

How to Build a Graph in n Days: Some Variants on Graph Assembly

Aria Dougherty, Nick Mayers, and Robert Short

Department of Mathematics, Lehigh University, Bethlehem, PA, 18015

July 24, 2018

Abstract

In a recent article by M. Bona and A. Vince, the authors introduced the concept of an assembly tree for a graph. Assembly trees act as record keeping devices for the construction of a given graph from its vertices. In this paper we extend the work initiated by M. Bona and A. Vince as well as define and examine a more generalized definition of assembly tree.

Contents

1	Introduction	1
2	Preliminaries	2
3	Enumeration of Assembly Trees	5
4	Time Dependent Assembly Trees	8
4.1	Connected Gluing Rule	10
4.2	Edge Gluing Rule	12
5	Questions	14

1 Introduction

As the title suggests, the subject matter of this paper is graph-theoretic, but the motivation for our objects of interest, in fact, comes from the study of viruses. A detailed discussion on viruses and their connection to graph theory can be found in a paper by Bona et al [1].

Encouraged by the behavior of viruses, Bona et al [1] introduced the notion of an assembly tree of a graph. An assembly tree for a graph, G , can be thought of as a record of how G can be “assembled” starting from the set of its vertices. But what rules should dictate how a graph is assembled from its vertices?

Bona and Vince [2] answer this question by defining “gluing rules”. They focus on one such rule, requiring a graph to be assembled in such a way that two groups of vertices are combined as long as they are connected by an edge. Using this restriction the authors determine explicit formulas or generating functions for the number of assembly trees for many classical families of graphs. In concluding their results, Bona and Vince offer a few reasonable alternative “gluing rules”.

In this paper we begin by analyzing one of the alternative “gluing rules” which they call the *connected gluing rule*. Given a graph G , using the connected gluing rule, at each stage of construction each specified grouping of vertices of G must form a connected induced subgraph of G . Investigating various classical families of graphs, we determine formulas and recursive relations for the number of such assembly trees. For some of these families our formulas are related to classic integer sequences in combinatorics, while for the others these sequences are new to the literature.

In the case of star graphs, the resulting integer sequence forms what is known as the sequence of Fubini numbers¹. Curiously, this sequence was studied by Cayley ([3],1859) while enumerating a certain family of trees. In this particular case, Cayley was studying a family of trees which could be realized as a generalization of assembly trees on paths where a notion of time or order is also tracked. In Section 4 we define such a generalized assembly tree and enumerate them for various families of graphs with both the edge and connected gluing rules. As before, we encountered a mix of both old and new integer sequences.

This paper is organized as follows. In Section 2 the preliminaries of graph theory needed for this paper are given along with a formal treatment of assembly trees and gluing rules. In Section 3 we prove our main results on the enumeration of assembly trees for the classical families of stars, paths, cycles, and complete graphs with the connected gluing rule. Following this, in Section 4 we introduce the notion of a time-dependent assembly tree and enumerate such trees for the same four families of graphs with the addition of both the edge and connected gluing rule. We conclude in Section 5 by discussing further research directions.

2 Preliminaries

Throughout this paper all graphs G are assumed to be simple, i.e., will have no loops or multiple edges. Let $G = (V, E)$ be the graph with vertex set V and edge set E . In the definition of an assembly tree T for a graph G , each vertex of T is labeled by a subset of V . No distinction will be made between a vertex and its label. For a vertex U in a rooted tree, $c(U)$ denotes the children of U .

¹The Fubini numbers (A000670), so named by Louis Comtet, count the number of different ways to rearrange the orderings of sums or integrals in Fubini’s Theorem.

Definition 2.1. Let G be a connected graph on n vertices. An assembly tree for G is a rooted tree, each vertex of which is labeled by a subset $U \subseteq V$ such that

1. the label of the root is $[n] = \{1, 2, \dots, n\}$,
2. each internal vertex U has at least two children and (the label of) $U = \bigcup c(U)$,
3. there are n leaves which are labeled $1, 2, 3, \dots, n$, respectively.

The following Figure 1 illustrates an assembly tree on a graph of seven vertices. Here, there are three internal nodes: $U_1 = \{1, 3, 5, 7\}$, $U_2 = \{4, 2, 6\}$, and $U_3 = \{2, 6\}$.

