Combinatorial Species and a Proof of the Lagrange Inversion Formula

By Adrian Fry

Mentored By Saud Molaib

Abstract

The theory of Combinatorial species allows us to derive the generating functions of discrete structures. By characterizing these objects as mappings which take sets to sets with structure (ex. binary-trees or linear orderings), we are able to find the generating functions for those discrete structures. We can then perform operations on these combinatorial species, which correspond naturally to operations on generating functions.

I will show how this theory can be used to prove the Lagrange Inversion Formula, a fundamental result in complex analysis.

1 Generating Functions

1.1 Ordinary Generating Functions

Definition 1.1. For a sequence (a_n) , an ordinary generating function is a representation of the sequence as the coefficients in a formal power series

$$\sum a_n x^n$$

So the ith term in the sequence is the coefficient of the x^i term in the power series.

"A generating function is a clothesline on which we hang up a sequence of numbers for display."

- Herbert Wilf, Generatingfunctionology"

This representation of a sequence of numbers can prove especially useful when we are trying to count something.

Example 1.2. How many ways can we make 11 cents using pennies, nickels, dimes, and quarters?

- 1. To start off, let's try to determine what the generating function for each coin is.
 - a) The generating function for pennies is $\sum_{i=0}^{\infty} x^i$, since there is only 1 way to make n cents using pennies.
 - **b)** For nickels, it's $1 + x^5 + x^{10} + x^{15} + \cdots$

- c) For dimes, $1 + x^{10} + x^{20} + x^{30} + \cdots$
- **d)** For guarters, $1 + x^{25} + x^{50} + x^{75} + \cdots$

The *i*th term of each function is the number of cents we want to make using that coin (so when i = 0, we want to choose zero quarters)

- 2. How do we use these generating functions to solve the problem? Notice that when we multiply these generating functions together, the coefficient of the x^{11} term is the number of ways to get to 11 using these coins.
- 3. So we have

$$(1+x+x^2+\cdots)(1+x^5+x^{10}+\cdots)(1+x^{10}+\cdots)(1+x^{25}+\cdots)$$

= 1+x+x^2+x^3+x^4+2x^5+2x^6+2x^7+2x^8+2x^9+4x^{10}+4x^{11}+\cdots

So there are 4 ways to get 11 cents.

One can see how this can get unwieldy pretty quickly, but luckily, many power series have closed form solutions, e.g. $\sum x^n = \frac{1}{1-x}$. More important to the scope of this project, is to remember that generating functions are useful tools to count things, and that it is valuable to be able to find the generating functions of simple combinatorial objects if we want to count more complicated ones.

1.2 Exponential Generating Functions

Definition 1.3. An **exponential generating function** is a representation of a sequence (b_n) as the coefficients in a formal power series

$$\sum b_n \frac{x^n}{n!}$$

These are very similar to ordinary generating functions. Consider

$$\sum \frac{x^n}{n!}$$

This is an ordinary generating function. It is also an exponential generating function for a sequence of 1s. Exponential generating functions are used because it can be easier to do operations with them, and they can be more likely to converge.

Proposition 1.4 (Multiplication of Exponential Generating Functions.). Given two sequences (a_n) , (b_n) with corresponding exponential generating functions f, g respectively, the coefficients of fg are

$$h_n = \sum_r \binom{n}{r} a_n b_{n-r}$$

Lets look at an example where it serves us to use exponential generating functions.

Example 1.5 (Derangements). A derangement is a permutation with no fixed elements. Let

 D_n be the number of derangements of n letters, and

$$D(x) = \sum D_n \frac{x^n}{n!}$$

. The number of derangements with a specific set of k fixed points is D_{n-k} . There are $\binom{n}{k}$ ways to pick this set of fixed points, so there are $\binom{n}{k}D_{n-k}$ derangements with k points. Every permutation is a a permutation with $k \geq 0$ fixed points, so

$$\sum_{k} \binom{n}{k} D_{n-k} = n!$$

Taking the exponential generating functions of both sides, we have by proposition 1.4

$$\left(\sum \frac{x^n}{n!}\right) \left(D_n \frac{x^n}{n!}\right) = \sum x^n$$

. These all have closed form solutions, so we have

$$e^x D(x) = \frac{1}{1-x}$$

SO

$$D(x) = \frac{1}{e^x(1-x)}$$

Clearly, exponential generating series are valuable in their own right, and as we will see, expanding on the concept of performing operations on these generating series (we multiplied generating functions in the example above) leads to many interesting results.

