How to Count k-Paths

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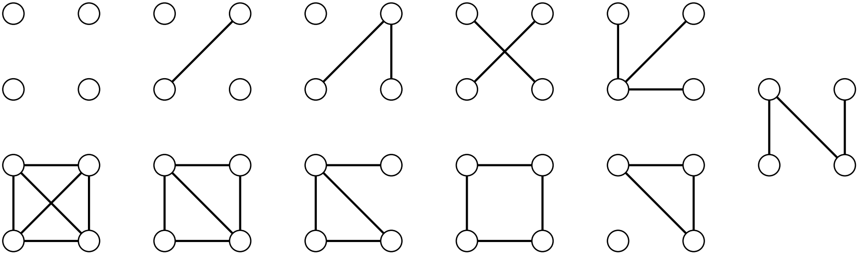
Counting Graphs

- One common problem in graph theory in counting the graphs in a given class.
- There are two variations of this problem.
- A labeled graph has distinct labels (say 1, ... , n) on its vertices.
- Unlabeled graphs do not. (They may be considered as isomorphism classes of labeled graphs.)
- Counting labeled graphs is usually easier since the isomorphism classes may have different sizes.

Counting Graphs

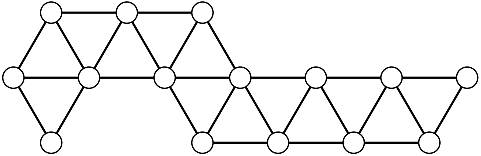
- A graph with order n has $\binom{n}{2}$ possible edges.
- There are $2^{\binom{n}{2}}$ labeled graphs with order n.
- There is no known closed formula for the number of unlabeled graphs with order n.
- Generating functions can be used to show that the formula is asymptotic to $\frac{2^{\binom{n}{2}}}{n!}$.
- There are 11 unlabeled graphs of order 4.



- Paths are a well-known class of graphs. They can be generalized.

Definition

A k-**path graph** G is an alternating sequence of distinct k- and $k+1$-cliques $e_0, t_1, e_1, t_2, \ldots, t_p, e_p$, starting and ending with a k-clique and such that t_i contains exactly two k-cliques e_{i-1} and e_i.



- Note that k-paths are also known a linear k-trees [2017]. They are closely related to pathwidth [1999]; in particular, they are the maximal graphs with proper pathwidth k.

k-Paths

- There is a simple characterization of k-paths.

Definition

A clique K_k of order $k \geq 1$ is a k-**tree**, and any k-tree of order $n+1$ can be obtained from a k-tree of order $n \geq k$ by adding a new vertex adjacent to all vertices of a clique of order k, which is called the **root** of the newly added vertex.

Theorem

(MJP [2006]) *Let G be a k-tree with $n > k+1$ vertices. Then G is a k-path graph if and only if G has exactly two vertices of degree k.*

- We consider the number of unlabeled 2-paths of order n. The first few values ($n \geq 3$) of the sequence are 1, 1, 1, 2, 3, 6, 10, ...

Theorem

There are $2^{n-6}+2^{\lfloor \frac{n-6}{2} \rfloor}$ 2-paths of order $n \geq 5$.

Proof.

A 2-path can be constructed from $K_4 - e$ with 2-leaves u and v by maintaining u as a 2-leaf and adding a new 2-leaf adjacent to v and one of its two neighbors. Then each time a 2-leaf is added, there are two choices, which we may call right (R) and left (L) since 2-paths are planar. Note that if the first choice is L, we could flip over the graph to make it R. Thus construting each 2-path of order n yields a string of Ls and Rs of length $n-4$ beginning with R. There are 2^{n-5} such strings. However, a 2-path may correspond to more than one string, since it can be constructed from either 2-leaf. Constructing from the other 2-leaf reverses the string, since L or R in the string corresponds to a copy of $P_4 + K_1$ in the 2-path.

2-Paths

Proof.

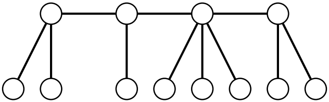
The 2-path may have a nontrivial automorphism. If it can be rotated onto itself, the string ends with L. Then contructing from the other end yields the same string, since each L and R are interchanged (flippped). If it can be reflected onto itself, the string ends with R. Then contructing from the other end yields the same string after flipping so that it begins with R.