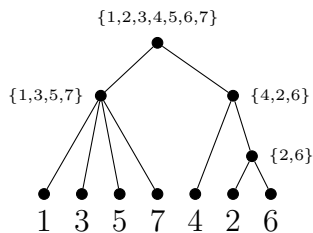


Figure 1: An assembly tree on a graph of seven vertices

Evidently, all graphs with the same number of vertices have the same set of assembly trees. Thus, it seems beneficial to add additional constraints which force properties of the graph to have an impact on the structure of the corresponding assembly tree. For this reason Bona and Vince [2] defined additional “gluing rules” which dictate the pairs of subsets of vertices that can be combined.

Bona and Vince focused on what they called the “edge gluing rule”. Given a graph $G = (V, E)$, an assembly tree T for G satisfies the *edge gluing rule* if each internal vertex $v \in T$ has exactly two children U_1 and U_2 such that there is an edge $v_1v_2 \in E$, called the the *gluing edge*, such that $v_1 \in U_1$ and $v_2 \in U_2$. In Figure 2, the assembly trees of the complete graph on 3 vertices, K_3 , are given assuming the addition of the edge gluing rule.

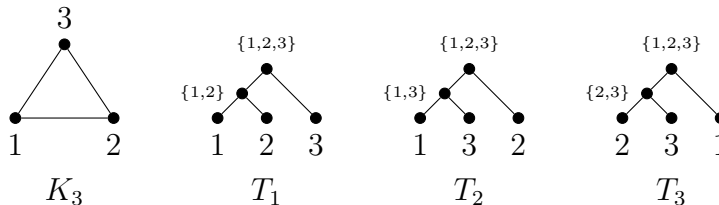


Figure 2: Edge Gluing Assembly Trees for K_3

While focusing their investigation on assembly trees satisfying the edge gluing rule, in their conclusion Bona and Vince offer some alternative reasonable options of “gluing rules”.

Among these alternative rules is the “connected gluing rule”. If $G = (V, E)$ is a graph, then $V' \subseteq V$ defines an *induced subgraph* consisting of V' and the set of all edges defined by elements of V' . We say that an assembly tree satisfies the *connected gluing rule* if for each internal node, the graph induced by the vertices in the label is connected. In Figure 3, the assembly trees of K_3 are given, this time assuming the addition of the edge gluing rule.

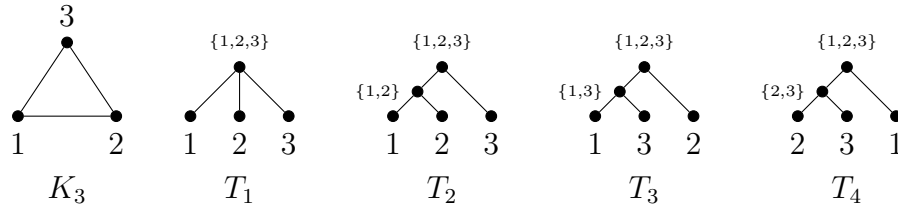


Figure 3: Connected Gluing Assembly Trees for K_3

The connected gluing rule is far less restrictive than the edge gluing rule. The edge gluing rule produces only binary trees whereas the connected gluing rule allows for non-binary trees.

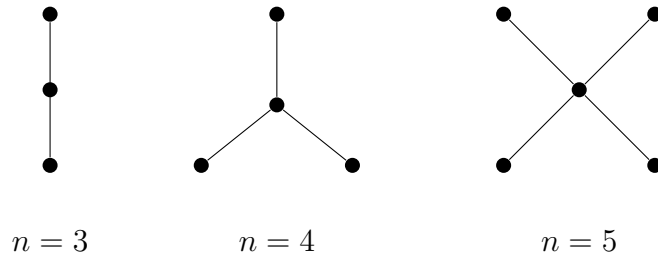
In the next section assembly trees with the addition of the connected gluing rule will be enumerated for the families of star, path, cycle, and complete graphs illustrated below for 1-5 vertices:

$n = 1, 2$ for all:

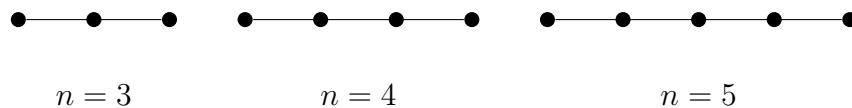


$n = 3, 4, 5$:

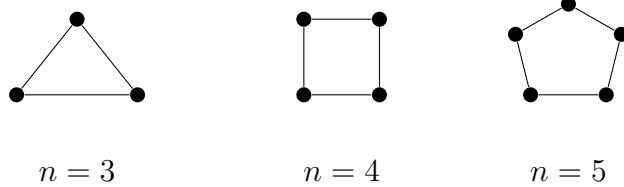
Star Graphs:



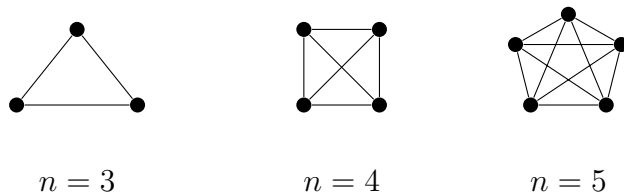
Path Graphs:



Cycle Graphs:



Complete Graphs:



We denote the star graph on n vertices by S_n , the path graph on n vertices by P_n , the cycle graph on n vertices by C_n , and the complete graph on n vertices by K_n .