2 Species of Structures

The theory of combinatorial species is a method for deriving generating functions of **discrete structures**.

Definition 2.1. A structure is a **construction** γ which is performed on a set U. It consists of a pair $s = (\gamma, U)$. U is called the **underlying set** of s.

Example 2.2. Below is a simple graph *G*



We can describe G as

$$(\gamma, U) = (\{\{a,b\}, \{a,d\}, \{b,c\}, \{b,d\}\}, \{a,b,c,d\})$$

How is the above structure related to this graph F below?



The underlying set of G is $U=\{a,b,c,d\}$. Replace the elements of U with the elements of $V=\{1,2,3,4\}$ through the bijection $\sigma:U\to V$ for which $a\mapsto 1,b\mapsto 2,c\mapsto 3,d\mapsto 4$. We say that

$$G = \sigma \cdot U$$

.

If we ignore the elements of the underlying sets, G and F are the same. We call these structures **isomorphic**¹.

Remark 2.3. Notice that if we apply the permutation τ with cycle notation (ad), then $\tau \cdot G = G$

Definition 2.4. A species is a functor \mathcal{F} from the category of FINSET with bijections to itself. If you don't know category theory, just think of it as a rule \mathcal{F} such that.

- For any set U, there is a finite set $\mathcal{F}[U]$ (the set of \mathcal{F} -structures on U).
- For any bijection $\sigma: U \to V$, there is a function $\mathcal{F}[\sigma]: \mathcal{F}[U] \to \mathcal{F}[V]$

and it satisfies the (functorial) properties

- $\sigma: U \to V$ and $\tau: V \to W$ implies $\mathcal{F}[\tau \circ \sigma] = \mathcal{F}[\tau] \circ \mathcal{F}[\sigma]$
- For the identity map $\operatorname{Id}_U:U o U$, $\mathcal{F}[\operatorname{Id}_U]=\operatorname{Id}_{\mathcal{F}[U]}$

An element $s \in F[U]$ is called an F-Structure on U.

To clarify this concept, here are some examples.

Example 2.5. Here are some examples of species, along with some information about their corresponding structures and bijections.

- Species of linear orderings \mathcal{L}
 - The construction of a \mathcal{L} -structure on the set [n] is some total order on it's elements, i.e.

$$1 < 2 < \cdots < n$$

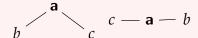
- There is a bijection from the induced total order on [n] by $\mathbb N$ to any other order on this set.
- The set $\mathcal{L}[3]$ has six elements

¹And say that other isomorphic structures have the same isomorphism type

- Species of rooted trees \mathcal{A}
 - The construction of a A-structure on the set [n] with a root i is the ordered pair $\{i\}$, followed by a construction of a graph as described in example 2.2, where the graph is connected and contains no cycles.
 - There are three rooted trees on [3].
- ullet Species of permutations ${\cal S}$
 - The construction of a S-structure on the set [n] is an element of S_n , the symmetric group. In particular, an element of this species is a group action.
 - $-((1\ 3\ 2)(5\ 4),[5])$ and $((3\ 2\ 1)(5\ 4),[5])$ are the same structure on [5].
 - Applying a permutation σ on a finite set U corresponds to the function $\mathrm{Id}_{\mathcal{S}[U]}$, since permutations are bijections from a set to itself.

Warning 2.6

Depictions of (rooted) trees can be suggestive, yet these



are the same structure.

2.1 A rigorous description of an Octopus

An octopus is drawn in figure 10.

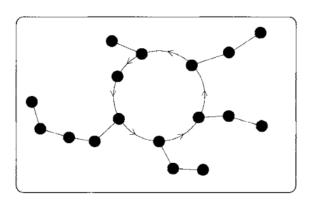


Fig. 10. An octopus.

The set of Octopuses on a set U, where the tentacles are trees is described as follows:

$$Oct[U] = \{((P, S, c), U) \mid P \in Par[U], S = \{A(p) \mid p \in Par[U]\}, c \in (Cyc(S))\}$$

But if instead the tentacles are just non-oriented chains, we have the following description:

$$Oct[U] = \{((P, S, c), U) \mid P \in Par[U], S = \{Cha(p) \mid p \in Par[U]\}, c \in (Cyc(S))\}$$

3 Series

We can now associate to each species of structures an exponential generating function.

