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On Cubical Graphs

M. R. GAREY AND R. L. GRAHAM

Bell Laboratories, Murray Hill, New Jersey 07974

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It is frequently of interest to represent a given graph G as a subgraph of a graph H which has some special structure. A particularly useful class of graphs in which to embed G is the class of n-dimensional cubes. This has found applications, for example, in coding theory, data transmission, and linguistics. In this note, we study the structure of those graphs G, called *cubical* graphs (not to be confused with *cubic* graphs, those graphs for which all vertices have degree 3), which can be embedded into an n-dimensional cube. A basic technique used is the investigation of graphs which are critically nonembeddable, i.e., which can not be embedded but all of whose subgraphs can be embedded.

INTRODUCTION

It is frequently of interest to represent a given graph[1] G as a subgraph of a graph H which has special structure. A particularly important class of graphs in which to embed G is the class of n-dimensional cubes. This has found application, for example, in coding theory [6, 10], data transmission [8], and linguistics [4]. In this note, we study the structure of those graphs G, called *cubical* graphs, which can be embedded in some n-dimensional cube. It is convenient however to approach the analysis indirectly, examining instead the simplest graphs which *cannot* be embedded in any n-dimensional cube. Such graphs, called *critical* graphs, are the "forbidden subgraphs" for cubical graphs; in fact, a graph is cubical if and only if it contains no critical subgraph. Thus the critical graphs play a crucial role in determining the structure of cubical graphs. After some preliminary results, directly concerning cubical graphs, we focus exclusively on the structure of critical graphs.

[1] See [5] for graph theory terminology.

Notation

For a set S, define[2] a graph $Q(S)$, called the *cube on* S, as follows. The vertices of $Q(S)$ are the finite subsets of S; the pair of subsets $\{S_1, S_2\}$ is an *edge* of $Q(S)$ iff the symmetric difference of S_1 and S_2 consists of a single element, i.e., $|S_1 \Delta S_2| = 1$. To each $T \subseteq S$, one can associate the characteristic function $\chi_T : S \to \{0, 1\}$. For a finite set $S_n = \{s_1, ..., s_n\}$, χ can be used to coordinate $Q(S_n)$ by assigning to each $T \subseteq S_n$, the binary n-tuple $A(T) = (a_1, ..., a_n)$ where $a_k = 1$ iff $s_k \in T$. This is the standard description of the n-cube $Q(S_n) = Q(n)$. Note that $Q(n)$ has 2^n vertices and $n \cdot 2^{n-1}$ edges.

An embedding of a graph G into $Q(n)$ is an injective mapping of the vertices of G into the vertices of $Q(n)$ which maps the edges of G into edges of $Q(n)$. We let $\mathcal{Q}_n$ denote the set of graphs which can be embedded into $Q(n)$; we let $\mathcal{Q}$ denote $\bigcup_{n>0} \mathcal{Q}_n$, the set of cubical graphs. Unless otherwise stated G_n will denote a graph on n vertices.

Preliminary Facts

Fact 1. If $G_n \in \mathcal{Q}$ then $G_n \in \mathcal{Q}_{n-1}$.

Proof. If G_n is disconnected then this follows easily by induction on n. If G_n is connected, fix an embedding of G_n such that every coordinate position varies at least once. Repeatedly removing all edges along which coordinate position i varies, for $i = 1, 2, ..., n - 1$, we see that each step must increase the number of connected components remaining. But this implies that no edges can remain in G_n after step $n - 1$, so that no other coordinate position can vary and $G_n \in \mathcal{Q}_{n-1}$. ∎

A set of edges E of a connected graph G is said to form a *cutset* for G if their removal disconnects G but no proper subset of E has this property. A cutset E is said to be *simple* if no two edges of E have a common vertex. G is said to be *completely decomposable* if any connected subgraph of G (including G itself) has a simple cutset. Let $\mathcal{D}$ denote the set of completely decomposable graphs.