Throughout this paper we assume that the vertices of P_n are labeled by the elements of $[n]$ in increasing order from left to right. We also assume that the vertices of C_n are labeled by the elements of $[n]$ in increasing clockwise order. Given the structure of K_n there is no need to force any particular labeling for these graphs.

3 Enumeration of Assembly Trees

For a graph G , define $a^C(G)$ to be the number of assembly trees associated to G satisfying the connected gluing rule. We start our enumeration of assembly trees by first focusing on graphs with relatively simple connectivity structure. In particular we consider star, path, and cycle graphs.

We begin with star graphs, S_{n+1} . For our treatment of star graphs we label the middle vertex by 0, and the others by $[n]$ as illustrated in Figure 4. Let $S_2(n, k)$ denote the Stirling numbers of the second kind.

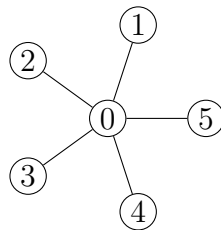


Figure 4: Labeled S_6

Theorem 3.1. *The number of assembly trees for S_{n+1} is $a^C(S_{n+1}) = \sum_{k=1}^n k! S_2(n, k)$.*

Proof. For a subset of vertices of S_{n+1} to correspond to a connected induced subgraph, the subset must contain the vertex labeled 0. Thus, given an appropriate labeling of the non-leaf vertices of an assembly tree U_1, \dots, U_k we have $U_1 \subset U_2 \subset \dots \subset U_k$. Therefore, $U_1 - \{0\}, (U_2 \setminus U_1) - \{0\}, \dots, (U_k \setminus \bigcup_{i=1}^{k-1} U_i) - \{0\}$ forms an ordered partition of $[n]$. Hence, assembly trees of S_{n+1} are in bijection with ordered partitions of $[n]$ which are enumerated by $\sum_{k=1}^n k! S_2(n, k)$. \square

As stated in the introduction, this sequence of values is known as the sequence of Fubini numbers. Cayley [3] determined a generating function for this sequence of values given in the corollary below.

Corollary 3.2. *Let $s_n = a^C(S_{n+1})$, then $\sum_{k=1}^{\infty} \frac{s_k}{k!} x^k = \frac{x}{2-e^x}$.*

Interestingly, when Cayley derived this generating function he was counting assembly trees satisfying the connected gluing rule for S_n . We return to this realization at the end of this section.

Next, we focus on path graphs. For the following result let $SC(n)$ denote n th super Catalan number (A001003).

Theorem 3.3. *The number of assembly trees for the path graph P_n is $a^C(P_n) = SC(n)$.*

Proof. Note, we can always arrange the leaves of an assembly tree of P_n to be in increasing order from left to right; this follows from the fact that two vertices in P_n are connected by an edge if and only if they are labeled by consecutive integers in our fixed labeling. Thus, there exists a bijection between assembly trees for P_n and plane trees with n leaves and with all internal vertices having two or more children. The latter is counted by the super Catalan numbers. \square

The generating function for the $SC(n)$, and thus the $a^C(P_n)$, is also well-known and given below as a corollary.

Corollary 3.4. *Let $p_n = a^C(P_n)$, then $\sum_{k=1}^{\infty} p_k x^k = \frac{1+x-\sqrt{1-6x+x^2}}{4x}$.*

Now, since the cycle graph C_n is just the path graph P_n with an extra edge connecting its vertices of degree 1, we consider assembly trees for C_n next.

Theorem 3.5. *The number of assembly trees for C_n is*

$$\sum_{k=2}^n \left[\sum_{i_1+\dots+i_k=n} i_1 \prod_{j=1}^k SC(i_j) \right].$$

Proof. Given the fixed labeling of the vertices of C_n by $[n]$, connected components consist of either a consecutive block of $[n]$ or a consecutive block ending in n and a consecutive block beginning with 1.