In each case, the first half of the string determines the second half, and if n is odd, the middle term is the same. Each case yields $\frac{1}{2}2^{\lfloor \frac{n-4}{2} \rfloor}$ strings, so there are $2^{\lfloor \frac{n-4}{2} \rfloor}$ total strings with symmetry. These strings have a bijection with symmetric 2-paths. Otherwise, each 2-path corresponds to two strings. Thus the number of 2-paths of order n is

$$2^{\lfloor \frac{n-4}{2} \rfloor} + \frac{1}{2}\left(2^{n-5} - 2^{\lfloor \frac{n-4}{2} \rfloor}\right) = 2^{n-6} + 2^{\lfloor \frac{n-6}{2} \rfloor}.$$

□

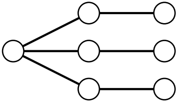
- A **caterpillar** is a tree such that the deletion of all its leaves results in a path.

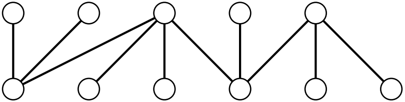


- Harary and Schwenk [1973] showed that there are $2^{n-4} + 2^{\lfloor \frac{n-4}{2} \rfloor}$ caterpillars of order $n \geq 3$.
- This suggests that there is a connection between 2-paths and caterpillars.

Caterpillars

- There are several useful characterizations of caterpillars.
- (Harary/Schwenk [1971]) A tree is a caterpillar if and only if it does not contain the tree shown below left.





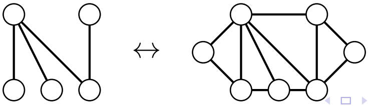
- (Harary/Schwenk [1972]) A tree is a caterpillar if and only if it can be drawn so that its vertices are on two parallel lines and its edges are straight lines that don't cross (see above right).

Theorem

The number of 2-paths of order n equals the number of caterpillars of order $n-2$.

Proof.

We show that there is a bijection between 2-paths of order n and caterpillars of order $n-2$. Given a drawing of a caterpillar with vertices on two parallel lines, add edges between consecutive vertices on each parallel line. Add a vertex neighboring the two leftmost vertices on the lines, and one neighboring the two rightmost vertices. This uniquely produces a 2-path.
Consider constructing a 2-path from $K_4 - e$. As new vertices are added, keep the 2-leaves on the exterior region, and put the other vertices on two parallel lines (a former 2-leaf may be moved to the appropriate line). Consider the graph T induced by the edges not on the exterior region. Adding a new vertex to the 2-path adds one pendant edge to T, so it is a tree. The drawing is a caterpillar. □



Constructing k-Paths

- The fact that 2-paths can be constructed with vertices on two parallel lines suggests a generalization for k-paths.
- A k-path can be constructed from $K_k + \overline{K_2}$ with k-leaves u and v by maintaining u as a k-leaf and adding a new k-leaf adjacent to v and $k-1$ of its k neighbors. Label the k neighbors of u 1 through k (in any way). Each time a k-leaf x is added adjacent to (old) k-leaf w, label w with the label of its neighbor that does not neighbor x.
- Define a string of length $n-k-2$ with the labels added after the first k.
- Call this a **construction string**.

Labeled k-Paths

Theorem

(BNS [2018]) *The number of labeled k-paths of order $n \geq k+3$ is*

$$\frac{n! \cdot k^{n-k-2}}{2 \cdot k!}.$$

Proof.

There are k^{n-k-2} construction strings for k-paths of order n. There are $k!$ ways to label $N(u)$ initially, so $k!$ strings can be produced this way. A given k-path may also be constructed starting at its other leaf. Constructing from the other k-leaf reverses the string, since each number in the string corresponds to a copy of $P_4 + K_{k-1}$ in the k-path. The n labels can be permuted in $n!$ ways. Thus the number of labeled k-paths of order $n \geq k+3$ is as stated. $\square$

Unlabeled k-Paths

- What about unlabeled k-paths?
- The k-path may have a nontrivial automorphism.
- One possibility is that its end may be interchanged.

Definition

A **dominating vertex** of a graph is a vertex adjacent to all other vertices.