For each positive integer k, let $w(k)$ denote the number of 1's in the binary expansion of k; let $W(k)$ denote $\sum_{i=1}^{k} w(i)$. Thus, $W(k) \sim \frac{1}{2}k \log_2 k$. In [7], the following result is proved.

Theorem. *If $G_n \in \mathcal{D}$ then G_n has at most $W(n - 1)$ edges.*

Since $Q(n) \in \mathcal{D}$ for all n then $\mathcal{Q} \subseteq \mathcal{D}$ and we obtain.

[2] This definition is due to R. Rado; see [4].

FACT 2. If $G_n \in \mathscr{Q}$ then G_n has at most $W(n-1)$ edges.

We note that the bound $W(n-1)$ is best possible since the subgraph D_n of $Q(n)$ induced by the n vertices with coordinates corresponding to the binary expansions of the integers in $[0, n-1]$ has exactly $W(n-1)$ edges.

For vertices v_1 and v_2 of a connected graph G, let $d_G(v_1, v_2)$ denote the distance between v_1 and v_2 in G, i.e., the number of edges in the shortest path in G connecting v_1 and v_2. If, for the embedding $f: G \to Q(n)$, it is true that

$$d_G(v_1, v_2) = d_{Q(n)}(f(v_1) f(v_2)),$$

then we say that f is an *isometric* embedding. A recent result of Djoković [2] elegantly characterizes those graphs G which can be isometrically embedded into some $Q(n)$.

THEOREM 2. *Let $C(v_1, v_2)$ denote the set of all vertices x of G such that $d_G(v_1, x) < d_G(v_2, x)$. A connected graph G has an isometric embedding into some $Q(n)$ iff*

(i) *G is bipartite (i.e., no odd circuits),*
(ii) *For every edge $\{v_1, v_2\}$ of G and for all $x, z \in C(v_1, v_2)$*

$$d_G(x, y) + d_G(y, z) = d_G(x, z) \Rightarrow y \in C(v_1, v_2).$$

Thus, (i) and (ii) are sufficient conditions for G to be cubical. While (i) is also necessary, (ii) is not, as the example in Fig. 1 shows.

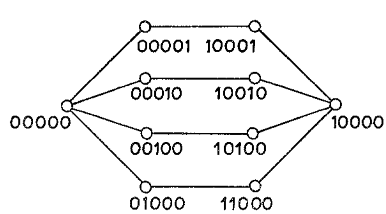

FIG. 1. A cubical graph with no isometric embedding

We now proceed to a discussion of the minimal subgraphs which prevent a graph from being cubical.

CRITICAL GRAPHS

DEFINITION. A graph G is called *critical* if:

(i) $G \notin \mathscr{Q}$,
(ii) For all proper subgraphs H of G, $H \in \mathscr{Q}$.

We let $\mathscr{C}$ denote the set of critical finite graphs.

The importance of critical graphs is derived from the following result.

FACT 3. $G \notin \mathscr{Q}$ if and only if, for some subgraph H of G, $H \in \mathscr{C}$.

Proof. For an edge e of G, let $G^{(e)}$ denote the graph formed by deleting e from G. Then either $G^{(e)} \in \mathscr{Q}$ for all edges e of G, in which case $G \in \mathscr{C}$, or for some edge e of G, $G^{(e)} \notin \mathscr{Q}$. The assertion now follows by repeated application of this argument.

In Fig. 2, we give several examples of critical graphs.

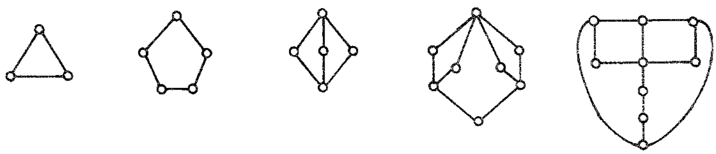

FIG. 2. Some critical graphs

It is clear that any odd cycle C_{2n+1} is critical. The smallest bipartite graph which is critical is the complete bipartite graph $K_{3,2}$. Of course, no critical graph can be a subgraph of any other critical graph.