Let U_1 through U_k for $2 \leq k \leq n$ be the vertices adjacent to the root of an assembly tree of C_n . Now, assume that U_1 contains 1, U_2 contains the least element of $[n] \setminus U_1, \dots$, and U_k

contains the least element of $[n] \setminus \bigcup_{i=1}^{k-1} U_i$. Note, that $|U_1| + \dots + |U_k|$ forms a composition of n . Now, fix each $|U_i|$. Given the structure of C_n , the induced subgraphs of the U_i will be paths. By Theorem 4.3, the number of assembly trees for the induced subgraph of U_i is $SC(|U_i|)$. Notice that with $|U_1|$ fixed, there are $|U_1|$ choices for the subset U_1 . Furthermore, once U_1 has been fixed, all other U_i get fixed as well. Thus, given a fixed U_1 there are $\prod_{i=1}^k SC(|U_i|)$ such assembly trees. Hence, there are $|U_1| \prod_{j=1}^k SC(|U_j|)$ assembly trees of C_n with the given values for the $|U_i|$. Summing over all compositions with at least 2 parts the result follows. \square

All choices of families of graphs up to this point have had simple connectivity structure in the sense that the number of edges was relatively minimal. For the final family of graphs we consider complete graphs, which also have simple connectivity structure. In the complete case, the simplicity derives from the fact that all vertices are adjacent and so the number of edges is maximal. To do this we use an approach similar to that of C_n . In this case we obtain a recursive relation.

Theorem 3.6. *For the complete graph on n vertices, K_n , we have*

$$a^C(K_n) = \sum_{k=2}^n \left[\sum_{\substack{i_1 + \dots + i_k = n \\ i_1 \geq i_2 \geq \dots \geq i_k}} \frac{\binom{n}{i_1, \dots, i_k}}{Q!} \prod_{j=1}^k a^C(K_{i_j}) \right]$$

where Q is the number of 1's in our partition $i_1 \geq i_2 \geq \dots \geq i_k$.

Proof. Begin by considering the vertices adjacent to the root of a given assembly tree of K_n , say V_1, \dots, V_k . Given the structure of K_n , any subset of the vertices produces a connected induced subgraph. In fact, for each V_j the induced subgraph is $K_{|V_j|}$. Now, let's assume that $|V_1| \geq \dots \geq |V_k|$ with $|V_1| + \dots + |V_k| = n$. Since the induced subgraph of V_j must be $K_{|V_j|}$, we know that there are $a^C(K_{|V_j|})$ choices of assembly tree for the induced subgraph of V_j . Thus, there are $\prod_{j=1}^k a^C(K_{|V_j|})$ choices of assembly trees for the induced subgraphs of V_1, \dots, V_k . Furthermore, there are $\frac{\binom{n}{|V_1|, \dots, |V_k|}}{Q!}$ choices of V_1, \dots, V_k with $|V_1| \geq \dots \geq |V_k|$. Replacing $|V_j|$ by i_j the result follows. \square

Returning to star graphs, in determining the generating function for the sequence of values $a^C(C_n)$ Cayley was enumerating a different variety of trees with certain restrictions on the degree of each node. This includes the enumeration of trees with n leaves – “knots” in Cayley’s terminology – recursively constructed from such trees on $< n$ leaves by adjoining branches emanating from the old leaves to the new leaves [3]. Examples for $n = 1, 2, 3$ are illustrated below in Figure 5.

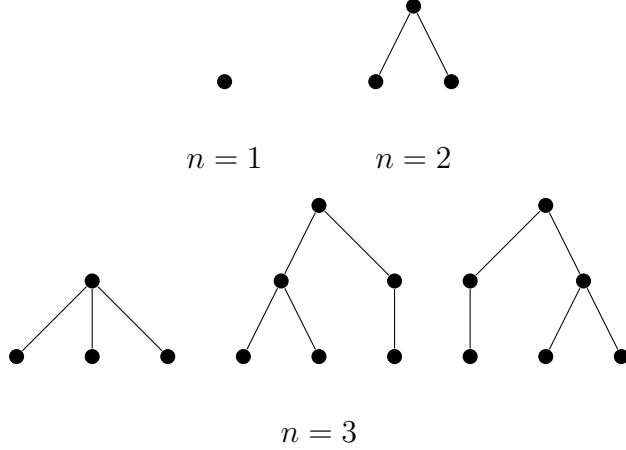


Figure 5: Cayley's recursive trees

One can view this family of trees as a generalization of assembly trees on path graphs where there is a notion of time or order. In the next section we define such a generalization and enumerate the number of such assembly trees with both the edge and connected gluing rules for the same four families of graphs considered above.

