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ABSTRACT

In this paper we study the problem of optimal ordering of Gaussian elimination of a structurally symmetric matrix using the concept of triangulations of a graph. Results on minimal triangulations and an efficient algorithm for finding such triangulations are presented. The algorithm is illustrated with an example.

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I. INTRODUCTION

In solving $Ax = b$, in which A is a large sparse matrix, using Gaussian elimination, it is advantageous to have an order of elimination such that the number of nonzeros (fill-ins) produced is minimized [1]. In most network problems, A is structurally symmetric and positive definite [2], [3], [4]. For this class of matrices, symmetric Gaussian elimination is used to simplify the programming. The problem of finding an order of elimination which creates the minimum number of fill-ins is still not completely solved for this class of matrices.

Ogbuobiri et. al. [3] propose an algorithm for decomposing a graph into clusters which are then optimally ordered by some simple schemes. This algorithm provides a partial solution to the minimum fill-in problem.

Rose [4], [5] studies the same problem using the concept of triangulated graph.¹ It is shown there that Gaussian elimination on a matrix, which is equivalent to vertex-elimination [3] of the graph associated with the matrix,² can be viewed as a process of finding a triangulation³ for the graph. This allows us to speak of Gaussian elimination on a matrix and triangulation of a graph interchangeably. The number of fill-ins is directly related to the size of the triangulation. In [4], Rose gives an algorithm for finding a minimal subset of a given triangulation such that this minimal set is also a triangulation. Rose's algorithm has several drawbacks. It is an indirect algorithm for getting a minimal triangulation⁴ because we have to find a triangulation by some scheme before applying the algorithm. Besides, the algorithm is inefficient in that successive "pass" of the algorithm has to be executed if the triangulation is not minimal after a "pass". Above all, the algorithm is incomplete in that it may never

terminate in some cases.⁵

Though minimal triangulation may not give the minimum fill-ins in the Gaussian elimination, it does give fairly good results if incorporated into some practical schemes like those listed in [3]. The importance of minimal triangulation is not difficult to see as it provides a step-stone to the problem of minimum triangulation. Besides this, minimal triangulation guarantees us that we can derive an ordering for the Gaussian elimination process, which is our ultimate aim. There is clear indication that a minimum triangulation algorithm, if one can be found, is going to be fairly involved and hence is not so practical as the existing heuristic schemes [3], [6]. However, sound theoretical insight into this may help us find out new ways of attacking the problem. Besides, the algorithm can be used as a basis for testing the relative performance of the existing practical schemes.

In this paper, we study the problem of minimal triangulation for an undirected graph in depth. Section III shows that sometimes we may not be able to derive an elimination order from a triangulation if the triangulation is not minimal. This important fact is not clearly indicated in Rose's work [4], [5]. The complexity of a minimal triangulation algorithm is indicated in Section IV, where it is shown that "local information" of a graph is insufficient for the success of a Rose-type algorithm. In Section V, we present results on minimal triangulation, which are used to derive an efficient algorithm for finding a minimal triangulation.

II. DEFINITIONS AND NOTATIONS

A graph is a pair, $G = (X, E)$, where X is a finite set of vertices and E is a set of edges, each of which connects two distinct vertices of X ,

and no more than one edge connecting the same pair of vertices. G is assumed to be connected in this paper. Given $x \in X$, $\text{Adj}(x)$ is the set of all vertices of X adjacent to x . For distinct vertices, $x, y \in X$, a chain from x to y (of length ℓ) is an ordered set of distinct vertices

$$\mu = [p_1, p_2, \dots, p_{\ell+1}] ; p_1 = x, p_{\ell+1} = y$$

such that $p_{i+1} \in \text{Adj}(p_i)$, $i = 1, \dots, \ell$. For any $x \in X$ and any two distinct vertices $y, z \in \text{Adj}(x)$, an x -external chain from y to z is a chain from y to z which does not go through any vertices of $x \cup \text{Adj}(x)$.

