Algorithmic Tools for the Asymptotics of Diagonals

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Lattice walks at the Interface of Algebra, Analysis and Combinatorics

September 19, 2017

Asymptotics & Univariate Generating Functions

counts the number of objects of size *n*

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

captures some structure

(a_n) P-recursive $\iff$ **A(z) D-finite**

$$p_0(n) a_{n+k} + \cdots + p_k(n) a_n = 0 \qquad q_0(z) A^{(\ell)}(z) + \cdots + q_\ell(z) A(z) = 0$$

1. Possible exponential growth $(a_n \approx \rho^n, \rho \neq 0)$

ρ root of the characteristic polynomial of the leading coeff of the recurrence wrt *n*

$$q_0(1/\rho) = 0$$

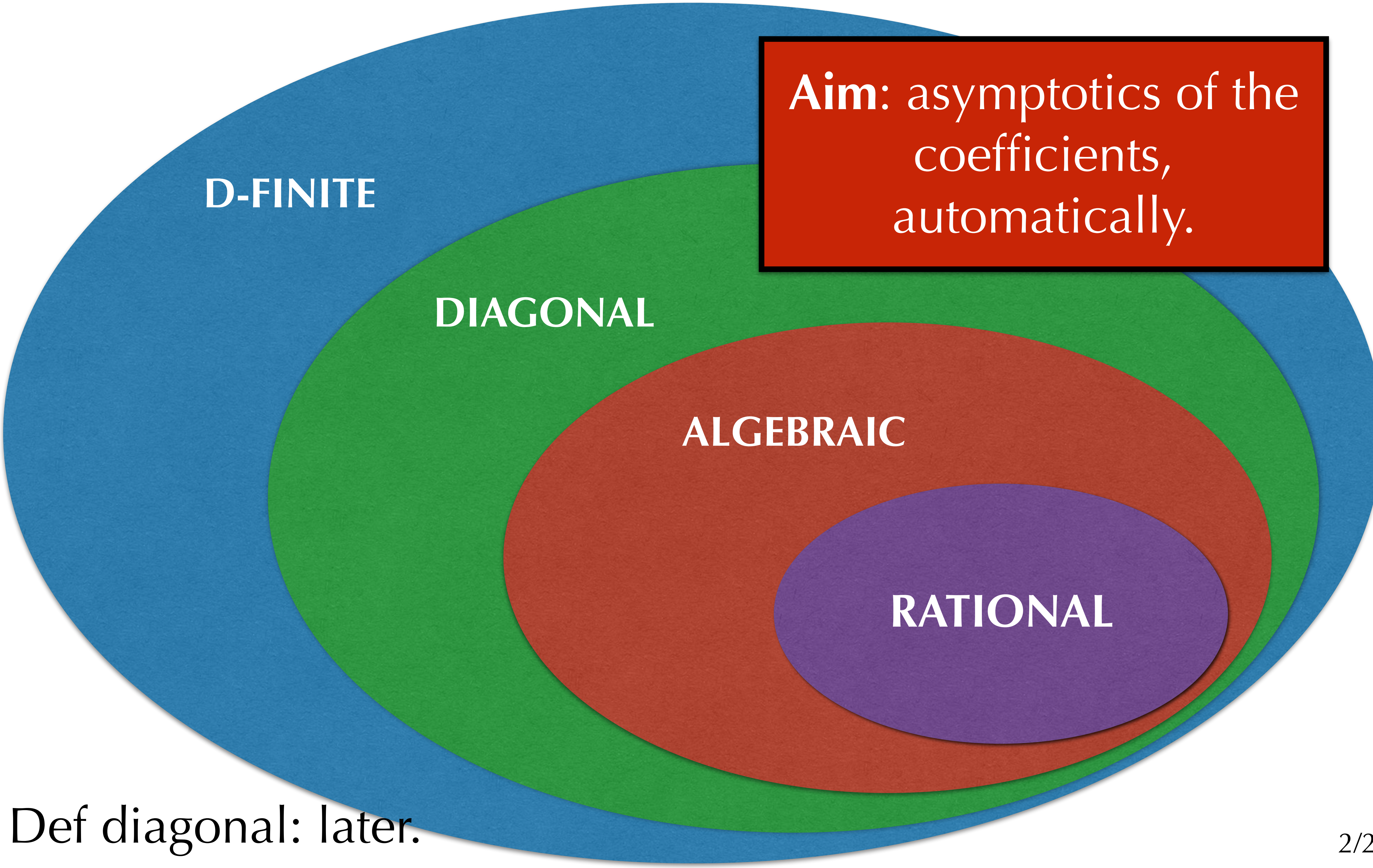
2. Possible sub-exponential growth $\left(a_n \sim c \rho^n \phi(n), \ \frac{\phi(n+1)}{\phi(n)} \to 1\right)$

a basis can be computed and then *c* approximated

Qu.: How can we get ρ, ϕ, c ? and how fast?

