

# Applications of Analytic Combinatorics to the Analysis of Algorithms: An Introduction

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# What is this course about?

**Analytic Combinatorics** seeks to develop mathematical techniques that help us to count combinatorial structures with given properties.

This is a shared goal with **Combinatorics** at large; results in this particular subfield have proved immensely useful and fruitful in many applications, e. g., **Analysis of Algorithms**, **Analytic Number Theory**, **Enumerative Combinatorics**, . . .

# What is this course about?

The key concept is that of **generating function**: Analytic Combinatorics exploits GFs both as formal power series (algebra, combinatorics) and as analytic functions on the complex plane (analysis).

# Outline of the course

Part I: Combinatorial methods

Part II: Complex analysis techniques

Part III: Applications

# Outline of the course

Part I: Combinatorial methods + Applications

Part II: Complex analysis techniques + Applications

# What is this course about?

It's probably better to understand what is this course about by looking at a few problems that we can tackle using AC . . .

## Some examples: Example #1

- A **derangement** is a permutation without fixed points, that is,  $\sigma$  is a derangement iff  $\sigma(i) \neq i$  for all  $i$
- To randomly generate a derangement, generate a random permutation and check if it is a derangement; if not, discard and repeat (**rejection method**)
- Can we generate derangements uniformly at random better? How?
- What's the average number of times we have to produce a random permutation before we get a derangement?
- How many derangements of size  $n$  there are?

## Some examples: Example #2

Ensure:  $n > 0$

```
procedure Maximum( $A, n$ )  
   $max \leftarrow A[1]$   
  for  $i \leftarrow 2$  to  $n$  do  
    if  $A[i] > max$  then  
       $max \leftarrow A[i]$   
    end if  
  end for  
  return  $max$   
end procedure
```

How many times do we update  $max$ ? The worst- and best-case scenarios are easy, but what happens **on average**?

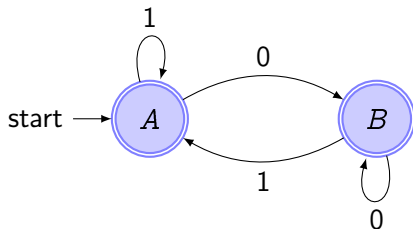


## Some examples: Example #3

- Modern hardware executes instructions in a pipeline fashion; in order to avoid getting stalled at conditional jumps, it tries to guess the most likely outcome of the condition
- But if the prediction is wrong (**branch misprediction**), it is costly to roll back
- Simple predictors can be modeled using finite automata

## Some examples: Example #3

- For example, in 1-bit prediction we have two states:



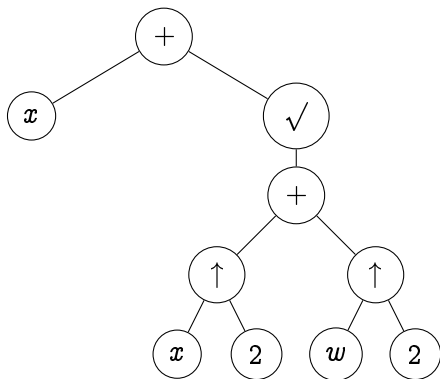
- In state A, we predict branch will be **taken**; if it is actually taken we remain there, if not we “pay” a branch misprediction and move to state B
- In state B we predict **not taken**; if not taken we remain there, else we “pay” and change to state A

## Some examples: Example #3

- Given a sequence of bits (0 = taken, 1 = not taken) of length  $n$  with exactly  $t$  0's, what's the probability of exactly  $r$  mispredictions? What's the average number of mispredictions?

## Some examples: Example #4

- Mathematical expressions such as  $x + \sqrt{x^2 + w^2}$  can be conveniently represented by trees



## Some examples: Example #4

- What is the complexity of performing several symbolic manipulations on them, say, derivatives?
- Many symbolic operations are easy to analyze as they involve traversal of the tree, with simple computations at each node  
 $\implies \Theta(n)$  cost
- Many interesting computations do not traverse all the tree, and the computation to be done at each node depends on the size of the subtree beneath

## Some examples: Example #5

The expected cost of a partial match in  $s$  dimensions in relaxed  $K$ -d trees (a data structure to store  $K$ -dimensional points) satisfies the following recurrence

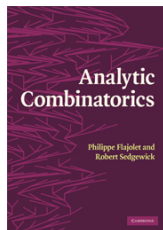
$$P_n = 1 + \frac{s}{K} \frac{2}{n} \sum_{0 \leq k < n} \frac{k}{n} P_k + \left(1 - \frac{s}{K}\right) \frac{2}{n} \sum_{0 \leq k < K} P_k,$$

where  $0 < s < K$ .

The goal is to find an asymptotic estimate of  $P_n$ . An elementary proof yields  $P_n = O(n)$ , but more precise information would be needed.

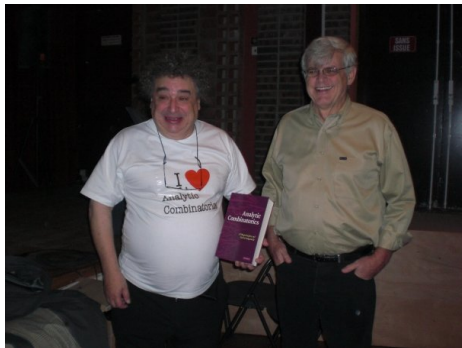
# What is this course about?

There are many excellent papers, surveys, books, etc. on the subject. However, the most authoritative work is the recent *Analytic Combinatorics* by Philippe Flajolet and Robert Sedgewick, two researchers who have made fundamental contributions to the field and have actually “shaped” it.



P. Flajolet, R. Sedgewick: *Analytic Combinatorics*. Cambridge Univ. Press, 2008. It is freely downloadable from <http://algo.inria.fr/flajolet/Publications/AnaCombi/anacomb>

## Philippe Flajolet: In memoriam



Philippe Flajolet (December 1st, 1948–March, 22nd, 2011) and Robert Sedgewick during the presentation of their book *Analytic Combinatorics* on the occasion of Flajolet's 60th Anniversary in Paris, December 2008



# Combinatorial Methods

# Two basic counting principles

Let  $\mathcal{A}$  and  $\mathcal{B}$  be two finite sets.

## The Addition Principle

If  $\mathcal{A}$  and  $\mathcal{B}$  are disjoint then

$$|\mathcal{A} \cup \mathcal{B}| = |\mathcal{A}| + |\mathcal{B}|$$

## The Multiplication Principle

$$|\mathcal{A} \times \mathcal{B}| = |\mathcal{A}| \times |\mathcal{B}|$$

## Definition

A **combinatorial class** is a pair  $(\mathcal{A}, |\cdot|)$ , where  $\mathcal{A}$  is a finite or denumerable set of values (combinatorial objects, combinatorial structures),  $|\cdot| : \mathcal{A} \rightarrow \mathbb{N}$  is the **size** function and for all  $n \geq 0$

$$\mathcal{A}_n = \{x \in \mathcal{A} \mid |x| = n\} \quad \text{is finite}$$

## Example

- $\mathcal{A}$  = all finite strings from a binary alphabet;  
 $|s|$  = the length of string  $s$
- $\mathcal{B}$  = the set of all permutations;  
 $|\sigma|$  = the order of the permutation  $\sigma$
- $\mathcal{C}_n$  = the partitions of the integer  $n$ ;  $|p| = n$  if  $p \in \mathcal{C}_n$

# Labelled and unlabelled classes

- In **unlabelled** classes, objects are made up of indistinguishable **atoms**; an atom is an object of size 1
- In **labelled** classes, objects are made up of distinguishable atoms; in an object of size  $n$ , each of its  $n$  atoms bears a distinct label from  $\{1, \dots, n\}$

# Counting generating functions

## Definition

Let  $a_n = \#\mathcal{A}_n$  = the number of objects of size  $n$  in  $\mathcal{A}$ . Then the formal power series

$$A(z) = \sum_{n \geq 0} a_n z^n = \sum_{\alpha \in \mathcal{A}} z^{|\alpha|}$$

is the (ordinary) generating function of the class  $\mathcal{A}$ .  
The coefficient of  $z^n$  in  $A(z)$  is denoted  $[z^n]A(z)$ :

$$[z^n]A(z) = [z^n] \sum_{n \geq 0} a_n z^n = a_n$$

# Counting generating functions

Ordinary generating functions (OGFs) are mostly used to enumerate unlabelled classes.

## Example

$$\begin{aligned}\mathcal{L} &= \{w \in (0 + 1)^* \mid w \text{ does not contain two consecutive } 0\text{'s}\} \\ &= \{\epsilon, 0, 1, 01, 10, 11, 010, 011, 101, 110, 111, \dots\}\end{aligned}$$

$$\begin{aligned}L(z) &= z^{|\epsilon|} + z^{|0|} + z^{|1|} + z^{|01|} + z^{|10|} + z^{|11|} + \dots \\ &= 1 + 2z + 3z^2 + 5z^3 + 8z^4 + \dots\end{aligned}$$

Exercise: Can you guess the value of  $L_n = [z^n]L(z)$ ?

# Counting generating functions

## Definition

Let  $a_n = \#\mathcal{A}_n$  = the number of objects of size  $n$  in  $\mathcal{A}$ . Then the formal power series

$$\hat{A}(z) = \sum_{n \geq 0} a_n \frac{z^n}{n!} = \sum_{\alpha \in \mathcal{A}} \frac{z^{|\alpha|}}{|\alpha|!}$$

is the **exponential generating function** of the class  $\mathcal{A}$ .



