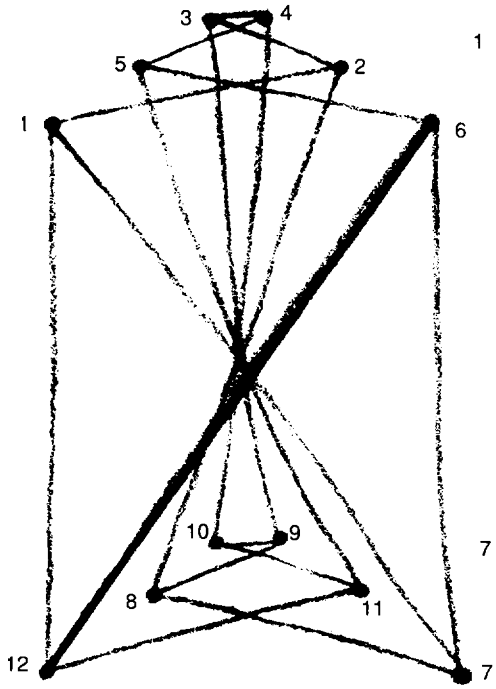
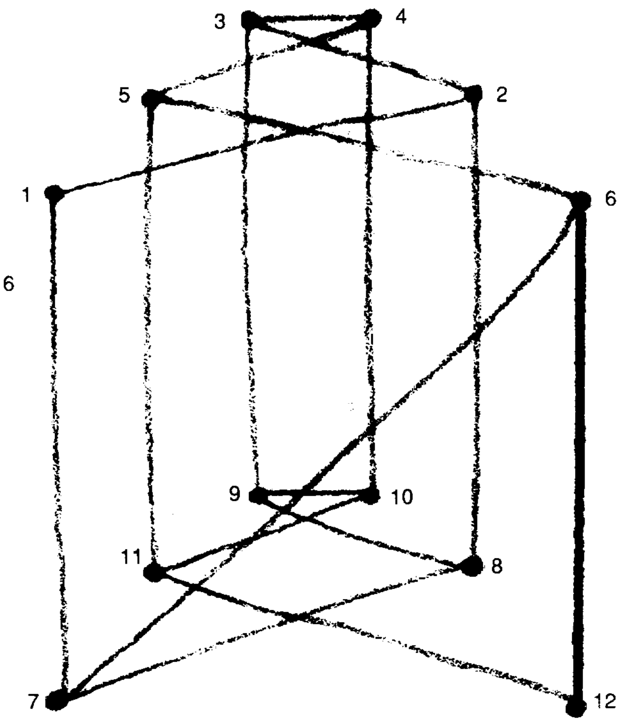
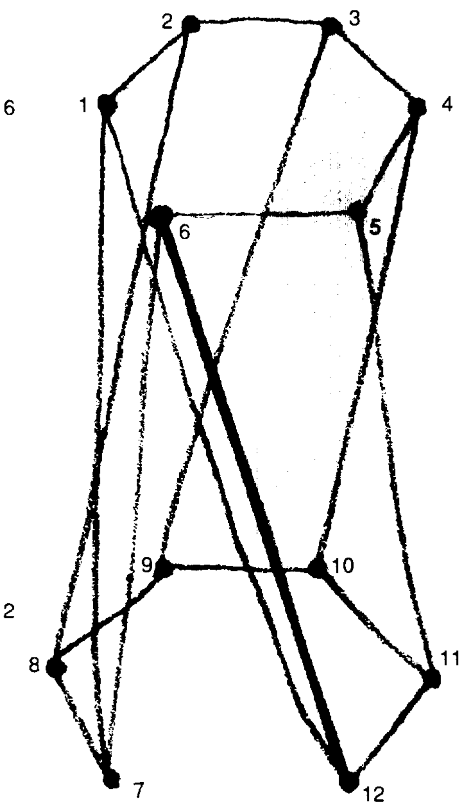


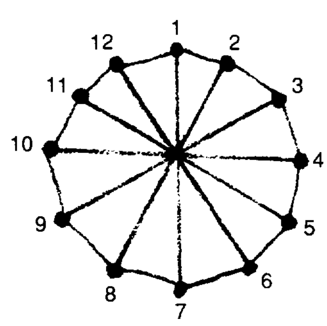




A Similarity Measure for Graphs–

reflections on a theme of Ulam

by Ronald L. Graham



Among a variety of fundamental themes running through Stan Ulam's mathematical research, one that particularly intrigued him was that of *similarity.* He was constantly fascinated by the problem of quantifying exactly how *alike* (or different) two mathematical objects or structures were, and during his career he discovered many ingenious ways of doing so. A good example is the well-known Ulam distance between finite sequences, which has recently been applied so effectively in analysis of DNA sequences and recognition of speech (Sankoff and Kruskal 1983). (Also see "Sequence Analysis: Contributions by Ulam to Molecular Biology" in this issue.)