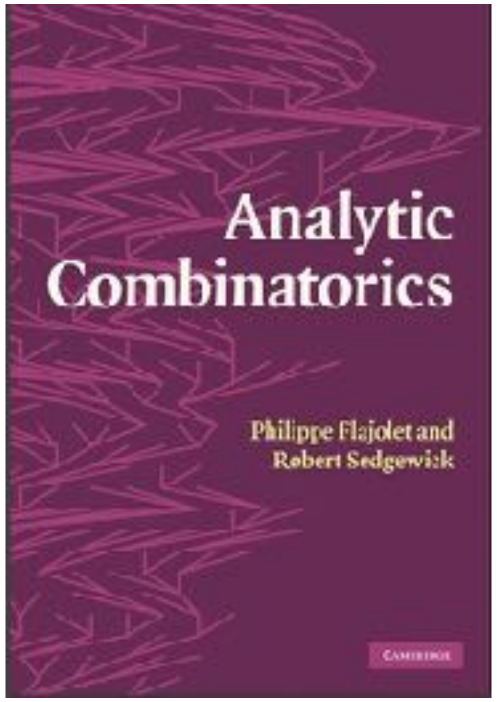
Univariate Generating Functions

Aim: asymptotics of the coefficients, automatically.



Def diagonal: later.

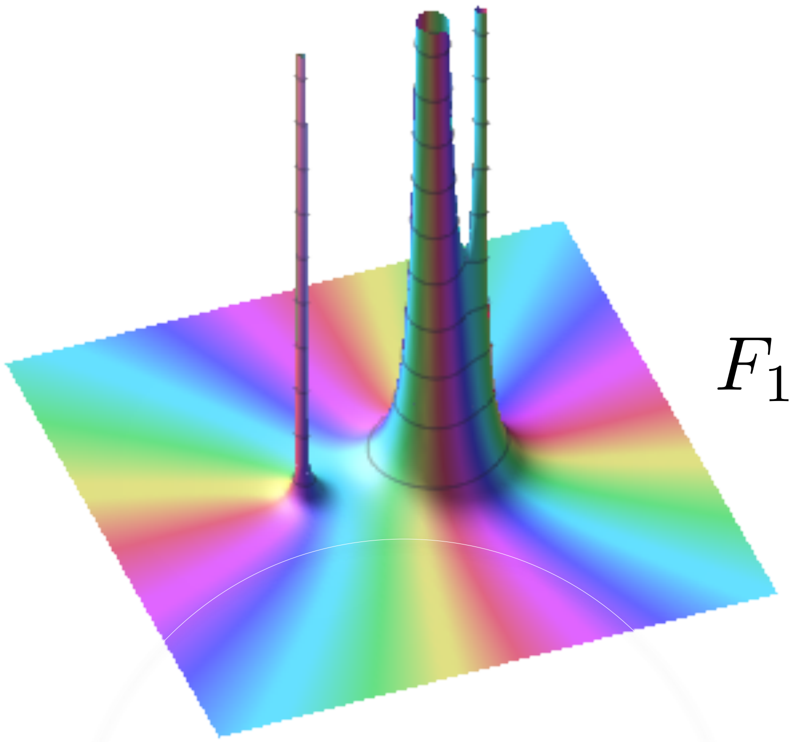
I. A Quick Review of Analytic Combinatorics in One Variable



Principle:

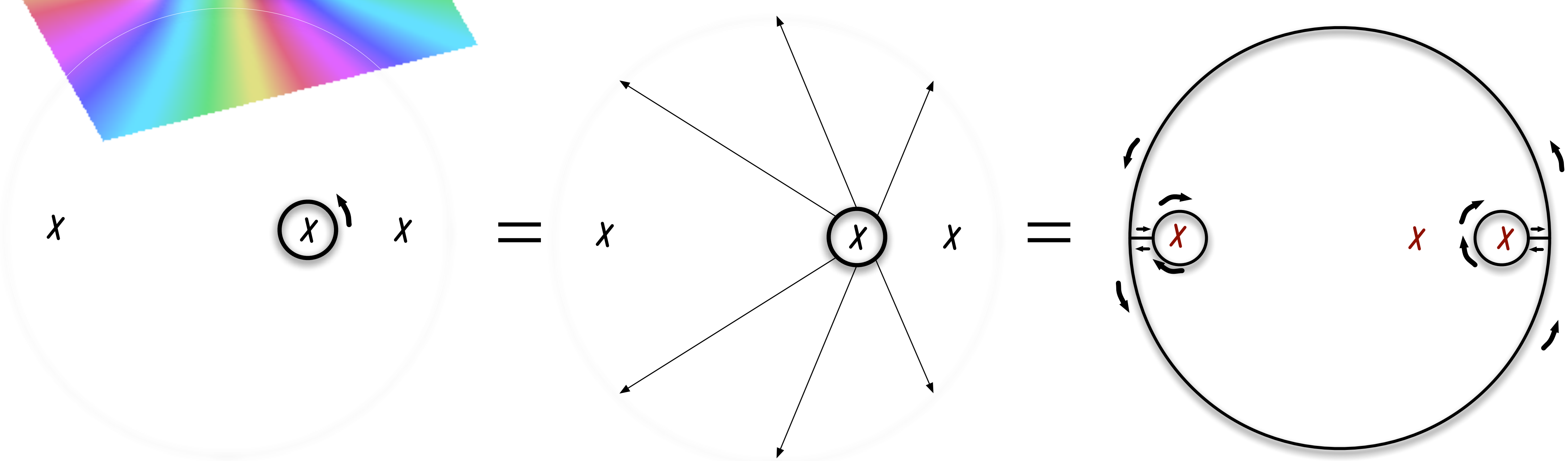
Dominant singularity ⟷ *exponential behaviour*
local behaviour ⟷ *subexponential terms*

Coefficients of Rational Functions



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

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



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

As n increases, the smallest singularities dominate.

Conway's sequence

1,11,21,1211,111221,...

Generating function for lengths:

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

with deg Q=72.