# Counting generating functions

Exponential generating functions (EGFs) are used to enumerate labelled classes.

## Example

$\mathcal{C}$  = circular permutations

=  $\{\epsilon, 1, 12, 123, 132, 1234, 1243, 1324, 1342, 1423, 1432, 12345, \dots\}$

$$\hat{C}(z) = \frac{1}{0!} + \frac{z}{1!} + \frac{z^2}{2!} + 2\frac{z^3}{3!} + 6\frac{z^4}{4!} + \dots$$

$$c_n = n! \cdot [z^n] \hat{C}(z) = (n-1)!, \quad n > 0$$

# Disjoint union

Let  $C = \mathcal{A} + \mathcal{B}$ , the disjoint union of the unlabelled classes  $\mathcal{A}$  and  $\mathcal{B}$  ( $\mathcal{A} \cap \mathcal{B} = \emptyset$ ). Then

$$C(z) = A(z) + B(z)$$

And

$$c_n = [z^n]C(z) = [z^n]A(z) + [z^n]B(z) = a_n + b_n$$

## Cartesian product

Let  $\mathcal{C} = \mathcal{A} \times \mathcal{B}$ , the Cartesian product of the unlabelled classes  $\mathcal{A}$  and  $\mathcal{B}$ . The size of  $(\alpha, \beta) \in \mathcal{C}$ , where  $a \in \mathcal{A}$  and  $\beta \in \mathcal{B}$ , is the sum of sizes:  $|(\alpha, \beta)| = |\alpha| + |\beta|$ .

Then

$$C(z) = A(z) \cdot B(z)$$

Proof.

$$\begin{aligned} C(z) &= \sum_{\gamma \in \mathcal{C}} z^{|\gamma|} = \sum_{(\alpha, \beta) \in \mathcal{A} \times \mathcal{B}} z^{|\alpha| + |\beta|} = \sum_{\alpha \in \mathcal{A}} \sum_{\beta \in \mathcal{B}} z^{|\alpha|} \cdot z^{|\beta|} \\ &= \left( \sum_{\alpha \in \mathcal{A}} z^{|\alpha|} \right) \cdot \left( \sum_{\beta \in \mathcal{B}} z^{|\beta|} \right) = A(z) \cdot B(z) \end{aligned}$$



# Cartesian product

The  $n$ th coefficient of the OGF for a Cartesian product is the *convolution* of the coefficients  $\{a_n\}$  and  $\{b_n\}$ :

$$\begin{aligned}c_n &= [z^n]C(z) = [z^n]A(z) \cdot B(z) \\ &= \sum_{k=0}^n a_k b_{n-k}\end{aligned}$$

# Sequences

Let  $\mathcal{A}$  be a class without any empty object ( $\mathcal{A}_0 = \emptyset$ ). The class  $\mathcal{C} = \text{Seq}(\mathcal{A})$  denotes the class of **sequences** of  $\mathcal{A}$ 's.

$$\begin{aligned}\mathcal{C} &= \{(\alpha_1, \dots, \alpha_k) \mid k \geq 0, \alpha_i \in \mathcal{A}\} \\ &= \{\epsilon\} + \mathcal{A} + (\mathcal{A} \times \mathcal{A}) + (\mathcal{A} \times \mathcal{A} \times \mathcal{A}) + \dots = \{\epsilon\} + \mathcal{A} \times \mathcal{C}\end{aligned}$$

Then

$$C(z) = \frac{1}{1 - A(z)}$$

Proof.

$$C(z) = 1 + A(z) + A^2(z) + A^3(z) + \dots = 1 + A(z) \cdot C(z)$$




## Example

Let  $\mathcal{A} = \{0, 1\}$ . Then  $\mathcal{C} = \text{Seq}(\mathcal{A}) = \{\epsilon, 0, 1, 00, 01, 10, 11, \dots\}$  is the class of the sequences (strings) of bits.

$$A(z) = 2z \implies C(z) = \frac{1}{1-2z} = 1 + 2z + (2z)^2 + (2z)^3 + \dots$$
$$[z^n]C(z) = 2^n$$

## Example

A general tree consists of a root to which we attach a sequence of general trees.


$$\mathcal{G} = \{\circ, \circ, \circ, \circ, \circ, \circ, \circ, \dots\}$$

$$\mathcal{G} = Z \times \text{Seq}(\mathcal{G}), \quad Z \equiv \{\circ\}$$

$$G(z) = z \frac{1}{1 - G(z)} = \begin{cases} \frac{1 - \sqrt{1 - 4z}}{2}, & z \neq 0, \\ 0, & z = 0. \end{cases}$$

## Example

$\mathcal{B}$  = binary trees

$$\mathcal{B} = \{\square\} + \{o\} \times \mathcal{B} \times \mathcal{B}$$

$$B(z) = 1 + zB^2(z) = \begin{cases} \frac{1 - \sqrt{1 - 4z}}{2z}, & z \neq 0, \\ 1, & z = 0. \end{cases}$$

$$zB(z) = G(z) \quad \leftarrow \mathcal{Z} \times \mathcal{B} \text{ is isomorphic to } \mathcal{G}$$



## Example

$$\begin{aligned}\mathcal{L} &= \{w \in (0 + 1)^* \mid w \text{ does not contain two consecutive } 0\text{'s}\} \\ &= \text{Seq}(\{1\} + \{01\}) \times (\{\epsilon\} + \{0\})\end{aligned}$$

$$L(z) = \frac{1}{1 - (z + z^2)}(1 + z) = \frac{1 + z}{1 - z - z^2}$$

## Example: Formal languages

### Example

$$\begin{aligned}L(z) &= \frac{1+z}{1-z-z^2} \\ &= \frac{1}{\sqrt{5}} \left( -\phi_2^2 \frac{1}{1-z/\phi_1} + \phi_1^2 \frac{1}{1-z/\phi_2} \right), \\ [z^n]L(z) &= -\frac{1}{\sqrt{5}} \phi_2^2 \phi_1^{-n} + \frac{1}{\sqrt{5}} \phi_1^2 \phi_2^{-n} \sim \frac{1}{\sqrt{5}} \left( \frac{1+\sqrt{5}}{2} \right)^{n+2} \\ &\approx 1.17 \cdot 1.618^n\end{aligned}$$

$$\phi_1 = \frac{-\sqrt{5}-1}{2}, \phi_2 = \frac{\sqrt{5}-1}{2}$$

## Labelled objects

Disjoint unions of labelled classes are defined as for unlabelled classes and  $\hat{C}(z) = \hat{A}(z) + \hat{B}(z)$ , for  $C = A + B$ . Also,  $c_n = a_n + b_n$ .

To define labelled products, we must take into account that for each pair  $(\alpha, \beta)$  where  $|\alpha| = k$  and  $|\alpha| + |\beta| = n$ , we construct  $\binom{n}{k}$  distinct pairs by consistently relabelling the atoms of  $\alpha$  and  $\beta$ :

$$\begin{aligned}\alpha &= (2, 1, 4, 3), & \beta &= (1, 3, 2) \\ \alpha \times \beta &= \{(2, 1, 4, 3, 5, 7, 6), (2, 1, 5, 3, 4, 7, 6), \dots, \\ & \quad (5, 4, 7, 6, 1, 3, 2)\} \\ \#(\alpha \times \beta) &= \binom{7}{4} = 35\end{aligned}$$

The size of an element in  $\alpha \times \beta$  is  $|\alpha| + |\beta|$ .

For a class  $\mathcal{C}$  that is labelled product of two labelled classes  $\mathcal{A}$  and  $\mathcal{B}$

$$\mathcal{C} = \mathcal{A} \times \mathcal{B} = \bigcup_{\substack{\alpha \in \mathcal{A} \\ \beta \in \mathcal{B}}} \alpha \times \beta$$

the following relation holds for the corresponding EGFs

$$\begin{aligned} \hat{C}(z) &= \sum_{\gamma \in \mathcal{C}} \frac{z^{|\gamma|}}{|\gamma|!} = \sum_{\alpha \in \mathcal{A}} \sum_{\beta \in \mathcal{B}} \binom{|\alpha| + |\beta|}{|\alpha|} \frac{z^{|\alpha| + |\beta|}}{(|\alpha| + |\beta|)!} \\ &= \sum_{\alpha \in \mathcal{A}} \sum_{\beta \in \mathcal{B}} \frac{1}{|\alpha|! |\beta|!} z^{|\alpha| + |\beta|} = \left( \sum_{\alpha \in \mathcal{A}} \frac{z^{|\alpha|}}{|\alpha|!} \right) \cdot \left( \sum_{\beta \in \mathcal{B}} \frac{z^{|\beta|}}{|\beta|!} \right) \\ &= \hat{A}(z) \cdot \hat{B}(z) \end{aligned}$$

The  $n$ th coefficient of  $\hat{C}(z) = \hat{A}(z) \cdot \hat{B}(z)$  is also a convolution

$$c_n = [z^n] \hat{C}(z) = \sum_{k=0}^n \binom{n}{k} a_k b_{n-k}$$

## Marking (pointing)

Given a class  $\mathcal{A}$ , the class  $\Theta\mathcal{A}$  is the class that we obtain by marking an atom in each object, in all possible ways:

$$\mathcal{A} = \{01, 10, 11, 010, 011, 101, \dots\}$$

$$\Theta\mathcal{A} = \{\underline{0}1, 0\underline{1}, \underline{1}0, 1\underline{0}, \underline{1}1, 1\underline{1}, \underline{0}10, 0\underline{1}0, 01\underline{0}, \dots\}$$

Marking works for both labelled and unlabelled objects. Since the class  $\Theta\mathcal{A}$  has  $na_n$  objects of size  $n$  ( $a_n = \#\mathcal{A}_n$ ), we have

$$C(z) = z \frac{d}{dz} A(z),$$

$$\hat{C}(z) = z \frac{d}{dz} \hat{A}(z)$$

We overload  $\Theta$  to denote the operator  $z \frac{d}{dz}$  too

Sequences of labelled objects are defined as in the case of unlabelled objects. The construction  $\mathcal{C} = \text{Seq}(\mathcal{A})$  is well defined if  $\mathcal{A}_0 = \emptyset$ .