If G has no simple cutset but every proper subgraph of G does have a (possible empty) simple cutset then G is said to be *primitive* (cf. [7]). Let $\mathscr{P}$ denote the set of primitive graphs. The classes of graphs $\mathscr{D}$ and $\mathscr{P}$ bear roughly the same relationship to one another as the pair $\mathscr{Q}$ and $\mathscr{C}$ do. For example, if $G \notin \mathscr{D}$ (or $\mathscr{Q}$) then G contains a subgraph $H \in \mathscr{P}$ (or $\mathscr{C}$). The pairs are also interrelated as we have seen in the previous section, namely, $\mathscr{Q} \subseteq \mathscr{D}$. Since $C_5 \notin \mathscr{Q}$ and $C_5 \in \mathscr{D}$, the inclusion is proper.

In [7], constructions were given which combined two primitive graphs to form a new one. Although no such general construction is currently known for $\mathscr{C}$, a method is known for constructing exponentially many critical graphs on n vertices.

THEOREM 1. *Let T denote the transformation shown in Fig. 3. Then G is critical if and only if $T(G)$ is critical.*

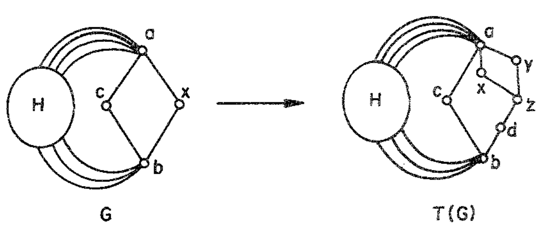

FIGURE 3

Proof. (i) Suppose $G \in \mathscr{C}$ and assume $T(G) \in \mathscr{Q}$. Let $A(a)$, $A(x)$, etc., denote the vertices of $Q(n)$ into which $T(G)$ is embedded. We may assume without loss of generality that:

$$A(a) = (0, 0, 0, 0,...),$$
$$A(c) = (1, 0, 0, 0,...),$$
$$A(b) = (1, 1, 0, 0,...).$$

Suppose neither $A(x)$ nor $A(y)$ is equal to (0, 1, 0, 0,...). Then we may assume

$$A(x) = (0, 0, 1, 0,...),$$
$$A(y) = (0, 0, 0, 1,...).$$

But this implies $A(z) = (0, 0, 1, 1,...)$ so that $d_{Q(n)}(A(z), A(b)) = 4$ which is impossible.

Hence, one of the quantities, say, $A(x)$, must be equal to (0, 1, 0, 0,...). Then we may assume $A(y) = (0, 0, 1, 0,...)$, $A(z) = (0, 1, 1, 0,...)$ and $A(d) = (1, 1, 1, 0,...)$. But this implies that $G \in \mathscr{Q}$. For we may simply map all the vertices of G in just the same way that they were mapped as vertices of $T(G)$.

Hence, $T(G) \notin \mathscr{Q}$. However, if any edge is deleted from $T(G)$ then it is not difficult to check that the resulting graph is in $\mathscr{Q}$ (by deleting an appropriate edge from G and embedding this graph in some $Q(n)$). This implies $T(G) \in \mathscr{C}$.

The implication in the other direction, $T(G) \in \mathscr{C}$ implies $G \in \mathscr{C}$, follows in a similar manner. ∎

Theorem 1 can be used to show that there are exponentially many critical graphs on n vertices.

COROLLARY 1. *For $n \geqslant 8$ there are at least $2^{(n-17)/3}$ nonisomorphic critical graphs on n vertices.*

Proof. Consider the three critical graphs in Fig. 4. They have, respectively, 9, 13 and 17 vertices. Note that each of these graphs has a unique 4-cycle (v_1, v_2, v_3, v_4); furthermore, the 4-cycle satisfies

$$\deg v_1 > 3, \qquad \deg v_2 = \deg v_4 = 2, \qquad \deg v_3 = 3. \tag{*}$$

For any such graph G, the transformation T can be applied in two ways, as shown in Fig. 5. Observe that G_1 and G_2 are nonisomorphic, since they differ in the number of vertices of degree 3. Furthermore, G_1 and G_2 each have a unique 4-cycle and this 4-cycle satisfies (*).

