Diagonals: Combinatorics, Asymptotics and Computer Algebra

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Inria & ENS de Lyon

aofa2017

June 19-23, Princeton, USA

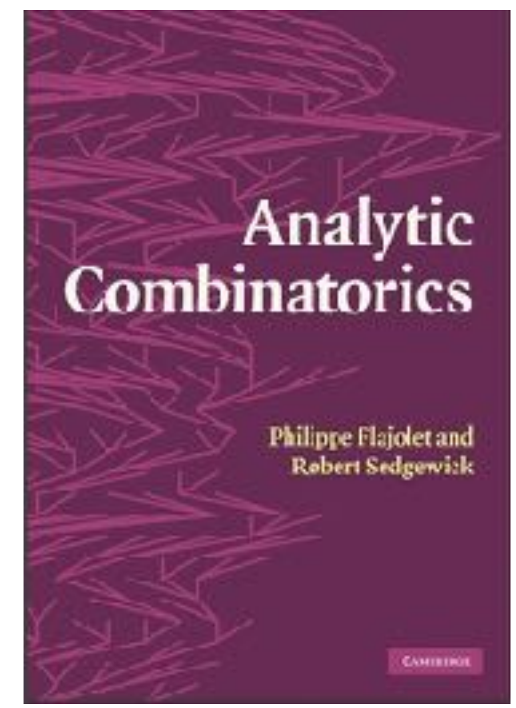
Families of Generating Functions

$$(a_n) \mapsto A(z) := \sum_{n\geq 0} a_n z^n$$

counts the number of objects of size *n*

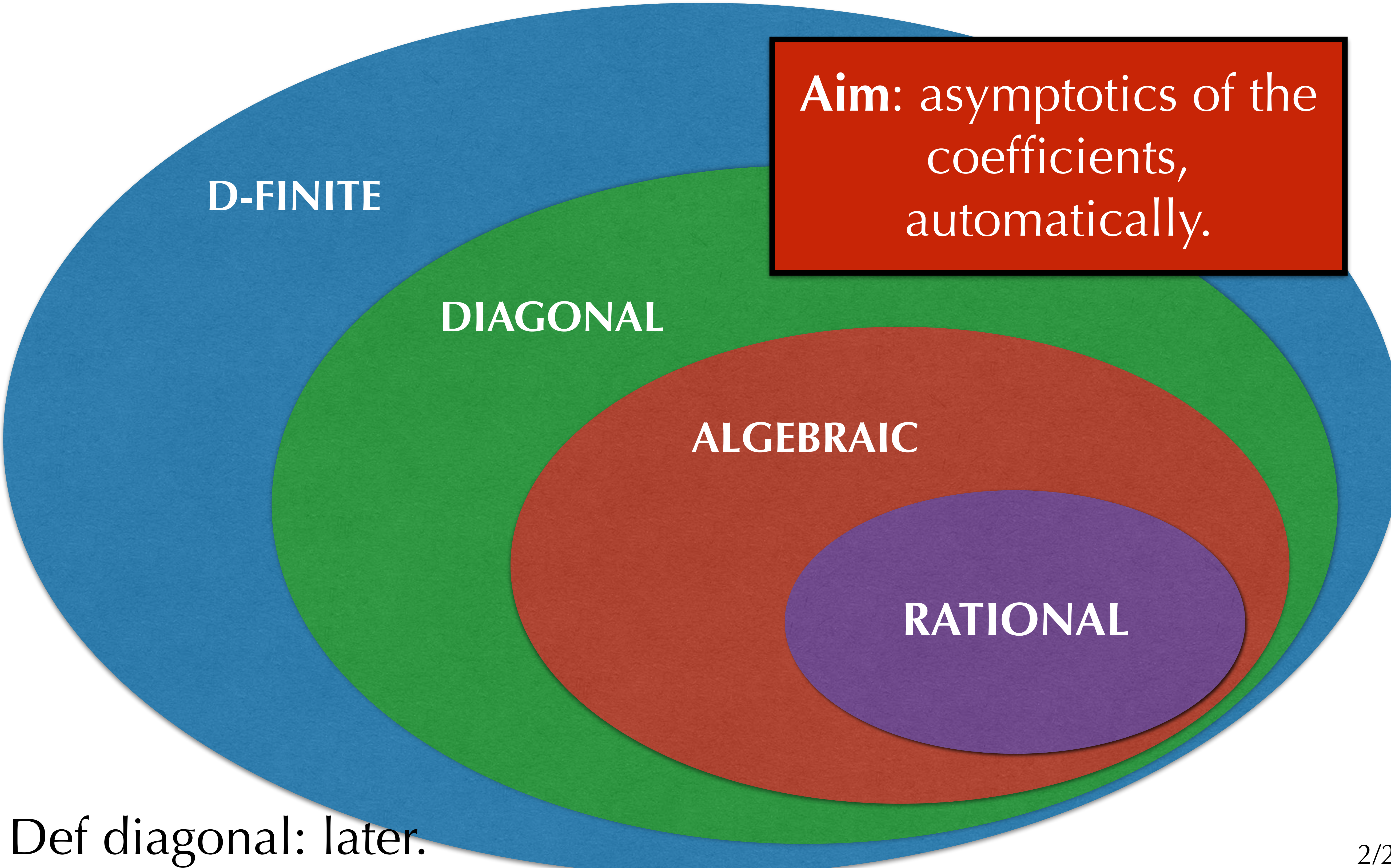
captures some structure

If (a_n)	**then A(z) is**
. counts the number of words of length *n* in a regular language	rational
. in a nonambiguous context-free language	algebraic (*satisfies a polynomial equation* P(z,A)=0)
. satisfies a linear recurrence with polynomial coefficients	differentially finite (*satisfies a LDE with polynomial coefficients*)



hundreds of examples

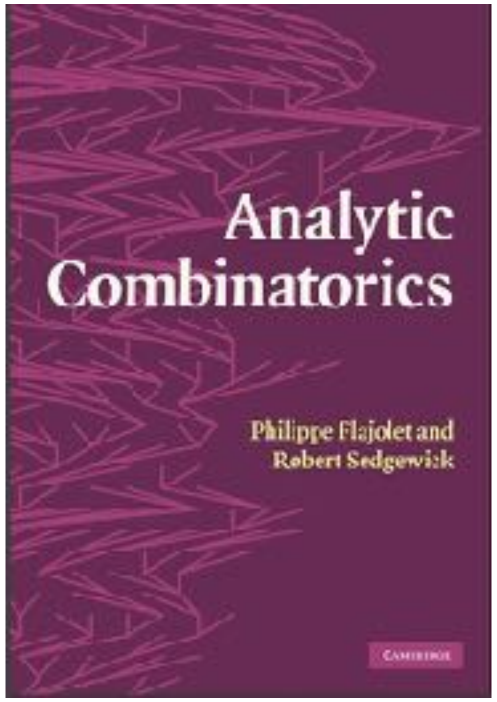
Univariate Generating Functions



Aim: asymptotics of the coefficients, automatically.

Def diagonal: later.