If  $\mathcal{C} = \text{Seq}(\mathcal{A}) = \{\epsilon\} + \mathcal{A} \times \mathcal{C}$  then

$$\hat{C}(z) = \frac{1}{1 - \hat{A}(z)}$$

## Example

Permutations are labelled sequences of atoms,  $\mathcal{P} = \text{Seq}(\mathcal{Z})$ . Hence,

$$\hat{P}(z) = \frac{1}{1 - z} = \sum_{n \geq 0} z^n$$

$$n! \cdot [z^n] \hat{P}(z) = n!$$

Given a labelled class  $\mathcal{A}$  with no object of size 0,  $\mathcal{C} = \text{Set}(\mathcal{A})$  is the class of all finite subsets whose elements are objects from  $\mathcal{A}$ :

$$\mathcal{C} = \{\{\alpha_1, \dots, \alpha_k\} \mid k \geq 0, \alpha_i \in \mathcal{A}\}$$

Since the objects must be labelled, the labels  $\{1, \dots, n\}$  are distributed among the components of a set  $\gamma = \{\alpha_1, \dots, \alpha_k\} \in \mathcal{C}$  of size  $n = |\alpha_1| + \dots + |\alpha_k|$  and the atoms of each  $\alpha_i$  are consistently relabelled.

Despite we may have  $\alpha_i = \alpha_j$  for some  $i \neq j$ , after assigning labels to  $\alpha_i$  and  $\alpha_j$ , they will be distinct (they'll have the same "shape" but not the same labels)



Let  $\mathcal{C} = \text{Set}(\mathcal{A})$ . If we mark one of the atoms of one of the components of a set in  $\mathcal{C}$ , we tell this component apart and the remaining components form a set. Since the marked component belongs to  $\Theta\mathcal{A}$

$$\Theta\mathcal{C} = \Theta\mathcal{A} \times \mathcal{C}$$

Solving the corresponding differential equation with  $\hat{C}(0) = 1$ , we have

$$\hat{C}(z) = \exp(\hat{A}(z))$$

Alternatively, let  $\equiv$  denote the equivalence relation between two sequences  $(\alpha_1, \dots, \alpha_k) \equiv (\alpha'_1, \dots, \alpha'_k)$  if and only if one is a permutation of the other.

Then

$$\mathcal{C} = \{\emptyset\} + (\mathcal{A}/\equiv) + (\mathcal{A}^2/\equiv) + (\mathcal{A}^3/\equiv) + \dots + (\mathcal{A}^k/\equiv) + \dots$$

and

$$\hat{\mathcal{C}}(z) = 1 + \hat{\mathcal{A}}(z) + \frac{\hat{\mathcal{A}}^2(z)}{2!} + \frac{\hat{\mathcal{A}}^3(z)}{3!} + \dots + \frac{\hat{\mathcal{A}}^k(z)}{k!} + \dots = \exp(\hat{\mathcal{A}}(z))$$

## Example: The number of derangements

A derangement  $\sigma$  is a permutation without fixed points, i. e.,  $\sigma(i) \neq i$ . Therefore, if  $\mathcal{D}$  is the class of all derangements

$$\mathcal{P} = \mathcal{D} \times \text{Set}(Z)$$

(a permutation = a derangement  $\times$  a set of fixed points)

$$\hat{P}(z) = \frac{1}{1-z} = \hat{D}(z) \cdot \exp(z)$$

$$\hat{D}(z) = \frac{e^{-z}}{1-z} = \sum_{\ell \geq 0} \frac{(-1)^\ell z^\ell}{\ell!} \sum_{m \geq 0} z^m = \sum_{n \geq 0} z^n \left( \sum_{k=0}^n \frac{(-1)^k}{k!} \right)$$

$$\begin{aligned} n! \cdot [z^n] \hat{D}(z) &= n! \sum_{k=0}^n \frac{(-1)^k}{k!} = n! \left( \frac{1}{0!} - \frac{1}{1!} + \frac{1}{2} - \frac{1!}{3!} + \frac{1}{4!} - \frac{1}{5!} + \dots \right) \\ &\sim \frac{n!}{e} \end{aligned}$$

## Example: The number of derangements

The probability that a random permutation is a derangement quickly tends to  $\sim \frac{1}{e} = 0.3678\dots$

If we want to generate random derangements of size  $n$  with the rejection method, the number of iterations follows a **geometric distribution** of parameter  $p = D_n/n! \sim e^{-1}$ .

The expected number of iterations to produce a derangement is  $\sim e = 2.71828\dots$

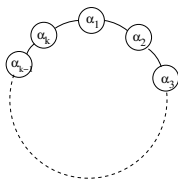
$$\begin{aligned}\mathbb{E}[\# \text{ of iterations}] &= \sum_{k>0} kp(1-p)^{k-1} = p \frac{d}{dx} \sum_{k>0} x^k \Big|_{x=1-p} \\ &= p \frac{d}{dx} \left( \frac{1}{1-x} - 1 \right) \Big|_{x=1-p} = \frac{1}{p}\end{aligned}$$

# Cycles

Given a labelled class  $\mathcal{A}$  with no object of size 0,  $\mathcal{C} = \text{Cycle}(\mathcal{A})$  is the class of all non-empty cycles whose elements are objects from  $\mathcal{A}$ :

$$\mathcal{C} = \{ \langle \alpha_1, \dots, \alpha_k \rangle \mid k > 0, \alpha_i \in \mathcal{A} \}$$

Here  $\langle \alpha_1, \dots, \alpha_k \rangle$  denotes a cycle of length  $k$  and size  $|\alpha_1| + \dots + |\alpha_k|$



Let  $\mathcal{C} = \text{Cycle}(\mathcal{A})$ . If we mark one of the atoms of one of the components of a cycle in  $\mathcal{C}$ , we tell this component apart and the remaining components form a sequence—we break the ring/necklace at that point. Since the marked component belongs to  $\Theta\mathcal{A}$

$$\Theta\mathcal{C} = \Theta\mathcal{A} \times \text{Seq}(\mathcal{A})$$

Solving the corresponding differential equation with  $\hat{C}(0) = 0$ , we have

$$\hat{C}(z) = \ln \left( \frac{1}{1 - \hat{A}(z)} \right)$$

Alternatively, let  $\equiv$  denote the equivalence relation between two sequences  $(\alpha_1, \dots, \alpha_k) \equiv (\alpha'_1, \dots, \alpha'_k)$  if and only if one is a cyclic permutation of the other, that is,  $\alpha_1 = \alpha'_i, \alpha_2 = \alpha'_{i+1}, \dots, \alpha_{k-i+1} = \alpha'_k, \alpha_{k-i+2} = \alpha'_1, \dots$ . Then

$$C = (\mathcal{A}/\equiv) + (\mathcal{A}^2/\equiv) + (\mathcal{A}^3/\equiv) + \dots + (\mathcal{A}^k/\equiv) + \dots$$

and

$$\hat{C}(z) = \hat{A}(z) + \frac{\hat{A}^2(z)}{2} + \frac{\hat{A}^3(z)}{3} + \dots + \frac{\hat{A}^k(z)}{k} + \dots = \ln \left( \frac{1}{1 - \hat{A}(z)} \right)$$

## Remark

$$\int dz \sum_{n \geq 0} z^n = \sum_{n \geq 0} \frac{z^{n+1}}{n+1} = \sum_{n > 0} \frac{z^n}{n}$$
$$\int \frac{dz}{1-z} = \ln \left( \frac{1}{1-z} \right) + \kappa$$

# Examples

A permutation is a set of cycles. For example, the permutation

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

can be (uniquely) represented by the set of cycles  $\{\langle 1, 3, 4 \rangle, \langle 2, 7, 8, 6 \rangle, \langle 5 \rangle\}$ .

Thus

$$\mathcal{P} = \text{Set}(\text{Cycle}(Z)) \implies \hat{P}(z) = \exp\left(\ln\left(\frac{1}{1-z}\right)\right) = \frac{1}{1-z}$$



## Restricted cardinalities

Restrictions in the cardinalities (number of components) of sequences, sets and cycles are easy to deal with.