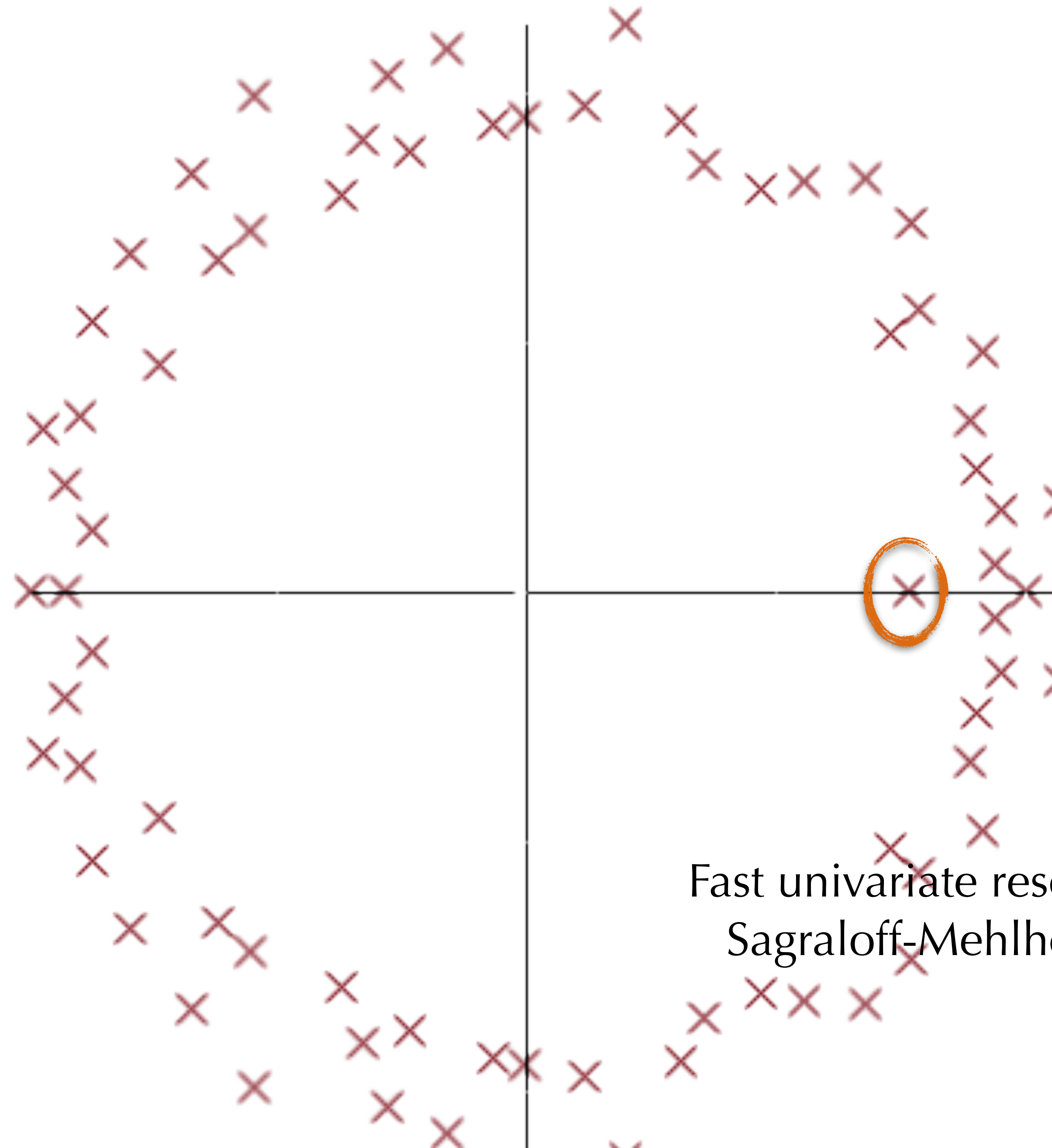
Smallest singularity:

$\delta(f) \simeq 0.7671198507$

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

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

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



Fast univariate resolution:
Sagraloff-Mehlhorn16

remainder exponentially small

Singularity Analysis

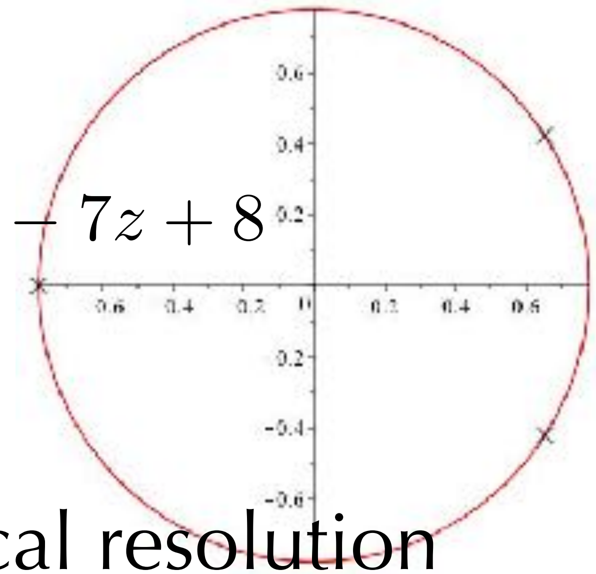
A 3-Step Method:

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

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

Ex: Rational Functions

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



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

Useful property [Pringsheim Borel]

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

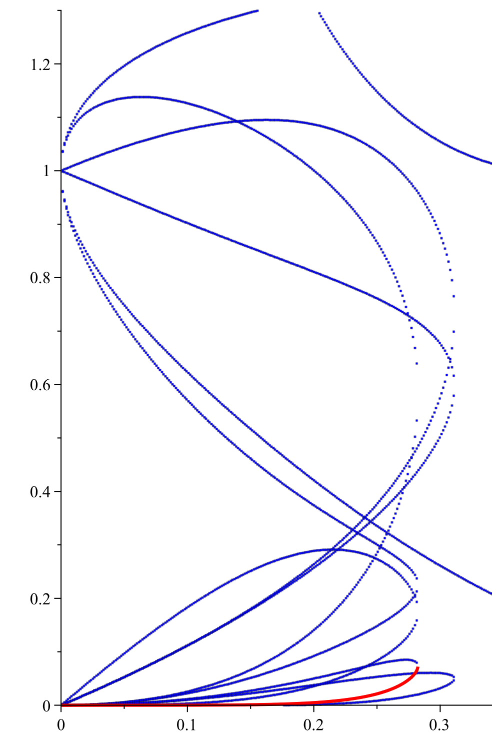
Algebraic Generating Functions

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

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]