4 Time Dependent Assembly Trees

In this section a generalization of the assembly tree defined in Section 2 is defined where the order or time at which vertices of G are grouped is taken into account. Recall that for a vertex U in a rooted tree, $c(U)$ denotes the children of U .

Definition 4.1. A *time-dependent assembly tree* for a connected graph G on n vertices is a rooted tree, each node of which is labeled by a subset $U \subseteq V$ and a nonnegative integer i such that

1. there are leaves labeled $(v, 0)$, for each vertex $v \in V$,
2. each internal (non-leaf) node has at least two children,
3. the label on the root is (V, m) for $1 \leq m \leq n - 1$,
4. for each node (U, i) with $i < m$, $U = \bigcup \{v\}$ for all $(v, 0) \in c((U, i))$,
5. if (U, i) and (U', i') are adjacent nodes with $U \subseteq U'$, then $i < i'$,
6. for each $0 \leq i \leq m$, there exists a node (U, i) with $U \subseteq V$.

An example of a time-dependent assembly tree is given below for an arbitrary graph on seven vertices.

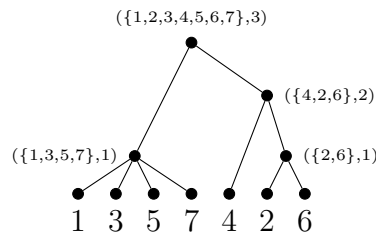


Figure 6: A time-dependent assembly tree

To be clear, when we use the term assembly graph without the prefix time-dependent, we are referring to the object defined in Section 2.

Note, that a time-dependent assembly tree of a graph G is a mechanism which records not only the sequence in which the vertices are combined but also the time or stage at which they are combined in a given assembly of G . Thus, one assembly tree can correspond to multiple time-dependent assembly trees. This is illustrated in Figure 7 where the assembly tree drawn above corresponds to all three time-dependent assembly trees drawn below it. To unclutter the assembly trees in Figure 7 the labels have been removed from the internal nodes and it is assumed that the leaves are labeled in increasing order from left to right; thus, the subsets corresponding to each node should be clear. Furthermore, the time integer labels for the time-dependent assembly trees are given by the horizontal dashed line on which the given node rests.

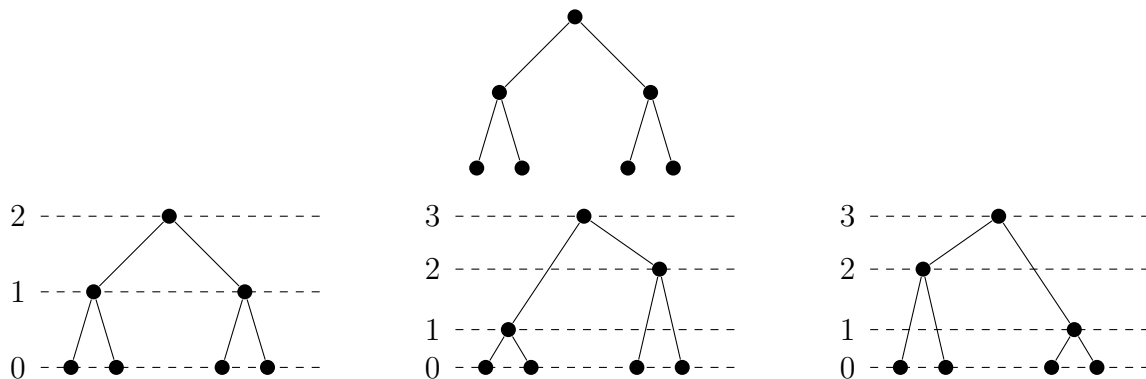


Figure 7: Assembly Trees v. Time-Dependent Assembly Trees

Just as in the case of assembly trees without additional gluing rules any two graphs with the same number of vertices have the exact same collection of time-dependent assembly trees. In the next few sections time-dependent assembly trees with the addition of the edge and connected gluing rules are enumerated for the families of star, path, cycle, and complete

graphs. We will adopt the following helpful notation: Given a time-dependent assembly tree T of a graph $G = (V, E)$ with n vertices let

$$U_j(T) = \{U_i \subseteq V \mid \text{for } s \leq j, (U_i, s) \text{ is assigned to a node of } T\}.$$

Observe that $U_j(T)$ consists of all subsets of V assigned to a vertex of T corresponding to a nonnegative integer $i \leq j$. Now, we can define

$$\mathcal{P}_j(T) = U_j(T) \setminus \{U_i \in U_j(T) \mid \exists U_s \in U_{j,T} \text{ such that } U_i \subseteq U_s\}.$$

Thus, $\mathcal{P}_j(T)$ contains all of the maximal subsets contained in $U_j(T)$ under inclusion. Note that $\mathcal{P}_j(T)$ forms a set partition of $[n]$.