For example, the generating function for sequences of  $\mathcal{A}$ 's with at least  $m$  components ( $\mathcal{C} = \text{Seq}(\mathcal{A}, \text{card} \geq m)$ ) is

$$\hat{C}(z) = \hat{A}^m(z) + \hat{A}^{m+1}(z) + \dots = \frac{\hat{A}^m(z)}{1 - \hat{A}(z)}$$

### Example

An *involution* is a permutation  $\sigma$  such that  $\sigma^2 = \text{Id}$ . Such a permutation is a set of cycles, each with only one or two elements.

$$\mathcal{I} = \text{Set}(\text{Cycle}(Z, \text{card} \leq 2))$$

Hence,

$$\hat{I}(z) = \exp\left(z + \frac{z^2}{2}\right)$$

# Set partitions

The  $n$ th Bell number  $B_n$  is the number of partitions of a set of size  $n$  (with no empty parts). For instance, some of the  $B_4 = 15$  partitions of the set  $\{1, \dots, 4\}$  are

$\{\{1\}, \{2, 3, 4\}\}, \{\{2\}, \{1, 3, 4\}\}, \{\{1, 3\}, \{2, 4\}\}, \dots$

Thus, a partition is a set of non-empty sets of atoms. The class of set partitions can be specified as

$$\mathcal{S} = \text{Set}(\text{Set}(\mathcal{Z}, \text{card} > 0))$$

Hence the EGF for  $\mathcal{S}$  is

$$\hat{S}(z) = \exp(\exp(z) - 1) = \sum_{n \geq 0} B_n \frac{z^n}{n!}$$

## Theorem

Let  $y(z)$  a GF such that

$$y(z) = z\phi(y(z))$$

for some analytic function  $\phi(w)$  with  $\phi(0) \neq 0$ .

Then

$$[z^n]y(z) = \frac{1}{n}[w^{n-1}]\phi(w)^n$$

## Theorem

Let  $y(z)$  a GF such that

$$y(z) = z\phi(y(z))$$

for some analytic function  $\phi(w)$  with  $\phi(0) \neq 0$ .

Then, if  $g(w)$  is an arbitrary analytic function,

$$[z^n]g(y(z)) = \frac{1}{n}[u^{n-1}](g'(u)\phi(u)^n)$$

## Example: Cayley trees

A *Cayley tree* is a labelled rooted tree; it is either a single root node, or a root with a set of subtrees attached to it.

$$\mathcal{T} = Z \times \text{Set}(\mathcal{T})$$

$$\hat{T}(z) = z \exp(\hat{T}(z))$$

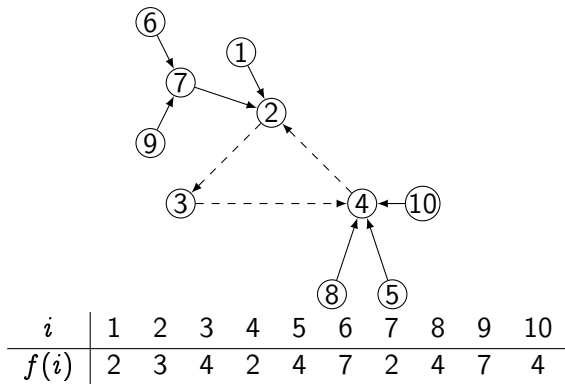
Using Lagrange's inversion formula with  $\phi(w) = e^w$

$$[z^n] \hat{T}(z) = \frac{1}{n!} n^{n-1} e^{nu} \Big|_{u=0} = \frac{n^{n-1}}{n!}$$

$$\hat{T}(z) = \sum_{n>0} n^{n-1} \frac{z^n}{n!}$$

# Examples

Given a function  $f : [1..n] \rightarrow [1..n]$ , its functional graph has  $n$  nodes and there is an arc  $(i, j)$  whenever  $f(i) = j$ . Such a graph consists in a collection of (weakly) connected components, each one a directed cycle of directed trees.



## Example: Functional graphs

The class  $\mathcal{F}$  of functional graphs is hence

$$\mathcal{F} = \text{Set}(\mathcal{C})$$

$$\mathcal{C} = \text{Cycle}(\mathcal{T})$$

$$\mathcal{T} = \mathbb{Z} \times \text{Set}(\mathcal{T})$$

The EGF is

$$\begin{aligned}\hat{F}(z) &= \exp\left(\ln \frac{1}{1 - \hat{T}(z)}\right) \\ &= \frac{1}{1 - \hat{T}(z)}\end{aligned}$$

Exercise: Functional graphs are isomorphic to sequences of Cayley trees. Why? Find a bijection.

## Unlabelled sets and cycles

Since atoms in unlabelled objects are indistinguishable, we consider two different combinatorial constructs: multisets and powersets. The class  $\mathcal{C} = \text{MSet}(\mathcal{A})$  is the set of multisets of objects from  $\mathcal{A}$ . A multiset  $\gamma = \{\alpha_1, \dots, \alpha_k\}$  may contain several repetitions of some object in  $\mathcal{A}$ , say  $\alpha_1 = \alpha_2 = \alpha_3$ .

Thus

$$\mathcal{C} = \text{MSet}(\mathcal{A}) = \prod_{\alpha \in \mathcal{A}} \text{Seq}(\{\alpha\}),$$

that is, a finite object in  $\mathcal{C}$  is a tuple where each  $\alpha \in \mathcal{A}$  may appear any number of times (including zero), but only a finite number of  $\alpha$ 's appear one or more times.

From there

$$C(z) = \prod_{\alpha \in \mathcal{A}} \frac{1}{1 - z^{|\alpha|}}$$



Taking logarithms and interchanging summations

$$\begin{aligned}\ln C(z) &= \sum_{\alpha \in \mathcal{A}} \ln \frac{1}{1 - z^{|\alpha|}} \\ &= \sum_{\alpha \in \mathcal{A}} \sum_{k > 0} \frac{(z^{|\alpha|})^k}{k} \\ &= \sum_{k > 0} \frac{1}{k} \sum_{\alpha \in \mathcal{A}} (z^k)^{|\alpha|} \\ &= \sum_{k > 0} \frac{A(z^k)}{k}\end{aligned}$$

Hence

$$C(z) = \exp \left( \sum_{k > 0} \frac{A(z^k)}{k} \right)$$

## Example

Integer partitions

$\mathcal{I} = \text{Seq}(\mathbb{Z}, \text{card} \geq 1)$ , Positive integers,

$\mathcal{P} = \text{MSet}(\mathcal{I})$ , Integer partitions,

$$I(z) = \frac{z}{1-z},$$

$$\begin{aligned} P(z) &= \prod_{j>0} \frac{1}{1-z^j} = \exp\left(\sum_{k>0} \frac{1}{k} \frac{z^k}{1-z^k}\right) \\ &= 1 + z + 2z^2 + 3z^3 + 5z^4 + 7z^5 + \dots \end{aligned}$$

## Unlabelled sets and cycles

The construction  $\mathcal{C} = \text{PSet}(\mathcal{A})$  gives the class of sets of objects in  $\mathcal{A}$ , that is, with no repetitions.

We have

$$\mathcal{C} = \prod_{\alpha \in \mathcal{A}} (\{\epsilon\} + \{\alpha\})$$

using a reasoning analogous to that before, but now each  $\alpha \in \mathcal{A}$  either appears (once) or does not in a given set in  $\mathcal{C}$ .

The OGF is then

$$C(z) = \prod_{\alpha \in \mathcal{A}} (1 + z^{|\alpha|}) = \exp \left( \sum_{k>0} (-1)^k \frac{A(z^k)}{k} \right),$$

where the last equality can be proved using the  $\exp - \log$  trick.

# Unlabelled sets and cycles

Unlabelled cycles (necklaces) are is one of the most complicated combinatorial constructions to enumerate.

The OGF for  $\mathcal{C} = \text{Cycle}(\mathcal{A})$  is

$$C(z) = \sum_{k>0} \frac{\phi(k)}{k} \ln \frac{1}{1 - A(z^k)},$$

where  $\phi(k) = \#\{i < n \mid \gcd(i, n) = 1\}$  is Euler's *totient* function.

The proof relies on Pólya's theory for the enumeration of combinatorial structures that remain invariant under the symmetric group of transformations.

# Admissible combinatorial classes

A combinatorial operator  $\Phi$  over combinatorial classes is called **admissible** if  $\mathcal{C} = \Phi(\mathcal{A}_1, \dots, \mathcal{A}_j)$  implies that there exists some operator  $\Psi$  over OGF (or EGFs) such that  $C(z) = \Psi(A_1(z), \dots, A_j(z))$ .

We have seen that disjoint unions, products, sequences, marking, multisets, powersets, and cycles are all admissible.

A class is called **admissible** if it is an  $\epsilon$ -class (contains a single object of size 0), or it is an atomic class (contains a single object of size 1), or it can be finitely specified by application of admissible operators on admissible classes.

# A dictionary of admissible unlabelled operators

Class	OGF	Name
$\epsilon$	1	Epsilon
$\mathcal{Z}$	$z$	Atomic
$\mathcal{A} + \mathcal{B}$	$A(z) + B(z)$	Disjoint union
$\mathcal{A} \times \mathcal{B}$	$A(z) \cdot B(z)$	Product
$\text{Seq}(\mathcal{A})$	$\frac{1}{1-A(z)}$	Sequence
$\Theta\mathcal{A}$	$\Theta A(z) = zA'(z)$	Marking
$\text{MSet}(\mathcal{A})$	$\exp\left(\sum_{k>0} A(z^k)/k\right)$	Multiset
$\text{PSet}(\mathcal{A})$	$\exp\left(\sum_{k>0} (-1)^k A(z^k)/k\right)$	Powerset
$\text{Cycle}(\mathcal{A})$	$\sum_{k>0} \frac{\phi(k)}{k} \ln \frac{1}{1-A(z^k)}$	Cycle

# A dictionary of admissible labelled operators

Class	EGF	Name
$\epsilon$	1	Epsilon
$Z$	$z$	Atomic
$\mathcal{A} + \mathcal{B}$	$\hat{A}(z) + \hat{B}(z)$	Disjoint union
$\mathcal{A} \times \mathcal{B}$	$\hat{A}(z) \cdot \hat{B}(z)$	Product
$\text{Seq}(\mathcal{A})$	$\frac{1}{1 - \hat{A}(z)}$	Sequence
$\Theta \mathcal{A}$	$\Theta \hat{A}(z) = z \hat{A}'(z)$	Marking
$\text{Set}(\mathcal{A})$	$\exp(\hat{A}(z))$	Set
$\text{Cycle}(\mathcal{A})$	$\ln\left(\frac{1}{1 - \hat{A}(z)}\right)$	Cycle

# Bivariate generating functions

We need often to study some characteristic of combinatorial structures, e. g., the number of left-to-right maxima in a permutation, the height of a rooted tree, the number of complex components in a graph, etc.