- Another possibility is that it has multiple dominating vertices that may be permuted. The numbers assigned to dominating vertices will not appear in the string.
- Thus we must count strings of length $n-k-2$ using at most k numbers which are equivalent under reversal and permutation (**reversal symmetry**).
- We split the strings into those that have reversal symmetry and those that do not.

Unlabeled k-Paths

$$N = \left|\begin{array}{c} k-paths\ with \\ reversal\ symmetry \end{array}\right| + \left|\begin{array}{c} k-paths\ without \\ reversal\ symmetry \end{array}\right|$$

$$= \sum_i \left|\begin{array}{c} k-paths\ with \\ reversal\ symmetry \\ using\ exactly\ i\ numbers \end{array}\right| + \sum_i \left|\begin{array}{c} k-paths\ without \\ reversal\ symmetry \\ using\ exactly\ i\ numbers \end{array}\right|$$

$$= \sum_i \frac{\left|\begin{array}{c} strings\ with \\ reversal\ symmetry \\ using\ exactly\ i\ numbers \end{array}\right|}{i!} + \sum_i \frac{\left|\begin{array}{c} strings\ without \\ reversal\ symmetry \\ using\ exactly\ i\ numbers \end{array}\right|}{2(i!)}$$

$$= \sum_{i=1}^{k} \frac{a^*(i,x)}{i!} + \sum_{i=1}^{k} \frac{b(i,x)-a^*(i,x)}{2(i!)}$$

- Let the number of strings of length $x = n-k-2$ using exactly i numbers that have reversal symmetry be $a^*(i,x)$.
- Let the total number of strings of length $x = n-k-2$ using exactly i specified numbers of k numbers be $b(i,x)$.

Counting Onto Functions

- Let the total number of strings of length $x = n - k - 2$ using exactly i specified numbers of k numbers be $b(i,x)$.
- Equivalently, this is the number of onto functions from $\{1, ..., k\}$ to $\{1, ..., i\}$.
- There is a well-known formula for this, proved using Inclusion-Exclusion (Rosen [2011] p.561), showing

$$b(i,x) = \sum_{j=1}^{i} (-1)^{i-j} \binom{i}{j} j^x.$$

Unlabeled k-Paths

- The number of strings with reversal symmetry depends on whether $x = n - k - 2$ is even or odd.
- Let the number of strings of length $x = n - k - 2$ using exactly i numbers that have reversal symmetry be $a(i,x)$ for $n - k$ even, and $a'(i,x)$ for $n - k$ odd. Certainly $a(1,x) = a'(1,x) = 1$.
- A string with reversal symmetry can have its numbers permuted to produce the original string.
- Such a permutation must be an involution.

- A permutation that is self-inverse is called an **involution**.
- It must have cycles of length one or two only.
- We will need the sequence $s(n)$ of involution numbers. This sequence (OEIS A000085) begins 1, 2, 4, 10, 26, 76, 232, 764, 2620, ...
- Suppose there are r 2-cycles in an involution. Pick a number and match it to its image in $2r-1$ ways. The next number can be matched in $2r-3$ ways.
- Divide by 2^r to eliminate the order of these choices.
- We choose $2r$ of n numbers and sum over all values of r. Thus

$$s(n) = \sum_{r=0}^{\lfloor n/2 \rfloor} \binom{n}{2r} (2r-1)!! = \sum_{r=0}^{\lfloor n/2 \rfloor} \frac{n!}{2^r (n-2r)! r!}$$

Unlabeled k-Paths

- Assume $n-k$ is even, so the length of the string is even.
- To find how many strings with reversal symmetry use exactly i numbers, we find how many use at most i numbers and subtract out those that use fewer than i.
- There are $i^{\lceil \frac{x}{2} \rceil}$ choices for the first half of the string, and $s(i)$ involutions produce the second half of the string.
- Thus there are $s(i) \cdot i^{\lceil \frac{x}{2} \rceil}$ strings with reversal symmetry that use at most i numbers.

- There are $\binom{i}{j}$ choices of j numbers that appear in a string using exactly j of i numbers.
- The number of involutions of the remaining $j-i$ numbers is $s(j-i)$, so each string using exactly j of i numbers will appear $\binom{i}{j}a(j,x)s(i-j)$ times in the $s(i)\cdot i^{\lceil \frac{x}{2} \rceil}$ strings.
- Thus we have the recursive formula $a(i,x)=s(i)\cdot i^{\lceil \frac{x}{2} \rceil}-\sum_{j=1}^{i-1}\binom{i}{j}a(j,x)s(i-j)$.