A cycle (of length ℓ) is an ordered set of ℓ distinct vertices

$$\mu = [p_1, p_2, \dots, p_\ell, p_1]$$

such that $p_{i+1} \in \text{Adj}(p_i)$; $i = 1, \dots, \ell - 1$ and $p_1 \in \text{Adj}(p_\ell)$.

For graph $G = (X, E)$ and subset $A \subseteq X$, the section graph $G(A)$ is the subgraph

$$G(A) = (A, E(A)); E(A) = \{\{x, y\} \in E : x, y \in A\} .$$

A separator of a graph $G = (X, E)$ is a subset $S \subset X$ such that the section graph $G(X - S)$ consists of two or more connected components, say $C_i = (X_i, E_i)$.

The section graphs $G(S \cup X_i)$ are the leaves of G with respect to S .

A minimal separator is a separator no subset of which is also a separator.

Given $a, b \in X$ with $a \notin \text{Adj}(b)$ an a, b separator is a separator such that a and b are in distinct components, say C_a and C_b , respectively. A clique

of a graph is a subset of vertices which are pairwise adjacent, and a

separation clique is a separator which is also a clique.

Let $G = (X, E)$ be a graph with $|X| = n$. An ordering of X is a bijective map

$$\alpha : \{1, 2, \dots, n\} \leftrightarrow X .$$

If X is ordered by α , then $G_\alpha = (X, E, \alpha)$ is an ordered graph associated with α . The deficiency $D(x)$ of a vertex $x \in X$, is the set of all pairs of $\text{Adj}(x)$ which are not themselves adjacent; i.e.,

$$D(x) = \{\{y, z\} : y, z \in \text{Adj}(x) \text{ \& } y \notin \text{Adj}(z)\}.$$

In case of ambiguity, we use $[D(x)]_G$ to denote $D(x)$ in graph G . Similarly for $[\text{Adj}(x)]_G$.

Given a vertex x of a graph G , the graph G_x obtained from G by
 (i) deleting x and its incident edges and
 (ii) adding edges such that all vertices in the set $\text{Adj}(x)$ are adjacent
 is the x - elimination graph of G . (i) and (ii) constitute a vertex - elimination step. Thus

$$G_x = (X - \{x\}, E(X - \{x\}) \cup D(x)).$$

For an ordered graph $G_\alpha = (X, E, \alpha)$ the order sequence of elimination graphs G_1, G_2, \dots, G_{n-1} is defined recursively by $G_1 = G_{x_1}$ and

$$G_i = (G_{i-1})_{x_i} ; \quad i = 2, \dots, n - 1.$$

The elimination process on a graph $G = (X, E)$ with ordering α is the ordered set

$P(G; \alpha) = [G = G_0, G_1, \dots, G_{n-1}]$. The elimination process is perfect if

$$G_i = G(X - \bigcup_{j=1}^i \{x_j\}).$$

The ordered graph $G_\alpha = (X, E, \alpha)$ is monotone transitive iff $P(G; \alpha)$ is a perfect elimination process.

If the ordered graph $G_\alpha = (X, E, \alpha)$ is not monotone transitive, we

define the monotone transitive extension $G_{MTE\alpha}$ as

$$G_{MTE\alpha} = (X, \bigcup_{i=0}^{n-1} E_i)$$

where E_i is the set of edges in the elimination graph G_i . We define

$$T(\alpha) = \bigcup_{i=0}^{n-1} E_i - E \text{ as the } \underline{\text{triangulation induced by ordering } \alpha} \text{ on } X.$$

If $G = (X, E)$ is non-triangulated and T is a triangulation for G , then the triangulated extension G_T of G by T is

$$G_T \underline{\Delta} (X, E \cup T).$$

A minimal order $\hat{\alpha}$ is an order such that no other order α gives $T(\alpha)$ which is a proper subset of $T(\hat{\alpha})$.