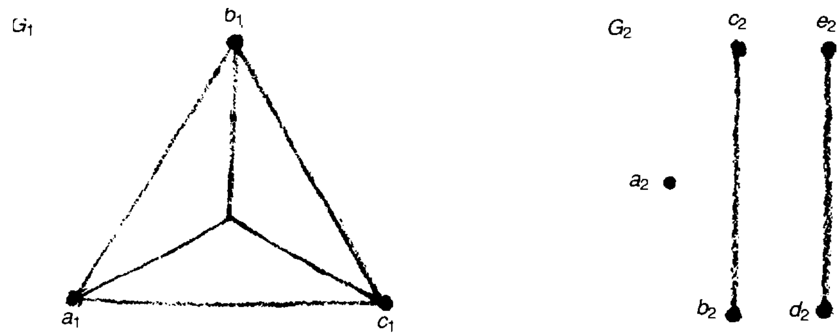
Here I will describe another measure of similarity suggested by Stan, one applicable to a wide assortment of combinatorial structures. Like many seeds planted by his fertile imagination, this similarity measure has taken root and flowered in the modem mathematical jungle.

The story begins one morning in late July of 1977, during one of my aperiodic visits to Stan and Francoise's marvelous house on the outskirts of Santa Fe. Stan and I had just finished playing tennis, which not only generated a plentiful supply of perspiration (and consequent thirst) but also inevitably led to a lively discussion of the differences in the game at an altitude of over 7000 feet, where the balls are effectively more highly pressurized, the air resistance is diminished, less oxygen is available for demanding lungs, and so on.

Perhaps stimulated by trying to get a better grasp on understanding just how various aspects of the game (such as the

EXAMPLES OF GRAPHS

Fig. 1. Shown here are the pictorial and mathematical representations of two simple graphs. G_1 has the maximum number of edges for a given number n of vertices (namely, $\binom{n}{2}$, or $\frac{1}{2}n(n-1)$). G_2 is an example of a graph consisting of disjoint subgraphs. (For simplicity in this and all other figures, the edges of graphs are depicted as straight lines.)



$V_1 = \{a_1, b_1, c_1, d_1\}$

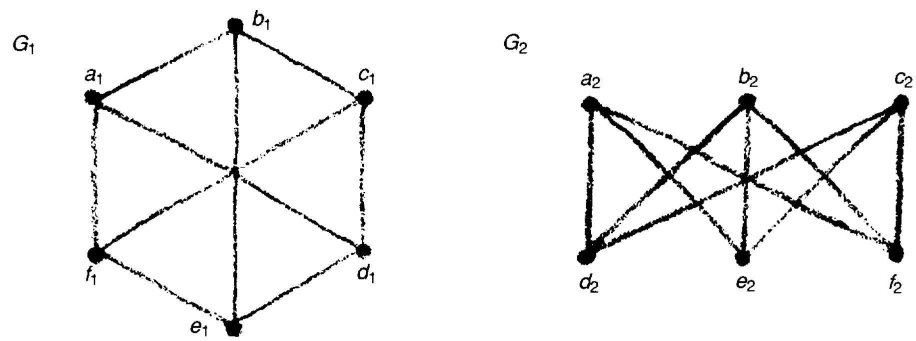
$E_1 = \{(a_1, b_1), (a_1, c_1), (a_1, d_1), (b_1, c_1), (b_1, d_1), (c_1, d_1)\}$

$V_2 = \{a_2, b_2, c_2, d_2, e_2\}$

$E_2 = \{(b_2, c_2), (d_2, e_2)\}$

ISOMORPHISM OF GRAPHS

Fig. 2. Let T be the following one-to-one transformation of V_1 onto V_2: $a_1 \to a_2$, $b_1 \to d_2$, $c_1 \to b_2$, $d_1 \to e_2$, $e_1 \to c_2$, and $f_1 \to f_2$. Since $T(E_1) = E_2$, G_1 is isomorphic to G_2, or, symbolically, $G_1 \cong G_2$. Note that a necessary condition for isomorphism of two graphs is that they have the same number of vertices and edges. The relation of isomorphism, like that of equality in arithmetic, is reflexive, symmetric, and transitive. That is, $G \cong G$; if $G_1 \cong G_2$, then $G_2 \cong G_1$; and if $G_1 \cong G_2$ and $G_1 \cong G_3$, then $G_2 \cong G_3$.



$V_1 = \{a_1, b_1, c_1, d_1, e_1, f_1\}$

$E_1 = \{(a_1, b_1), (a_1, d_1), (a_1, f_1), (b_1, c_1), (b_1, e_1), (c_1, d_1), (c_1, f_1), (d_1, e_1), (e_1, f_1)\}$

$V_2 = \{a_2, b_2, c_2, d_2, e_2, f_2\}$

$E_2 = \{(a_2, d_2), (a_2, e_2), (a_2, f_2), (b_2, d_2), (b_2, e_2), (b_2, f_2), (c_2, d_2), (c_2, e_2), (c_2, f_2)\}$

serve, the stroke, and the strategy) might change under varying conditions, Stan suddenly suggested, "Why not measure the difference between objects by trying to break them up into as few as possible pairwise equal pieces?" At first I didn't see quite what Stan was driving at (which happened fairly often), but after we talked it over, it became clear that here was an entirely new way of defining a measure of similarity between two (or more) combinatorial structures. In fact, it is very much akin to comparing two complex molecules by breaking them up into a number of pairwise identical fragments—the smaller the number of pieces needed, the more similar are the molecules.

Our first application of the approach was to a class of mathematical objects known as *graphs.* Simply speaking, a graph G consists of a set V of elements called the *vertices* of G and a set E of certain pairs of elements of V called the edges of G. Graphs are often pictured by representing the vertices in V as points and the edges as lines between the pairs of points in E (Fig. 1).

