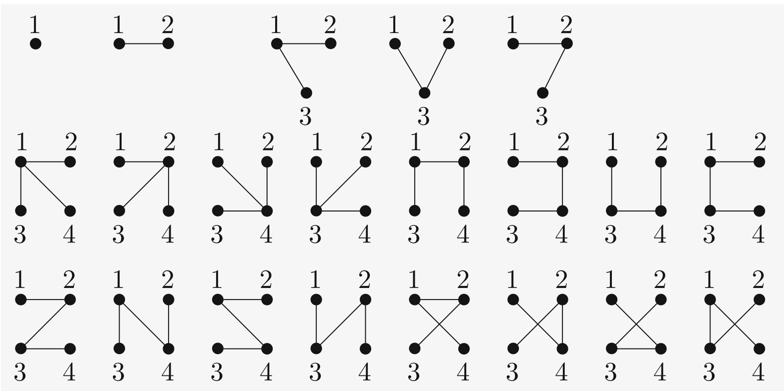
Cayley's formula for the number of trees

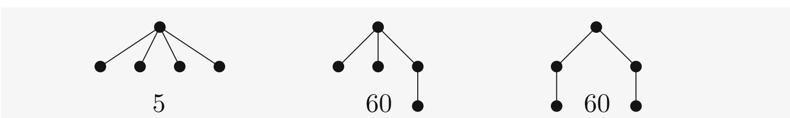
Chapter 33

One of the most beautiful formulas in enumerative combinatorics concerns the number of labeled trees. Consider the set $N = \{1, 2, \ldots, n\}$. How many different trees can we form on this vertex set? Let us denote this number by T_n. Enumeration "by hand" yields $T_1 = 1$, $T_2 = 1$, $T_3 = 3$, $T_4 = 16$, with the trees shown in the following table:



Arthur Cayley

Note that we consider *labeled* trees, that is, although there is only one tree of order 3 in the sense of graph isomorphism, there are 3 different labeled trees obtained by marking the inner vertex 1, 2 or 3. For $n = 5$ there are three nonisomorphic trees:



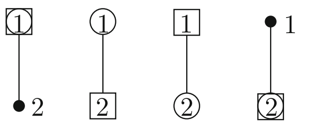
For the first tree there are clearly 5 different labelings, and for the second and third there are $\frac{5!}{2} = 60$ labelings, so we obtain $T_5 = 125$. This should be enough to conjecture $T_n = n^{n-2}$, and that is precisely Cayley's result.

Theorem. *There are n^{n-2} different labeled trees on n vertices.*

This beautiful formula yields to equally beautiful proofs, drawing on a variety of combinatorial and algebraic techniques. We will outline three of them before presenting the proof which is to date the most beautiful of them all.

M. Aigner, G. M. Ziegler, *Proofs from THE BOOK*, https://doi.org/10.1007/978-3-662-57265-8_33

■ **First proof (Bijection).** The classical and most direct method is to find a bijection from the set of all trees on n vertices onto another set whose cardinality is known to be n^{n-2}. Naturally, the set of all ordered sequences $(a_1, \ldots, a_{n-2})$ with $1 \leq a_i \leq n$ comes into mind. Thus we want to uniquely encode every tree T by a sequence $(a_1, \ldots, a_{n-2})$. Such a code was found by Prüfer and is contained in most books on graph theory.



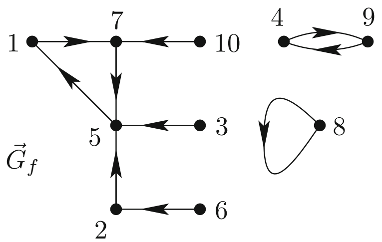
The four trees of $\mathcal{T}_2$

Here we want to discuss another bijection proof, due to Joyal, which is less known but of equal elegance and simplicity. For this, we consider not just trees t on $N = \{1, \ldots, n\}$ but trees together with two distinguished vertices, the *left end* $\bigcirc$ and the *right end* $\square$, which may coincide. Let $\mathcal{T}_n = \{(t; \bigcirc, \square)\}$ be this new set; then, clearly, $|\mathcal{T}_n| = n^2 T_n$.

Our goal is thus to prove $|\mathcal{T}_n| = n^n$. Now there is a set whose size is known to be n^n, namely the set N^N of all mappings from N into N. Thus our formula is proved if we can find a bijection from N^N onto $\mathcal{T}_n$.