Finally, we define an optimal set X^* for graph G as

$$X^* \underline{\Delta} \{x \in X : \exists \text{ a minimal order } \alpha \text{ such that } \alpha^{-1}(x) = 1\}.$$

III. MINIMAL TRIANGULATION AND TRANSITIVE ORDERING

Rose has shown [4], [5] that with respect to any ordering α on X of a graph G , the set of edges $T(\alpha)$ is a triangulation for G . Now suppose we have found a triangulation T for $G = (X, E)$, we want to know if we can find an ordering α on X such that

$$G_{MTE\alpha} = G_T.$$

If such an ordering can be found, then corresponding to the triangulation T , we have an ordering for the Gaussian elimination [4], [5]. The following lemma gives a sufficient condition for the existence of α .

[Lemma 1]

Let $G = (X, E)$ be non-triangulated and T be a minimal triangulation.

Then there exists an ordering α on X such that $G_{\text{MTE}\alpha} = G_T$.

Proof

Since G_T is a triangulated graph, by Theorem 1 of [5], there exists an ordering α on X such that $(G_T)_\alpha = (X, E \cup T, \alpha)$ is monotone transitive. Let $\alpha(i) = x_i$; $i = 1, 2, \dots, n$, $|X| = n$.

First show that $T(\alpha) \subseteq T$. Since G is a subgraph of G_T , then $[\text{Adj}(x_1)]_G \subseteq [\text{Adj}(x_1)]_{G_T}$ implies $[D(x_1)]_G \subseteq E \cup T$. Therefore, the set of edges added in G_{x_1} is a subset of T . Hence G_{x_1} is a subgraph of $(G_T)_{x_1}$

which is still monotone transitive with monotone transitive ordering

$$\alpha(i) = x_i ; i = 2, 3, \dots, n.$$

Repeating the process of vertex-elimination, we see that $T(\alpha) \subseteq T$.

Suppose $T(\alpha) \subset T$ (strict inclusion), then $T(\alpha)$ is a triangulation which is a proper subset of a minimal triangulation. This is a contradiction. Hence $T(\alpha) = T$, that is $G_{\text{MTE}\alpha} = G_T$ □

Thus if T is a minimal triangulation, then any monotone transitive order of G_T will be an ordering for Gaussian elimination with number of fill-ins directly related to $|T|$. In Fig. 1, we give an example for the nonexistence of ordering α such that $G_{\text{MTE}\alpha} = G_T$. Note that T is not minimal because either $\{a\}$ or $\{b\}$ is also a triangulation.

From lemma 1, we can derive

[Lemma 2]

Let $G = (X, E)$ be non-triangulated and α be a minimal order. Then $T(\alpha)$ is a minimal triangulation.

Proof

If $T(\alpha)$ is not minimal, there exists a proper subset of T , denoted

by T' , that is a minimal triangulation. From Lemma 1, there exists an order α' such that $T' = T(\alpha') \subset T(\alpha)$. This contradicts the minimality of order α . □

From the above two lemmas, the following theorem is immediate

[Theorem 1]

Let $G = (X, E)$ be non-triangulated. A triangulation T is minimal (minimum) iff there exists a minimal (minimum) order α such that $T = T(\alpha)$. □

Theorem 1 indicates to us a way of testing whether a given triangulation is minimal (minimum). However it does not give us an algorithm for constructing a minimal triangulation.

IV. INSUFFICIENCY OF LOCAL INFORMATION FOR MINIMAL TRIANGULATION

Let $G = (X, E)$ and T be a triangulation for G . The Rose-algorithm [4], p. 4.24, is supposed to derive a minimal triangulation \hat{T} from T . The transformation from T to \hat{T} is actuated by a process of vertex-elimination. The algorithm produces an ordering $\alpha(i) = x_i$ such that $\hat{G} = (X, E \cup \hat{T}(\alpha))$ is triangulated, \hat{T} is minimal and $\hat{T} \subset T$.

Step 1. Set $i = 0$; $G_0 = (X, E \cup T)$;

$$X_0 = X; \hat{T} = T.$$

Step 2. Set $G_i = (X_i, E(X_i) \cup T)$

In G_i , Find $S_i = \{y_1, y_2, \dots, \ell\}$ with $D(y_j) = \phi$.