Suppose  $X : \mathcal{A}_n \rightarrow \mathbb{N}$  is a characteristic under study. Let

$$a_{n,k} = \#\{\alpha \in \mathcal{A} \mid |\alpha| = n, X(\alpha) = k\}$$

We can view the restriction  $X_n : \mathcal{A}_n \rightarrow \mathbb{N}$  as a **random variable**. Then under the usual uniform model

$$\mathbb{P}[X_n = k] = \frac{a_{n,k}}{a_n}$$



# Bivariate generating functions

Define

$$\begin{aligned}A(z, u) &= \sum_{n, k \geq 0} a_{n, k} z^n u^k \\ &= \sum_{\alpha \in \mathcal{A}} z^{|\alpha|} u^{X(\alpha)}\end{aligned}$$

Then  $a_{n, k} = [z^n u^k] A(z, u)$  and

$$\mathbb{P}[X_n = k] = \frac{[z^n u^k] A(z, u)}{[z^n] A(z, 1)}$$

# Bivariate generating functions

We can also define

$$\begin{aligned} B(z, u) &= \sum_{n, k \geq 0} \mathbb{P}[X_n = k] z^n u^k \\ &= \sum_{\alpha \in \mathcal{A}} \mathbb{P}[\alpha] z^{|\alpha|} u^{X(\alpha)} \end{aligned}$$

and thus  $B(z, u)$  is a generating function whose coefficient of  $z^n$  is the **probability generating function** of the r.v.  $X_n$

$$\begin{aligned} B(z, u) &= \sum_{n \geq 0} P_n(u) z^n \\ P_n(u) &= [z^n] B(z, u) = \sum_{k \geq 0} \mathbb{P}[X_n = k] u^k \\ &= \sum_{\alpha \in \mathcal{A}_n} \mathbb{P}[\alpha] u^{X(\alpha)} \end{aligned}$$

## Proposition

*If  $P(u)$  is the probability generating function of a random variable  $X$  then*

$$P(1) = 1,$$

$$P'(1) = \mathbb{E}[X],$$

$$P''(1) = \mathbb{E}[X^2] = \mathbb{E}[X(X - 1)],$$

$$\mathbb{V}[X] = P''(1) + P'(1) - (P'(1))^2$$

## Bivariate generating functions

We can study the moments of  $X_n$  by successive differentiation of  $B(z, u)$  (or  $A(z, u)$ ). For instance,

$$\bar{B}(z) = \sum_{n \geq 0} \mathbb{E}[X_n] z^n = \left. \frac{\partial B}{\partial u} \right|_{u=1}$$

For the  $r$ th factorial moments of  $X_n$

$$B^{(r)}(z) = \sum_{n \geq 0} \mathbb{E}[X_n^{\underline{r}}] z^n = \left. \frac{\partial^r B}{\partial u^r} \right|_{u=1}$$

$$X_n^{\underline{r}} = X_n(X_n - 1) \cdots (X_n - r + 1)$$

# The number of left-to-right maxima in a permutation

Consider the following specification for permutations

$$\mathcal{P} = \{\emptyset\} + \mathcal{P} \times \mathcal{Z}$$

The BGF for the probability that a random permutation of size  $n$  has  $k$  left-to-right maxima is

$$M(z, u) = \sum_{\sigma \in \mathcal{P}} \frac{z^{|\sigma|}}{|\sigma|!} u^{X(\sigma)},$$

where  $X(\sigma) = \#$  of left-to-right maxima in  $\sigma$

# The number of left-to-right maxima in a permutation

With the recursive decomposition of permutations and since the last element of a permutation of size  $n$  is a left-to-right maxima iff its label is  $n$

$$M(z, u) = \sum_{\sigma \in \mathcal{P}} \sum_{1 \leq j \leq |\sigma|+1} \frac{z^{|\sigma|+1}}{(|\sigma|+1)!} u^{X(\sigma) + \llbracket j = |\sigma|+1 \rrbracket}$$

$\llbracket P \rrbracket = 1$  if  $P$  is true,  $\llbracket P \rrbracket = 0$  otherwise.

# The number of left-to-right maxima in a permutation

$$\begin{aligned}M(z, u) &= \sum_{\sigma \in \mathcal{P}} \frac{z^{|\sigma|+1}}{(|\sigma| + 1)!} u^{X(\sigma)} \sum_{1 \leq j \leq |\sigma|+1} u^{\llbracket j = |\sigma|+1 \rrbracket} \\ &= \sum_{\sigma \in \mathcal{P}} \frac{z^{|\sigma|+1}}{(|\sigma| + 1)!} u^{X(\sigma)} (|\sigma| + u)\end{aligned}$$

Taking derivatives w.r.t.  $z$

$$\frac{\partial}{\partial z} M = \sum_{\sigma \in \mathcal{P}} \frac{z^{|\sigma|}}{|\sigma|!} u^{X(\sigma)} (|\sigma| + u) = z \frac{\partial}{\partial z} M + uM$$

Hence,

$$(1 - z) \frac{\partial}{\partial z} M(z, u) - uM(z, u) = 0$$

# The number of left-to-right maxima in a permutation

Solving, since  $M(0, u) = 1$

$$M(z, u) = \left( \frac{1}{1-z} \right)^u = \sum_{n, k \geq 0} \begin{bmatrix} n \\ k \end{bmatrix} \frac{z^n}{n!} u^k$$

where  $\begin{bmatrix} n \\ k \end{bmatrix}$  denote the (signless) Stirling numbers of the first kind, also called Stirling cycle numbers.

Taking the derivative w.r.t.  $u$  and setting  $u = 1$

$$m(z) = \left. \frac{\partial}{\partial z} M(z, u) \right|_{u=1} = \frac{1}{1-z} \ln \frac{1}{1-z}$$

Thus the average number of left-to-right maxima in a random permutation of size  $n$  is

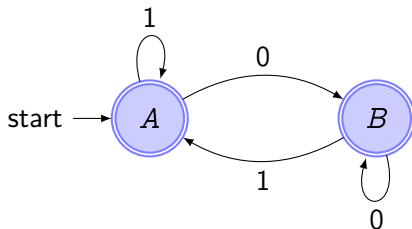
$$[z^n] m(z) = \mathbb{E}[X_n] = H_n = 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n} = \ln n + \gamma + O(1/n)$$

$$\frac{1}{1-z} \ln \frac{1}{1-z} = \sum_{\ell} z^{\ell} \sum_{m > 0} \frac{z^m}{m} = \sum_{n > 0} z^n \sum_{k=1}^n \frac{1}{k}$$



# Analyzing branch mispredictions

In the analysis of the 1-bit prediction scheme for branch mispredictions, we need to analyze how many times we will jump from state A to state B and viceversa for a random bit string of length  $n$



## Analyzing branch mispredictions

Let  $A_{n,k}$  be the number of bitstrings of length  $n$  with  $k$  mispredictions that end at state  $A$  (they end with a 1). Similarly,  $B_{n,k}$  for bitstrings ending at state  $B$  (ending with a 0). Define  $A(z, u)$  and  $B(z, u)$  the corresponding BGF with  $z$  marking the size and  $u$  the number of mispredictions. Then

$$\begin{aligned}A &= 1 + Az + Bzu, \\B &= Bz + Azu\end{aligned}$$

Solving the linear system

$$A = \frac{1 - z}{(1 - z)^2 - z^2 u^2}, \quad B = \frac{zu}{(1 - z)^2 - z^2 u^2},$$

## Analyzing branch mispredictions

The BGF for all bitstrings is

$$\begin{aligned}C(z, u) &= A(z, u) + B(z, u) = \frac{1}{1 - z(1 + u)} = \sum_{n \geq 0} (z(1 + u))^n \\ &= \sum_{n \geq 0} z^n \sum_{k=0}^n \binom{n}{k} u^k\end{aligned}$$

Hence, the number of bitstrings of length  $n$  that incur  $k$  branch mispredictions is

$$\binom{n}{k}$$

The PGF for the r.v.

$X_n = \#$  of branch mispredictions in a random bitstring of length  $n$  is

$$\frac{[z^n]C(z, u)}{2^n} = \frac{(1 + u)^n}{2^n}$$

## Analyzing branch mispredictions

The average number number of branch mispredictions is

$$\begin{aligned}\frac{1}{2^n} [z^n] \frac{\partial}{\partial u} C(z, u) \Big|_{u=1} &= \frac{1}{2^n} [z^n] \frac{z}{(1-z-zu)^2} \Big|_{u=1} \\ \frac{1}{2^n} [z^n] \frac{z}{(1-2z)^2} &= \frac{1}{2^n} [z^n] \frac{1}{2} \ominus \frac{1}{1-2z} = \frac{n}{2}\end{aligned}$$

Other moments can be computed easily as well. Notice that  $X_n$  has binomial distribution with parameters  $n$  and  $p = 1/2$ .

