Multivariate Algebraic Generating Functions: Asymptotics and Examples

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Generating Functions

Consider a closed-form generating function F for a multidimensional array $\{a_{n_1,n_2,\ldots,n_d}\}$:

$$F(\mathbf{z}) = \sum_{n_1,n_2,\ldots,n_d} a_{n_1,n_2,\ldots,n_d} z_1^{n_1} \cdots z_d^{n_d}$$

Goal: Extract information about $\{a_{\mathbf{n}}\}$ as the indices approach infinity.

Tool: Singularity Analysis

- The location of singularities of F will determine the exponential decay of $[\mathbf{z^n}]F(\mathbf{z})$.
- The behavior of F near the singularities determines the subexponential behavior.

Algebraic Singularities

Generating functions with algebraic singularities common.

- Catalan numbers
- SCFGs, Enumerating RNA secondary structures
- Random colorings in K_n

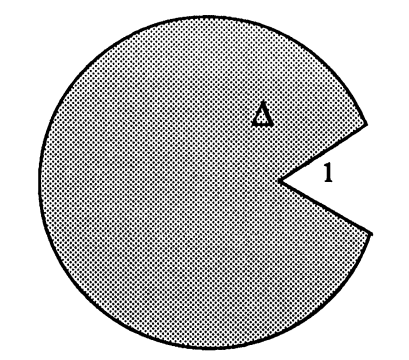
Previous Results

- Flajolet & Odlyzko (1990) analyzed a large class of univariate algebraic generating functions.
- Gao and Richmond (1992) and Hwang (1996) extended FO results to restricted classes of bivariate functions.
- Drmota (1997) and others looked at distributional results.
- Today: asymptotics for a broad class of algebraic singularities, via the multivariate Cauchy integral formula and Pemantle and Wilson techniques.

Univariate Generating Functions: Example Theorem

Theorem

(Flajolet & Odlyzko, 1990.) Consider a generating function F with $F(z) = O(|1 - z|^{\alpha})$ as $z \to 1$. If F is analytic in the region below, then $[z^n]F(z) = O(n^{-\alpha-1})$.



Proof

- Cauchy Integral Formula:

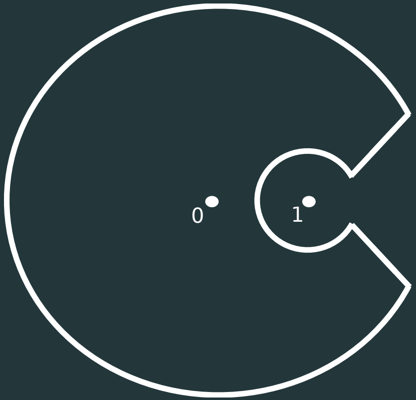
$$[z^n]F(z) = \frac{1}{2\pi i} \int_{\mathcal{C}} F(z) z^{-n-1} dz$$

- Since $F(z) = O(|1-z|^{\alpha})$, compare:

$$\frac{1}{2\pi i} \int_{\mathcal{C}} F(z) z^{-n-1} dz \quad \text{versus} \quad \frac{1}{2\pi i} \int_{\mathcal{C}} (1-z)^{\alpha} z^{-n-1} dz$$

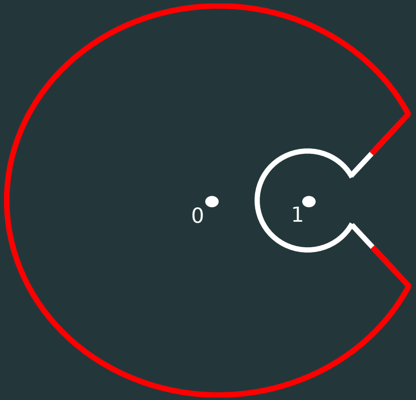
$$\frac{1}{2\pi i}\int_{\mathcal{C}} F(z)z^{-n-1}dz \quad \text{versus} \quad \frac{1}{2\pi i}\int_{\mathcal{C}} (1-z)^{\alpha}z^{-n-1}dz$$

Expand $\mathcal{C}$ to the contour below:



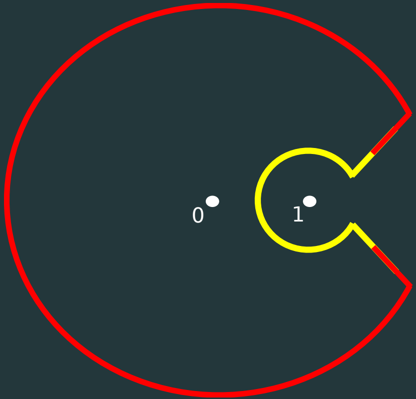
$$\frac{1}{2\pi i}\int_{\mathcal{C}} F(z) z^{-n-1} dz \quad \text{versus} \quad \frac{1}{2\pi i}\int_{\mathcal{C}} (1-z)^{\alpha} z^{-n-1} dz$$

Both are small away from 1.