Step 3. Find a $j \in \{1, 2, \dots, \ell\}$ such that y_j has some T edges incident with it i.e.

$$\tilde{T} = \{e = (y_j, z) \mid z \in \text{Adj}(y_j)\} \cap T \neq \phi$$

If $\tilde{T} = \phi$, go to Step 5.

Step 4. Set $T = T - \tilde{T}$

$$\hat{T} = \hat{T} - \tilde{T}$$

Go to Step 2.

Step 5. Set $i = i + 1$;

If $i > n$, go to Step 6; else

Set $x_i = y_1$;

Set $T = T - \{(u, v) \mid u, v \in \text{Adj}(y_1)\}$;

$$X_i = X_{i-1} - x_i$$

Go to Step 2.

Step 6. End of algorithm.

From the algorithm, it can be seen that at Step 5 of the process, the choice of a vertex, say y_1 , to be eliminated next is based on the following "local" information:

(i) $D(y_1)$

(ii) $\text{Adj}(y_1)$

(iii) Whether there is any member of T incident with y_1 .

Thus we may fail to eliminate a suitable vertex when we come to the situation of having more than one vertex carrying the same information.

This is illustrated in Fig. 2. In this example, vertices 1, 2, 3 carry the same information listed above. If vertex 1 is eliminated first, then \hat{T} will contain a. Hence in this case the Rose-algorithm would not reduce

$T = \{a, b, c\}$ to a minimal triangulation \hat{T} , which in this example is

$$\hat{T} = \{b, c\}.$$

In fact, failure in producing a minimum triangulation is common in most existing practical schemes [3], [6] which depend on local information.

V. MINIMAL TRIANGULATION

In this section, we shall present useful results which will lead to the construction of a minimal triangulation algorithm. We make use of Theorem 2 of [5] which is stated below.

[Lemma 3]

Let $\hat{G} = (X, F)$ be triangulated with subgraph $G = (X, E)$; $E \subset F$. Then G is triangulated iff for each $(x, y) \in F - E$, there exists an $x - y$ separation clique of G . □

This lemma leads us to the following theorem.

[Theorem 2]

A triangulation T of $G = (X, E)$ is minimal iff for each $(x, y) \in T$, every $x - y$ separator C of G is not a clique of the triangulated extension $G_T = (X, E \cup T)$.

Proof

"if part" We assume there exists a triangulated subgraph $G'_T = (X, E \cup T')$; $T' \subset T$ of G_T . From Lemma 3, there should exist, for each $(x, y) \in T - T'$, an $x - y$ separation clique C of G'_T . Since C is an $x - y$ separator of G and also a clique of G_T , it is a contradiction.

"only if part" We assume that there exists an $x - y$ separator C of G , which is also a clique of G_T . Let $T_C \subset T$ be the set of $(u, v) \in T$ such that C is also a $u - v$ separator. Then C is a $u - v$ separation clique of $G_{T_C} = (X, E \cup T - T_C)$, which, by Lemma 3, is still triangulated. Hence T is not minimal. □

Now we give a more algorithmic characterization of minimal triangulation.

[Theorem 3]

Let $G = (X, E)$ and X^* be the optimal set for G . $x \in X^*$ iff, for each

$(u, v) \in D(x)$, $S = \{x\} \cup \text{Adj}(x) - \{u, v\}$ is not a $u - v$ separator.

(Note that if $D(x) = \phi$, obviously $x \in X^*$).

Proof

"if part" Let β be a minimal ordering of $X - \{x\}$ with respect to the x - elimination graph $G_x = (X - \{x\}, E \cup D(x) - E(x))$, where $E(x)$ is the set of edges incident at x and $T_x(\beta)$ be a triangulation of G_x produced by β . Now considering the ordering α of X produced by

$$\alpha(1) = x, \alpha(2) = \beta(1), \dots, \alpha(n) = \beta(n-1).$$

Obviously, $T(\alpha) = D(x) \cup T_x(\beta)$ is a triangulation of G . It suffices to show that $T(\alpha)$ is minimal. We assume $T(\alpha)$ is not minimal, then as shown in Theorem 2, for at least one $(y, z) \in T(\alpha)$ there should exist a $y - z$ separator C of G such that C is a clique of $G_{T(\alpha)} = (X, E \cup T(\alpha))$. We have two cases.