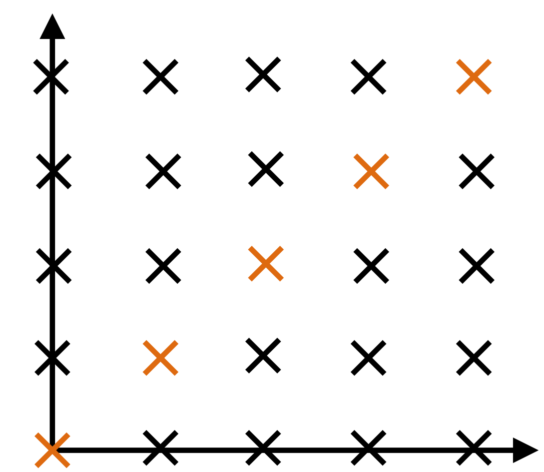
II. Diagonals

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

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

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

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

Diagonals & Multiple Binomial Sums

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

Thm. Diagonals ≡ binomial sums with 1 free index.

defined properly

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

has for diagonal the generating function of S_n

[Bostan-Lairez-S.17]

Multiple Binomial Sums

over a field $\mathbb{K}$

Sequences constructed from

- Kronecker's δ: $n \mapsto \delta_n$;
- geometric sequences $n \mapsto C^n$, $C \in \mathbb{K}$;
- the binomial sequence $(n, k) \mapsto \binom{n}{k}$;

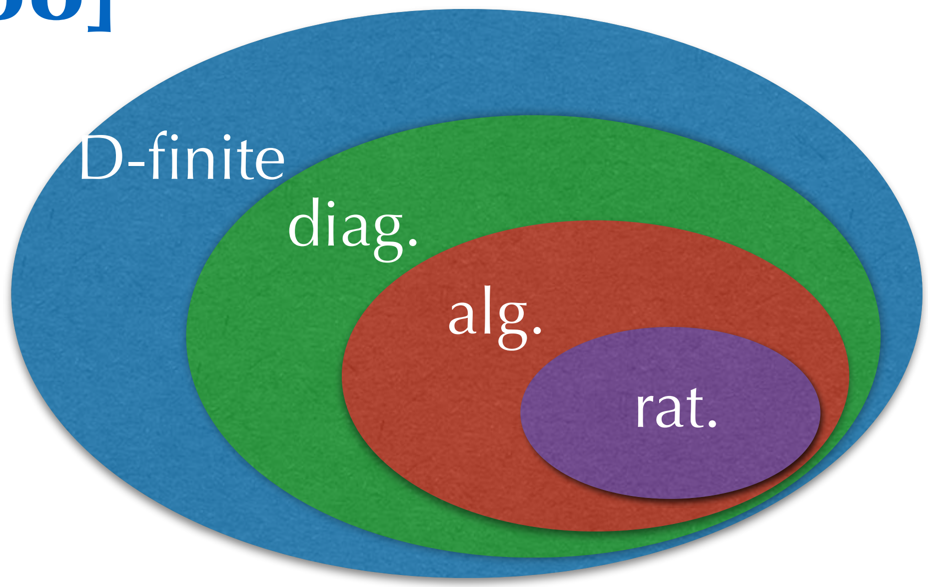
using algebra operations and

- affine changes of indices $(u_{\underline{n}}) \mapsto (u_{\lambda(\underline{n})})$;
- indefinite summation $(u_{\underline{n},k}) \mapsto \left(\sum_{k=0}^{m} u_{\underline{n},k}\right)$.

Diagonals are Differentially Finite

[Christol84,Lipshitz88]

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



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.