I. A Quick Review of Analytic Combinatorics in One Variable

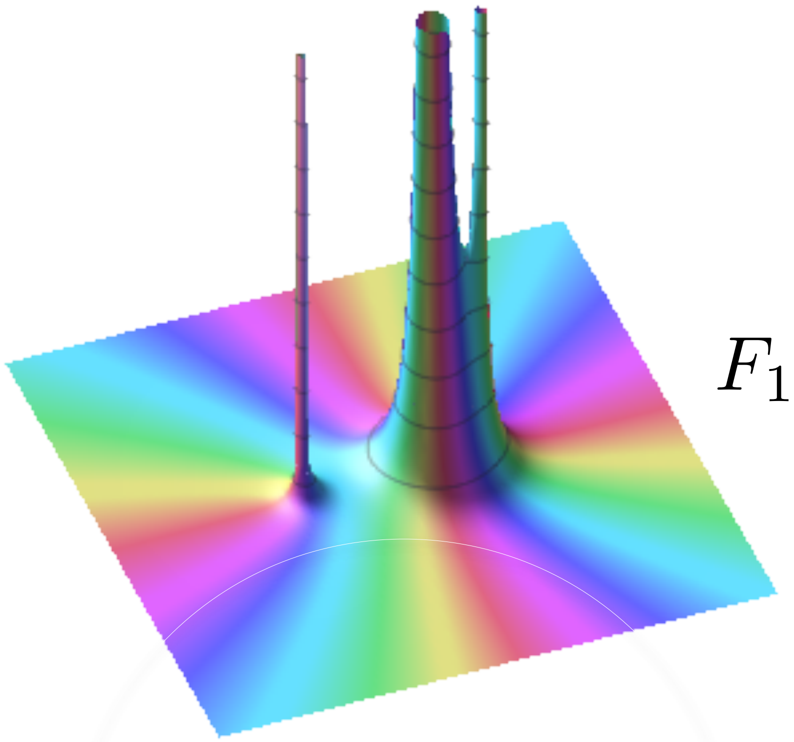


Principle:

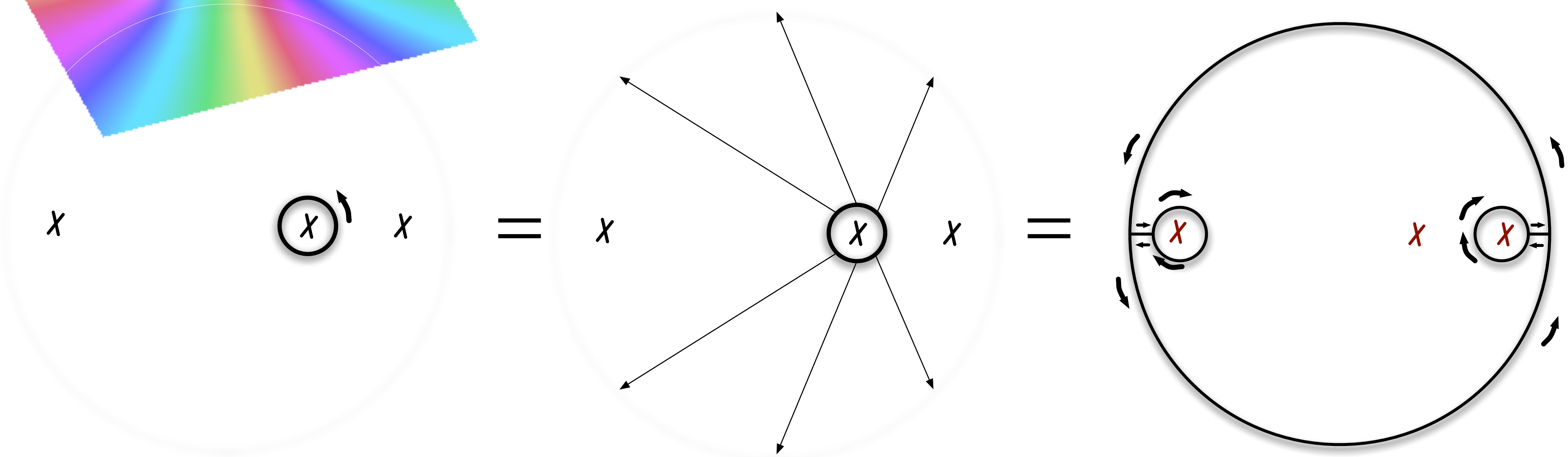
Dominant singularity $\longleftrightarrow$ *exponential behaviour*
local behaviour $\longleftrightarrow$ *subexponential terms*

Coefficients of Rational Functions

$$a_n = \frac{1}{2\pi i}\int_\gamma \frac{f(z)}{z^{n+1}}dz$$



$$F_1 = 1 = \frac{1}{2\pi i}\oint \frac{1}{1-z-z^2}\frac{dz}{z^2}$$



As n increases, the smallest singularities dominate.

$$F_n = \frac{\phi^{-n-1}}{1+2\phi} + \frac{\overline{\phi}^{-n-1}}{1+2\overline{\phi}}$$