Before proceeding to the main topic of the article, we need two more basic definitions-those for *isomorphism* of graphs and for a *partition* of the edge set of a graph.

Two graphs G_1 and G_2 are said to be isomorphic ($G_1 \cong G_2$) if, as shown in Fig. 2, a one-to-one transformation of V_1 onto V_2 effects a one-to-one transformation of E_1 onto E_2.

By a partition of the edge set E of a graph G is meant a set of pairwise disjoint subsets E_i of E such that $\bigcup_i E_i = E$ (Fig. 3). (The number of ways to partition an edge set depends, in a complicated way, on the number of edges of the graph, $e(G)$.)

We now come to the key definitions. Let G and G' be two graphs having the same number of edges. An *Ulam decomposition* of G and G' is a pair of par-

PARTITIONS OF THE EDGE SET OF A GRAPH

Fig. 3. The edge set E of the graph G can be partitioned (divided into subsets E_i such that $\bigcup_i E_i = E$) in numerous ways, two of which are illustrated here.

$$E = \{(v_1, v_2), (v_1, v_3), (v_1, v_4), (v_2, v_3), (v_2, v_4), (v_3, v_4)\}$$

Partition P

$E_1 = \{(v_1, v_2), (v_1, v_3), (v_2, v_3)\}$

$E_2 = \{(v_1, v_4), (v_2, v_4), (v_3, v_4)\}$

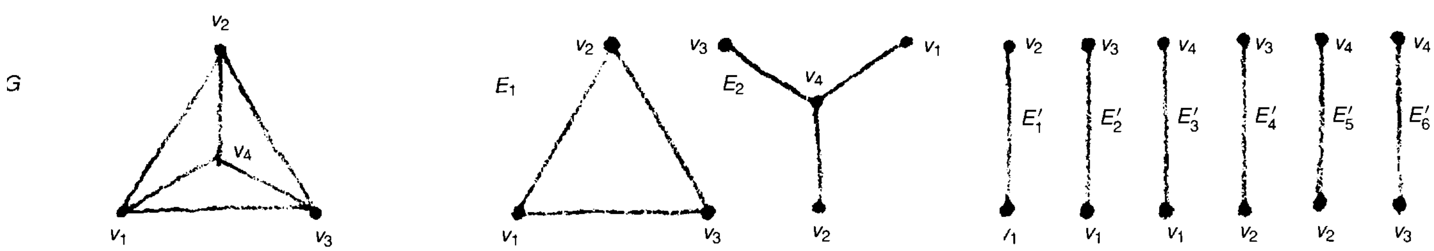
$E_1 \cup E_2 = E$

Partition P'

$E'_1 = \{(v_1, v_2)\}$ $E'_2 = \{(v_1, v_3)\}$ $E'_3 = \{(v_1, v_4)\}$

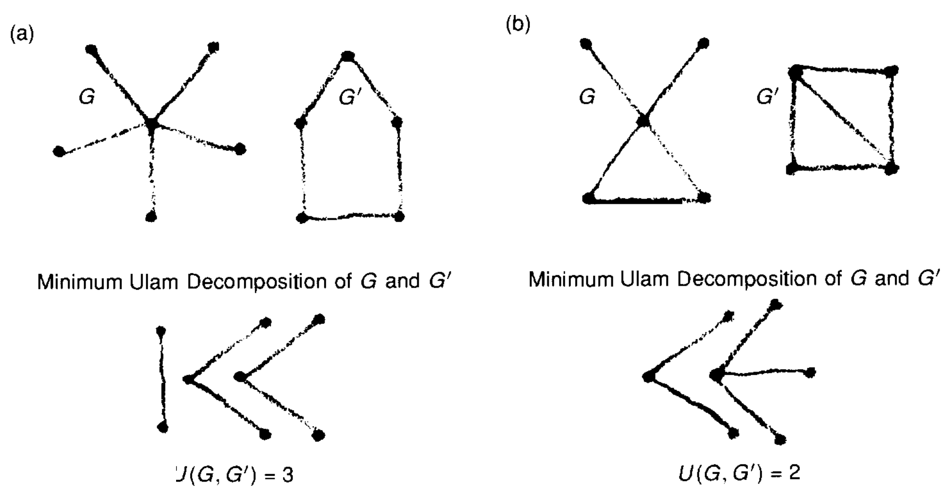
$E'_4 = \{(v_2, v_3)\}$ $E'_5 = \{(v_2, v_4)\}$ $E'_6 = \{(v_3, v_4)\}$

$E'_1 \cup E'_2 \cup E'_3 \cup E'_4 \cup E'_5 \cup E'_6 = E$



EXAMPLES OF MINIMUM ULAM DECOMPOSITIONS

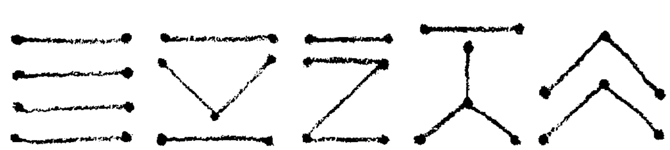
Fig. 4. The minimum Ulam decompositions shown here illustrate that $U(G, G')$ is a measure of similarity for a pair of graphs that agrees with our intuitive notion of their resemblance to each other in the sense of connections among vertices: the two graphs in (a) bear less resemblance in that sense than do the two graphs in (b).