Let $f : N \longrightarrow N$ be any map. We represent f as a directed graph $\vec{G}_f$ by drawing arrows from i to $f(i)$.

For example, the map



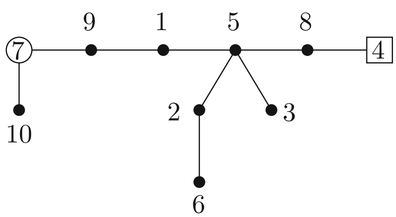
$$f = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 7 & 5 & 5 & 9 & 1 & 2 & 5 & 8 & 4 & 7 \end{pmatrix}$$

is represented by the directed graph in the margin.

Look at a component of $\vec{G}_f$. Since there is precisely one edge emanating from each vertex, the component contains equally many vertices and edges, and hence precisely one directed cycle. Let $M \subseteq N$ be the union of the vertex sets of these cycles. A moment's thought shows that M is the *unique* maximal subset of N such that the restriction of f onto M acts as a bijection on M. Write $f|_M = \begin{pmatrix} a & b & \ldots & z \\ f(a) & f(b) & \ldots & f(z) \end{pmatrix}$ such that the numbers $a, b, \ldots, z$ in the first row appear in natural order. This gives us an ordering $f(a), f(b), \ldots, f(z)$ of M according to the second row. Now $f(a)$ is our left end and $f(z)$ is our right end.

The tree t corresponding to the map f is now constructed as follows: Draw $f(a), \ldots, f(z)$ in this order as a *path* from $f(a)$ to $f(z)$, and fill in the remaining vertices as in $\vec{G}_f$ (deleting the arrows).

In our example above we obtain $M = \{1, 4, 5, 7, 8, 9\}$



$$f|_M = \begin{pmatrix} 1 & 4 & 5 & 7 & 8 & 9 \\ 7 & 9 & 1 & 5 & 8 & 4 \end{pmatrix}$$

and thus the tree t depicted in the margin.

It is immediate how to reverse this correspondence: Given a tree t, we look at the unique path P from the left end to the right end. This gives us the set M and the mapping $f|_M$. The remaining correspondences $i \to f(i)$ are then filled in according to the unique paths from i to P. $\square$

■ **Second proof (Linear Algebra).** We can think of T_n as the number of spanning trees in the complete graph K_n. Now let us look at an arbitrary connected simple graph G on $V = \{1, 2, \ldots, n\}$, denoting by $t(G)$ the number of spanning trees; thus $T_n = t(K_n)$. The following celebrated result is Kirchhoff's *matrix-tree theorem* (see [1]). Consider the incidence matrix $B = (b_{ie})$ of G, whose rows are labeled by V, the columns by E, where we write $b_{ie} = 1$ or 0 depending on whether $i \in e$ or $i \notin e$. Note that $|E| \geq n - 1$ since G is connected. In every column we replace one of the two 1's by -1 in an arbitrary manner (this amounts to an orientation of G), and call the new matrix C. $M = CC^T$ is then a symmetric $n \times n$ matrix with the degrees $d_1, \ldots, d_n$ in the main diagonal.

Proposition. *We have $t(G) = \det M_{ii}$ for all $i = 1, \ldots, n$, where M_{ii} results from M by deleting the i-th row and the i-th column.*

■ **Proof.** The key to the proof is the Binet–Cauchy theorem proved in the previous chapter: When P is an $r \times s$ matrix and Q an $s \times r$ matrix, $r \leq s$, then $\det(PQ)$ equals the sum of the products of determinants of corresponding $r \times r$ submatrices, where "corresponding" means that we take the same indices for the r columns of P and the r rows of Q.

For M_{ii} this means that

$$\det M_{ii} \;=\; \sum\nolimits_N \det N \cdot \det N^T \;=\; \sum\nolimits_N (\det N)^2,$$

where N runs through all $(n-1)\times(n-1)$ submatrices of $C\backslash\{\text{row } i\}$. The $n-1$ columns of N correspond to a subgraph of G with $n-1$ edges on n vertices, and it remains to show that

$$\det N = \begin{cases} \pm 1 & \text{if these edges span a tree} \\ 0 & \text{otherwise.} \end{cases}$$

Suppose the $n-1$ edges do not span a tree. Then there exists a component which does not contain i. Since the corresponding rows of this component add to 0, we infer that they are linearly dependent, and hence $\det N = 0$.