(Case 1): $(y, z) \in D(x)$

From the definition of the theorem, C should contain x and at least one vertex, say w , in $X - \{x\} - \text{Adj}(x)$. But from the definition of α , $(x, w) \notin T(\alpha)$, which contradicts the fact that C is a clique of $G_{T(\alpha)}$.

(Case 2): $(y, z) \in T_x(\beta)$

From Lemma 1, $T_x(\beta)$ is a minimal triangulation of G_x . And there exists no vertex pair $(u, v) \in D(x)$ such that C is also a $u - v$ separator of G , since otherwise it causes the same contradiction as in Case 1.

Therefore, $C - \{x\}$ is a $y - z$ separator of G_x and is also a clique of $\hat{G}_x = (X - \{x\}, E \cup D(x) - E(x) \cup T_x(\beta))$. Thus from Theorem 2, $T_x(\beta)$ cannot be a minimal triangulation of G_x , which is a contradiction.

"only if part" We assume there exists a $(u, v) \in D(x)$ such that $S = \{x\} \cup \text{Adj}(x) - \{u, v\}$ is a $u - v$ separator of G . Since any ordering α such that $\alpha(1) = n$ has the property that $D(x) \subseteq T(\alpha)$, S is a clique of

$G_{T(\alpha)} = (X, E \cup T(\alpha))$ for any α such that $\alpha(1) = x$. Theorem 2 shows that any $T(\alpha)$ with $\alpha(1) = x$ is not minimal. Hence $x \notin X^*$. \square

Hence if for each elimination graph G_{i-1} ; $i = 1, \dots, n-1$ with $G_0 = G$, we eliminate a vertex $x_i \in X_{i-1}^*$, where X_{i-1}^* is the optimal set of vertices for G_{i-1} , then $(\bigcup_{i=0}^{n-1} E_i) - E$ is a minimal triangulation for G . Theorem 3 can be stated in terms of external chains as follows.

[Corollary 1]

Let $G = (X, E)$ and X^* be the optimal set for G . $x \in X^*$ iff there exists an x - external chain between any pair of vertices in $\text{Adj}(x)$.

Proof

It is obvious that for $(u, v) \in D(x)$, $S = \{x\} \cup \text{Adj}(x) - \{u, v\}$ is not a $u - v$ separator iff we have an x - external chain from u to v . For $(u, v) \notin D(x)$, we have an edge between u and v which is a trivial external chain. \square

Theorem 3 or Corollary 1 can be used to find the optimal set X^* at each stage of vertex-elimination. However, it is not necessary to test all vertices in order to find X_i^* if we know X_{i-1}^* . The following lemmas allow us to simplify the testing procedure.

[Lemma 3]

Let y be such that $G_i = (G_{i-1})_y$; $i = 1, 2, \dots, n-1$. Then $(x \in X_{i-1}^* \Rightarrow x \in X_i^*)$ if in G_{i-1} , $y \notin \text{Adj}(x)$.

Proof Consider G_{i-1} . Let $x \in X_{i-1}^*$ and $u, v \in \text{Adj}(x)$. Suppose in G_{i-1} , the x - external chain from u to v passes through y . Then in $G_i = (G_{i-1})_y$, these exists an x - external chain from u to v through the deficiency edge of y .

Suppose, in G_{i-1} , the x - external chain between u, v does not go

through y . This chain remains unchanged in G_i . In both cases,

$$x \in X_i^*$$

□

Parallel to Lemma 3, we have

[Lemma 4]

Let y be such that $G_i = (G_{i-1})_y$, $i = 1, 2, \dots, n - 1$.

Then $(x \notin X_{i-1}^* \Rightarrow x \notin X_i^*)$ if in G_{i-1} , $y \notin \text{Adj}(x)$.