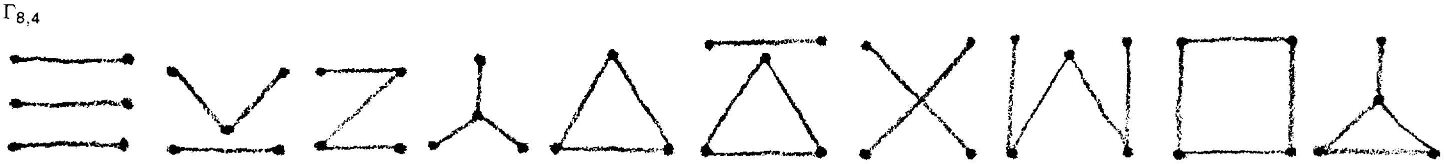
EXAMPLES OF $\Gamma_{n,e}$

Fig. 5. Two examples of $\Gamma_{n,e}$, the set of graphs each of which has e edges and at most n vertices. (Graphs with isolated vertices are not shown.) In both examples $n = 2e$, the maximum number of vertices for a given number of edges. $\Gamma_{n,e}$ for $n < 2e$ is a subset of $\Gamma_{2e,e}$.

$\Gamma_{6,3}$



$\Gamma_{8,4}$



titions $\{E_1, \ldots, E_r\}$ and $\{E'_1, \ldots, E'_r\}$ of the respective edge sets of G and G' such that, as graphs, $E_i \cong E'_i$ for $1 \le i \le r$. Such a decomposition always exists since we can always choose each E_i (and E'_i) to be a single edge (and by hypothesis $e(G) = e(G')$). Further, define $U(G, G')$ to be the *least* value of r for which an Ulam decomposition of G and G' into r parts exists. (Figure 4 shows such minimum Ulam decompositions for two pairs of graphs.) Thus $U(G, G')$ is a similarity measure for pairs of graphs: the smaller $U(G, G')$ is, the more alike G and G' are. In particular, $U(G, G') = 1$ exactly when G and G' are isomorphic (that is, when they differ only in the way their vertices are labeled).

We now extend our view from a single pair of graphs with the same number of edges to sets of graphs $\Gamma_{n,e}$ with e edges and at most n vertices (Fig. 5) and define the function $U(n)$:

$$U(n) \equiv \max_{G, G' \in \Gamma_{n,e}} U(G, G').$$

So in $U(n)$ we have a measure of the maximum dissimilarity among all pairs of graphs in $\Gamma_{n,e}$.

A fundamental question about $U(n)$ that occurs at the outset is this: How large can $U(n)$ ever be? To whet your appetite for the answer to this question, let us determine $U(G, G')$ for two examples. ($U(n)$ is of course equal to or greater than $U(G, G')$.) In the first example G is a k-rayed "star" (that is, it consists of one vertex joined to each of k others), and G' consists of k disjoint edges (Fig. 6a). Here $e = k$ and $n = 2k$. For such a pair of graphs, the only Ulam decomposition comes from taking each E_i and E'_i to be a single edge. Therefore

$$U(n) \ge U(G, G') = k = \frac{1}{2}n.$$

In the second, slightly more sophisticated example G consists of a 3k-rayed star, and G' consists of k disjoint triangles (Fig. 6b). Here $e = 3k$ and $n = 3k + 1$. What is $U(G, G')$ for such pairs of graphs? It is not difficult to see that the best we can do is to decompose each graph into k disjoint 2-rayed stars and k disjoint edges. Thus