# Complex Analysis Techniques

# Why complex analysis?

We now look to GFs as functions in the complex plane. The behavior of a GF in the complex plane gives valuable information about its coefficients (which are the quantities we actually are interested in). For many counting GFs we have

$$[z^n]F(z) = R^n \psi(n)$$

where  $\limsup_{n \rightarrow \infty} |\psi(n)|^{1/n} = 1$  and  $R > 0$ .

**First principle:** The exponential growth  $R^n$  of the coefficients is determined by the location of the **singularities** of  $F(z)$

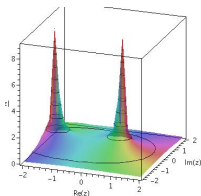
**Second principle:** The subexponential factor  $\psi(n)$  is dictated by the “nature” (local behavior) of  $F(z)$  around the singularities

## Example

Recall that the OGF for the language of all words without two consecutive 0's was

$$L(z) = \frac{1+z}{1-z-z^2}$$

A plot of  $|L(z)|$



The two peaks (singularities) occur at the roots of the denominator  $z = \phi_2 = \frac{\sqrt{5}-1}{2}$  and  $z = \phi_1 = -1/\phi_2$

# Example

The exponential growth is dictated by the “singularity” of smallest modulus  $z = \phi_2$

$$[z^n]L(z) \asymp \phi_2^{-n}$$

$$a_n \asymp K^n$$

means  $a_n \geq (K - \epsilon)^n$  infinitely often and  $a_n \leq (K + \epsilon)^n$  almost everywhere, for all  $\epsilon > 0$



## Example: Surjections

A *surjection* is a function  $f$  from  $A$  to  $B$  such that for all  $b \in B$  there exists at least one  $a$  such that  $f(a) = b$ .

A surjection from  $[1..n]$  to  $[1..r]$  with  $r \leq n$  can be put into one-to-one correspondence with a sequence (actually an  $r$ -tuple) of non-empty sets; we have a set for the antiimages of every element in  $[1..r]$ . The “size” of such a surjection is  $n$ .

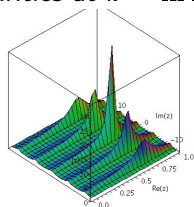
$$\mathcal{S} = \text{Seq}(\text{Set}(Z, \text{card} \geq 1))$$
$$\hat{S}(z) = \frac{1}{1 - (e^z - 1)} = \frac{1}{2 - e^z}$$

## Example: Surjections

The EGF

$$\hat{S}(z) = \frac{1}{2 - e^z}$$

has infinitely many singularities at  $z = \ln 2 + 2\pi ik$ ,  $k \in \mathbb{Z}$ .



The one of smallest modulus is  $z = \ln 2$  and

$$[z^n] \hat{S}(z) \asymp \left( \frac{1}{\ln 2} \right)^n$$

Thus, the number  $S_n$  of surjections from  $[1..n]$  onto another set is  $n!(\ln 2)^{-n} \psi(n)$ , for some subexponential function  $\psi(n)$

## Definition

A function  $f : \mathbb{C} \rightarrow \mathbb{C}$  defined in some region  $\Omega$  is **analytic at  $z_0$**  iff there exists an open disc  $D \subset \Omega$  centered at  $z_0$  such that  $f(z)$  is representable by a convergent series for all  $z \in D$ , i. e.,

$$f(z) = \sum_{n \geq 0} f_n (z - z_0)^n, \quad z \in D$$

By a **region** we mean an open connected subset of  $\mathbb{C}$

## Proposition

A function  $f : \mathbb{C} \rightarrow \mathbb{C}$  defined in some region  $\Omega$  is analytic at  $z_0$  iff  $f$  is differentiable at  $z_0$

## Fact

If  $f$  is analytic at  $z_0$  then it is infinitely differentiable at  $z_0$ ; furthermore, for  $z$  in a small neighborhood of  $z_0$

$$f(z) = \sum_{n \geq 0} \frac{f^{(n)}(z_0)}{n!} (z - z_0)^n$$

## Fact

If  $f$  and  $g$  are analytic at  $z_0$  then  $f + g$ ,  $f \cdot g$ , and  $\frac{df}{dz}$  are analytic at  $z_0$ ; furthermore, if  $f$  is analytic at  $g(z_0)$  then  $f \circ g$  is analytic at  $z = z_0$  too

# Analitycity and combinatorial structures

The counting GF (OGF or EGF) of admissible combinatorial classes are analytic at  $z = 0$

This can be proved by structural induction. It is easy for disjoint unions, products, sequences, labelled sets and cycles, and more involved for unlabelled multisets, powersets and cycles.

# Analitycity

## Definition

A function  $f$  is analytic in a region  $\Omega$  iff it is analytic for all  $z \in \Omega$

## Analytic continuation

If  $f$  is analytic in  $\Omega$ , then there is at most an analytic function in  $\Omega' \supset \Omega$  equal to  $f$  in  $\Omega$

## Example

The function  $f(z) = 1/(1 - z)$  is analytic in  $\mathbb{C} \setminus \{1\}$ ; even though the representation

$$\sum_{n \geq 0} z^n$$

only holds in the open disc  $|z| < 1$ , the function  $f(z)$  can be “continued” everywhere except for  $z = 1$ .

# Singularities

## Definition

A function  $f$  has a **singularity** at  $z_0$  if it is not analytic at  $z_0$

## Example

Function	Singularities	Why?
Polynomial	$\emptyset$	
$\exp(z)$	$\emptyset$	
$\frac{1}{1-z}$	$\{1\}$	$f(z)$ infinite
$\frac{1-\sqrt{1-4z}}{2}$	$\{1/4\}$	$f'(z)$ infinite
$1/z$	$\{0\}$	$f(z)$ infinite

## Definition

- The point  $z = \alpha$  is a **pole** (or polar singularity) of  $f(z)$  if there exists  $M > 0$  such that  $(1 - z/\alpha)^M \cdot f(z)$  is analytic at  $z = \alpha$ . The pole is said to be of order  $M$  if  $M$  is the least positive such integer.
- If  $f(z)$  has a pole of order  $M$  at  $z = \alpha$  then

$$f(z) = \sum_{n \geq -M} f_n (z - \alpha)^n$$

The **residue** of  $f(z)$  at  $z = \alpha$  is the coefficient  $f_{-1}$ ; we denote it  $\text{Res}(f, \alpha)$

- A function  $f(z)$  is **meromorphic** in a region  $\Omega$  if the only singularities of  $f(z)$  in  $\Omega$  are polar.



## Example

- The OGF for binary strings  $1/(1 - 2z)$  is meromorphic with a pole of order 1 at  $z = 1/2$
- The EGF for derangements  $e^{-z}/(1 - z)$  is meromorphic with a pole of order 1 at  $z = 1$
- The OGF for the language of bitstrings without two consecutive 0's is meromorphic with poles of order one at  $z = \phi_2 = (\sqrt{5} - 1)/2$  and  $z = -1/\phi_2$

# Dominant singularities

We know that an analytic function  $f(z)$  at  $z = 0$  can be represented by a convergent power series

$$f(z) = \sum_{n \geq 0} f_n z^n$$

in some open disc  $D = \{z \in \mathbb{C} \mid |z| < R\}$  for some  $R > 0$  or  $R = +\infty$ .

The radius of the largest such disc is called the **radius of convergence** of  $f(z)$ .

## Theorem

If  $f(z)$  is analytic at  $z = 0$  and has a finite radius of convergence  $R$  then  $f(z)$  has at least a singularity at  $|z| = R$ , and it is analytic in the region  $\{z \mid |z| < R\}$ .

This theorem is easily proved by *reductio ad absurdum* and using Cauchy's coefficient formula (we'll see that later).

## Theorem (Pringsheim's Theorem)

*If  $f(z)$  is representable at the origin by a convergent power series with non-negative coefficients and radius of convergence  $R$  then  $z = R$  is a singularity of  $f(z)$ .*

Pringsheim's Theorem is very useful since combinatorial GFs have non-negative coefficients; therefore we can focus the search for singularities in the real axis.

# Dominant singularities

## Definition

A singularity in the boundary of the disc of convergence of the series

$$\sum_{n \geq 0} f_n z^n$$

is called a **dominant singularity**

## Theorem

*If  $f(z)$  is analytic at  $z = 0$  and the radius of convergence  $R$  of the power series representation*

$$f(z) = \sum_{n \geq 0} f_n z^n$$

*is finite then*

$$f_n \asymp R^{-n}$$

# Dominant singularities

## Sketch of the proof

The theorem formalizes our previous observations. By definition of radius of convergence  $f_n(R - \epsilon)^n$  must tend to 0 for any small  $\epsilon > 0$  —otherwise the series wouldn't converge in  $z = R - \epsilon$  and it does. In particular,  $f_n(R - \epsilon)^n < 1$  for all  $n$  large enough, that is

$$f_n \leq (R - \epsilon)^{-n}$$

almost everywhere.

The other bound follows from the fact that  $f_n(R + \epsilon)^n$  cannot be bounded; otherwise,  $f_n(R + \epsilon/2)^n$  would be convergent. Thus  $f_n(R + \epsilon)^n > 1$  infinitely often.