Definition 3.1. The generating series of a species of structures \mathcal{F} a formal power series

$$\mathcal{F}(x) = \sum_{n=0}^{\infty} f_n \frac{x^n}{n!}$$

with f_n the number of \mathcal{F} -structures on [n].

Example 3.2 (Permutations vs. Linear Orderings). How many permutations are there on a set of n elements? The first element can go to n different places, the second has n-1 choices, and so on, so we get

$$S(x) = \sum_{n=0}^{\infty} n! \frac{x^n}{n!} = \frac{1}{1-x}$$

How many linear orderings are there on a set of n elements? There are n choices for the smallest element, n-1 for the second smallest, and so on and so similarly,

$$\mathcal{L}(x+=\sum_{n=0}^{\infty}n!\frac{x^n}{n!}=\frac{1}{1-x}$$

Example 3.3. The exponential generating series for X the species of singletons is

$$X(x) = 0 + x + 0 + \cdots$$

3.1 Cycle index series

Recall that if we ignore the elements of the underlying sets, two \mathcal{F} -structures are isomorphic if we can pass from one construction to the other by a bijection of the underlying sets. Say we want to find the number of isomorphism types of a structure.

Definition 3.4 (Equivalence class of isomorphism type). We define an equivalence relation \sim , where for any $s,t\in\mathcal{F}[n],\,s\sim t$ if there exists a permutation $\pi:[n]\to[n]$ such that $\mathcal{F}[\pi](s)=t$.

Each equivalence class of \mathcal{F} -structures of order n is an unlabeled \mathcal{F} -structures of order n.

Definition 3.5. The type generating series of a species \mathcal{F} is the formal power series

$$\tilde{\mathcal{F}}(x) = \sum \tilde{f}_n x^n$$

where $ilde{f_n}$ is the number of unlabeled $\mathcal{F} ext{-structures}$ of order n.

Note that the set of isomorphism types is the set of orbits of $\mathcal{F}[n]$ when acted on naturally by S_n , i.e., the orbits of

$$S_n \times \mathcal{F}[n] \to \mathcal{F}[n]$$

Calculating the type generating series of a species is difficult, since it requires the use of the **cycle index series**. This is a formal power series which holds more information than the generating series or the type generating series.

Definition 3.6. The cycle index series of a species \mathcal{F} is the formal power series

$$Z_{\mathcal{F}}(x_1, x_2, x_3, \dots) = \sum_{n \geq 0} \frac{1}{n!} \Big(\sum_{\sigma \in \mathcal{S}_n} |\{u \in U \mid \sigma(u) = u\} | x_1^{\sigma_1} x_2^{\sigma_2} x_3^{\sigma_3} \dots \Big)$$

where S_n is the group of permutation of [n] and the cardinality of $\{u \in U \mid \sigma(u) = u\}$ is the number of \mathcal{F} -structures on [n] for which σ is an automorphism.

This series is only reasonable to calculate with computers. It's value to us, however, comes in the form of the following theorem.

Theorem 3.7.

$$\mathcal{F}(x) = Z_{\mathcal{F}}(x, 0, 0, \dots)$$

$$\tilde{\mathcal{F}}(x) = Z_{\mathcal{F}}(x, x^2, x^3, \dots)$$

Exercise 3.1. In example 3.2, we showed that the species of linear orderings and the species of permutations have the same generating series. Calculate the cycle index series and the type generating series of the first few terms of S and L.

Once you calculate these, if you plug in values of x_1, x_2, \ldots as given in Theorem 3.7, you will obtain the generating and type generating series for permutations and linear orderings.

4 Operations

Finally, we get to the most important part: we can perform operations on species in order to construct new species.

Definition 4.1 (Sum of Species). We aim to define the number of $\mathcal{F} + \mathcal{G}$ structures on n elements such that the resulting generating functions is the sum of the series $\mathcal{F}(x) + \mathcal{G}(x)$. Then we say

$$(\mathcal{F} + \mathcal{G})[U] = \mathcal{F}[U] + \mathcal{G}[U]$$

So a $(\mathcal{F}+\mathcal{G})$ -structure on U is either a \mathcal{F} -structure or a \mathcal{G} -structure on U.

Example 4.2. As an example, consider the species of k-element sets E_k . E_k maps U to \emptyset unless |U| = k. It's generating series is

$$E_k(x) = 0 + \dots + 0 + \frac{x^k}{k!} + 0 + \dots$$

Then the sum

$$\sum E_k = E$$

where E is the species of sets, with $E[U] = \{U\}$, the singleton set containing U.