$$U(n) \ge U(G, G') = 2k = \frac{2}{3}(n-1) \approx \frac{2}{3}n.$$

CALCULATION OF LOWER BOUNDS ON $U(n)$

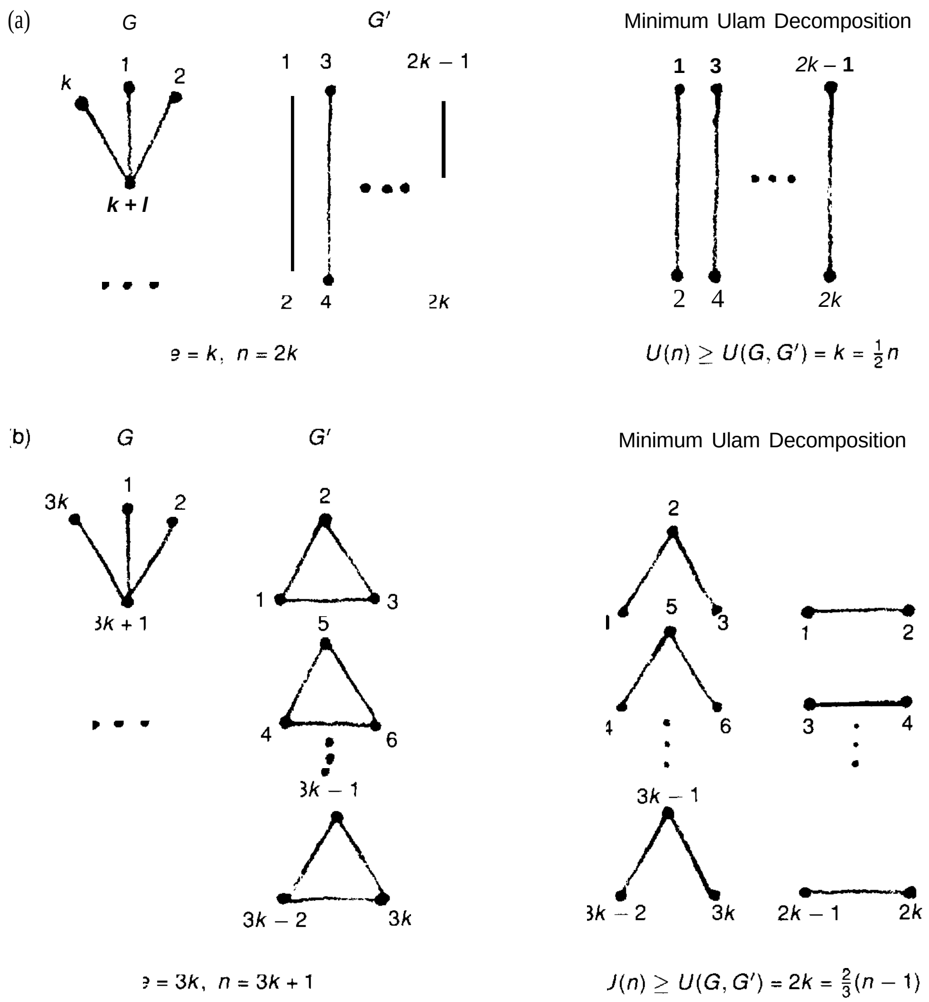


Fig. 6. By considering pairs of graphs of the general form shown in (a), $U(n)$ is found to be equal to or greater than $\frac{1}{2}n$, whereas by considering pairs of graphs of the general form shown in (b), $U(n)$ is found to be greater than $\frac{2}{3}(n-1)$, which is greater than $\frac{1}{2}n$ (for $n > 4$). This situation might lead one to conclude that $U(n)$ has no upper bound other than $\binom{n}{2}$, the greatest possible number of edges possessed by any graph with n vertices. However, as demonstrated in the text, $U(n)$ has an upper bound that is linear in n.

At this point one may well wonder whether further search will produce even more complicated examples from which even larger lower bounds on $U(n)$ can be deduced. That this *cannot* happen is the content of Theorem 1, which was the main result in our first paper on the subject (Chung, Erdös, Graham, Ulam, and Yao 1979).

Theorem 1. For a suitable fixed constant c, $U(n) \leq \frac{2}{3}n + c$ for all n.

Our proof of Theorem 1 uses several ideas that are now standard items in the toolbox of every combinatorialist. One is the idea of a *greedy algorithm*. It seems only natural to try to remove the *largest* subgraph common to each of the two graphs for which one is seeking a minimum Ulam decomposition (although in many situations that myopic approach is far from optimal). Indeed, such a technique is quite effective for the problem at hand. However, it leads to the next question: Just how large can we expect (or guarantee) such a common subgraph to be? Here the second technique we want to mention comes in, namely, the so-called *probabilistic method*, which was pioneered so effectively by Paul Erdös. Suppose G and G' each have n vertices and e edges. What we will show is that they must share a common subgraph H having at least $2e^2/n(n-1)$ edges. However, we won't be able to specify what H is or how to get it—just that it exists! How do we do this? Every mathematical paper should have at least one proof, so here comes ours.

Label the vertices of G and G' by, say, $V = \{x_1, \ldots, x_n\}$ and $V' = \{x'_1, \ldots, x'_n\}$. Let Λ denote the set of one-to-one mappings of V onto V'. Thus, Λ has $n!$ elements. If $y = \{x_i, x_j\}$ and $y' = \{x'_k, x'_l\}$ are given elements in V and V', respectively, there are exactly $2(n-2)!$ elements $\lambda \in \Lambda$ that map y onto y'. (The factor of 2 counts the two possibilities $\lambda(x_i) = x'_k, \lambda(x_j) = x'_l$ and $\lambda(x_i) = x'_l, \lambda(x_j) = x'_k$.) Define the *indicator function* $i_\lambda(y, y')$:

$$i_\lambda(y, y') = \begin{cases} 1 & \text{if } \lambda \text{ maps } y \text{ onto } y'; \\ 0 & \text{otherwise.} \end{cases}$$

Now sum $i_\lambda(y, y')$ over all $\lambda \in \Lambda$ and all $y \in E, y' \in E'$:

$$\begin{aligned} S &\equiv \sum_{\lambda \in \Lambda} \sum_{y, y'} i_\lambda(y, y') \\ &= \sum_{y, y'} \sum_{\lambda \in \Lambda} i_\lambda(y, y') \\ &= \sum_{y, y'} 2(n-2)! \\ &= 2e^2(n-2)!. \end{aligned}$$

In the first step we have interchanged the order of summation, and in the second we have used the previously noted fact about the number of $\lambda \in \Lambda$ that map any given $y \in E$ onto any given $y' \in E'$.