As an example, consider the time-dependent assembly tree illustrated in Figure 6, call it T . For T ,

$$U_2(T) = \{\{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{6\}, \{7\}, \{1, 3, 5, 7\}, \{2, 6\}, \{2, 4, 6\}\}$$

so that

$$\mathcal{P}_2(T) = \{\{1, 3, 5, 7\}, \{2, 4, 6\}\}.$$

4.1 Connected Gluing Rule

For a graph G , define $a_t^C(G)$ to be the number of time-dependent assembly trees associated to G satisfying the connected gluing rule.

As in Section 3, star graphs are investigated first. Given the structure of star graphs, it is clear that time-dependent assembly trees satisfying the connected gluing rule correspond exactly to assembly trees satisfying the connected gluing rule. We state the following proposition for completeness.

Proposition 4.2. $a_t^C(S_{n+1}) = \sum_{k=1}^n k! S_2(n, k)$.

For completeness we also state the associated generating function result.

Corollary 4.3. If $s_n = a_t^C(S_n)$, then $\sum_{k=1}^{\infty} \frac{s_k}{k!} x^k = \frac{x}{2 - e^x}$.

Remark: It is important to note that if we are given a time-dependent assembly tree, say T , of a graph G with $|G| = n$, then by Part 1 of the definition of time-dependent assembly trees we must have $1 \leq |\mathcal{P}_1(T)| < n$.

As in Section 3, we now consider path graphs. We begin with a recurrence result for such time-dependent assembly trees.

Proposition 4.4. $a_t^C(P_n) = \sum_{j=1}^{n-1} \binom{n-1}{j-1} a_t^C(P_j)$ where $a_t^C(P_1) = a_t^C(P_2) = 1$.

Proof. As stated in Theorem 3.3, connected components of P_n correspond to sets of consecutive integers. Thus, the collection of set partitions $\mathcal{P}_1(T)$ for time-dependent assembly trees T of P_n with $|\mathcal{P}_1(T)| = j$ is in bijection with the set of compositions of n into j parts; this can be seen by mapping the set partition $\{\{1, \dots, n_1\}, \dots, \{n - n_j + 1, \dots, n\}\}$ to the composition $n_1 + \dots + n_j = n$. The number of such compositions is $\binom{n-1}{j-1}$. Now, given the connectivity structure of the subsets in $\mathcal{P}_1(T)$, there are $a_t^C(P_j)$ ways to complete the assembly of P_n . Thus, the number of time-dependent assembly trees T of P_n with $|\mathcal{P}_1(T)| = j$ is $\binom{n-1}{j-1} a_t^C(P_j)$. \square

As mentioned earlier, Cayley [3, 4] derived a generating function for the sequence $a_t^C(P_n)$, given in Corollary 4.3. In the vernacular of assembly trees: the number of time-dependent assembly trees satisfying the connected gluing rule for path graphs is also the number of time-dependent assembly trees satisfying the connected gluing rule for star graphs. This is not an obvious result.

Next we examine the family of cycle graphs.

Proposition 4.5. $a_t^C(C_n) = 1 + \sum_{j=2}^{n-1} \binom{n}{j} a_t^C(C_j)$ where $a_t^C(C_1) = a_t^C(C_2) = 1$.

Proof. Note that connected components of C_n correspond to non-crossing partitions of $[n]$ under our fixed labeling of the vertices of C_n by $[n]$. Now, if all vertices of C_n are not assembled at once, then $2 \leq |\mathcal{P}_1(T)| = j \leq n - 1$. Using our bijection with non-crossing partitions we find that the number of choices for such $\mathcal{P}_1(T)$ is $\binom{n}{j}$. Now, given the connectivity structure of the subsets in $\mathcal{P}_1(T)$, there are $a_t^C(C_j)$ ways to complete the assembly of C_n . Thus, the number of such time-dependent assembly trees T of C_n with $|\mathcal{P}_1(T)| = j$ is $\binom{n}{j} a_t^C(C_j)$. The result follows by noting that there is only one way to assemble all vertices of C_n at once. \square

The fact that the coefficients in the recursive relation of Proposition 4.5 all have numerator $n!$ suggests that an exponential generating function for $a_t^C(C_n)$ is existent. Indeed, this is so:

Corollary 4.6. Let $c_n = a_t^C(C_n)$, then $\sum_{k=1}^{\infty} \frac{c_k}{k!} x^k = \frac{x - xe^x + e^x - 1}{2 - e^x}$.