Unlabeled k-Paths

i	$a(i,x)$
1	1
2	$2\cdot 2^{\lceil \frac{x}{2}\rceil} - 2$
3	$4\cdot 3^{\lceil \frac{x}{2}\rceil} - 6\cdot 2^{\lceil \frac{x}{2}\rceil}$
4	$10\cdot 4^{\lceil \frac{x}{2}\rceil} - 16\cdot 3^{\lceil \frac{x}{2}\rceil} + 8$
5	$26\cdot 5^{\lceil \frac{x}{2}\rceil} - 50\cdot 4^{\lceil \frac{x}{2}\rceil} + 40\cdot 2^{\lceil \frac{x}{2}\rceil} - 10$
6	$76\cdot 6^{\lceil \frac{x}{2}\rceil} - 156\cdot 5^{\lceil \frac{x}{2}\rceil} + 160\cdot 3^{\lceil \frac{x}{2}\rceil} - 60\cdot 2^{\lceil \frac{x}{2}\rceil} - 36$
7	$232\cdot 7^{\lceil \frac{x}{2}\rceil} - 532\cdot 6^{\lceil \frac{x}{2}\rceil} + 700\cdot 4^{\lceil \frac{x}{2}\rceil} - 280\cdot 3^{\lceil \frac{x}{2}\rceil} - 252\cdot 2^{\lceil \frac{x}{2}\rceil} + 112$

Unlabeled k-Paths

- If $n-k$ is odd, the length of the string is odd.
- As before, to find how many strings with reversal symmetry use exactly i numbers, we find how many use at most i numbers and subtract out those that use fewer than i.
- Now the middle element must be fixed in any involution, so $s(i-1)$ involutions produce the second half of the string.
- Thus there are $s(i-1) \cdot i^{\lceil \frac{x}{2} \rceil}$ strings with reversal symmetry that use at most i numbers.
- As before, we have the recursive formula $a'(i,x) = s(i-1) \cdot i^{\lceil \frac{x}{2} \rceil} - \sum_{j=1}^{i-1} \binom{i}{j} a'(j,x) s(i-j)$.

Unlabeled k-Paths

i	$a'(i,x)$
1	1
2	$2^{\lceil \frac{x}{2} \rceil} - 2$
3	$2 \cdot 3^{\lceil \frac{x}{2} \rceil} - 3 \cdot 2^{\lceil \frac{x}{2} \rceil}$
4	$4 \cdot 4^{\lceil \frac{x}{2} \rceil} - 8 \cdot 3^{\lceil \frac{x}{2} \rceil} + 8$
5	$10 \cdot 5^{\lceil \frac{x}{2} \rceil} - 20 \cdot 4^{\lceil \frac{x}{2} \rceil} + 20 \cdot 2^{\lceil \frac{x}{2} \rceil} - 10$
6	$26 \cdot 6^{\lceil \frac{x}{2} \rceil} - 60 \cdot 5^{\lceil \frac{x}{2} \rceil} + 80 \cdot 3^{\lceil \frac{x}{2} \rceil} - 30 \cdot 2^{\lceil \frac{x}{2} \rceil} - 36$
7	$76 \cdot 7^{\lceil \frac{x}{2} \rceil} - 182 \cdot 6^{\lceil \frac{x}{2} \rceil} + 280 \cdot 4^{\lceil \frac{x}{2} \rceil} - 140 \cdot 3^{\lceil \frac{x}{2} \rceil} - 126 \cdot 2^{\lceil \frac{x}{2} \rceil} + 112$

Unlabeled k-Paths

- Thus the number of strings without reversal symmetry is $b(i,x) - a(i,x)$ or $b(i,x) - a'(i,x)$, depending on parity.
- Thus the number of k-paths with $x = n - k - 2$ even is

$$\sum_{i=1}^{k} \frac{a(i,x)}{i!} + \sum_{i=1}^{k} \frac{b(i,x) - a(i,x)}{2(i!)} = \sum_{i=1}^{k} \frac{b(i,x) + a(i,x)}{2(i!)}.$$