Now we note that since S is a sum of $n!$ terms of the form $\sum_{y,y'} i_\lambda(y, y')$ (one for each $\lambda \in \Lambda$), at least one of those terms must equal or exceed their *average*, which of course is just $2e^2(n-2)!/n!$, or $2e^2/n(n-1)$. In other words, for *some* $\lambda \in \Lambda$, say λ_0, we have

$$\sum_{y, y'} i_{\lambda_0}(y, y') \geq \frac{2e^2}{n(n-1)}$$

Having proved that the two graphs G and G' have a common subgraph H with at least $2e^2/n(n-1)$ edges, suppose now that we remove H from G and G', producing the graphs G_1 and G'_1, which have at most $e_1 = e - 2e^2/n(n-1)$ edges. Our theorem says that those graphs also have in common a subgraph H_1 with at least $2e_1^2/n(n-1)$ edges. Remove H_1 to produce G_2 and G'_2, and so on. It is not hard to show that after repeating the process k times, we have graphs G_k and G'_k with at most $n(n-1)/2k$ edges. That in turn can be used to show that $U(n) < \sqrt{2}n$. To squeeze the last bit of juice out of the argument and show that $U(n) \leq \frac{2}{3}n + c$ requires more complicated considerations that we will not go into here.

It was only natural that we began to wonder next about what happens if instead of starting with two graphs, we start with *three* (or more). Indeed, defining $U(G_1, G_2, G_3)$ as the minimum value of r for which an Ulam decomposition of G_1, G_2, and G_3 exists and $U_3(n)$ as $\max_{G_1, G_2, G_3 \in \Gamma_{n,e}} U(G_1, G_2, G_3)$, we soon saw that $U_3(n)$ was going to be larger than $U_2(n) \equiv U(n)$ by considering the example shown in Fig. 7. For those triplets of graphs, just as for the pairs of graphs shown in Fig. 6, the minimum Ulam decomposition consists of a certain number (approximately $\frac{1}{4}n$) of 2-rayed stars and a certain number (approximately $\frac{1}{2}n$) of disjoint edges. Thus

$$U_3(n) \geq U(G_1, G_2, G_3) \geq \frac{3}{4}n.$$

It has been shown (this time by much more complicated arguments) that $U_3(n)$, like $U_2(n)$, possesses an upper bound (Chung, Erdös, and Graham 1981):

Theorem 2. For a suitable fixed constant c, $U_3(n) \leq \frac{3}{4}n + c$ for all n.

As mathematicians are prone to do, we naturally began to look beyond $U_3(n)$ to the general case, namely

$$U_k(n) \equiv \max_{G_1, \ldots, G_k \in \Gamma_{n,e}} U(G_1, \ldots, G_k).$$

Here, however, something completely unexpected happened. We had been guessing what the coefficient of n was going to be in the bound for $U_4(n)$ (why not $\frac{4}{5}$?) and more generally for $U_k(n)$ (could it be $\frac{k}{k+1}$?). We were quite unprepared for the following result, which was finally proved with the full arsenal of techniques we were rapidly accumulating (Chung, Erdös, and Graham 1981):

Theorem 3. For each $k \geq 3$, there is a fixed constant c_k such that $U_k(n) \leq \frac{3}{4}n + c_k$ for all n.

In other words, the constant factor of $\frac{3}{4}$ that appears in the bound for $U_3(n)$ *does not increase* for values of k greater than 3. It is as though the space of n-vertex graphs is in some sense "three-dimensional," and once you have three graphs that are maximally separated, then adding further graphs can cause no real additional trouble. In fact, the most striking result we were finally able to establish dealt with trying to decompose *all* graphs on n vertices simultaneously into mutually isomorphic subgraphs. If $U^*(n)$ denotes the smallest number of subgraphs needed for such an Ulam decomposition, then we have the ultimate generalization of Theorem 1 (Chung, Erdos, and Graham 1983):

Theorem 4. For a suitable fixed constant c^*, $U^*(n) \leq \frac{3}{4}n + c^*$ for all n.

A key concept arising in these investigations is that of an *unavoidable* subgraph of a graph. To be precise, we say that H is (n, e)-unavoidable if any graph with n vertices and e edges contains H as a subgraph. For example, *any* n-vertex graph is $(n, \binom{n}{2})$-unavoidable (since there is only one graph with n vertices and $\binom{n}{2}$ edges and that graph includes all possible edges). Also, a d-rayed star is $(n, \frac{1}{2}n(d-1)+1)$-unavoidable, where $n \geq d+1$ and n must be even if d is even (Fig. 8). Many beautiful results on unavoidable graphs have been proved in recent years; indeed, that subject is developing, primarily under the leadership of F. R. K. Chung, into a central area of graph theory.

We mention finally the concept of a universal graph, a concept related to that of an unavoidable graph and one motivated in part by the problem of finding Ulam decompositions. If $\mathbf{F}$ is a family of graphs, we say that a graph G is $\mathbf{F}$-universal if every $F \in \mathbf{F}$ occurs as a subgraph of G. The connection between these two ideas is the following. Let $\bar{G}$ denote the complementary graph of the graph G; that is, $\bar{G}$ is a graph with the same vertices as G and exactly (and only) the edges that G does not have. Thus, for a graph with n vertices,

$$e(G) + e(\bar{G}) = \binom{n}{2}.$$

Now if $\mathbf{F}(i,j)$ denotes the family of all graphs with i vertices and j edges, then the statement

$$H \text{ is } (n, e)\text{-unavoidable}$$

is equivalent to the statement

$$\bar{H} \text{ is } \mathbf{F}(n, \tbinom{n}{2} - e)\text{-universal.}$$

Figure 9 illustrates this equivalence.