A permutation of a set U can be decomposed into all the elements that are invariant and all the elements which aren't, that is, those which are a derangement.

Definition 4.3 (Multiplication of species). When we multiply two species, the resulting species $F \cdot G$ is defined as follows

$$(F \cdot G)[U] := \sum_{\substack{U_1, U_2:\ U_1 \cap U_2 = \emptyset \ U_1 \cup U_2 = U}} F[U_1] \times G[U_2]$$

This counts the number of \mathcal{F} -structures times the number of \mathcal{G} -structures on all pairs of subsets which partition U into two parts.

So a permutation can be defined as

$$\mathcal{S} = E \cdot \mathsf{Der}$$

where E denotes the species of sets, defined as $E[U] = \{U\}^2$

Example 4.4. Consider the product $(\mathcal{L} \cdot \mathcal{L})[n]$. The associated series is is

$$(\mathcal{L} \cdot \mathcal{L})[n] = \sum_{n \in \mathbb{Z}_{>0}} \sum_{i=0}^{n} i!(n-i)! \frac{x^n}{n!}$$

We imagine a resultant \mathcal{L}^2 -structure as dividing the set in two and giving each subset a linear order.

A classroom where the boys and girls are each organized by age is one such structure.

Proposition 4.5. The number of E^k -structures is

$$E^k[n] = k^n$$

Corollary 4.6. The species \wp of subsets is the product $(E \cdot E)$.

Proof.

$$E^{2}[n] = 2^{n}$$
$$= \wp[n]$$

This means the generating series

$$\wp(x) = (E \cdot E)(x)$$

$$= \sum_{n=1}^{\infty} \frac{x^n}{n!} \cdot \sum_{n=1}^{\infty} \frac{x^n}{n!}$$

$$= e^x \cdot e^x$$

$$= e^{2x}$$

²Note that this isn't the set U, but rather the singleton set containing the set U.

Definition 4.7 (Composition of species). Consider two species \mathcal{F}, \mathcal{G} . An $\mathcal{F} \circ \mathcal{G}$ structure on U is an \mathcal{F} -structure on some partition π of U, with a \mathcal{G} structure on each $p \in \pi$. The composition of structures is defined by

$$(\mathcal{F}\circ\mathcal{G})[U]\coloneqq\sum_{\pi(U)}\mathcal{F}[\pi] imes\prod_{p\in\pi}\mathcal{G}[p]$$

with π a partition of U.

This corresponds to composition of generating functions, that is, $\mathcal{F}[\mathcal{G}[U]]$.

Example 4.8. The species $Oct[U] = C(A)[U] = -\log(1 - A_+)$, where C is the species of cycles, and A_+ is the species of nonempty rooted trees. See how much simpler this definition of an octopus is compared to earlier?

So we can see how knowing some "basic" structures³ can allow us to define more complicated ones.

The derivative of an exponential generating function $F(x) = \sum b_n \frac{x^n}{n!}$ is

$$\sum b_{n+1} \frac{x^n}{n!}$$

Definition 4.9 (Derivative). An \mathcal{F}' -structure on a set U is an \mathcal{F} structure on $U \cup \{*\}$, where $\{*\}$ is an element outside of U.

$$F'[U] = F[U \cup \{*\}]$$

As it turns out, these structures can have unexpected relationships using the derivative.

Example 4.10. $C' = \mathcal{L}$. A C'-structure on some set U is a cycle on $U \cup \{*\}$. Of course, $\{*\}$ is not an actual element of C, so we imagine this cycle with a "hole". But that's just a linear ordering.

While we have so far searched for operations on species by performing operations on generating functions, we can also come up with operations on species and then understand what they correspond to on generating functions. One example of this concept is the operation of **pointing**.

Definition 4.11 (Pointing). Pointing distinguishes an element of a species. It corresponds to the operation $x \frac{d}{dx}$, i.e.,

$$x\frac{d}{dx}\sum f_n\frac{x^n}{n!}=\sum f_n\frac{x^n}{(n-1)!}$$

Let ${\mathcal F}$ be a species of structures. An ${\mathcal F}^{ullet}$ -structure on U is the pair (f,u), where f is an

^aA canonical way to find $\{*\}$ is to let $\{*\} = \{U\}$, since a set can't contain itself.