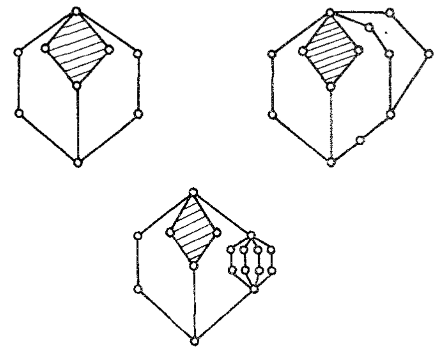

FIGURE 4

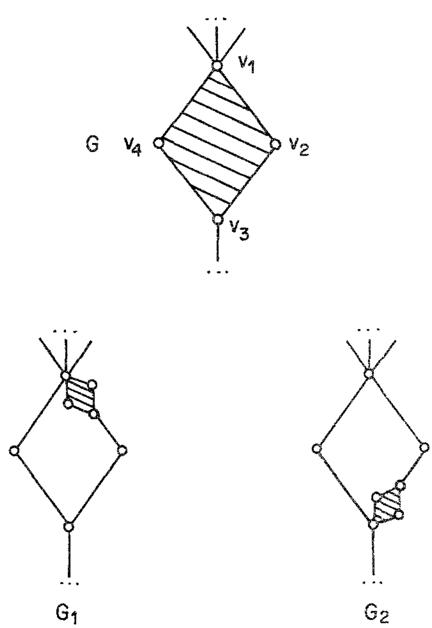

FIGURE 5

Thus, if $\mathscr{G}$ is a family of nonisomorphic graphs on n vertices, each satisfying (*), then we can form a new family $T(\mathscr{G})$ of graphs on $n + 3$ vertices by applying T to each $G \in \mathscr{G}$ in the two ways shown in Fig. 5. Note that $|T(\mathscr{G})| = 2|\mathscr{G}|$ since any two elements of $T(\mathscr{G})$ with different "predecessors" must be nonisomorphic. (Because of (*) each graph in $T(\mathscr{G})$ has a unique predecessor.) By applying this construction repeatedly, starting with the graphs shown in Fig. 4, the desired result follows in case $n \geqslant 17$.

For the range $8 \leqslant n < 17$, $n \neq 10$, the transformation T may be applied repeatedly to the critical graphs shown in Fig. 6 to produce at least one critical graph on n vertices. A critical graph on 10 vertices appears in Fig. 9. This completes the proof of the corollary. ∎

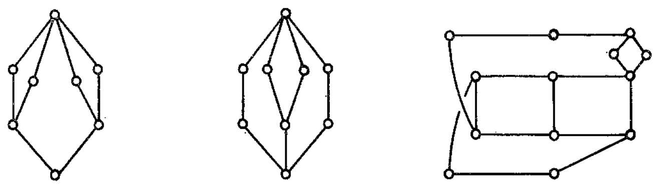

FIGURE 6

Since the transformation T increases the number of vertices of G by 3 and the number of edges of G by 4, we can construct arbitrarily large critical graphs with edge-to-vertex ratio arbitrarily close to 4/3.

In the other direction, we have the following result.

THEOREM 2. *Suppose G_n is critical and has e edges. Then*

$$e/n \leqslant W(n-2)/(n-2)$$

Proof. Suppose $e/n > W(n-2)/(n-2)$. Some vertex v of G must have degree $\leqslant 2e/n$. Form the graph G' by removing the vertex v and all edges incident to it. Then G' has $n-1$ vertices and $> W(n-2)$ edges. But G' must belong to $\mathscr{Q}$ and this contradicts Fact 2. ∎

The bound in Theorem 2 shows that for all $\epsilon > 0$

$$\frac{e}{n} < \left(\frac{1}{2} + \epsilon\right) \frac{\log n}{\log 2}, \qquad n \text{ large.}$$

However, all known critical graphs with n vertices and e edges have $e/n < 4/3$.