# “Chasing” dominant singularities

The following rules of thumb help us locate dominant singularities

Function	Dominant singularity $\Delta(f)$
$\exp(f)$	$\Delta(f)$
polynomial	$\emptyset$
$1/(1-f)$	$\min(\Delta(f), \{z \mid f(z) = 1\})$
$\log(1/(1-f))$	$\min(\Delta(f), \{z \mid f(z) = 1\})$
$f \cdot g, f + g$	$\min(\Delta(f), \Delta(g))$
$f/g$	$\min(\Delta(f), \Delta(g), \{z \mid g(z) = 0\})$
$f^{-\alpha}, \alpha \in \mathbb{R}^+$	$\min(\Delta(f), \{z \mid f(z) = 0\})$

# Dominant singularities

Sometimes there are several dominant singularities (there might even be an infinite number!)  $\implies$  periodic fluctuations, cancellations of the main exponential growth, irregular oscillating behaviors ...

## Example

$$A(z) = \sum_{n \geq 0} (-1)^n z^{2n} = 1 - z^2 + z^4 - z^6 + z^8 \dots$$

$$B(z) = \sum_{n \geq 0} z^{3n} = 1 + z^3 + z^6 + \dots$$

$$[z^n]A(z) + B(z) = \begin{cases} 0 & \text{if } 2 \nmid n \text{ and } 3 \nmid n, \text{ or } n = 6m, m \text{ odd} \\ \neq 0 & \text{otherwise} \end{cases}$$

$A(z) + B(z)$  has dominant singularities at  $z = \pm i$  and the cubic roots of unity  $z = 1, z = e^{\frac{2\pi i}{3}}, z = e^{\frac{4\pi i}{3}}$ ; all of modulus 1.



# Inverse functions

In many instances, we do not have explicit forms for GFs, but only functional equations they satisfy, e. g., the tree function  $\hat{T}(z) = ze^{\hat{T}(z)}$  that counts Cayley trees.

Given a function  $\phi$  analytic at  $y_0$  and  $z_0 = \phi(y_0)$ , what is the behavior of its inverse, that is, the solution  $y(z)$  of the equation  $z = \phi(y(z))$ ?

## Lemma (Analytic Inversion)

*Let  $\phi$  analytic at  $y_0$  and  $z_0 = \phi(y_0)$ . Assume  $\phi'(y_0) \neq 0$ . Then there exists a function  $y(z)$  which is analytic in a small neighborhood of  $z_0$  such that  $\phi(y(z)) = z$  and  $y(z_0) = y_0$ .*

Solutions to systems of equations stemming from admissible combinatorial specifications are analytic in a neighborhood of the origin.

## Theorem (Implicit Function Theorem)

*The system of  $n$  equations*

$$\vec{y}(z) = \vec{\Phi}(z, \vec{y}(z))$$

*admits an analytic solution at  $z_0$  if*

- 1  $\vec{\Phi}(z, \vec{y})$  is analytic (in  $n + 1$  variables) at  $(z_0, \vec{y}_0)$  with  $\vec{y}_0 = \vec{y}(z_0)$ .
- 2  $\vec{\Phi}(z_0, \vec{y}_0) = \vec{y}_0$  and  $\det(I - \frac{\partial \vec{\Phi}}{\partial \vec{y}}) \neq 0$  at  $(z_0, \vec{y}_0)$

## Example

$$\hat{T}(z) = ze^{\hat{T}(z)}$$

Here,  $y(z) \equiv \hat{T}(z)$  and  $\Phi(z, y) = ze^y$ . take  $z_0 = 0$ . The conditions of the theorem hold, in particular,  $1 - ze^y \neq 0$  at  $z = 0$ . Actually, the only singularity occurs when  $1 - ze^y = 1 - y = 0$ , that is,  $y = 1$ , hence  $z = e^{-1}$  and

$$T_n = \# \text{ of Cayley trees of size } n \\ \asymp n!e^n$$

# Complex integration

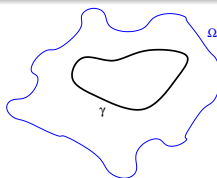
## Theorem

If  $f(z)$  is analytic in  $\Omega$  and  $\gamma$  is a simple closed path in  $\Omega$  then

$$\int_{\gamma} f(z) dz = 0$$

Furthermore for any two homotopic paths  $\gamma_1$  and  $\gamma_2$  (we can continuously deform one into the other inside  $\Omega$ ) then

$$\int_{\gamma_1} f(z) dz = \int_{\gamma_2} f(z) dz$$



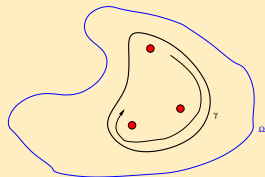
# Residue Theorem

## Theorem

If  $f$  is meromorphic in  $\Omega$  and  $\gamma$  is a simple closed path that encircles clockwise and only once the poles  $\alpha_1, \dots, \alpha_k$  of  $f(z)$  then

$$\int_{\gamma} f(z) dz = 2\pi i \sum_j \text{Res}(f; \alpha_j)$$

## Sketch of the proof



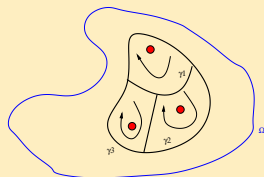
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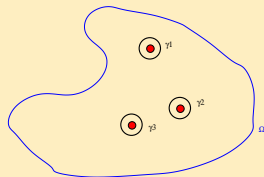
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## Sketch of the proof



## Sketch of the proof (cont'd)

$$\begin{aligned}\int_{\gamma} f(z) dz &= \sum_j \int_{\gamma_j} f(z) dz = \sum_j \int_{\gamma_j} \sum_{n \geq M_j} f_{n,j} (z - \alpha_j)^n dz \\ &= \sum_j \left[ \sum_{\substack{n \geq M_j \\ n \neq -1}} f_{n,j} \int_{\gamma_j} (z - \alpha_j)^n dz + f_{-1,j} \int_{\gamma_j} \frac{dz}{z - \alpha_j} \right] \\ &= \sum_j \left[ \sum_{\substack{n \geq M_j \\ n \neq -1}} f_{n,j} \frac{(z - \alpha_j)^{n+1}}{n+1} \Big|_{\gamma_j} + f_{-1,j} \int_{\gamma_j} \frac{dz}{z - \alpha_j} \right]\end{aligned}$$



# Residue Theorem

## Sketch of the proof (cont'd)

$$\begin{aligned}\int_{\gamma} f(z) dz &= \sum_j \int_{\gamma_j} f(z) dz = \sum_j \int_{\gamma_j} \sum_{n \geq M_j} f_{n,j} (z - \alpha_j)^n dz \\ &= \sum_j \left[ \sum_{\substack{n \geq M_j \\ n \neq -1}} f_{n,j} \int_{\gamma_j} (z - \alpha_j)^n + f_{-1,j} \int_{\gamma_j} \frac{dz}{z - \alpha_j} \right] \\ &= \sum_j \left[ \underbrace{\sum_{\substack{n \geq M_j \\ n \neq -1}} f_{n,j} \frac{(z - \alpha_j)^{n+1}}{n+1} \Big|_{\gamma_j}}_{=0} + f_{-1,j} \int_{\gamma_j} \frac{dz}{z - \alpha_j} \right]\end{aligned}$$

# Residue Theorem

## Sketch of the proof (cont'd)

$$\begin{aligned}\int_{\gamma} f(z) dz &= \sum_j \int_{\gamma_j} f(z) dz = \sum_j \int_{\gamma_j} f_{-1,j} \frac{dz}{z - \alpha_j} \\ &= \sum_j \operatorname{Res}(f; \alpha_j) \int_{\gamma_j} \frac{dz}{z - \alpha_j} = \sum_j \operatorname{Res}(f; \alpha_j) \int_0^{2\pi} i d\theta \\ &= 2\pi i \sum_j \operatorname{Res}(f; \alpha_j)\end{aligned}$$

We take each  $\gamma_j$  a circle centered at  $\alpha_j$  of radius  $r$  small enough;  
 $z = \alpha_j + re^{i\theta}$ ,  $dz = ire^{i\theta} d\theta$

# Cauchy's formula

## Theorem

If  $f(z)$  is analytic in a region  $\Omega$  enclosing the origin, then for any simple closed curve inside  $\Omega$  that encircles clockwise and only once the origin

$$f_n = [z^n]f(z) = \frac{1}{2\pi i} \oint f(z) \frac{dz}{z^{n+1}}$$

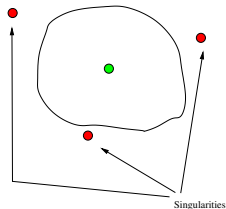
## Proof.

- $f(z)/z^{n+1}$  is meromorphic in  $\Omega$  with a pole of order 1 at  $z = 0$
- $\text{Res}(f(z)/z^{n+1}; z = 0) = f_n$
- Apply Residue Theorem



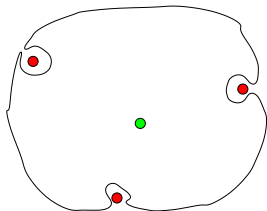
# Applying Cauchy's formula

The idea is to extend the contour of integration so that the integral can be approximated by the behavior of the integrand very close to the singularities and the rest  $\rightarrow 0$



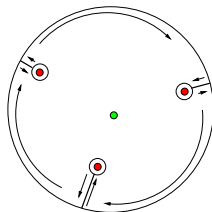
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## Cauchy's formula and surjections

$$\hat{S}(z) = \frac{1}{2 - e^z}$$

The dominant singularity is  $z = \log 2 \approx 0.69314$

At this singularity, one finds

$$\hat{S}(z) \sim -\frac{1}{2} \times \frac{1}{z - \log 2}$$

Take as Cauchy contour a circle centered at the origin and of radius  $\log 2 + \epsilon$ .