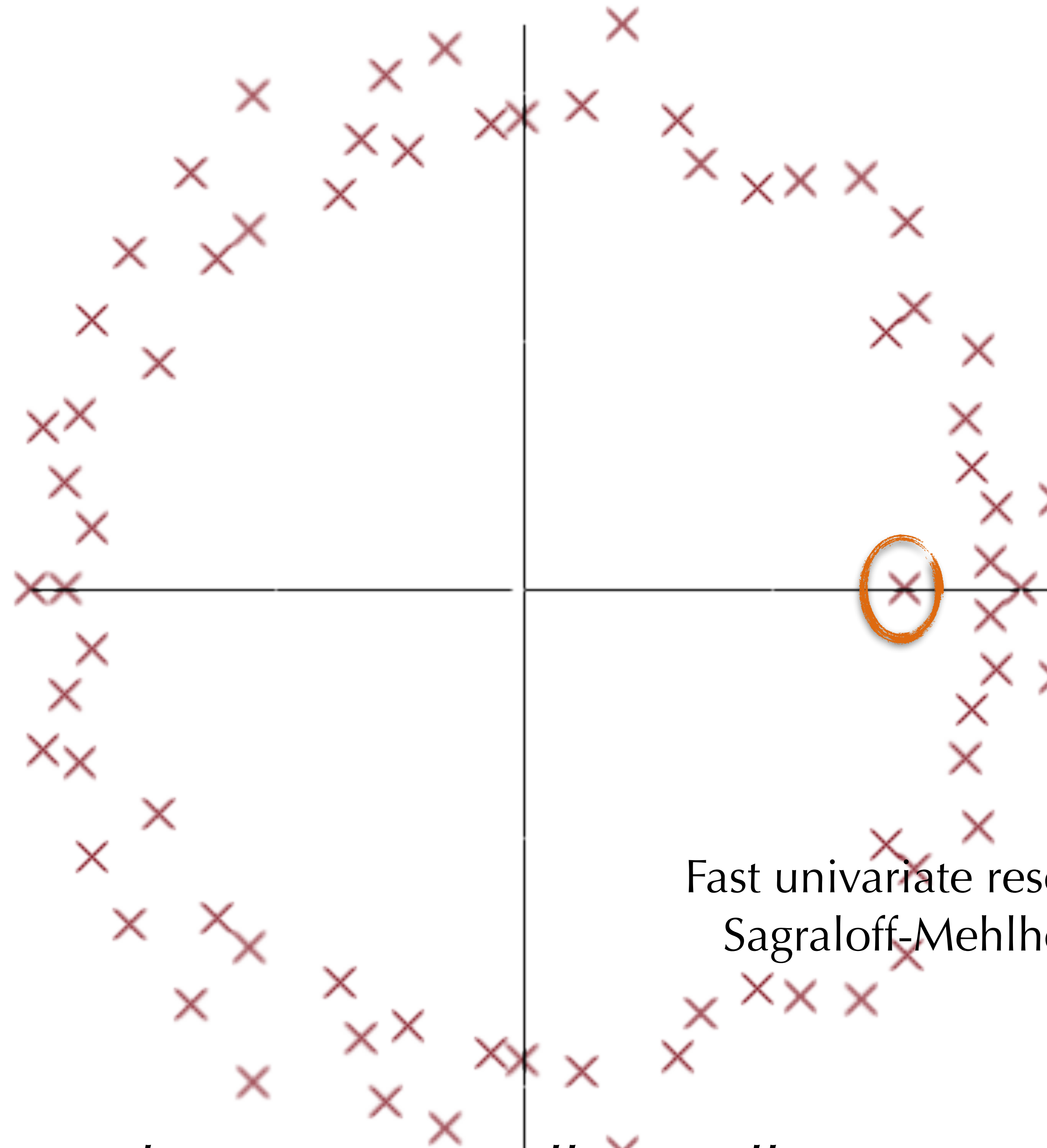
Conway's sequence

1,11,21,1211,111221,…

Generating function for lengths:

$$f(z)=P(z)/Q(z)$$

with deg Q=72.



Smallest singularity:
$\delta(f) \simeq 0.7671198507$

$\rho = 1/\delta(f) \simeq 1.30357727$

$$\ell_n \simeq 2.04216\, \rho^n$$

$\rho\ \mathrm{Res}(f, \delta(f))$

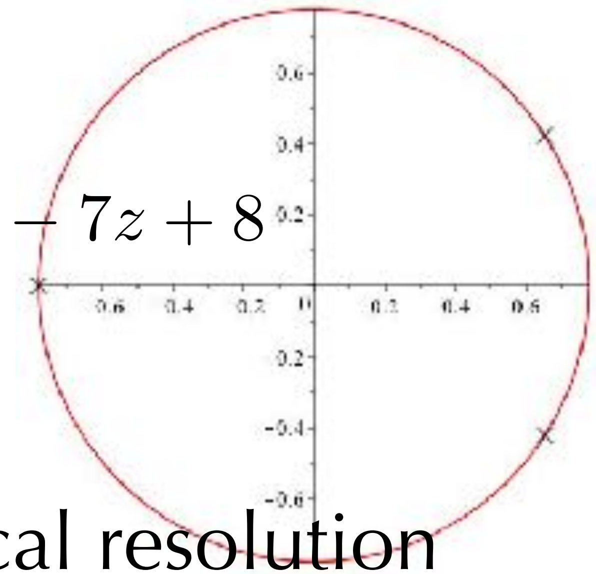
Fast univariate resolution:
Sagraloff-Mehlhorn16

remainder exponentially small

Singularity Analysis

Ex: Rational Functions

$17z^3 - 9z^2 - 7z + 8$



1. Numerical resolution with sufficient precision + algebraic manipulations
2. Local expansion (easy).
3. Easy.

A 3-Step Method:

1. Locate dominant singularities
   a. singularities; b. dominant ones
2. Compute local behaviour
3. Translate into asymptotics

$$(1-z)^\alpha \log^k \frac{1}{1-z} \mapsto \frac{n^{-\alpha-1}}{\Gamma(-\alpha)} \log^k n, \qquad (\alpha \notin \mathbb{N}^\star)$$

Useful property [Pringsheim Borel]

$a_n \geq 0$ for all $n \Longrightarrow$ real positive dominant singularity.

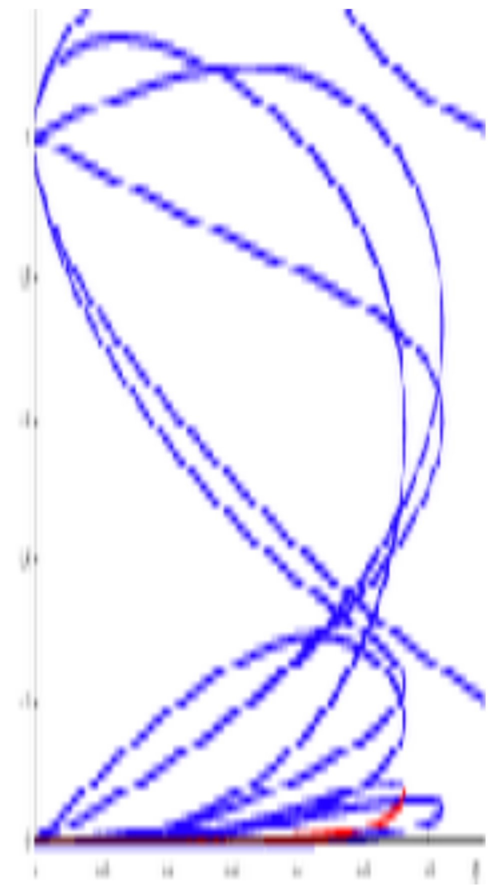
Algebraic Generating Functions

$$P(z, y(z)) = 0$$

Numerical resolution
with sufficient precision
+ algebraic manipulations

1a. Location of possible singularities
Implicit Function Theorem:

$$P(z, y(z)) = \frac{\partial P}{\partial y}(z, y(z)) = 0$$



1b. Analytic continuation finds the dominant ones:
not so easy [FlSe NoteVII.36].

2. Local behaviour (Puiseux): $(1-z)^{\alpha}, \quad (\alpha \in \mathbb{Q})$

3. Translation: easy.

Differentially-Finite Generating Functions

$$a_n(z)y^{(n)}(z) + \cdots + a_0(z)y(z) = 0, \quad a_i \text{ polynomials}$$

1a. Location of possible singularities.
Cauchy-Lipshitz Theorem:

$$a_n(z) = 0$$

Numerical resolution
with sufficient precision
+ algebraic manipulations

1b. Analytic continuation finds the dominant ones:
only numerical in general.
Sage code exists [Mezzarobba2016].

2. Local behaviour at regular singular points:

$$(1-z)^\alpha \log^k \frac{1}{1-z}, \quad (\alpha \in \overline{\mathbb{Q}}, k \in \mathbb{N})$$

3. Translation: easy.

Example: Apéry's Sequences

$$a_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2, \qquad b_n = a_n \sum_{k=1}^{n} \frac{1}{k^3} + \sum_{k=1}^{n} \sum_{m=1}^{k} \frac{(-1)^m \binom{n}{k}^2 \binom{n+k}{k}^2}{2m^3 \binom{n}{m} \binom{n+m}{m}}$$

and $c_n = b_n - \zeta(3) a_n$ have generating functions that satisfy

vanishes at 0,
$\alpha = 17 - 12\sqrt{2} \simeq 0.03,$
$\beta = 17 + 12\sqrt{2} \simeq 34.$

$$z^2(z^2 - 34z + 1)y''' + \cdots + (z-5)y = 0$$

In the neighborhood of $\alpha,$ all solutions behave like

$$\text{analytic} - \mu\sqrt{\alpha - z}(1 + (\alpha - z)\text{analytic}).$$

Mezzarobba's code gives $\mu_a \simeq 4.55, \quad \mu_b \simeq 5.46, \quad \mu_c \simeq 0.$

Slightly more work gives $\mu_c = 0$, then $c_n \approx \beta^{-n}$
and eventually, a proof that $\zeta(3)$ is irrational.