For a lower bound on e/n, C_{2n+1} has an edge-to-vertex ratio of 1 which is the least possible for a critical graph. Even if G_n is required to be bipartite, it is still possible to have $e/n < 1 + \epsilon$. To see this, consider the graph G_k shown in Fig. 7. G_k is bipartite, critical and has $\frac{1}{3}(8k^3 + 34k + 6)$ vertices and $\frac{1}{3}(8k^3 + 6k^2 + 40k - 6)$ edges, as may be verified by the patient reader.

We now give another method for constructing critical graphs. For a graph G, let $T_k(G)$ denote a graph formed from G by replacing some fixed edge by k disjoint paths of length 3 (see Fig. 8).

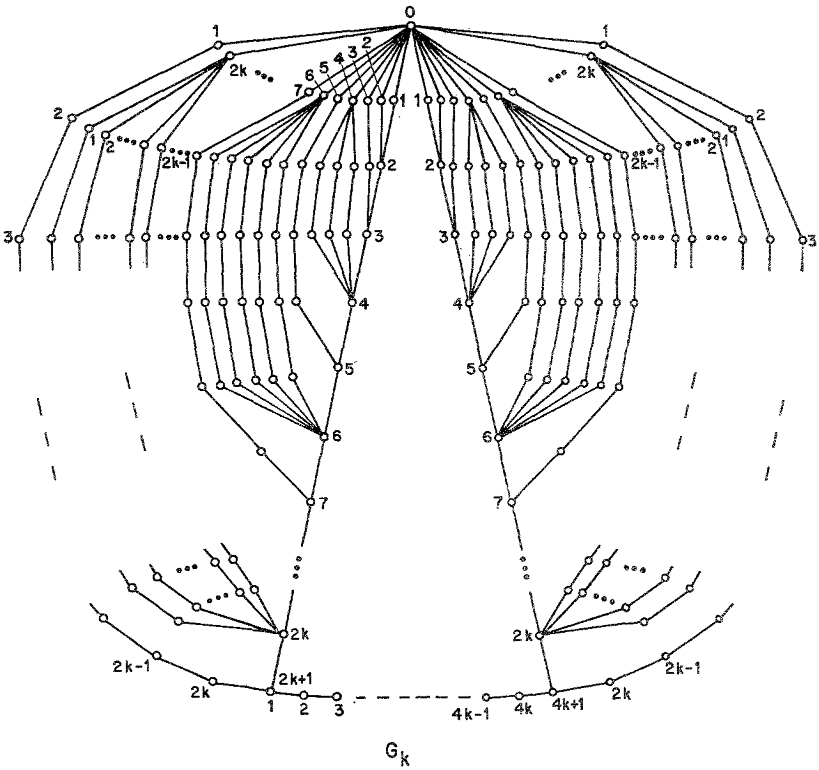

FIG. 7. A bipartite critical graph with small e/n

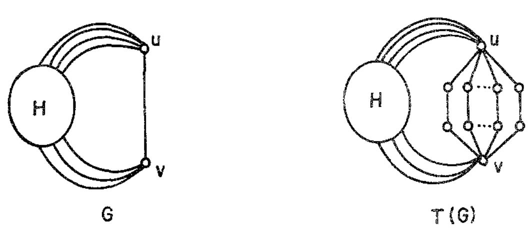

FIGURE 8

THEOREM 3. *If $G \in \mathscr{C}$ then $T_k(G) \in \mathscr{C}$ for exactly one value of $k = 1, 2,$ 3 or 4.*

Proof. Suppose $G \in \mathscr{C}$ and $T_4(G) \in \mathscr{Q}$. Then $A(u)$ and $A(v)$ must differ in 3 coordinate positions since if they differed in just 1 position, then G would have an induced embedding in some $Q(n)$. Thus, all 8 interior vertices on the 4 paths between u and v in $T_4(G)$ must have coordinates which differ only in those positions in which $A(u)$ and $A(v)$ differ. Clearly this is impossible and so $T_4(G) \notin \mathcal{Q}$.