□

Thus at each stage of vertex elimination, all we have to do is to test vertices adjacent to the one just eliminated and update the optimal set X^* accordingly.

The schematic for obtaining a minimal ordering α is shown by a flow-chart in Fig. 3. It should be noted that no matter which x_i is chosen from X_{i-1}^* ; $i = 1, 2, \dots, n$, we always get some minimal ordering α and the corresponding minimal triangulation $T(\alpha)$ for G . It is obvious that some minimal orderings $\hat{\alpha}$ are also minimum ones. In the steps marked with an asterisk, we have some flexibility in picking $x_i \in X_{i-1}^*$, $i = 1, 2, \dots, n$. If some additional criterion is imposed on the choice of x_i , like choosing

$$\hat{x}_i \text{ such that } \left| [D(x_i)]_{G_{i-1}} \right| = \min_{x_i \in X_{i-1}^*} \left| [D(x_i)]_{G_{i-1}} \right|$$

then we get a smaller family of minimal orderings. Whether this additional criterion would lead to a triangulation with a smaller cardinality is still an open problem. We illustrate the minimal triangulation algorithm with the following example.

Example

In Fig. 4(a), we have a graph [4] consisting of 11 vertices. Fig. 4(b) shows that vertex $a \in X^*$ of G_0 because $(b, g) \in D(a)$ and $\{b, h, g\}$ is an a -external chain going between b and g . Similarly

for $(c, g) \in D(a)$, we have an a -external chain from c to g .

The algorithm successively gives the following optimal sets for the elimination graphs. In each optimal set, we pick the vertex which introduces the minimum number of edges.

X_0^*	= {a, b, c, d, e, f};	pick	$x_1 = a$
X_1^*	= {b, c, d, e, f};		$x_2 = b$
X_2^*	= {c, d, e, f};		$x_3 = c$
X_3^*	= {d, e, f, h};		$x_4 = h$
X_4^*	= {d, e, f, k};		$x_5 = k$
X_5^*	= {d, e, f, i, j, g};		$x_6 = g$
X_6^*	= {d, f, i, j};		$x_7 = i$
X_7^*	= {d, f, j, e};		$x_8 = d$
X_8^*	= {f, j, e};		$x_9 = f$
X_9^*	= {j, e};		$x_{10} = j$
X_{10}^*	= {e};		$x_{11} = e$.

Thus $\alpha\{1, 2, \dots, 11\} = \{a, b, c, h, k, g, i, d, f, j, e\}$

with $T(\alpha) = \{(b, g), (c, g), (h, c), (g, i), (e, i), (e, j), (d, j)\}$.

In Fig. 4(c), we show the triangulated extension $G_{T(\alpha)}$.

VI. CONCLUSION

The concept of triangulation of a graph is used to find an optimal ordering for the symmetric Gaussian elimination of a structurally symmetric matrix. It is shown that when the triangulation is minimal, it is always possible to derive from the triangulation an elimination ordering. Results on minimal triangulation and an efficient direct algorithm for constructing it are presented. It is hoped that these results may help us solve the minimum triangulation problem.

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FOOTNOTES

1. A graph G is triangulated if for every cycle μ of length $l > 3$, there is an edge of G joining two nonconsecutive vertices of μ ; such edges are called chords of the cycle [5].
2. When we say the graph associated with a structurally (i.e. zero-non-zero) symmetric matrix we mean an undirected graph constructed in the way shown in [3] or [4].
3. Triangulation T for a graph $G = (X, E)$ is a set of edges such that the new graph with vertices X and edges $E \cup T$ is triangulated.
4. A minimal triangulation for a graph G is a triangulation such that no proper subset of it is also a triangulation. A minimum triangulation \hat{T} is a triangulation such that $|\hat{T}| \leq |T|$, where T is any triangulation for G ; $|T|$ denotes the cardinality of set T .
5. This will be clarified in Section IV.

