Math 155 (Lecture 8)

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Definition 1. Let G be a graph. A *path* in G is a sequence of vertices $v_0, \ldots, v_n$ such that v_i is adjacent to v_{i-1} for $1 \leq i \leq n$. In this case, we also say $(v_0, \ldots, v_n)$ is a *path from v_0 to v_n*. We say that a path is *simple* if the vertices v_i are disjoint. We say that a simple path $(v_0, \ldots, v_n)$ is a *cycle* if $n \geq 2$ and v_0 is adjacent to v_n.

We say that a graph G is *connected* if every pair of vertices can be connected by a path. We say that G is a *tree* if it is connected and contains no cycles.

The problem we will consider in this lecture is the following:

Question 2. How many trees are there having the set of vertices $\{1, \ldots, n\}$?

The answer turns out to be n^{n-2}. There are many different proofs of this result. In this lecture, we will give a proof using the composition formula for exponential generating functions. First, it is convenient to introduce a slight variation on Question 2.

Question 3. How many ways are there to choose a tree having the set of vertices $\{1, \ldots, n\}$, together with an ordered pair of (possibly identical) vertices of the tree?

It is clear that the answer to Question 3 differs from the answer to Question **??** by a factor of n^2. We will show that the answer to Question 3 is n^n. We already know another counting problem whose answer is n^n: namely, it is the number of maps from the set $\{1, 2, \ldots, n\}$ to itself. To discuss these counting problems in more detail, it is convenient to introduce some species:

Definition 4. Let S_{End} denote the *species of endomorphisms*: for each finite set I, $S_{\mathrm{End}}[I]$ is the set of all maps from I to itself.

We define a species $S_{2-\mathrm{tree}}$ as follows:

- If I is nonempty, then $S_{2-\mathrm{tree}}[I]$ is the collection of all triples (T, i, j) where i and j are elements of I, and T is a tree with vertex set I.
- If $I = \emptyset$, then $S_{2-\mathrm{tree}}[I] = \{*\}$.

We would like to show that for every nonempty finite set I, the sets $S_{\mathrm{End}}[I]$ and $S_{2-\mathrm{tree}}[I]$ have the same number of elements (our ad-hoc definition of $S_{2-\mathrm{tree}}[\emptyset]$ was made to ensure that this is also correct when I is empty). Equivalently, we would like to show that the exponential generating functions of S_{End} and $S_{2-\mathrm{tree}}$ coincide.

Warning 5. The species S_{End} and $S_{2-\mathrm{tree}}$ are *not* isomorphic. For example, when $I = \{1, 2\}$, then the sets $S_{\mathrm{End}}[I]$ and $S_{2-\mathrm{tree}}[I]$ are acted on by the symmetric group Σ_2. This action has no fixed points on $S_{2-\mathrm{tree}}[I]$, but has two fixed points on $S_{\mathrm{End}}[I]$. This is what makes Question 2 interesting: though it has a simple answer, there is no obvious bijective approach.

Let's begin by analyzing the species S_{End}. Suppose that I is a finite set and we are given a map $\pi : I \to I$. What could I look like? It might be a permutation of I. Let S_{perm} denote the species of permutations, so that $S_{\mathrm{perm}}[I]$ is the set of permutations of I. However, there are many maps from I to itself which are not permutations. For example, at the other extreme, there are constant maps from I to itself.

Definition 6. Let π be a map from a finite set I to itself. We will say that π is *nilpotent* if some power of π is a constant map. In other words, π is nilpotent if there exists an element $i \in I$ such that for each $j \in I$, we have $\pi^n(j) = i$ for all sufficiently large n. We let S_{nil} denote the *species of nilpotent endomorphisms*: for every finite set I, we let $S_{\text{nil}}[I]$ denote the set of all nilpotent maps from I to itself.

Remark 7. If $\pi : I \to I$ is a nilpotent map, then there is a unique element $i \in I$ such that $\pi^n(j) = i$ for $n \gg 0$. We will call i the *attractor* of π.

Note that if I has more than one element, then no map $\pi : I \to I$ can be both a permutation and nilpotent (otherwise, some power of π would be a constant permutation). We now show that, in some sense, every map is made out of nilpotent maps and permutations.