Proof. Let $A(x)$ denote the desired generating function. Translating the recursive relation of Proposition 4.5 into a relation satisfied by $A(x)$ gives the following:

$$A(x) - x - \frac{x^2}{2} = (A(x) - x)(e^x - 1) + e^x - x - \frac{x^2}{2} - 1.$$

Solving for $A(x)$ completes the proof. \square

Finally, we consider complete graphs. The next proposition provides a recursive relation for the $a_t^C(K_n)$.

Proposition 4.7. $a_t^C(K_n) = \sum_{j=1}^{n-1} S_2(n, j) a_t^C(K_j)$ where $a_t^C(K_1) = a_t^C(K_2) = 1$.

Proof. Note that any subset of vertices of K_n forms a connected component. Thus, the collection of $\mathcal{P}_1(T)$ with $|\mathcal{P}_1(T)| = j$ for a time dependent assembly tree of T for K_n is in bijective correspondence with the collection of partitions of $[n]$ into j parts which is enumerated by $S_2(n, j)$. Now, given the connectivity structure of the subsets in $\mathcal{P}_1(T)$, there are $a_t^C(K_j)$ ways to complete the assembly of K_n . Therefore, the number of time-dependent assembly trees T of K_n with $|\mathcal{P}_1(T)| = j$ is $S_2(n, j)a_t^C(K_j)$. \square

4.2 Edge Gluing Rule

For a graph G , define $a_t^E(G)$ to be the number of time-dependent assembly trees associated to G with the addition of the edge gluing rule.

So we begin with star graphs. Due to a star graphs structure it is easy to see that the time-dependent assembly trees satisfying the edge gluing rule correspond exactly to assembly trees satisfying the edge gluing rule. The following proposition is essentially Proposition 1 of Vince and Bona [2].

Proposition 4.8. $a_t^E(S_n) = n!$.

The following corollary is immediate.

Corollary 4.9. Let $s_n = a_t^E(S_n)$, then $\sum_{k=1}^{\infty} \frac{s_k}{k!} x^k = \frac{1}{1-x}$.

Next, the family of path graphs are analyzed.

Proposition 4.10. $a_t^E(P_n) = \sum_{j=1}^{\lfloor n/2 \rfloor} \binom{n-j}{n-2j} a_t^E(P_{n-j})$ where $a_t^E(P_1) = a_t^E(P_2) = 1$.

Proof. Given our fixed labeling of the vertices of P_n , there exists a bijection between $\mathcal{P}_1(T)$ for time dependent assembly trees T of P_n with $|\mathcal{P}_1(T)| = n - j$ and compositions of n consisting of $n - j$ 1's and j 2's where $j > 1$. The bijection is as follows: a 2 occurs as the i th part of the composition if and only if $(\{i, i + 1\}, 1)$ is a node in the time-dependent assembly tree; otherwise, the i th part is a 1. Thus, the number choices for $\mathcal{P}_1(T)$ satisfying $|\mathcal{P}_1(T)| = n - j$ is $\binom{n-j}{n-2j}$. Any choice of $\mathcal{P}_1(T)$ for a time-dependent assembly tree T of P_n with $|\mathcal{P}_1(T)| = n - j$ can be completed to a full time-dependent assembly tree in $a_t^E(P_{n-j})$ ways. \square

Considering the bijection used in the proof of the recursion in Proposition 4.10, one is led to the following relation satisfied by the generating of the $a_t^E(P_n)$.

Corollary 4.11. Let $P(x)$ be the generating function for the $a_t^E(P_n)$, then $P(x) = \frac{x+P(x+x^2)}{2}$.

Proof. Replacing x by $x+x^2$ in $P(x)$ produces a series of terms of the form $a_t^E(P_k)x^n$, where n is the weight of a composition of length k consisting of 1's and 2's. Collecting the coefficients of x^n we get $\sum_{k=1}^n C_{1,2}(k, n)a_t^E(P_k)x^n$, where $C_{1,2}(k, n)$ is the number of compositions of n

into k parts consisting of 1's and 2's; note that $C_{1,2}(n, n) = 1$ and for $\lceil n/2 \rceil \leq k < n$ we have $C_{1,2}(k, n) = \binom{k}{2k-n}$. Thus, at $n = 1$ we get the term $a_t^E(P_1)x$. For $k > 1$, we get

$$\begin{aligned} \sum_{k=1}^n C_{1,2}(k, n) a_t^E(P_k) x^n &= \sum_{k=\lceil n/2 \rceil}^{n-1} \binom{k}{2k-n} a_t^E(P_k) x^n + a_t^E(P_n) x^n \\ &= \sum_{j=1}^{\lfloor n/2 \rfloor} \binom{n-j}{n-2j} a_t^E(P_{n-j}) x^n + a_t^E(P_n) x^n = a_t^E(P_n) x^n + a_t^E(P_n) x^n. \end{aligned}$$