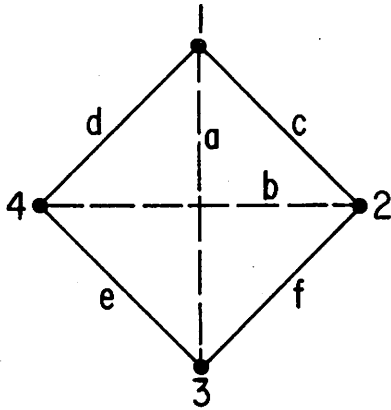


Fig. 1. Example showing nonexistence of ordering α which is such that $G_{MTE\alpha} = G_T$.
 $G = (\{1,2,3,4\}, \{c,d,e,f\}), T = \{a,b\}$.

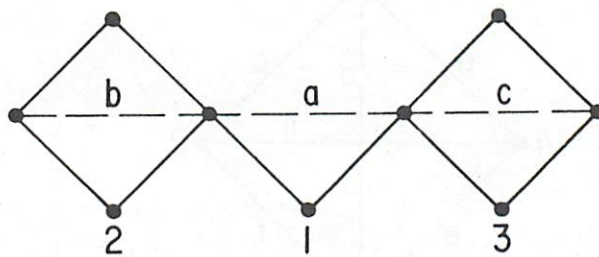


Fig. 2. Example showing failure of Rose's Algorithm.

Graph G is represented by solid lines.

$T = \{a, b, c\}$.