On the other hand, if any edge not on one of the 4 paths is removed from $T_4(G)$, then the resulting graph can be embedded into some $Q(n)$ by simply removing the corresponding edge from G and embedding this graph. Thus, if $T_4(G)$ is not critical, then the removal of one of the 4 paths from it results essentially in the graph $T_3(G)$ which does not belong to $\mathcal{Q}$. If $T_3(G)$ is not critical, then removing another path from it, we have essentially the graph $T_2(G) \notin \mathcal{Q}$, etc. This proves the theorem. ∎

We leave unstated the analog of Theorem 3 in which a path of length 2 is replaced by k paths of length 4, $1 \leqslant k \leqslant 5$.

Unfortunately, there seems to be no simple way to decide *which* of $T_1(G)$, $T_2(G)$, $T_3(G)$ or $T_4(G)$ is the critical graph. All four possibilities can occur as can be seen in Fig. 9. The example for T_1 was pointed out by L. Lovász [11].

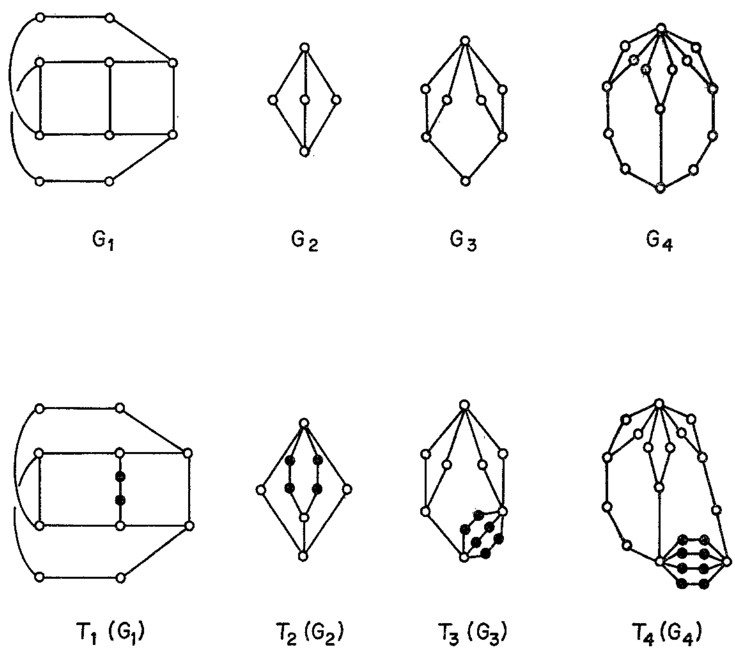

FIGURE 9

The graph $T_1(G_1)$ in Fig. 9 is an example of a bipartite critical graph with smallest circuit having length 6. More generally, we have the following result.

THEOREM 4. *For any m, there exist bipartite critical graphs with smallest circuit having length* $>m$.

Proof. By a result of Erdös [3], for any m, there exists $\epsilon_m > 0$, $c > 0$ such that for n sufficiently large, there exists a graph G with n vertices and at least $cn^{1+\epsilon_m}$ edges whose smallest circuit has length $> m$. Form the graph G' from G as follows. For each vertex v of G there are two vertices v_1, v_2 of G'; for each edge $\{u, v\}$ of G there are two edges $\{u_1, v_2\}$ and $\{u_2, v_1\}$ of G'. Thus, G' has $2n$ vertices, at least $2cn^{1+\epsilon_m}$ edges and is bipartite. Also, the smallest circuit in G' has length $> m$. But, by Fact 2, $G' \notin \mathcal{Q}$ for n sufficiently large. Thus, by Fact 4, G' contains a critical subgraph H. Since H cannot have a smaller circuit than G' and m was arbitrary, the theorem is proved. ∎

It should be noted that certain graphs are forbidden from occurring as subgraphs of critical graphs. For example, $Q(3)$ is such a graph. The reason is that there is essentially no freedom in embedding $Q(3)$ in $Q(n)$ so that even if an edge e of $Q(3)$ is removed, the resulting graph $Q(3)^{(e)}$ has no additional freedom. Thus, if a graph containing $Q(3)^{(e)}$ can be embedded in $Q(n)$, then so can the augmented graph containing $Q(3)$.