The result follows. \square

Interestingly, in the OEIS the sequence of values formed by the $a_t^E(P_n)$ are listed (A171792) only as the coefficients of the generating function satisfying the relation given in Corollary 4.11. Thus, Corollary 4.11 gives a previously unknown counting realization to the sequence A171792.

Now, just as before, given their similar structure to path graphs, cycle graphs are considered next.

Proposition 4.12. $a_t^E(C_n) = \sum_{j=1}^{\lfloor n/2 \rfloor} \left(\binom{n-j}{n-2j} + \binom{n-j-1}{n-2j} \right) a_t^E(C_{n-j})$ where $a_t^E(C_1) = a_t^E(C_2) = 1$.

Proof. Note that the only difference between cycles C_n and paths P_n is the edge $\{1, n\}$. If $(\{1, n\}, 1)$ is not a node, then as in the proof of Proposition 4.10 the number of such time-dependent assembly trees is $\sum_{j=1}^{\lfloor n/2 \rfloor} \binom{n-j}{n-2j} a_t^E(C_{n-j})$. On the other hand, if $(\{1, n\}, 1)$ is such a node, then applying similar reasoning we get $\binom{n-j-1}{n-2j}$ choices of $\mathcal{P}_1(T)$ with $|\mathcal{P}_1(T)| = j$ for a time-dependent assembly tree T of C_n . Thus, there are $\sum_{j=1}^{\lfloor n/2 \rfloor} \binom{n-j-1}{n-2j} a_t^E(C_{n-j})$ such time-dependent assembly trees. Putting these two cases together, the result follows. \square

Finally, we investigate complete graphs.

Proposition 4.13. $a_t^E(K_n) = \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{2^i i! (n-2i)!} a_t^E(K_{n-i})$ where $a_t^E(K_1) = a_t^E(K_2) = 1$.

Proof. Given the structure of K_n , the collection of set partitions formed by the $\mathcal{P}_1(T)$ for time-dependent assembly trees T of K_n with $|\mathcal{P}_1(T)| = i$ are in bijection with set partitions of $[n]$ into blocks of size 1 or 2 with i blocks of size 2. The number of such blocks is

$$\frac{\prod_{j=0}^{i-1} \binom{n-2j}{2}}{i!} = \frac{n!}{2^i i! (n-2i)!}.$$

Given $|\mathcal{P}_1(T)| = i$, the number of ways to complete such a time-dependent assembly tree of K_n is $a_t^E(K_{n-i})$. \square

5 Questions

In this preliminary investigation we find generating functions for the sequences $a^C(S_n)$, $a^C(P_n)$, $a_t^C(S_n)$, $a_t^C(P_n)$, $a_t^C(C_n)$, and $a_t^E(S_n)$. What about generating functions for $a^C(C_n)$, $a^C(K_n)$, $a_t^C(K_n)$, $a_t^E(P_n)$, $a_t^E(C_n)$, and $a_t^E(K_n)$? All recurrence relations determined involve some form of binomial coefficient which suggest a product of exponential generating functions (see Corollary 4.6).

Further research might also include the enumeration of both regular and time-dependent assembly trees for families of graphs with more complex structure. Of particular interest [2, p.15] is the enumeration of both regular and time-dependent assembly trees for caterpillar graphs (see Figure 8) for which no recurrence relation is known.

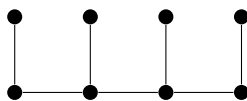


Figure 8: A caterpillar

References

- [1] M. Bóna, M. Sitharam, and A. Vince. Enumeration of viral capsid assembly pathways: tree orbits under permutation group action. Bulletin of mathematical biology, 73(4):726–753, 2011.
- [2] M. Bóna and A. Vince. The number of ways to assemble a graph. In Proceedings of the Meeting on Analytic Algorithmics and Combinatorics, pages 8–17. Society for Industrial and Applied Mathematics, 2013.
- [3] A. Cayley. Lviii. on the analytical forms called trees.–part ii. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 18(121):374–378, 1859.
- [4] A. Cayley. A theorem on trees. Quarterly Journal of Mathematics, 23:376–378, 1889.