Proposition 8. *There is an isomorphism of species* $S_{\text{End}} \simeq S_{\text{perm}} \circ S_{\text{nil}}$.

Proof. Let I be a finite set. By definition, an element of S_{perm} corresponds to the following data:

(a) An equivalence relation $\sim$ on the set I.

(b) A permutation σ of the set $I/\sim$ of equivalence classes.

(c) For each equivalence class $J \subseteq I$, a nilpotent map $\tau_J : J \to J$.

Let us first describe how, given this data, we can construct a map $\pi : I \to I$. Each of the nilpotent maps τ_J has an attractor, which we will denote by i_J. Let $I_0 \subseteq I$ be the collection of all these attractors. The composition $I_0 \to I \to I/\sim$ is a bijection (that is, I_0 contains exactly one element of each equivalence class), so we may regard σ as a permutation of the set I_0. We now set

$$\pi(i) = \begin{cases} \sigma(i) & \text{if } i \in I_0 \\ \tau_J(i) & \text{if } i \in J - \{i_J\}. \end{cases}$$

Conversely, suppose that we start with an arbitrary map $\pi : I \to I$. We will say that an element $i \in I$ is *periodic* if there exists an integer $n > 0$ such that $\pi^n(i) = i$. Let I_0 denote the collection of periodic elements of I. The map π carries periodic elements to periodic elements (note that if $\pi^n(i) = i$, then $\pi^n\pi(i) = \pi^{n+1}(i) = \pi(i)$), and restricts to a permutation on the subset $I_0 \subseteq I$. For each element $i \in I$, the sequence

$$i, \pi(i), \pi^2(i), \ldots$$

must eventually repeat (since I is finite), and therefore contains a periodic element of I. We will denote the first periodic element of the sequence by $r(i)$. The map r determines an equivalence relation on I: let us write $i \sim j$ if $r(i) = r(j)$. Note that each equivalence class contains a unique element of I_0. Let J be an arbitrary equivalence class containing an element $i_J \in I_0$. For each element $j \in I_0$, we have $\pi^n(j) = i_J$ for some integer $n \geq 0$, and $\pi^m(j) \notin I_0$ for $m < n$. If $j \neq i_J$, then $n > 0$, so that $\pi^{n-1}(\pi(j)) = i_J$ (and $\pi^m(\pi_j) \notin I_0$ for $m < n - 1$). It follows that $\pi(j) \in J$, so that π determines a map

$$\tau_J : J - \{i_J\} \to J.$$

This extends to a nilpotent map from J to itself, if we set $\tau_J(i_J) = i_J$. Then the triple $(\sim, \sigma, \{\tau_J\}_{J \in I/\sim})$ is an element of $(S_{\text{perm}} \circ S_{\text{nil}})[I]$.

The above constructions determine maps of species

$$S_{\text{perm}} \circ S_{\text{nil}} \to S_{\text{End}}$$

$$S_{\text{perm}} \circ S_{\text{nil}} \leftarrow S_{\text{End}}.$$

We leave it to the reader as an exercise to show that these maps really are inverse to one another, and therefore determine an isomorphism $S_{\text{perm}} \circ S_{\text{nil}} \simeq S_{\text{End}}$. □

We would now like to relate the above discussion to trees. First, we need a few basic facts from graph theory.

Lemma 9. *Let G be a tree containing vertices v and v'. Then there is a unique simple path $v = v_0, v_1, v_2, \ldots, v_n = v'$ from v to v'.*

Proof. Since G is connected, there is at least one path $v = v_0, v_1, \ldots, v_n = v'$ from v to v'. The number n is called the *length* of the path; let us assume that n has been chosen as small as possible. We claim that this path is automatically simple: if $v_i = v_j$ for $i < j$, then

$$v = v_0, \ldots, v_{i-1}, v_i = v_j, v_{j+1}, \ldots, v_n = v'$$

is a shorter path from v to v'. This proves existence.

Now we prove uniqueness. Choose a path $v = v_0, \ldots, v_n = v'$ of minimal length. We will use induction on n to show that every other simple path $v = w_0, \ldots, w_m = v'$ coincides with $(v_0, \ldots, v_n)$. The case $n = 0$ is trivial: if $v = v'$, then every simple path from v to v' is automatically of length 0 (since the vertices appearing in the path must be distinct).