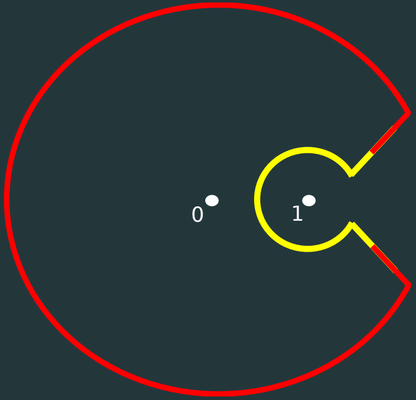
$$\frac{1}{2\pi i}\int_{\mathcal{C}} F(z) z^{-n-1} dz \quad \text{versus} \quad \frac{1}{2\pi i}\int_{\mathcal{C}} (1-z)^{\alpha} z^{-n-1} dz$$

$(1-z)^{\alpha}$ dominates near 1.



$$\frac{1}{2\pi i}\int_{\mathcal{C}} F(z) z^{-n-1} dz \quad \text{versus} \quad \frac{1}{2\pi i}\int_{\mathcal{C}} (1-z)^{\alpha} z^{-n-1} dz$$

Comparing the integrals shows $[z^n]F(z) = O(n^{-\alpha-1})$.



Multivariate Generating Functions with Algebraic Singularities

Start with:

$$H(\mathbf{x})^{-\beta} = \sum_{\mathbf{r} \geq 0} a_{\mathbf{r}} \mathbf{x}^{\mathbf{r}}$$

Can we estimate $a_{\mathbf{r}}$ as $\mathbf{r}$ approaches infinity, such that $\mathbf{r} \approx s \cdot \lambda$ for some $\lambda \in \mathbb{R}_+^d$ as $s \to \infty$? As before,

- The location of singularities of H will determine the exponential behavior of the coefficients.
- The behavior of H near the singularities determines the subexponential behavior.

Smooth critical points

- Determining relevant singularities of H more complicated for multivariate generating functions.
- We restrict to "smooth minimal critical points" $\mathbf{p}$ where:

1. For coefficients $a_{\mathbf{r}}$ as $\mathbf{r} = s\lambda$ with $s \to \infty$,

$$\begin{aligned}
\lambda_2 x_1 H_{x_1} &= \lambda_1 x_2 H_{x_2} \\
\lambda_3 x_1 H_{x_1} &= \lambda_1 x_3 H_{x_3} \\
&\vdots \\
\lambda_n x_1 H_{x_1} &= \lambda_1 x_n H_{x_n}
\end{aligned}$$

2. $H_{x_1}(\mathbf{p}) \neq 0$
3. No other singularities of H are closer to the origin than $\mathbf{p}$.

Result

Theorem (G.)

Let $H(\mathbf{x})$ have a smooth, minimal critical point, $\mathbf{p}$. Then, as $\mathbf{r}$ approaches infinity with $\frac{r_i}{r_j} = \frac{\lambda_i}{\lambda_j} + O(1)$ for a constant vector λ and all $1 \leq i \leq j \leq d$,

$$[\mathbf{x}^{\mathbf{r}}]\, H(\mathbf{x})^{-\beta} \sim \left(\frac{1}{2\pi i}\right)^{d-1} \mathbf{p}^{-\mathbf{r}-\mathbf{1}} \left[\frac{r_1^{\beta-1} p_1}{\Gamma(\beta)} \left\{(-H_{x_1}(\mathbf{p})p_1)^{-\beta}\right\}_P e^{-\beta(2\pi i\omega)}\right] \times \left[\frac{\left(\frac{\lambda_1}{r_1}\pi\right)^{\frac{d-1}{2}}}{\sqrt{\det\left(\frac{1}{2}\mathcal{H}\right)}}\right]$$