[Apéry1978]

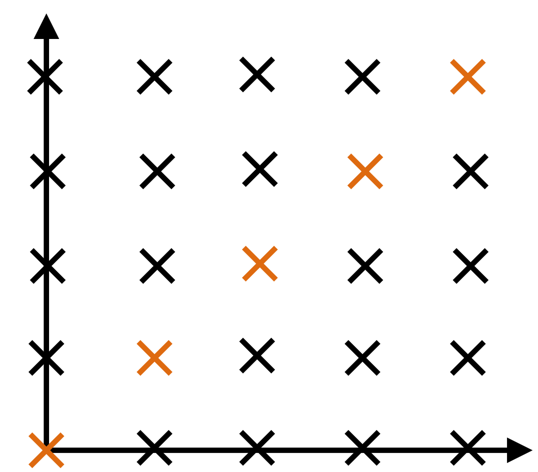
II. Diagonals

Definition

in this talk

If $F(\boldsymbol{z}) = \dfrac{G(\boldsymbol{z})}{H(\boldsymbol{z})}$ is a multivariate rational function with Taylor expansion

$$F(\boldsymbol{z}) = \sum_{\boldsymbol{i} \in \mathbb{N}^n} c_{\boldsymbol{i}} \boldsymbol{z}^{\boldsymbol{i}},$$



its **diagonal** is $\Delta F(t) = \sum_{k \in \mathbb{N}} c_{k,k,\ldots,k} t^k.$

$$\binom{2k}{k} : \qquad \frac{1}{1-x-y} = 1 + x + y + 2xy + x^2 + y^2 + \cdots + 6x^2y^2 + \cdots$$

$$\frac{1}{k+1}\binom{2k}{k} : \qquad \frac{1-2x}{(1-x-y)(1-x)} = 1 + y + 1xy - x^2 + y^2 + \cdots + 2x^2y^2 + \cdots$$

Apéry's a_k : $\dfrac{1}{1 - t(1+x)(1+y)(1+z)(1+y+z+yz+xyz)} = 1 + \cdots + 5xyzt + \cdots$

Multiple Binomial Sums

Ex. (from A=B) $S = \sum_{r\geq 0}\sum_{s\geq 0}(-1)^{n+r+s}\binom{n}{r}\binom{n}{s}\binom{n+s}{s}\binom{n+r}{r}\binom{2n-r-s}{n}$

Def.: expressions obtained from:

$$n \mapsto C^n, \quad (n,k) \mapsto \binom{n}{k}, \quad n \mapsto \delta_n \text{(Kronecker)}$$

using +, x, multiplication by constants, affine changes of indices and indefinite summation:

$$(\underline{m}, n) \mapsto \sum_{k=0}^{n} u_{\underline{m},k}.$$

Thm. Diagonals ≡ univariate binomial sums.

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> BinomSums[sumtores](S,u): (…)
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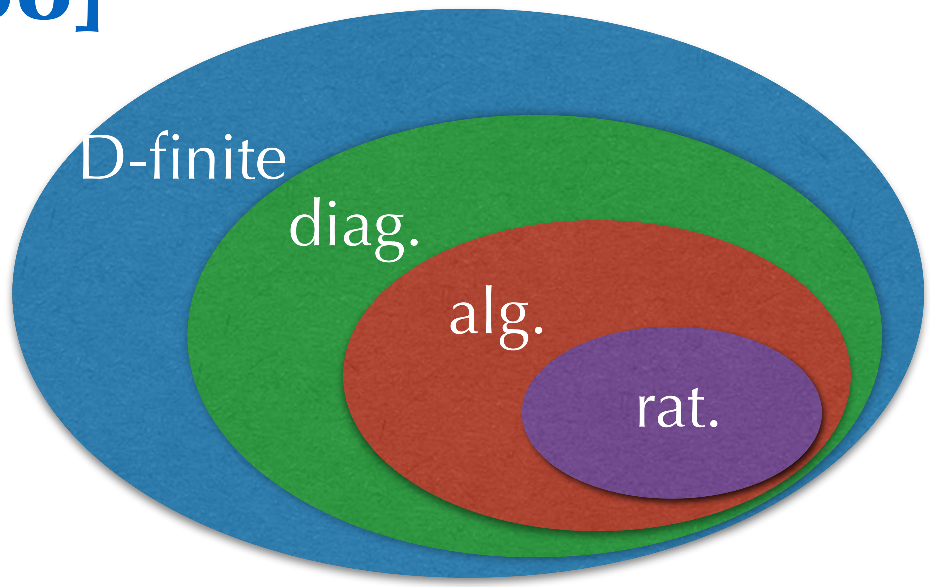
$$\frac{1}{1-t(1+u_1)(1+u_2)(1-u_1u_3)(1-u_2u_3)}$$

[Bostan-Lairez-S.17]

Diagonals are Differentially Finite
[Christol84,Lipshitz88]



Thm. If F has degree *d* in *n* variables, ΔF satisfies a LDE with
order $\approx d^n$, coeffs of degree $d^{O(n)}$.

+ algo in $\tilde{O}(d^{8n})$ ops.

Compares well with creative telescoping when both apply.

Christol's conjecture: All differentially finite power series with integer coefficients and radius of convergence in (0,∞) are diagonals.

[Bostan-Lairez-S.13,Lairez16]

Asymptotics

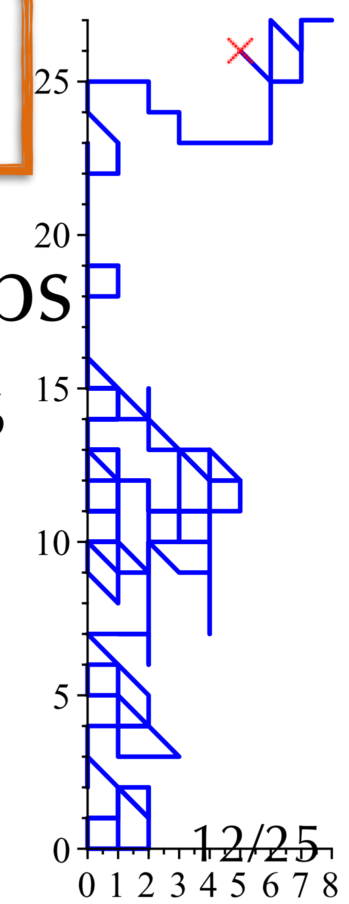
Thm. [Katz70,André00,Garoufalidis09]