By assumption, we have $v_n = v' = w_m$. Let i be the smallest positive integer such that $v_i \in \{w_1, \ldots, w_m\}$, and write $v_i = w_j$. Then the sequence

$$v_0, v_1, \ldots, v_i = w_j, w_{j-1}, \ldots, w_1$$

is a simple path from v_0 to w_1. If $i + j > 2$, this is a cycle. We must therefore have $i = j = 1$. This proves that $v_1 = w_1$. We then have two simple paths $(v_1, \ldots, v_n)$ and $(w_1, \ldots, w_m)$ from $v_1 = w_1$ to v', which must coincide by the inductive hypothesis. □

Definition 10. A *rooted tree* is a tree T together with a choice of vertex $r \in T$, called the *root* of T. We let $S_{1-\mathrm{tree}}$ denote the species of rooted trees: for each finite set I, we let $S_{1-\mathrm{tree}}[V]$ denote the set of pairs (r, T), where $r \in V$ and T is a tree with vertex set V.

Proposition 11. *The species $S_{1-\mathrm{tree}}$ and S_{nil} are isomorphic.*

Proof. Let V be a finite set. We will show that there is a canonical bijection between $S_{1-\mathrm{tree}}[V]$ and $S_{\mathrm{nil}}[V]$. First, suppose we are given a tree T with vertex set V and a choice of root r. We define a function $\pi : V \to V$ as follows. For each element $v \neq r$ in V, let $v = v_0, v_1, \ldots, v_n = r$ be the unique simple path from v to the root r. Then we set $\pi(v) = v_1$. If $v = r$, we let $\pi(r) = r$. It is easy to see that the function π is nilpotent (with attractor r).

Conversely, suppose that we are given a nilpotent function $\pi : V \to V$, and let r be the attractor of π. We can make V into a graph by declaring that a pair of distinct vertices v and w are adjacent if either $v = \pi(w)$ or $w = \pi(v)$. We claim that this graph is always a tree. To prove this, suppose we are given a cycle

$$v_0, v_1, \ldots, v_n.$$

For $1 \leq i \leq n$, we have either $v_i = \pi(v_{i-1})$ or $\pi(v_i) = v_{i-1}$. Note that in the second case, since $v_{i+1} \neq v_{i-1}$, we must also have $\pi(v_{i+1}) = v_i$. It follows that the path is given by

$$v_0, \pi(v_0), \pi^2(v_0), \ldots, \pi^p(v_0) = w_0, w_1, w_2, \ldots, w_q$$

where $p + q = n$ and the sequence $\{w_i\}$ satisfies $\pi(w_i) = w_{i-1}$. If the path is a cycle, then either $\pi(v_0) = w_q$ or $\pi(w_q) = v_0$. In the first case, we must have $p = 0$ (otherwise $v_1 = v_n$), so that $\pi^{q+1} w_q = w_q$, which implies that $w_q = r$ and therefore $q = 0$, a contradiction. In the second case we must have $q = 0$ (otherwise $v_0 = v_{n-1}$) in which case we have $\pi^{p+1} v_0 = v_0$, which implies that $v_0 = r$ so that $p = 0$, again a contradiction.

We again leave it to the reader to show that these constructions are inverse to one another, and give an isomorphism of species $S_{1-\mathrm{tree}} \simeq S_{\mathrm{nil}}$. □

Combining Propositions 8 and 11, we get an isomorphism of species

$$S_{\text{End}} \simeq S_{\text{perm}} \circ S_{1-\text{tree}}.$$

To complete our analysis, we will need the following analogous fact:

Proposition 12. *Let S_{lin} denote the species of linear orderings. There is an isomorphism of species $S_{2-\text{tree}} \simeq S_{\text{lin}} \circ S_{1-\text{tree}}$.*

Assuming Proposition 12 for the moment and using the composition formula, we obtain

$$F_{S_{\text{End}}}(x) = F_{S_{\text{perm}}}(F_{S_{1-\text{tree}}}(x))$$
$$F_{S_{2-\text{tree}}}(x) = F_{S_{\text{lin}}}(F_{S_{1-\text{tree}}}(x)).$$