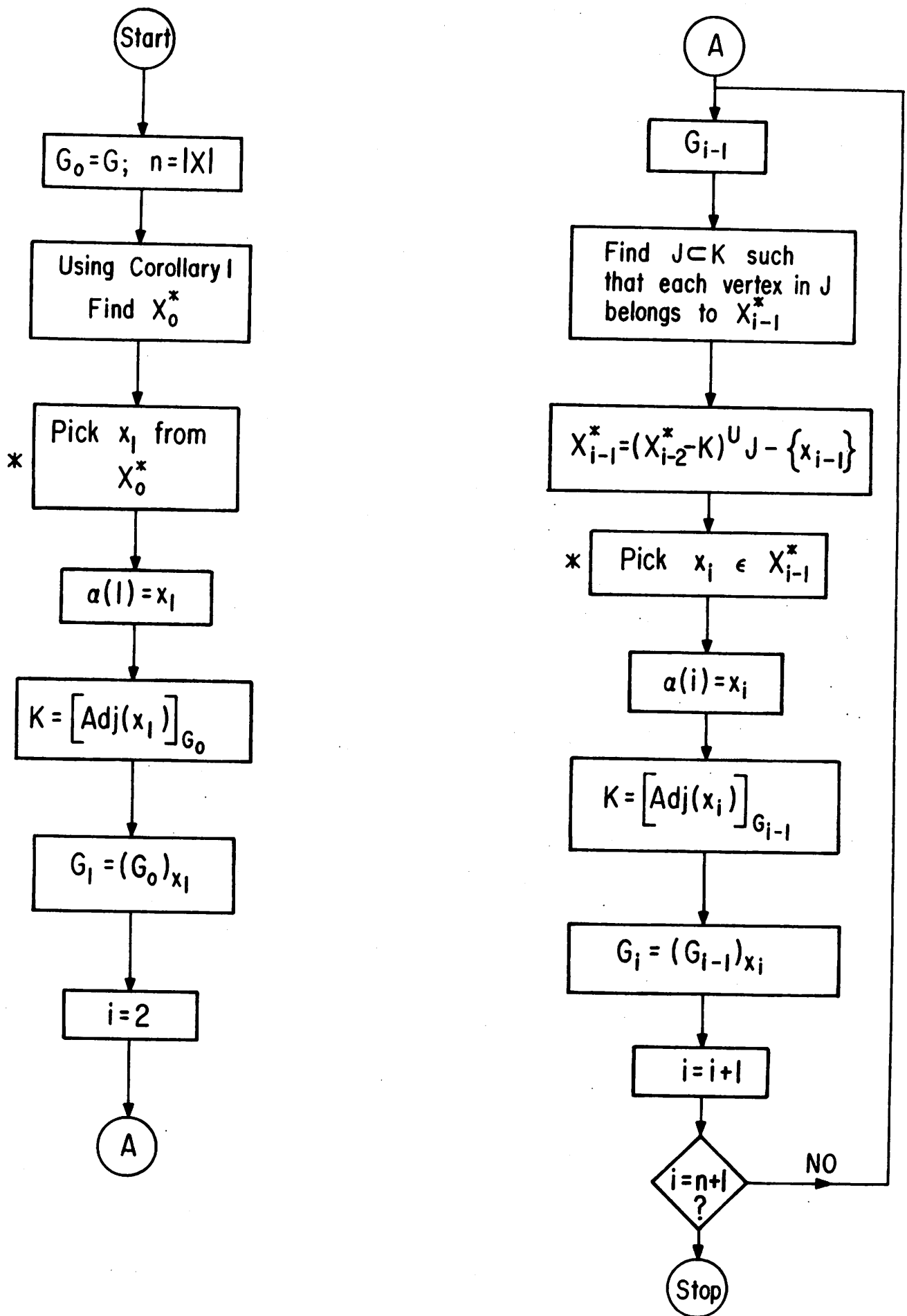


Fig. 3. Flow chart for finding ordering α .

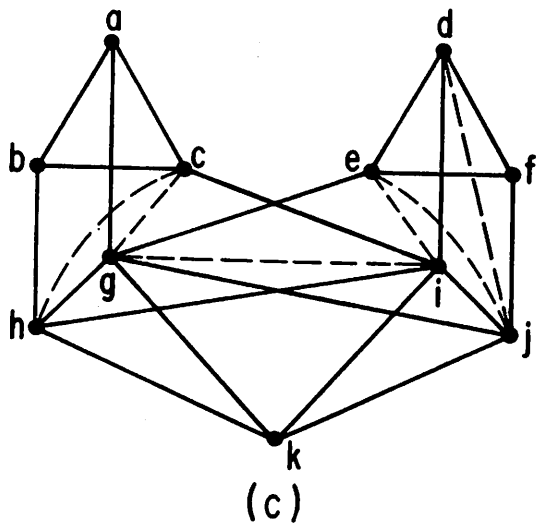
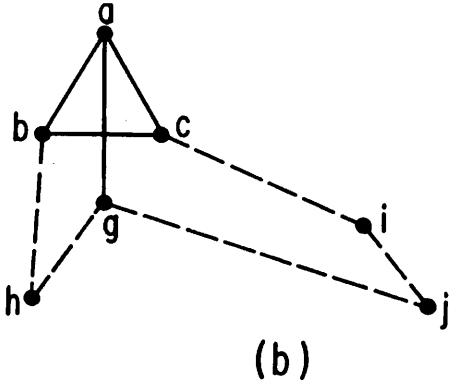
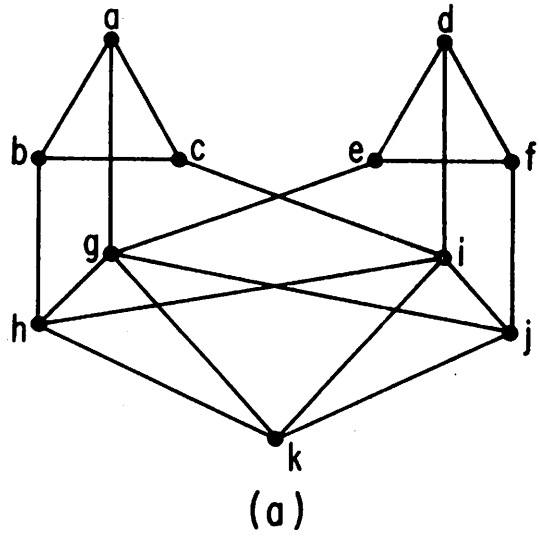


Fig. 4. Illustration for the minimal triangulation algorithm.
 (a) Graph G . (b) Two a -external chains. (c) The triangulated extension $G_{T(\alpha)}$, $T(\alpha)$ is represented by dashed lines.