 $^{^3}$ If you define octopuses with their tentacles as linear orders instead of rooted trees, you get $\mathcal{C}\circ\mathcal{L}_+$

 \mathcal{F} -structure on U, and u is an element of U. So

$$\mathcal{F}^{\bullet}[U] = \mathcal{F}[U] \times U$$

and for some
$$\sigma:U\to V$$
,
$$\mathcal{F}^{ullet}[\sigma](s)=(F[\sigma](f),\sigma(u))$$

where s is an \mathcal{F}^{\bullet} structure s=(f,u) on U.

Example 4.12. A an structure in the species of pointed trees is a rooted tree.

Lagrange Inversion Formula 5

Theorem 5.1 (Lagrange Inversion Formula). Let f be a formal power series. Assume f(0) = $0, f'(0) \neq 0$. Let $f^{(-1)}$ denote the composition inverse of f, that is, $f^{(-1)} \circ f = f \circ f^{(-1)} = f \circ f^{(-1)}$ z. One can write explicitly the coefficients of the inverse formal power series $f^{(-1)}(z)$ of

$$f^{-1}(z) = \sum_{n \ge 1} \left(\frac{d}{dt}\right)^{n-1} \left(\frac{t}{f(t)}\right)^n \Big|_{t=0} \frac{z^n}{n!}$$

Proof. We want to interpret this as combinatorial species, so first we want a situation in which we are applying operations to species. We see this $\frac{t}{f(t)}$ term, which isn't an operation we can apply to species, so we want to get rid of it. Towards this goal, let A(z) denote $f^{(-1)}(z)$ and set

 $R(z) = \frac{z}{f(z)}$

. Then

$$R(A(z)) = \frac{A(z)}{f(A(z))}$$

$$= \frac{A(z)}{z}$$

$$\implies zR(A(z)) = A(z)$$

We can now rewrite the Lagrange inversion formula as

$$A(z) = \sum_{n>1} a_n \frac{z^n}{n!} \tag{1}$$

where

$$a_n = \left(\frac{d}{dt}\right)^{n-1} R(t)^n \Big|_{t=0} \tag{2}$$

We will show that when R is a species, we can construct a species A such that

$$A = X \cdot R(A)$$
.

We see from the functional equation that the species A is recursively defined. More specifically, a A structure on a set U is obtained choosing an element of U and forming R-assembly of A structures on the rest of the elements. This suggests some sort of tree-like structure rooted at the chosen element, and inspires the following definition:

^aThere are n choices for u

Definition 5.2 (R-enriched rooted tree). An R-enriched rooted tree on a finite set U is

- 1. An arbitrary rooted tree α on U
- 2. An R-structure on the set of "children" of u for each vertex $u \in U$ in this rooted tree.

The leaves of the tree are the vertices who have no children. This means there are not 0 R-structures on the empty set, that is, $R(0) \neq 0$. The species of R-enriched rooted trees is denoted \mathcal{A}_R .

Thus, to prove the Lagrange inversion formula, it suffices to show that the generating series of \mathcal{A}_R is indeed (1), which means the number of \mathcal{A}_R structures on a set with n elements is given by (2), but with the corresponding operations on species. Remember that the number of F'-structures on a set with n elements is |F[n-1]|, so

$$|\mathcal{A}_R[n]| = |R^n[n-1]| \tag{3}$$

Definition 5.3 (R-enriched endofunctions). An R-enriched endofunction on a finite set U consists of

- 1. A function $s: U \to U$
- 2. An R-structure on $s^{-1}(u)$

An R-enriched partial endofunction replaces the condition 1. with

1. A function $s: V \to U$ with $V \subseteq U$

The species of R-enriched endofunctions is denoted End_R , and the species of R-enriched partial endofunctions is denoted End_R^\wp

Lemma 5.4. The number of R-enriched partial endofunctions with domain of size k is the same as the number of R^n -structures on a set of size k, that is,

$$|\{f \in \operatorname{End}_R^{\wp} \mid |\operatorname{dom}(f)| = k\}| = |R^n[k]|$$

WLOG, assume $V=[k]\subset U=[n].$ $f:V\to U$ is determined by a family $\{\xi_i\}_{i\in[n]}$, where

$$\xi_a \in R[f^{-1}(a)]$$

So ξ_i is an R-structure on $U_i = f^{-1}(i)$ corresponding to an R-structure on the fibers of i where $\bigcup_{i \in [n]} U_i = V$. This family $(\xi_1, \ldots, \xi_u) \in R^n[k]$. So there is a bijection between these sets.