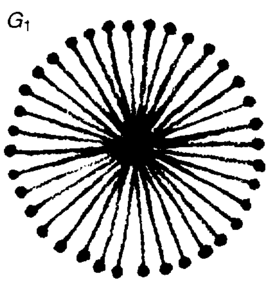
Much is now known about $\mathbf{F}$-universal graphs for special classes of $\mathbf{F}$. For example, if $\mathbf{F} = \mathbf{T}_n$, the family of all *trees* (connected graphs containing no closed loops) with n vertices, then the minimum possible number $s(\mathbf{T}_n)$ of edges in a $\mathbf{T}_n$-universal graph satisfies

$$\frac{1}{2}n \ln n < s(\mathbf{T}_n) < \frac{7}{\ln 4} n \ln n.$$

Fig. 7. By considering the graphs G_1 (a $9k^2$-rayed star), G_2 ($3k^2$ disjoint triangles), and G_3 ($\frac{1}{2}3k(3k+1)$ disjoint edges and a $3k$-sided polygon with each vertex connected to every other), one can deduce that $U_3(n)$ is equal to or greater than about $\frac{3}{4}n$. (The graphs shown here illustrate the case $k = 2$.)

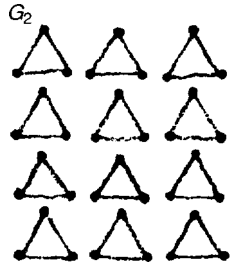
CALCULATION OF A LOWER BOUND ON $U_3(n)$

G_1



$e(G_1) = 9k^2$
$n(G_1) = 9k^2 + 1$

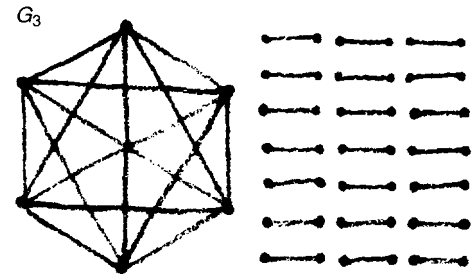
G_2



$e(G_2) = 9k^2$
$n(G_2) = 9k^2$

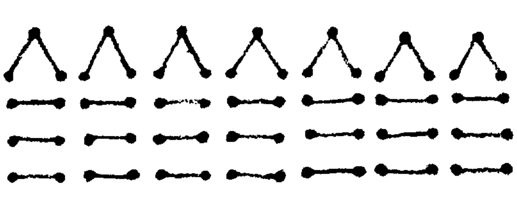
$e = 9k^2, \quad n = 3k(3k+2)$

G_3



$$e(G_3) = \frac{1}{2}3k(3k-1) + \frac{1}{2}3k(3k-1) = 9k^2$$
$$n(G_3) = 3k + 3k(3k+1) = 3k(3k+2)$$

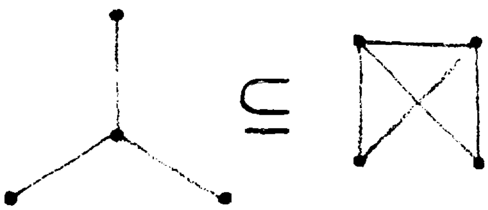
Minimum Ulam Decomposition of G_1, G_2, and G_3



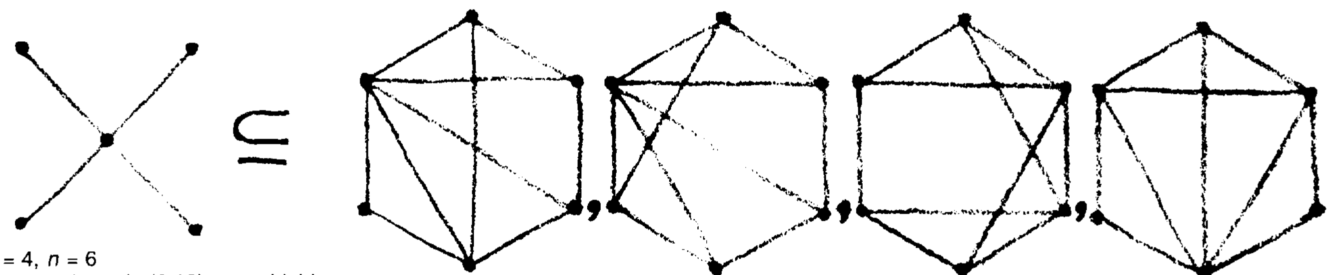
$$U(G_1, G_2, G_3) = \begin{cases} \frac{3}{4}k(3k-1) + \frac{3}{2}k(3k+1) = \frac{3}{4}(9k^2+k) & \text{if } k = 4j \text{ or } 4j-1 \\ \frac{3}{4}k(3k-1) - \frac{1}{2} + \frac{3}{2}k(3k+1) + 1 = \frac{3}{4}(9k^2+k) + \frac{1}{2} & \text{otherwise} \end{cases}$$

$$\approx \frac{3}{4}n$$

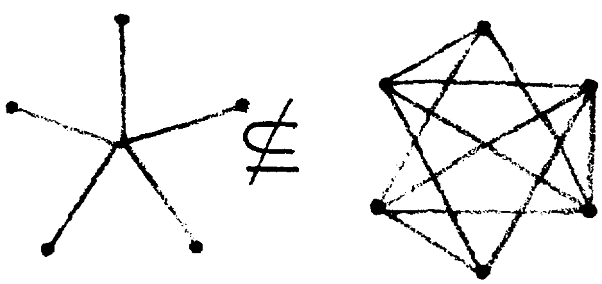
A d-RAYED STAR IS $(n, \frac{1}{2}n(d-1))$-UNAVOIDABLE