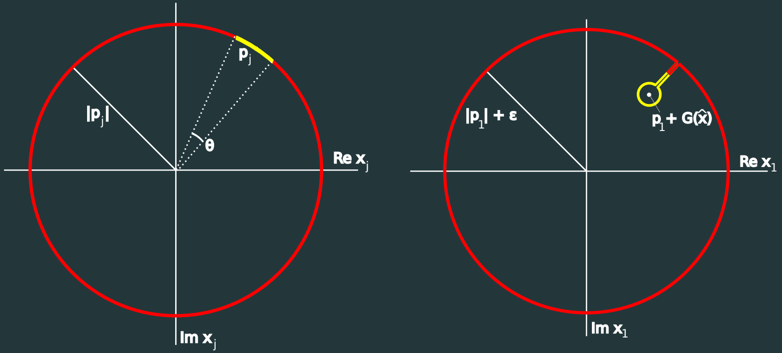
$\mathcal{H}$ is the Hessian of a $(d-1)$-dimensional phase function describing the zero set of H near $\mathbf{p}$.

Proof Overview

$$\left(\frac{1}{2\pi i}\right)^d \int_T H(\mathbf{x})^{-\beta} \mathbf{x}^{\mathbf{r}-1} d\mathbf{x}$$

- Determine how to expand the torus, T, using Flajolet-Odlyzko as motivation.
- Manipulate $H(\mathbf{x})$ to approximate the integral as a product of a univariate integral and a $(d-1)$-dimensional Fourier-Laplace integral.
- Estimate the remaining integrals.

Expanding the Torus



$G(\widehat{\mathbf{x}})$ is a parameterization of the zero set of H near $\mathbf{p}$.

Approximating $H(\mathbf{x})^{-\beta}$

Rewrite H as a power series near $\mathbf{p}$:

$$H(\mathbf{x}) = \sum_{\mathbf{r}} b_{\mathbf{r}}(\mathbf{x} - \mathbf{p})^{\mathbf{r}}$$

As long as $b_{\mathbf{r}} = 0$ for all $\mathbf{r}$ with $|\mathbf{r}| \leq 2$ except for coefficients corresponding to $x_1 - p_1$ and $(x_1 - p_1)(x_j - p_j)$, H can be approximated by a function in x_1 alone.

Change of Variables

Choose the change of variables:

$$\begin{aligned} u_1 &= x_1 + \sum_{j=2}^{d} k_j(x_j - p_j) + \sum_{j=2}^{d} q_j(x_j - p_j)^2 \\ &\quad + \sum_{2 \le j < \ell \le d} m_{j,\ell}(x_j - p_j)(x_\ell - p_\ell) \\ u_j &= x_j \text{ for } 2 \le j \le d \end{aligned}$$

k_j, q_j, and $m_{j,\ell}$ are constants in terms of the derivatives of H at $\mathbf{p}$.

The Integral after the Change of Variables

After applying the change of variables, we can show

$$\int_T H(\mathbf{x})^{-\beta}\mathbf{x}^{\mathbf{r}-1}d\mathbf{x}$$

is approximately

$$\int_{\mathcal{C}_\ell} [H_{x_1}(\mathbf{p})(u_1 - p_1)]^{-\beta}\left[1 - \frac{\psi(\widehat{\mathbf{u}})}{p_1}\right]^{-r_1-1} \mathbf{u}^{-\mathbf{r}-\mathbf{1}}\,\mathrm{d}\mathbf{u}$$

Here, $\psi(\widehat{\mathbf{u}})$ is related to a phase function and defined by

$$\psi(\widehat{\mathbf{u}}) = \sum_{j=2}^{d-1} k_j(u_j - p_j) + \sum_{j=2}^{d-1} q_j(u_j - p_j)^2 + \sum_{2\leq j<\ell\leq d} m_{j,\ell}(u_j - p_j)(u_\ell - p_\ell)$$

The Remaining Integrals

$$\int_U [H_{x_1}(\mathbf{p}) \cdot (u_1 - p_1)]^{-\beta} u_1^{-r_1-1}\, du$$

is a univariate Cauchy integral representing a binomial coefficient, approximated by:

$$\frac{2\pi i}{\Gamma(\beta)} r_1^{\beta-1} p_1^{-r_1} \left\{ (-H_x(\mathbf{p}) p_1)^{-\beta} \right\}_P e^{-\beta(2\pi i \omega)}$$