- The number of k-paths with $x = n - k - 2$ odd is

$$\sum_{i=1}^{k} \frac{a'(i,x)}{i!} + \sum_{i=1}^{k} \frac{b(i,x) - a'(i,x)}{2(i!)} = \sum_{i=1}^{k} \frac{b(i,x) + a'(i,x)}{2(i!)}.$$

Unlabeled k-Paths

Theorem

Let $a(1,x) = a'(1,x) = 1$, *and*
$a(i,x) = s(i) \cdot i^{\lceil \frac{x}{2} \rceil} - \sum_{j=1}^{i-1} \binom{i}{j} a(j,x) s(i-j)$
$a'(i,x) = s(i-1) \cdot i^{\lceil \frac{x}{2} \rceil} - \sum_{j=1}^{i-1} \binom{i}{j} a'(j,x) s(i-j)$
$b(i,x) = \sum_{j=1}^{i} (-1)^{i-j} \binom{i}{j} j^x$.
Then the number of k-paths of order $n \geq k+3$ *is*

$$\sum_{i=1}^{k} \frac{b(i,n-k-2) + a(i,n-k-2)}{2(i!)} \quad n-k \text{ even}$$

$$\sum_{i=1}^{k} \frac{b(i,n-k-2) + a'(i,n-k-2)}{2(i!)} \quad n-k \text{ odd}$$

Unlabeled k-Paths

- The problem of enumerating strings that are considered equivalent under reversal and permutation was previously studied by Nester [1999] using Polya enumeration.
- This produced a method for calculating small values of these sequences, but did not produce closed formulas for them.
- For small values of k, here are simplified formulas for the number $N(k,x)$ of k-paths of order $x = n-k-2$.
- $N(2,x) = \begin{cases} \frac{1}{4}2^x + \frac{1}{2}2^{\lceil \frac{x}{2} \rceil} & n\,even \\ \frac{1}{4}2^x + \frac{1}{4}2^{\lceil \frac{x}{2} \rceil} & n\,odd \end{cases} = 2^{n-6} + 2^{\lfloor \frac{n-6}{2} \rfloor}$
- $N(3,x) = \begin{cases} \frac{1}{12}3^x + \frac{1}{6}3^{\lceil \frac{x}{2} \rceil} + \frac{1}{4} & n\,even \\ \frac{1}{12}3^x + \frac{1}{3}3^{\lceil \frac{x}{2} \rceil} + \frac{1}{4} & n\,odd \end{cases}$
- $N(4,x) = \begin{cases} \frac{1}{48}4^x + \frac{5}{24}4^{\lceil \frac{x}{2} \rceil} + \frac{1}{8}2^x + \frac{1}{3} & n\,even \\ \frac{1}{48}4^x + \frac{1}{12}4^{\lceil \frac{x}{2} \rceil} + \frac{1}{8}2^x + \frac{1}{3} & n\,odd \end{cases}$