$a_0+a_1z+\dots$ D-finite, a_i in $\mathbb{Z}$, radius in $(0,\infty)$, then its singular points are regular with rational exponents

$$a_n \sim \sum_{\substack{(\lambda,\alpha,k)\in \text{ finite set} \\ \text{in } \overline{\mathbb{Q}}\times\mathbb{Q}\times\mathbb{N}}} \lambda^{-n} n^{\alpha} \log^k(n)\, f_{\lambda,\alpha,k}\left(\frac{1}{n}\right).$$

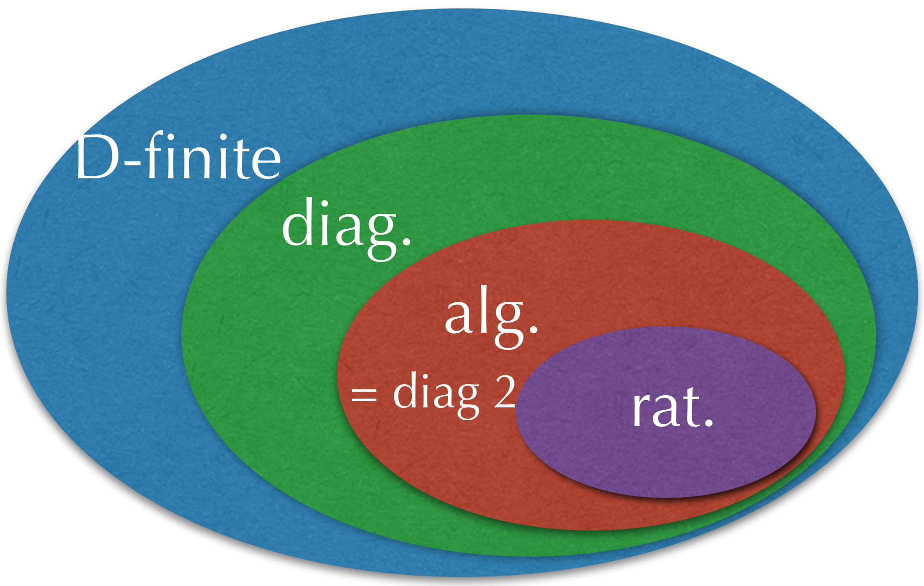
Ex. The number a_n of walks from the origin taking n steps *{N,S,E,W,NW}* and staying in the first quadrant behaves like $C\lambda^{-n}n^{\alpha}$ with $\alpha \notin \mathbb{Q}$ → not D-finite.

$$\alpha = -1 + \frac{\pi}{\arccos(u)}, \quad 8u^3-8u^2+6u-1=0, \quad u>0.$$



[Bostan-Raschel-S.14]

Bivariate Diagonals are Algebraic
[Pólya21,Furstenberg67]



Thm. F=A(x,y)/B(x,y), deg≤d in x and y, then ΔF cancels a polynomial of degree ≲ 4^d in y and t.

$$\Delta \frac{x}{1-x^2-y^3}$$ satisfies

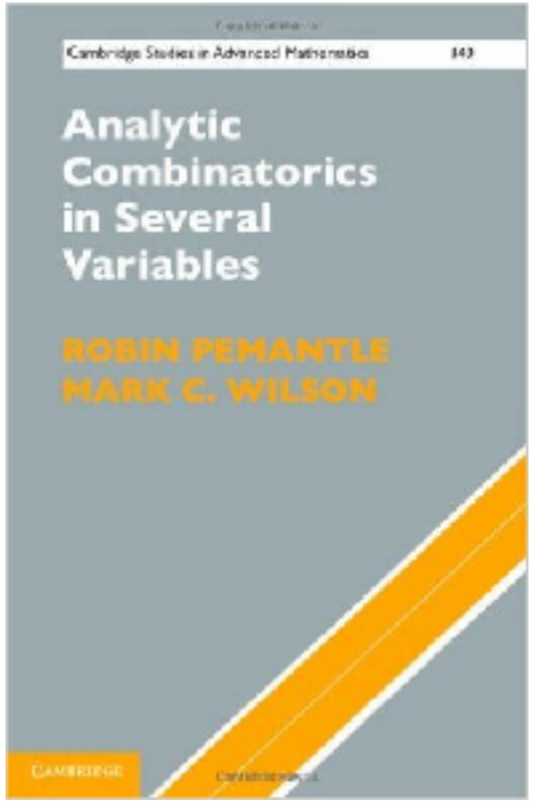
$$\begin{aligned}&\left(3125\,t^6-108\right)^3 y^{10}+81\left(3125\,t^6-108\right)^2 y^8\\&+50t^3\left(3125\,t^6-108\right)^2 y^7+\left(6834375\,t^6-236196\right) y^6\\&-t^3\left(34375\,t^6-3888\right)\left(3125\,t^6-108\right) y^5\\&+\left(-7812500\,t^{12}+270000\,t^6+19683\right) y^4\\&-54\,t^3\left(6250\,t^6-891\right) y^3+50\,t^6\left(21875\,t^6-2106\right) y^2\\&-t^3\left(50\,t^2+9\right)\left(2500\,t^4-450\,t^2+81\right) y\\&-t^6\left(3125\,t^6-1458\right)=0\end{aligned}$$

+ quasi-optimal algorithm.

→ *the differential equation is often better.*

[Bostan-Dumont-S.17]

III. Analytic Combinatorics in Several Variables



Here, we restrict to rational diagonals and simple cases

Starting Point: Cauchy's Formula

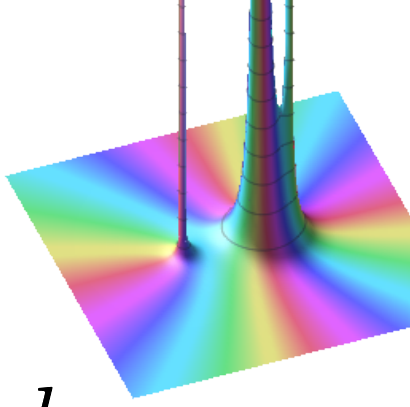
If $f = \sum_{i_1,\ldots,i_n \geq 0} c_{i_1,\ldots,i_n} z_1^{i_1} \cdots z_n^{i_n}$ is convergent in the neighborhood of 0, then

$$c_{i_1,\ldots,i_n} = \left(\frac{1}{2\pi i}\right)^n \int_T f(z_1,\ldots,z_n) \frac{dz_1 \cdots dz_n}{z_1^{i_1+1} \cdots z_n^{i_n+1}}$$

for any small torus T ($|z_j| = re^{i\theta_j}$) around 0.

Asymptotics: deform the torus to pass where the integral concentrates asymptotically.

Coefficients of Diagonals



$$F(\underline{z}) = \frac{G(\underline{z})}{H(\underline{z})} \qquad c_{k,\dots,k} = \left(\frac{1}{2\pi i}\right)^n \int_T \frac{G(\underline{z})}{H(\underline{z})} \frac{dz_1 \cdots dz_n}{(z_1 \cdots z_n)^{k+1}}$$

Critical points: minimize $z_1 \cdots z_n$ on $\mathcal{V} = \{\underline{z} \mid H(\underline{z}) = 0\}$

$$\operatorname{rank} \begin{pmatrix} \frac{\partial H}{\partial z_1} & \cdots & \frac{\partial H}{\partial z_n} \\ \frac{\partial (z_1 \cdots z_n)}{\partial z_1} & \cdots & \frac{\partial (z_1 \cdots z_n)}{\partial z_n} \end{pmatrix} \leq 1 \qquad \text{i.e.} \qquad z_1 \frac{\partial H}{\partial z_1} = \cdots = z_n \frac{\partial H}{\partial z_n}$$

Minimal ones: on the boundary of the domain of convergence of $F(\underline{z})$.