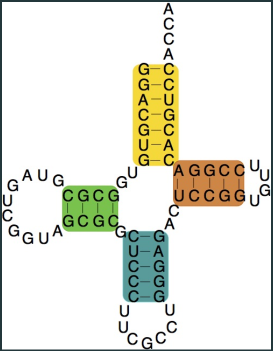
$$\iint_V \left[1 - \frac{\psi(\widehat{\mathbf{u}})}{p_1} \right]^{-r_1-1} \widehat{\mathbf{u}}^{-\widehat{\mathbf{r}}-\widehat{\mathbf{1}}}\, \mathrm{d}\widehat{\mathbf{u}}$$

is a Fourier-Laplace type integral. From Pemantle & Wilson, we can approximate by:

$$\widehat{\mathbf{p}}^{-\widehat{\mathbf{r}}-\widehat{\mathbf{1}}} \frac{\left(\frac{\lambda_1 \pi}{r_1}\right)^{\frac{d-1}{2}}}{\sqrt{\det\left(\frac{1}{2}\mathcal{H}\right)}}$$

Application: RNA Secondary Structures

RNA secondary structures reveal valuable functional information about RNA molecules.



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Stochastic Context Free Grammars for Secondary Structures

Knudsen-Hein 1999 Grammar:

S	$\rightarrow$	LS	with probability	p_1
		L	with probability	q_1
F	$\rightarrow$	(F)	with probability	p_2
		LS	with probability	q_2
L	$\rightarrow$	$.$	with probability	p_3
		(F)	with probability	q_3

Converting KH99 to Probability Generating Functions

- Find the GF, $S(x_1, x_2, x_3) = \sum_{n=0}^{\infty} p(n_1, n_2, n_3) x_1^{n_1} x_2^{n_2} x_3^{n_3}$
  - $p(n_1, n_2, n_3)$: probability of producing a structure with n_1 nucleotides, n_2 base pairs, and n_3 helices

- Production rules become recursions. For example, the rules,

$$\begin{array}{llll} F & \rightarrow & (F) & \text{with probability} \quad p_2 \\ & & LS & \text{with probability} \quad q_2, \end{array}$$

  become

$$F = p_2 x_1^2 x_2 x_3 F + q_2 LS.$$

KH99 Generating Function

Solving yields

$$S(\mathbf{x}) \quad = \quad \frac{p_1p_3q_2x_2x_1^3 - p_3x_2x_1^2 - p_1q_2x_1 + 1}{2p_2q_3x_1^2x_2x_3} - \frac{\sqrt{H(\mathbf{x})}}{2p_2q_3x_1^2x_2x_3}$$

where

$$H(\mathbf{x}) = (p_3x_1^2x_2 - 1)\times$$
$$(p_1^2p_3q_2^2x_1^4x_2 + 4p_2q_1q_2q_3x_1^3x_2x_3 - 2p_1p_3q_2x_1^3x_2 - p_1^2q_2^2x_1^2 + p_3x_1^2x_2 + 2p_1q_2x_1 - 1).$$

Heitsch and Poznanović used these methods to find distributions of single features.

Critical Points

The asymptotics are often controlled by a smooth minimal critical point, and the results from before apply. For example, let us choose $p_1 = p_2 = p_3 = \frac{1}{4}$ and $\lambda = (6, 2, 1)$.

- This approximates the probability of structures where there are six times as many nucleotides as helices, and twice as many base pairs as helices.
- Using the smooth critical point equations,

$$H = 0, \quad 2x_1 H_{x_1} = x_2 H_{x_2}, \quad 6x_1 H_{x_1} = x_3 H_{x_3}$$

  yields the critical point, $\left(\frac{16}{9}, \frac{81}{128}, \frac{4}{27}\right)$.

Asymptotics

Plugging into the asymptotic formula yields:

$$\left[x_1^{r_1}x_2^{r_2}x_3^{r_3}\right]\sqrt{H} \sim -\frac{64}{\pi^{3/2}r_1^{5/2}}\left(\frac{16}{9}\right)^{-r_1-1}\left(\frac{81}{128}\right)^{-r_2-1}\left(\frac{4}{27}\right)^{-r_2-1}$$

as r_1, r_2, and r_3 approach infinity in the ratio $6:2:1$. For $(r_1, r_2, r_3) = (60, 20, 10)$, the ratio of the approximation to the exact coefficient of H is 1.056.

We can plug this approximation back into the formula for S to approximate the probabilities we want.

Future Research

Analytic Combinatorics:

- Can the results be rewritten in a coordinate-free way?
- What about more general types of algebraic singularities?
- How about non-smooth points?

RNA:

- How well can this approach handle all directions λ and all probabilities p_1, p_2, p_3 simultaneously?
- Can we understand what types of rules control which types of features?