→ asymptotics from that LDE

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

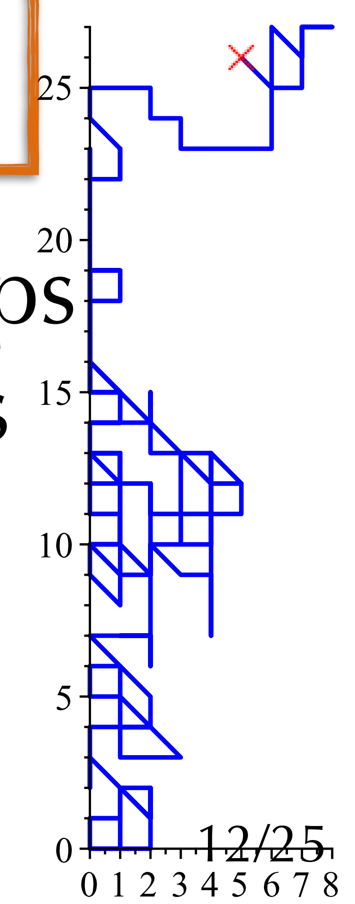
Thm. [Katz70,André00,Garoufalidis09]

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

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

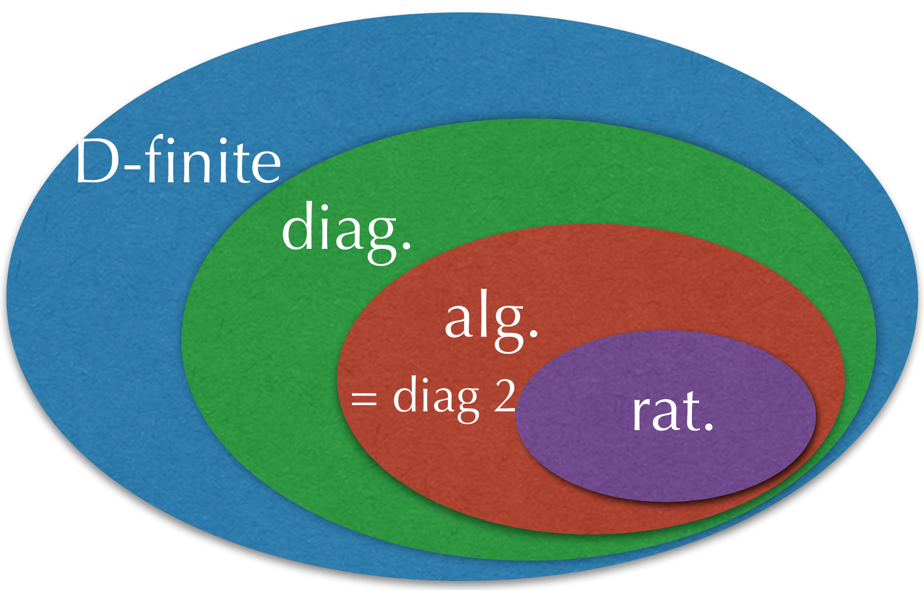
Ex. The number a_n of walks from the origin taking n steps *{N,S,E,W,NW}* and staying in the first quadrant behaves like $C\lambda^{-n}n^{\alpha}$ with $\alpha \notin \mathbb{Q}$ → not D-finite.

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



[Bostan-Raschel-S.14]

Bivariate Diagonals are Algebraic
[Pólya21,Furstenberg67]



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

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

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.

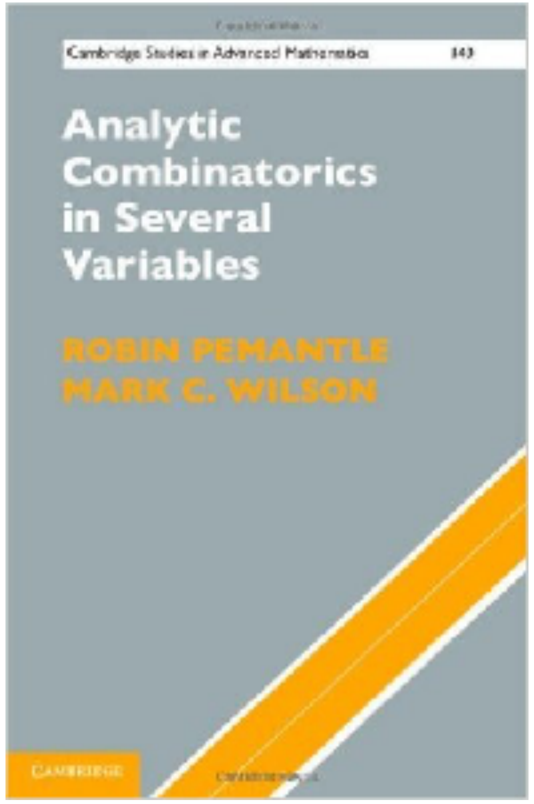
+ quasi-optimal algorithm.