A 3-step method

1a. locate the critical points (**algebraic** condition);
1b. find the minimal ones (**semi-algebraic** condition);
2. translate (easy in simple cases).

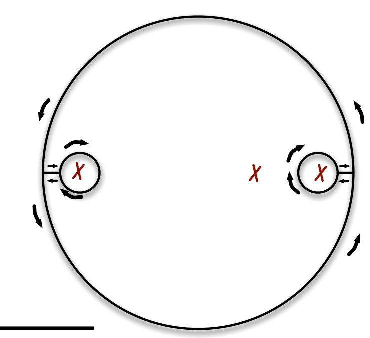
Ex.: Central Binomial Coefficients

$$\binom{2k}{k} : \qquad \frac{1}{1-x-y} = 1 + x + y + 2xy + x^2 + y^2 + \cdots + 6x^2y^2 + \cdots$$

(1). Critical points: $1 - x - y = 0, x = y \Longrightarrow x = y = 1/2.$

(2). Minimal ones. Easy. In general, this is the difficult step.

(3). Analysis close to the minimal critical point:



$$a_k = \frac{1}{(2\pi i)^2} \iint \frac{1}{1-x-y} \frac{dx\,dy}{(xy)^{k+1}} \approx \frac{1}{2\pi i} \int \frac{dx}{(x(1-x))^{k+1}}$$

$$\approx \frac{4^{k+1}}{2\pi i} \int \exp(4(k+1)(x-1/2)^2)\,dx \approx \frac{4^k}{\sqrt{k\pi}}.$$

residue

saddle-point approx

Kronecker Representation for the Critical Points

Algebraic part: ``compute'' the solutions of the system

$$H(\underline{z}) = 0 \qquad z_1 \frac{\partial H}{\partial z_1} = \cdots = z_n \frac{\partial H}{\partial z_n}$$

If $\quad \deg(H) = d, \quad \max \text{coeff}(H) \leq 2^h \quad D := d^n$

Under genericity assumptions, a probabilistic algorithm running in $\tilde{O}(hD^3)$ bit ops finds:

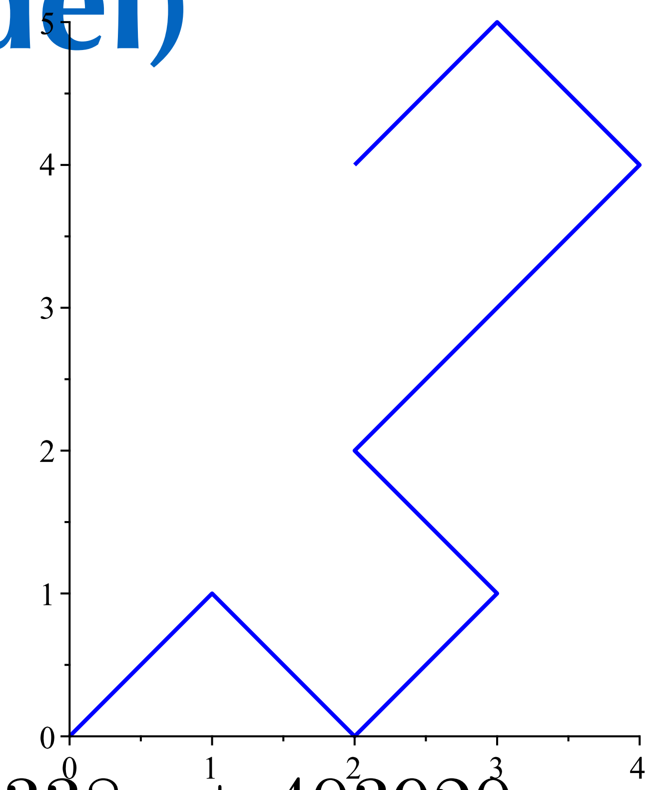
$$\left.\begin{aligned} P(u) &= 0 \\ P'(u)z_1 - Q_1(u) &= 0 \\ &\vdots \\ P'(u)z_n - Q_n(u) &= 0 \end{aligned}\right\} \quad \begin{aligned} &\text{Degree } \leq D \\ &\text{Height } \leq \tilde{O}(hD) \end{aligned}$$

History and Background: see Castro, Pardo, Hägele, and Morais (2001)

System reduced to a univariate polynomial.

[Giusti-Lecerf-S.01;Schost02;SafeySchost16]

Example (Lattice Path Model)



The number of walks from the origin taking steps *{NW,NE,SE,SW}* and staying in the first quadrant is

$$\Delta F, \quad F(x,y,t) = \frac{(1+x)(1+y)}{1-t(1+x^2+y^2+x^2y^2)}$$

Kronecker representation of the critical points:

$$P(u) = 4u^4 + 52u^3 - 4339u^2 + 9338u + 403920$$

$$Q_x(u) = 336u^2 + 344u - 105898$$

$$Q_y(u) = -160u^2 + 2824u - 48982$$

$$Q_t(u) = 4u^3 + 39u^2 - 4339u/2 + 4669/2$$

ie, they are given by:

$$P(u) = 0, \quad x = \frac{Q_x(u)}{P'(u)}, \quad y = \frac{Q_y(u)}{P'(u)}, \quad t = \frac{Q_t(u)}{P'(u)}$$

Which one of these 4 is minimal?