Corollary 5.5.

$$|\mathcal{A}_R \cdot \mathsf{End}_R[n]| = n \cdot |R^n[n-1]|$$

Let |U|=n, and choose a root $u_0\in U$. Notice that an $\mathcal{A}_R\cdot \mathsf{End}_R$ -structure on U is an R-enriched partial endofunction from

$$U\setminus\{u_0\}\to U$$

So we have

$$\begin{aligned} |\mathcal{A}_R \cdot \mathsf{End}_R[n]| &= n \cdot |\{f \in \mathsf{End}_R^{\wp} \mid \mathsf{dom}(f) = U \setminus \{u_0\}\}\}| \\ &= n \cdot |R^n[n-1]| \end{aligned}$$

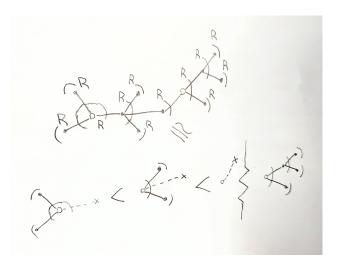
$$A_R^{\bullet} \cong \mathcal{L}(X \cdot R'(\mathcal{A}_R)) \cdot \mathcal{A}_R$$

An A_R^{\bullet} -structure is an A_R -structure with one element e distinguished.

Remark 5.7. Remember that each node (besides the root) in an *R*-enriched rooted tree has a parent. This means we can canonically give this tree direction, where each edge points to the parent-vertex in the parent-child relationship it represents. That is, each edge in the tree points to the root.

Take the shortest path L between the root and e. Since we are dealing with a tree, there are no cycles and this path is unique. Note that this path can just be a single vertex. By the remark above, this path has a direction, where e is the beginning and the root is the end.

For each vertex v on this path, we have an R-enriched rooted tree T_v where the root is said vertex, by excluding the edges in L. As in the diagram below, each of the vertices in L has an R-structure on its children vertices, which is one extra element than its children in T_v (except for the vertex e). But this is just an R'-structure an its child nodes. Recalling the recursive definition of $A_R = X \cdot R(A_R)$, we have for each vertex $v \in L \setminus \{e\}$ a $X \cdot R'(A_R)$ -structure T'_v .



These T_v' s have an induced linear ordering were $T_a' < T_b'$ if b is a descendant of a. Finally, the remaining tree rooted at e is just an R-enriched rooted tree on the rest of the elements, so we have that A_R^{\bullet} is isomorphic to

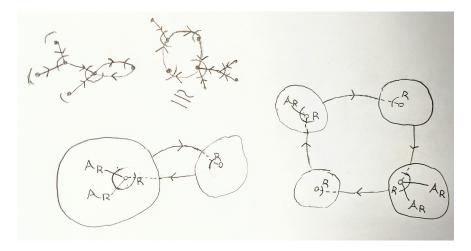
$$\mathcal{L}(X \cdot R'(\mathcal{A}_R)) \cdot \mathcal{A}_R$$

Lemma 5.8.

$$|\mathcal{S}(X \cdot R'(A_R))[n]| = |\mathsf{End}_R[n]|$$

By the same logic as above, we can decompose an R-enriched endofunction into $X \cdot R'(\mathcal{A}_R)$ -structures, but in this case they are ordered according to a permutation induced by the cycles in

the endofunction.



And we know the species of linear orderings has the same number of elements as the species of permutations, so this means

$$\begin{aligned} |\mathcal{A}_{R}^{\bullet}[n]| &= |\mathcal{S}(X \cdot R'(A_{R})) \cdot \mathcal{A}_{R}[n]| \\ &= |\mathcal{L}(X \cdot R'(A_{R})) \cdot \mathcal{A}_{R}[n]| \\ &= |\mathcal{A}_{R} \cdot \mathsf{End}_{R}[n]| \end{aligned}$$

Putting this all together, we have that

$$n \cdot |R^n[n-1]| = |\mathcal{A}_R \cdot \mathsf{End}_R[n]|$$
 (Corollary 6.5)
= $|\mathcal{A}_R^{ullet}[n]|$ (Lemma 6.6)
= $n \cdot |\mathcal{A}_R[n]|$

Then

$$|R^n[n-1]| = |\mathcal{A}_R[n]|$$

Which is exactly equation (3), so we're done.

6 References

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