We have already seen that, although the species S_{perm} and S_{lin} are different, they have the same exponential generating function $\sum_{n\geq 0} \frac{n!}{n!}x^n = \frac{1}{1-x}$. We therefore obtain

$$F_{S_{\text{End}}}(x) = \frac{1}{1 - F_{S_{1-\text{tree}}}(x)} = F_{S_{2-\text{tree}}}(x).$$

This proves that the number of elements of $S_{2-\text{tree}}[I]$ is the same as the number of elements of $S_{\text{End}}[I]$ for every finite set I, thereby giving n^{n-2} as the answer to Question 2.

Let us now prove Proposition 12. For each finite set V, we must construct a bijection from the set $S_{2-\text{tree}}[V]$ to the set $(S_{\text{lin}} \circ S_{1-\text{tree}})[V]$. It is clear what to do if V is empty (in that case, both sides have one element). Let us therefore assume that V is nonempty, so that an element of $S_{2-\text{tree}}[V]$ corresponds to a triple (T, v, v'), where T is a tree with vertex set V, and $v, v' \in V$ are elements. To this, we wish to associate the following data:

(a) An equivalence relation $\sim$ on the set V.

(b) A linear ordering of the set of equivalence classes $V/\sim$.

(c) For each equivalence class $W \subseteq V$, a rooted tree with vertex set W.

We first invoke Lemma 9: since T is a tree, there is a unique simple path

$$v = v_0, v_1, \ldots, v_n = v'$$

from v to v'. Let $V_0 = \{v_0, \ldots, v_n\}$ be the set of vertices along this path. For any vertex $w \in V$, there exists a simple path $w = w_0, \ldots, w_m$ which ends in a vertex w_m which belongs to V_0. In fact, we can assume that $w_i \notin V_0$ for $i < m$ (otherwise, end the path at w_i instead). In this case, we claim that the path $w_0, \ldots, w_m$ is unique. Suppose otherwise: that is, suppose that we have another simple path $w = w'_0, w'_1, \ldots, w'_{m'}$ with $w'_{m'} \in V_0$ and $w'_j \notin V_0$ for $j < m'$. If $w'_{m'} = w_m$, this contradicts Lemma 9. Otherwise, we may suppose that $w_m = v_i$ and $w'_{m'} = v_j$ for $i < j$. Let k be the largest integer such that w_k appears in the path $w'_0, \ldots, w'_{m'}$ (such an integer exists, since $w_0 = w = w'_0$). Writing $w_k = w'_{k'}$, we obtain a cycle $w_k, w_{k+1}, \ldots, w_m = v_i, v_{i+1}, \ldots, v_j = w'_{m'}, w'_{m'-1}, \ldots, w'_{k'+1}$, contradicting our assumption that T is a tree.

For each $w \in V$, let $\tau(w) \in V_0$ be the endpoint of the unique path constructed above. Let us define an equivalence relation on V by writing $w \sim w'$ if $\tau(w) = \tau(w')$. Then the composition $V_0 \to V \to V/\sim$ is a bijection: that is, V_0 contains a unique element of each equivalence class. Writing $V_0 = \{v_0, v_1, \ldots, v_n\}$, we obtain a linear ordering on the set $V/\sim$. Each equivalence class $W \in V/\sim$ has the form $\tau^{-1}\{v_i\}$ for some $0 \leq i \leq n$. Note that if $w \in \tau^{-1}v_i$, there is a simple path $w = w_0, \ldots, w_m = v_i$ from w to v_i which contains no other vertex of V_0. Each of the paths $w_j, w_{j+1}, \ldots, w_m$ has the same property, so that $\tau(w_j) = v_i$ for $0 \leq j \leq m$. It follows that w can be connected to v_i by a path lying entirely in W, so that W determines a connected subgraph of T. This subgraph cannot contain any cycles (since T does not contain any cycles) and is therefore a tree (which has a natural choice of root, given by the vertex $v_i \in V_0$).

We leave it to the reader to verify that this construction determines a bijection of $S_{2-\text{tree}}[V]$ with $(S_{\text{lin}} \circ S_{1-\text{tree}})[V]$ (if it is not clear, try drawing a picture for yourself).