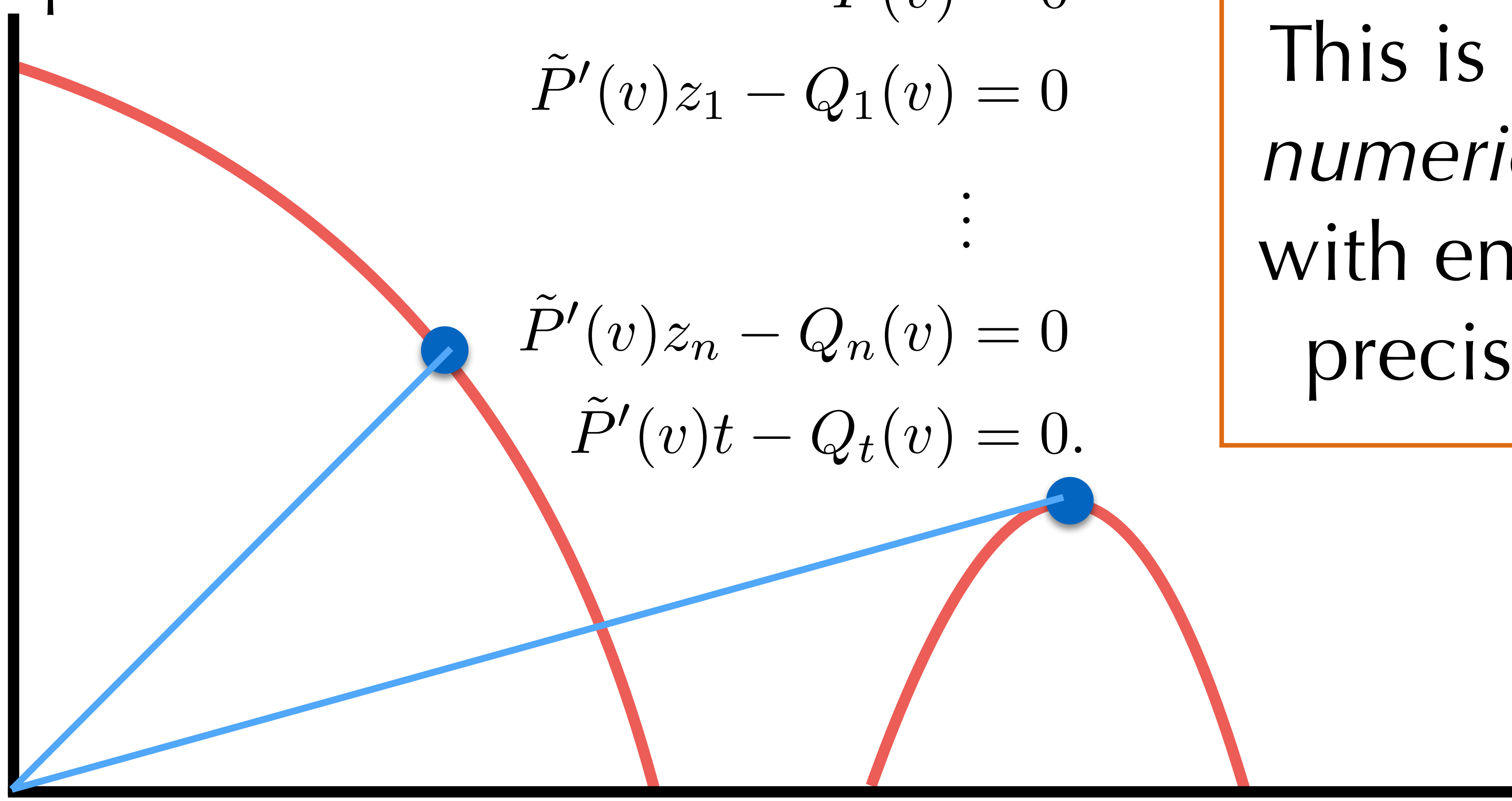
Testing Minimality

Def. $F(z_1,\ldots,z_n)$ is **combinatorial** if every coefficient is ≥ 0.

Prop. [PemantleWilson] In the combinatorial case, one of the minimal critical points has positive real coordinates.

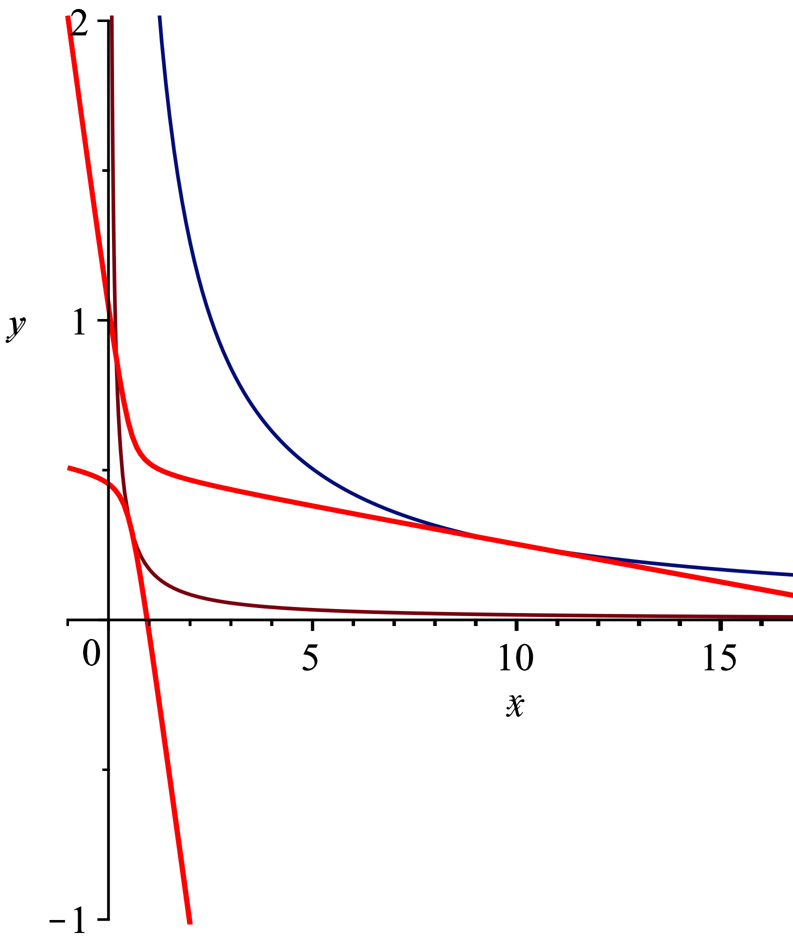
Thus, we add the equation $H(tz_1,\ldots,tz_n)=0$ for a new variable t and select the positive real point(s) $\mathbf{z}$ with no $t \in (0,1)$ from a new Kronecker representation:

$$
\begin{aligned}
\tilde{P}(v) &= 0 \\
\tilde{P}'(v)z_1 - Q_1(v) &= 0 \\
&\vdots \\
\tilde{P}'(v)z_n - Q_n(v) &= 0 \\
\tilde{P}'(v)t - Q_t(v) &= 0.
\end{aligned}
$$



This is done *numerically*, with enough precision.

Example



$$F = \frac{1}{H} = \frac{1}{(1-x-y)(20-x-40y)-1}$$

Critical point equation $x\frac{\partial H}{\partial x} = y\frac{\partial H}{\partial y}$:

$$x(2x+41y-21) = y(41x+80y-60)$$

→ 4 critical points, 2 of which are real:

$$(x_1, y_1) = (0.2528, 9.9971), \quad (x_2, y_2) = (0.30998, 0.54823)$$

Add $H(tx, ty) = 0$ and compute a Kronecker representation:

$$P(u) = 0, \quad x = \frac{Q_x(u)}{P'(u)}, \quad y = \frac{Q_y(u)}{P'(u)}, \quad t = \frac{Q_t(u)}{P'(u)}$$

Solve numerically and keep the real positive sols:

$$(0.31, 0.55, 0.99), (0.31, 0.55, 1.71), (0.25, 9.99, 0.09), (0.25, 0.99, 0.99)$$

(x_1, y_1) is not minimal, (x_2, y_2) is.

Algorithm and Complexity

Thm. If $F(\underline{z})$ is combinatorial, then under regularity conditions, the points contributing to dominant diagonal asymptotics can be determined in $\tilde{O}(hd^5D^4)$ bit operations. Each contribution has the form

$$A_k = \left(T^{-k}k^{(1-n)/2}(2\pi)^{(1-n)/2}\right)(C + O(1/k))$$

T, C can be found to $2^{-\kappa}$ precision in $\tilde{O}(h(dD)^3 + D\kappa)$ bit ops.

This result covers the easiest cases.
The complexity should be compared with the size of the result.
All conditions hold generically and can be checked within the same complexity, except combinatoriality.