Unlabeled k-Paths

- For small values of k, here are simplified formulas for the number of k-paths of order $x = n - k - 2$.
- $N(5,x) = \begin{cases} \frac{5^x}{240} + \frac{3^x}{24} + \frac{2^x}{12} + \frac{5^{\lceil \frac{x}{2} \rceil}}{24} + \frac{2^{\lceil \frac{x}{2} \rceil}}{12} + \frac{5}{16} & n \text{ even} \\ \frac{5^x}{240} + \frac{3^x}{24} + \frac{2^x}{12} + \frac{13 \cdot 5^{\lceil \frac{x}{2} \rceil}}{120} + \frac{2^{\lceil \frac{x}{2} \rceil}}{6} + \frac{5}{16} & n \text{ odd} \end{cases}$
- $N(6,x) =$
$$\begin{cases} \frac{6^x}{1440} + \frac{4^x}{96} + \frac{3^x}{36} + \frac{3 \cdot 2^x}{32} + \frac{19 \cdot 6^{\lceil \frac{x}{2} \rceil}}{360} + \frac{3^{\lceil \frac{x}{2} \rceil}}{9} + \frac{2^{\lceil \frac{x}{2} \rceil}}{8} + \frac{17}{60} & n \text{ even} \\ \frac{6^x}{1440} + \frac{4^x}{96} + \frac{3^x}{36} + \frac{3 \cdot 2^x}{32} + \frac{13 \cdot 6^{\lceil \frac{x}{2} \rceil}}{720} + \frac{3^{\lceil \frac{x}{2} \rceil}}{18} + \frac{2^{\lceil \frac{x}{2} \rceil}}{16} + \frac{17}{60} & n \text{ odd} \end{cases}$$
- $N(7,x) =$
$$\begin{cases} \frac{7^x}{10080} + \frac{5^x}{480} + \frac{4^x}{144} + \frac{3^x}{32} + \frac{11 \cdot 2^x}{120} + \frac{19 \cdot 7^{\lceil \frac{x}{2} \rceil}}{2520} + \frac{4^{\lceil \frac{x}{2} \rceil}}{36} + \frac{3^{\lceil \frac{x}{2} \rceil}}{24} + \frac{2^{\lceil \frac{x}{2} \rceil}}{20} + \frac{85}{288} \\ \frac{7^x}{10080} + \frac{5^x}{480} + \frac{4^x}{144} + \frac{3^x}{32} + \frac{11 \cdot 2^x}{120} + \frac{29 \cdot 7^{\lceil \frac{x}{2} \rceil}}{1260} + \frac{5 \cdot 4^{\lceil \frac{x}{2} \rceil}}{72} + \frac{3^{\lceil \frac{x}{2} \rceil}}{12} + \frac{2^{\lceil \frac{x}{2} \rceil}}{10} + \frac{85}{288} \end{cases}$$
- In general, the dominant term is always $\frac{1}{2(k!)} k^{n-k-2}$, and for $k \geq 5$, the next largest term is $\frac{1}{4 \cdot (k-2)!} (k-2)^{n-k-2}$.

Unlabeled k-Paths

- The following table lists the beginnings of the sequences, which occur in OEIS up to $k = 6$.

k	Sequence ($n \geq k+3$)	OEIS
2	1, 2, 3, 6, 10, 20, 36, 72, 136, 272, ...	A005418
3	1, 2, 4, 10, 25, 70, 196, 574, 1681, 5002, ...	A001998
4	1, 2, 4, 11, 31, 107, 379, 1451, 5611, 22187, ...	A056323
5	1, 2, 4, 11, 32, 116, 455, 1993, 9134, 43580, ...	A056324
6	1, 2, 4, 11, 32, 117, 467, 2135, 10480, 55091, ...	A056325
7	1, 2, 4, 11, 32, 117, 468, 2151, 10722, 58071, ...	

- All k-paths with order $k+3 \leq n \leq 2k+1$ have diameter 2, and so have a dominating vertex. If there are N k-paths with order $2k+2$, then there are N $k+r$-paths with order $2k+2+r$, since they have at least r dominating vertices.
- Thus the sequences in the table above approach a limiting sequence of 1, 2, 4, 11, 32, 117, 468, 2152, 10743, ... which appears to be A103293.

Thank You!

- A. Abiad, B. Brimkov, A. Erey, L. Leshock, X. Martínez-Rivera, S. O, S. Song, J. Williford, On the Wiener index, distance cospectrality and transmission-regular graphs, Discrete Appl. Math. 230 (2017), 1-10.
- J. Bastea, M. Noyb, I. Sau, On the number of labeled graphs of bounded treewidth, European J. Combin. 71 (2018), 12-21.
- F. Harary and A. Schwenk, Trees with Hamiltonian square, Mathematika, 18 (1971), 138-140.
- F. Harary and A. Schwenk, A new crossing number for bipartite graphs, Utilitas Math. 1 (1972), 203-209.
- F. Harary and A. Schwenk, The number of caterpillars, Discrete Math. 6 4 (1973), 359-365.
- L. Markenzona, C. M. Justelb, N. Paciornikc, Subclasses of k-trees: Characterization and recognition, Discrete Appl. Math. 154 5 (2006), 818-825.
- M. R. Nester, Mathematical investigations of some plant interaction designs. PhD Thesis. University of Queensland, Brisbane, Australia (1999).
- A. Proskurowski, J. Telle, Classes of graphs with restricted interval models Discrete Math. Theoret. Comput. Sci. 3 (1999), 167–176.
- K. Rosen, Discrete Mathematics and Its Applications Seventh Edition 7th Edition, McGraw Hill, 2011.