Assume now that the columns of N span a tree. Then there is a vertex $j_1 \neq i$ of degree 1; let e_1 be the incident edge. Deleting j_1, e_1 we obtain a tree with $n-2$ edges. Again there is a vertex $j_2 \neq i$ of degree 1 with incident edge e_2. Continue in this way until $j_1, j_2, \ldots, j_{n-1}$ and $e_1, e_2, \ldots, e_{n-1}$ with $j_i \in e_i$ are determined. Now permute the rows and columns to bring j_k into the k-th row and e_k into the k-th column. Since by construction $j_k \notin e_\ell$ for $k < \ell$, we see that the new matrix N' is lower triangular with all elements on the main diagonal equal to ± 1. Thus $\det N = \pm \det N' = \pm 1$, and we are done.

For the special case $G = K_n$ we clearly obtain

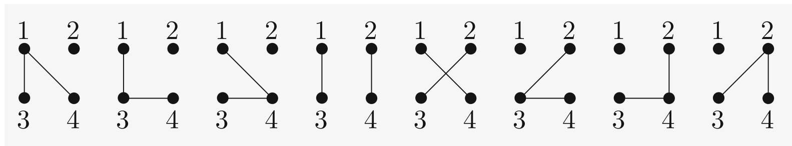
$$M_{ii} = \begin{pmatrix} n-1 & -1 & \ldots & -1 \\ -1 & n-1 & & -1 \\ \vdots & & \ddots & \vdots \\ -1 & -1 & \ldots & n-1 \end{pmatrix}$$

and an easy computation shows $\det M_{ii} = n^{n-2}$. □

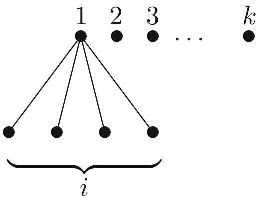
"A nonstandard method of counting trees: Put a cat into each tree, walk your dog, and count how often he barks."

■ **Third proof (Recursion).** Another classical method in enumerative combinatorics is to establish a recurrence relation and to solve it by induction. The following idea is essentially due to Riordan and Rényi. To find the proper recursion, we consider a more general problem (which already appears in Cayley's paper). Let A be an arbitrary k-set of the vertices. By $T_{n,k}$ we denote the number of (labeled) forests on $\{1, \dots, n\}$ consisting of k trees where the vertices of A appear in different trees. Clearly, the set A does not matter, only the size k. Note that $T_{n,1} = T_n$.

For example, $T_{4,2} = 8$ for $A = \{1, 2\}$



Consider such a forest F with $A = \{1, 2, \dots, k\}$, and suppose 1 is adjacent to i vertices, as indicated in the margin. Deleting 1, the i neighbors together with $2, \dots, k$ yield one vertex each in the components of a forest that consists of $k - 1 + i$ trees. As we can (re)construct F by first fixing i, then choosing the i neighbors of 1 and then the forest $F\backslash 1$, this yields



$$T_{n,k} \;=\; \sum_{i=0}^{n-k} \binom{n-k}{i} T_{n-1,k-1+i} \tag{1}$$

for all $n \geq k \geq 1$, where we set $T_{0,0} = 1$, $T_{n,0} = 0$ for $n > 0$. Note that $T_{0,0} = 1$ is necessary to ensure $T_{n,n} = 1$.

Proposition. *We have*

$$T_{n,k} \;=\; k\,n^{n-k-1} \tag{2}$$

and thus, in particular,

$$T_{n,1} \;=\; T_n \;=\; n^{n-2}.$$

■ **Proof.** By (1), and using induction, we find

$$\begin{aligned}
T_{n,k} &= \sum_{i=0}^{n-k} \binom{n-k}{i} (k-1+i)(n-1)^{n-1-k-i} \qquad (i \to n-k-i) \\
&= \sum_{i=0}^{n-k} \binom{n-k}{i} (n-1-i)(n-1)^{i-1} \\
&= \sum_{i=0}^{n-k} \binom{n-k}{i} (n-1)^{i} - \sum_{i=1}^{n-k} \binom{n-k}{i} i(n-1)^{i-1} \\
&= n^{n-k} - (n-k) \sum_{i=1}^{n-k} \binom{n-1-k}{i-1} (n-1)^{i-1} \\
&= n^{n-k} - (n-k) \sum_{i=0}^{n-1-k} \binom{n-1-k}{i} (n-1)^{i} \\
&= n^{n-k} - (n-k)n^{n-1-k} \;=\; k\,n^{n-1-k}.
\end{aligned}$$

□

■ **Fourth proof (Double Counting).** The following marvelous proof due to Arnon Avron and Nachum Dershowitz, which builds on an idea of Jim Pitman, gives Cayley's formula and its generalization (2) without induction or bijection — it is just clever counting in two ways.