We get

$$S_n \equiv n![z^n]\hat{S}(z) \sim \frac{n!}{2} \left(\frac{1}{\log 2}\right)^{n+1}$$

# Singularity Analysis

The plan:

- 1 Locate the dominant singularity\*
- 2 Obtain a local expansion of  $f(z)$  near the singularity
- 3 Transfer the asymptotic estimate of  $f(z)$  to coefficients

\* We will consider here the case of a single dominant singularity here. The techniques generalize to multiple dominant singularities.



## Example

- Cayley Trees with functional equation  $T(z) = ze^{T(z)}$ . The dominant (algebraic) singularity of  $\hat{T}(z)$  is at  $z = e^{-1}$
- Near  $z = e^{-1}$ ,

$$\hat{T}(z) \sim 1 - \sqrt{2 - 2ez} + \frac{2}{3}(1 - ez) + O((1 - ez)^{3/2})$$

- **Preview:**  $\hat{T}(z)$  behaves like  $\sqrt{1 - z}$  near the singularity; this transfers to a subexponential growth  $n^{-3/2}$

$$T_n = n![z^n]\hat{T}(z) \sim n! \cdot \frac{e^n}{\sqrt{2\pi}} n^{-3/2} (1 + O(1/n))$$

Using  $n! \sim n^n e^{-n} \sqrt{2\pi n}$ , we get

$$T_n \sim n^{n-1} \quad \text{Not too bad}$$

# Transfer lemma

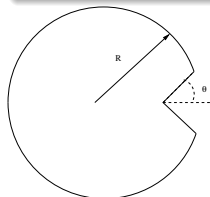
## Lemma (Flajolet, Odlyzko)

Let  $z = 1$  be the dominant singularity of  $f(z)$ , with  $f(z)$  analytic in the region  $\Omega(R, \theta)$ ,  $R > 1$  (see figure). If

$$f(z) \sim (1 - z)^{-\alpha} \log^{\beta} \frac{1}{1 - z}, \quad z \rightarrow 1$$

for some  $\alpha \notin \{-1, -2, -3, \dots\}$ , then

$$f_n = [z^n]f(z) = \frac{n^{\alpha-1}}{\Gamma(\alpha)} \log^{\beta} n \left(1 + O\left(\frac{1}{n}\right)\right)$$



# Singularity Analysis

- Similar results hold when we have  $O(\cdot)$  and  $o(\cdot)$  estimates of  $f(z)$  near  $z = 1$ .
- Furthermore, the complete version of the transfer lemma yields full asymptotic expansions of  $f_n$
- Other slow growing factors, e. .g.,  $(\log \log(1/(1 - z)))^\gamma$  can also be taken into account  
 $((\log \log(1/(1 - z))))^\gamma \rightarrow (\log \log n)^\gamma$
- There's a generalization to cope with any fixed number of dominant singularities
- If the dominant singularity of  $f(z)$  is located at  $z = \rho$ , the lemma can be applied with  $g(z) = f(z/\rho)$ , since  $[z^n]f(z) = \rho^{-n}[z^n]g(z)$  and  $g(z)$  has its dominant singularity at  $z = 1$

## Example

The OGF of binary trees is  $B(z) = (1 - \sqrt{1 - 4z})/2z$ .

The dominant singularity is at  $z = 1/4$ .

Locally around  $z \rightarrow 1/4$ ,

$$B(z) \sim -2\sqrt{1 - 4z}$$

Applying the transfer lemma with  $\alpha = -1/2$ , yields

$$B_n \sim 4^n \frac{n^{-3/2}}{\sqrt{\pi}} (1 + O(1/n))$$

## Example

The recurrence for the expected cost of partial matches in relaxed  $K$ -d trees is

$$P_n = 1 + \frac{s}{K} \frac{2}{n} \sum_{0 \leq k < n} \frac{k}{n} P_k + \left(1 - \frac{s}{K}\right) \frac{2}{n} \sum_{0 \leq k < K} P_k,$$

where  $0 < s < K$ , and  $P_0 = 0$ .

Multiplying both sides by  $z^n$  and summing over all  $n \geq 0$ , the recurrence translates to a second-order linear differential equation

$$zP''(z) - 2\frac{2z-1}{1-z}P'(z) - 2\frac{2-x-z}{(1-z)^2}P(z) = 2\frac{1}{(1-z)^3}$$

for  $P(z) = \sum_{n \geq 0} P_n z^n$  and  $x = s/K$ ; the initial conditions are  $P(0) = 0$  and  $P'(0) = 1$ .

## Example (cnt'd)

The ODE can be solved in this case, because it is hypergeometric; this yields

$$P(z) = \frac{1}{1-x} \left( \frac{{}_2F_1([a, b, 2]; z)}{(1-z)^{-\alpha}} - \frac{1}{1-z} \right),$$

where  ${}_2F_1(\cdot)$  is the hypergeometric function,  $a = 2 - \alpha$ ,  $b = 1 - \alpha$  and  $\alpha = (1 + \sqrt{9 - 8x})/2$ .

The dominant singularity of  $P(z)$  is at  $z = 1$ , since the hypergeometric function is analytic there. Then, as  $z \rightarrow 1$

$$P(z) \sim \frac{1}{1-x} {}_2F_1([a, b, 2]; 1)(1-z)^{-\alpha}$$

## Example (cnt'd)

Finally, applying the transfer lemma

$$P_n \sim \frac{1}{(1-x)\Gamma(\alpha)} {}_2F_1([a, b, 2]; 1) n^{\alpha-1}$$

For any value of  $x = s/K \in (0, 1)$ ,  $1 \leq \alpha \leq 2$ ; furthermore,  $\alpha - 1 \geq 1 - x$  for all  $x \in [0, 1]$ .

What if  $f(z)$  has no singularities?

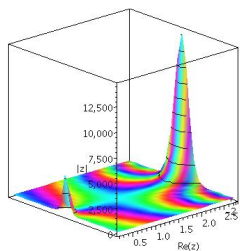
Saddle point methods estimate contour integrals by choosing a circle centered at the origin and passing through a **saddle point**

## Definition

A saddle point  $z_0$  of  $f(z)$  is a point such that  $f(z_0) \neq 0$  and  $f'(z_0) = 0$



# Saddle point methods



A plot of  $\left| \frac{\hat{S}(z)}{z^5} \right|$ , with  $\hat{S}(z) = \exp(\exp(z) - 1)$  (EGF of set partitions)

The “small” peak at the left is actually the singularity at  $z = 0$ ; the “peak” to the right is due to the rapid variation of the function

## Saddle point methods

Suppose  $f(z)$  has non-negative coefficients and it is *entire* (analytic in  $\mathbb{C}$ )

Take  $\exp(h(z)) = f(z)/z^{n+1}$ . Then the saddle point occurs at  $\zeta_n$  such  $h'(\zeta_n) = 0$ , that is,

$$\zeta_n \frac{f'(\zeta_n)}{f(\zeta_n)} = n + 1$$

Under suitable conditions we can use the expansion

$h(z) = h(\zeta_n) + 1/2 h''(\zeta_n)(z - \zeta_n)^2 + O((z - \zeta_n)^3)$  on a local neighborhood of  $\zeta_n$  and integrate termwise Cauchy's integral

$$\begin{aligned} f_n &\sim \frac{1}{2\pi i} \left( \exp(h(\zeta_n)) + \int_{\gamma^{(0)}} \exp \left[ \frac{1}{2} h''(\zeta_n)(z - \zeta_n)^2 \right] dz \right. \\ &\quad \left. + \int_{\gamma^{(1)}} \exp(h(z)) dz \right) \\ &\sim \frac{f(\zeta_n)}{\zeta_n^{n+1} \sqrt{2\pi h''(\zeta_n)}} \end{aligned}$$

## Example

Consider  $f(z) = \exp(z)$ . Then  $[z^n]f(z) = 1/n!$ . The saddle point method can be applied to  $f(z)$ , with  $h(z) = z - (n+1)\log z$ ,  $h'(z) = 1 - \frac{n+1}{z}$  and  $h''(z) = (n+1)/z^2$ .

The saddle point is at  $\zeta = n+1$ . Hence we get the estimate

$$\frac{1}{n!} \sim \frac{e^{n+1}}{(n+1)^n \sqrt{2\pi(n+1)}}$$

Since  $(1 + 1/n)^n \sim e$ ,

$$n! \sim e^{-n} n^n \sqrt{2\pi n}$$

## Example

The EGF of set partitions is  $\hat{S}(z) = \exp(\exp(z) - 1)$ . Hence,  $h(z) = e^z - 1 - (n + 1) \log z$  and the saddle point occurs at  $\zeta$ , the solution of  $\zeta e^\zeta = n + 1$ .

$$\zeta = \log n - \log \log n + o(1)$$

But we have

$$B_n = n! \cdot [z^n] \hat{S}(z) \sim \frac{n^n e^{e^\zeta - 1 - n}}{\zeta^{n+1/2}}$$

since the asymptotic estimate of  $\zeta$  cannot be used to get an asymptotic estimate of  $B_n$

However, taking  $\log$ 's

$$\frac{1}{n} \log B_n = \log n - \log \log n + O(1)$$