CONCLUDING REMARKS

As is apparent from the preceding sections, a plethora of questions remain unanswered. We mention several of these here.

(1) Must every critical graph have a vertex of degree 2? The corresponding question was raised in [7] for primitive graphs and answered in the negative by Bouwer and LeBlanc [1] by the graph shown in Fig. 10.

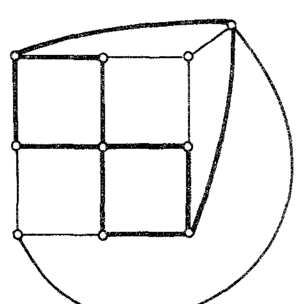

FIGURE 10

This graph is not critical, though. The subgraph shown with the darkened edges is critical; it contains a vertex of degree 2.

(2) The graphs shown in Fig. 11(a) are all critical. They were obtained by determining the critical subgraphs of the corresponding graphs in Fig. 11(b). What are the critical subgraphs of the general a by b "grid" with an edge connecting a pair of diagonally opposite vertices? What about the n-dimensional analog?

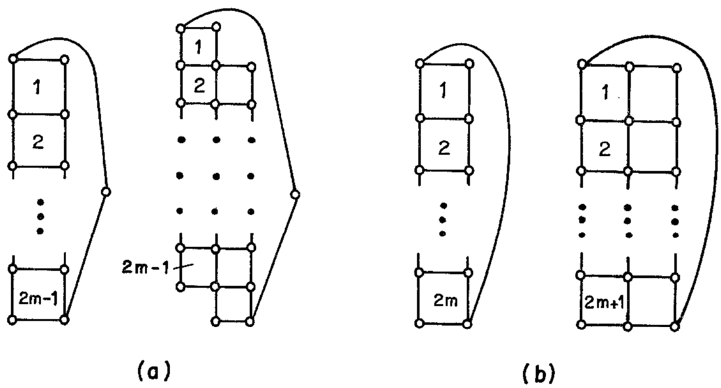

FIGURE 11

(3) Are there other simple transformations of the type occurring in Theorem 1 which map certain elements of $\mathscr{C}$ into $\mathscr{C}$? More generally, is there a way to combine 2 critical graphs and obtain a third critical graph?

(4) How can one determine *which* one of the graphs $T_k(G)$ in Theorem 3 is critical?

(5) Let $G \in \mathscr{C}$ with n vertices and e edges. Can e/n exceed 4/3? Is e/n unbounded? Can e/n exceed $c \log n$ for some $c > 0$ independent of n? (cf. Theorem 2)

(6) Is there an efficient algorithm (in the sense of Cook and Karp [9]) to determine whether or not G is critical? cubical? If $G \in \mathscr{Q}$ then it is necessary that G possesses what might be called a *segregated labeling*, i.e., a nontrivial[3] assignment of 0's and 1's to the vertices so that no symbol is adjacent to more than one symbol of the opposite type. Is there an efficient algorithm to assign a segregated labeling to G? Notice that G possesses a segregated labeling if and only if G has a simple cutset.

(7) How many critical graphs on n vertices are there? The corollary to Theorem 1 shows that there are quite a few, e.g., $>c^n$. How many cubical graphs on n vertices are there?

(8) Is there a characterization of cubical graphs similar in spirit to Djoković's theorem [2] for isometric embeddings? Based on the evidence in hand, the existence of such a characterization would be surprising.

[3] That is, at least one 0 and one 1 are assigned.

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