We consider labeled forests with vertex set $\{1, \dots, n\}$. A *rooted forest* is a forest together with a choice of a root in each component tree. Let $\mathcal{F}_{n,k}$ be the set of all rooted forests that consist of k rooted trees. Thus $\mathcal{F}_{n,1}$ is the set of all rooted trees. Let us set $F_{n,k} := |\mathcal{F}_{n,k}|$, and note that $F_{n,k} = \binom{n}{k} T_{n,k}$, with $T_{n,k}$ as in the third proof, since we may choose the k roots in $\binom{n}{k}$ possible ways.

Here is the crucial idea: We count in two ways the number of rooted forests on n vertices that consist of k trees and have one distinguished non-root vertex. This will yield the equality

$$(n-k)\, F_{n,k} \;=\; kn\, F_{n,k+1}. \tag{3}$$

The left side is clear: In every forest $F \in \mathcal{F}_{n,k}$, we may choose any one of the $n-k$ non-root vertices as the distinguished vertex.

For the expression on the right side, consider a forest $F' \in \mathcal{F}_{n,k+1}$. Choose one of the n vertices in F', say v, and attach to it any one of the k trees that do *not* contain v. The root of the chosen tree becomes the distinguished vertex. (This is illustrated in the figure.)

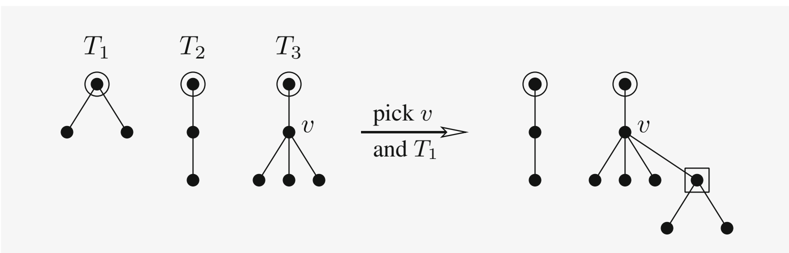


Illustration of the right side of (3).

As there are n choices for v and k choices for the tree that does not contain v, we get $knF_{n,k+1}$ choices altogether. All rooted forests in $\mathcal{F}_{n,k}$ with a distinguished non-root vertex arise uniquely in this process.

Iterating (3) $n-1$ times, we obtain

$$\begin{aligned} F_{n,1} &= \frac{1}{n-1} n\, F_{n,2} \;=\; \frac{1}{n-1}\frac{2}{n-2} n^2\, F_{n,3} \;=\; \cdots \\ &= \frac{1 \cdot 2 \cdots (k-1)}{(n-1)(n-2)\cdots(n-k+1)} n^{k-1}\, F_{n,k} \;=\; \cdots \\ &= \frac{1 \cdot 2 \cdots (n-1)}{(n-1)(n-2)\cdots 1} n^{n-1}\, F_{n,n} \;=\; n^{n-1}\, F_{n,n}. \end{aligned}$$

Since there is only one forest in $\mathcal{F}_{n,n}$ (each root being its own tree), we have $F_{n,n} = 1$ and conclude that $F_{n,1} = n^{n-1}$. □

We get even more out of this proof, namely that

$$F_{n,k} = \binom{n-1}{k-1} n^{n-k} = \binom{n}{k} k n^{n-k-1}.$$

With $F_{n,k} = \binom{n}{k} T_{n,k}$ we have reproved the formula $T_{n,k} = kn^{n-k-1}$ without recourse to induction.

Let us end with a historical note. Cayley's paper from 1889 was anticipated by Carl W. Borchardt (1860), and this fact was acknowledged by Cayley himself. An equivalent result appeared even earlier in a paper of James J. Sylvester (1857), see [3, Chapter 3]. The novelty in Cayley's paper was the use of graph theory terms, and the theorem has been associated with his name ever since.

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