(a) $d = 3$, $n = 4$
A 3-rayed star is (4,5)-unavoidable



(b) $d = 4$, $n = 6$
A 4-rayed star is (6,10)-unavoidable



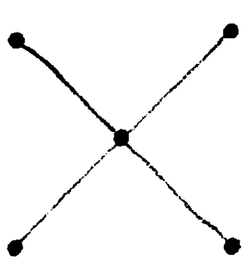
(c) $d = 5$, $n = 6$
A 5-rayed star is not (6,12)-unavoidable

Fig. 8. (a) Since a 3-rayed star is (4,5)-unavoidable, it is a subgraph of the single graph with 4 vertices and 5 edges. (b) Since a 4-rayed star is (6,10)-unavoidable, it is a subgraph of all four of the graphs with 6 vertices and 10 edges. (c) Since a 5-rayed star is *not* (6,12)-unavoidable, it is not a subgraph of some graph with 6 vertices and 12 edges.

UNAVOIDABLE AND UNIVERSAL GRAPHS

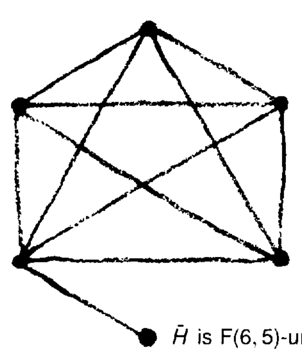
Fig. 9. The graph H and its complement $\bar{H}$ illustrate that H is (n, e)-unavoidable if and only if $\bar{H}$ is $F(n, \binom{n}{2} - e)$-universal. H is (6, 10)-unavoidable; that is, any graph with 6 vertices and 10 edges contains H as a subgraph (see Fig. 8). Therefore $\bar{H}$ is F(6, 5)-universal; that is, any graph with 6 vertices and 5 edges (such as a 5-rayed star) is contained in $\bar{H}$.

H



H is 6, 10)-unavoidable

$\bar{H}$



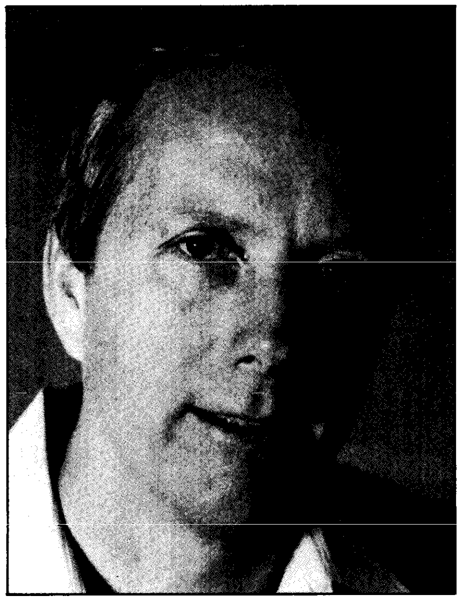
$\bar{H}$ is F(6, 5)-universal

That result, and many other similar results (which have interesting applications to the design of VLSI chips, for example) can be found in Chung and Graham 1978, 1979, 1983; Chung, Graham, and Pippenger 1978; Bhatt and Leighton 1984; and Bhatt and Ipsen 1985. The basic idea here is that a silicon chip (or wafer) can have a universal graph G for some class of graphs, say for all trees with twenty vertices. When a particular tree T is needed for connecting various components on the chip, the appropriate edges of G can be "activated" to realize T.

In the spirit of the current algorithmic trend in mathematics, we might ask how hard it is in practice to find the minimuml Ulam decomposition for two graphs G and G'. In general that is almost surely a difficult computational problem. More precisely, the question "Is $U(G,G') = 2$?" has been shown (Yao 1979) to belong to the notorious class of *NP-complete* problems, an intensively studied collection of thousands of computational problems, including the well-known traveling salesman and graph coloring problems (see Garey and Johnson 1979). Computer scientists believe, although no one has yet been able to prove, that an NP-complete problem is inherently intractable as the general instance size of the problem increases. The resolution of that question remains as perhaps the outstanding problem in theoretical computer science.

It's interesting to note that the related question "Is $U(G,G') = 1$?" (or "Is $G \cong G'$?") is *not* known to belong to the class of NP-complete problems, and indeed, many people believe that an efficient algorithm does exist for its solution. A fuller treatment of such matters can be found in Garey and Johnson.

In conclusion, all of the preceding questions can also be asked about numerous other combinatorial and algebraic structures, such as directed graphs, hypergraphs, partially ordered sets, finite metric spaces, and so on. Some work on those topics can be found in Chung, Graham, and Erdos 1981; Chung, Graham, and Shearer 198 1; Babai, Chung, Erdos, Graham, and Spencer 1982; Chung, Erdos, and Graham 1982; Chung 1983; and Chung and Erdos 1983. Clearly, however, that area of research remains mostly unexplored—and is one more example of the prolific mathematical legacy left to us by Stan Ulam. ■



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