[Melczer-S.16]

Example: Apéry's sequence

$$\frac{1}{1-t(1+x)(1+y)(1+z)(1+y+z+yz+xyz)} = 1 + \cdots + 5xyzt + \cdots$$

Kronecker representation of the critical points:

$$P(u) = u^2 - 366u - 17711$$

$$a = \frac{2u-1006}{P'(u)}, \quad b = c = -\frac{320}{P'(u)}, \quad z = -\frac{164u+7108}{P'(u)}$$

There are two real critical points, and one is positive. After testing minimality, one has proven asymptotics

```
> A, U := DiagonalAsymptotics(numer(F),denom(F),[t,x,y,z], u, k):
> evala(allvalues(subs(u=U[1],A)));
```

$$\frac{\left(17+12\sqrt{2}\right)^k \sqrt{2}\sqrt{24+17\sqrt{2}}}{8k^{3/2}\pi^{3/2}}$$

Example: Restricted Words in Factors

$$F(x,y) = \frac{1 - x^3y^6 + x^3y^4 + x^2y^4 + x^2y^3}{1 - x - y + x^2y^3 - x^3y^3 - x^4y^4 - x^3y^6 + x^4y^6}$$

words over {0,1} without 10101101 or 1110101

```
> A,U:=DiagonalAsymptotics(numer(F),denom(F),indets(F),u,k,true,u-T,T):
> A;
```

$$\left(\left(\frac{84u^{20}+240u^{19}-285u^{18}-1548u^{17}-2125u^{16}-1408u^{15}+255u^{14}+756u^{13}+2509u^{12}+2856u^{11}-605u^{10}+2020u^{9}+1233u^{8}-1760u^{7}+924u^{6}-492u^{5}-675u^{4}+632u^{3}-249u^{2}+24u+16}{-12u^{20}+30u^{19}+258u^{18}+500u^{17}+440u^{16}-102u^{15}-378u^{14}-1544u^{13}-2142u^{12}-550u^{11}-2222u^{10}-1644u^{9}+2860u^{8}-1848u^{7}+1230u^{6}+2160u^{5}-2686u^{4}+1494u^{3}-228u^{2}-320u+84}\right)^k\right.$$

$$\sqrt{2}\sqrt{\frac{84u^{20}+240u^{19}-285u^{18}-1548u^{17}-2125u^{16}-1408u^{15}+255u^{14}+756u^{13}+2509u^{12}+2856u^{11}+605u^{10}+2020u^{9}+1233u^{8}-1760u^{7}+924u^{6}-492u^{5}-675u^{4}+632u^{3}-249u^{2}+24u+16}{-162u^{18}-612u^{17}-902u^{16}-616u^{15}+254u^{14}+548u^{13}+2054u^{12}+2156u^{11}+898u^{10}-2268u^{9}+2462u^{8}-2088u^{7}+1312u^{6}-540u^{5}-1410u^{4}+1188u^{3}-290u^{2}+32}}$$

$$\left.(12u^{20}+36u^{19}-21u^{18}-170u^{17}-255u^{16}-190u^{15}-19u^{14}+46u^{13}+461u^{12}+628u^{11}+133u^{10}+374u^{9}+161u^{8}-384u^{7}+146u^{6}-138u^{5}-285u^{4}-40u^{3}+91u^{2}-30u+32)\right) \Big/ \left(2\sqrt{k}\sqrt{\pi}\,(84u^{20}\right.$$

$$\left.+240u^{19}-285u^{18}-1548u^{17}-2125u^{16}-1408u^{15}+255u^{14}+756u^{13}+2509u^{12}+2856u^{11}-605u^{10}+2020u^{9}+1233u^{8}-1760u^{7}+924u^{6}-492u^{5}-675u^{4}+632u^{3}-249u^{2}+24u+16)\right)$$

```
> U;
```

$$[\mathit{RootOf}(4\_Z^{21}+12\_Z^{20}-15\_Z^{19}-86\_Z^{18}-125\_Z^{17}-88\_Z^{16}+17\_Z^{15}+54\_Z^{14}+193\_Z^{13}+238\_Z^{12}+55\_Z^{11}+202\_Z^{10}+137\_Z^{9}-220\_Z^{8}+132\_Z^{7}-82\_Z^{6}-135\_Z^{5}+158\_Z^{4}-83\_Z^{3}+12\_Z^{2}+16\_Z-4, 0.25574184)]$$

```
> evalf(subs(u=U[1],A));
```

$$\frac{0.60294599\; 3.9101932^k}{\sqrt{k}}$$

Minimal Critical Points in the Noncombinatorial Case

Then we use even more variables and equations:

$$H(\underline{z}) = 0 \qquad z_1 \frac{\partial H}{\partial z_1} = \cdots = z_n \frac{\partial H}{\partial z_n}$$

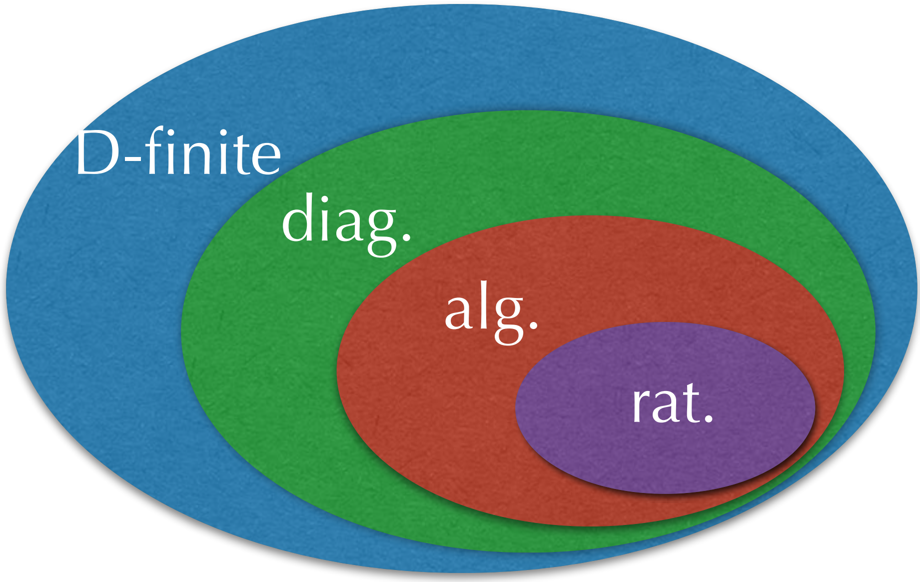
$$H(\underline{u}) = 0 \qquad |u_1|^2 = t|z_1|^2, \ldots, |u_n|^2 = t|z_n|^2$$

+ critical point equations for the projection on the *t* axis

And check that there is no solution with *t* in (0,1).

Prop. Under regularity assumptions, this can be done in $\tilde{O}(hd^4 2^{3n} D^9)$ bit operations.

Summary & Conclusion



- Diagonals are a nice and important class of generating functions for which we now have many good algorithms.
- ACSV can be made effective (at least in simple cases).
- Requires nice semi-numerical Computer Algebra algorithms.
- Without computer algebra, these computations are difficult.

Work in progress: extend beyond some of the assumptions (see Melczer's thesis).

The End