÔNE-ALPES
Inovallée
655 avenue de l'Europe Montbonnot
38334 Saint Ismier Cedex

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Inria
Domaine de Voluceau - Rocquencourt
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