→ *the differential equation is often better.*

[Bostan-Dumont-S.17]

III. Analytic Combinatorics in Several Variables, with Computer Algebra

Here, we restrict to rational diagonals and simple cases



Starting Point: Cauchy's Formula

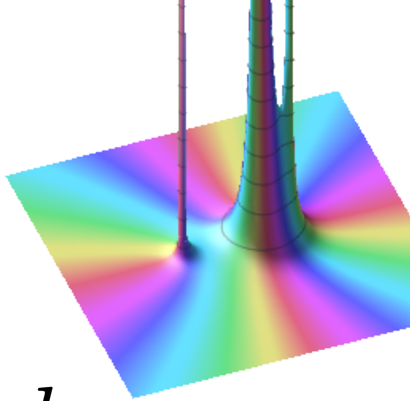
If $f = \sum_{i_1,\dots,i_n \geq 0} c_{i_1,\dots,i_n} z_1^{i_1} \cdots z_n^{i_n}$ is convergent in the neighborhood of 0, then

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

for any sufficiently 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 $\mathcal{V} = \{\underline{z} \mid H(\underline{z}) = 0\}$

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

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).

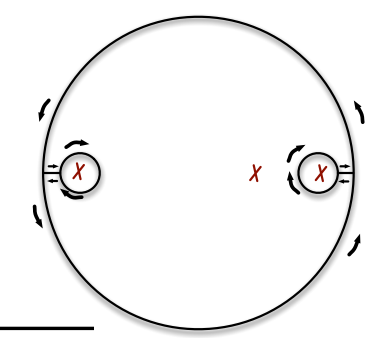
Ex.: Central Binomial Coefficients

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

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

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

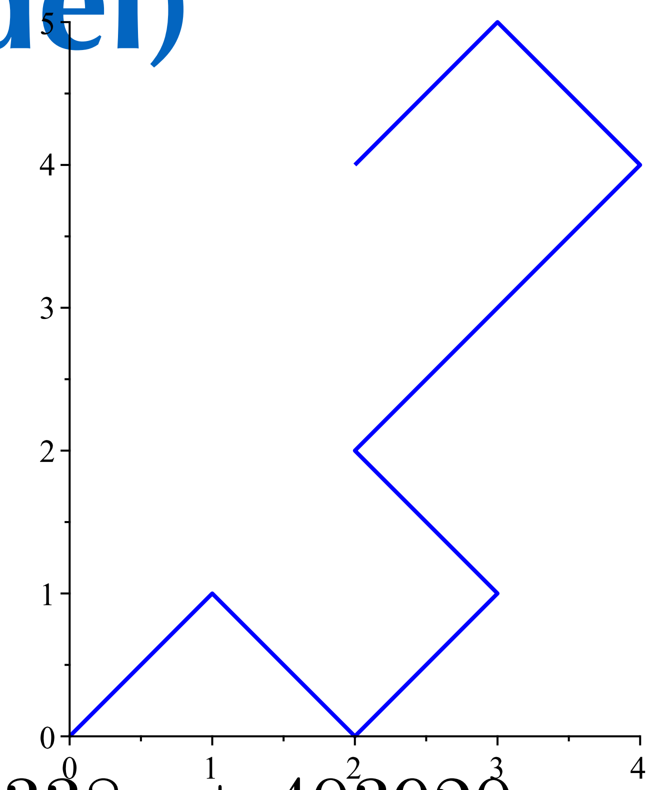
$$\left.\begin{aligned} P(u) &= 0 \\ P'(u)z_1 - Q_1(u) &= 0 \\ &\vdots \\ P'(u)z_n - Q_n(u) &= 0 \end{aligned}\right\} \quad \begin{aligned} &\text{Degree } \leq D \\ &\text{Height } \leq \tilde{O}(hD) \end{aligned}$$

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

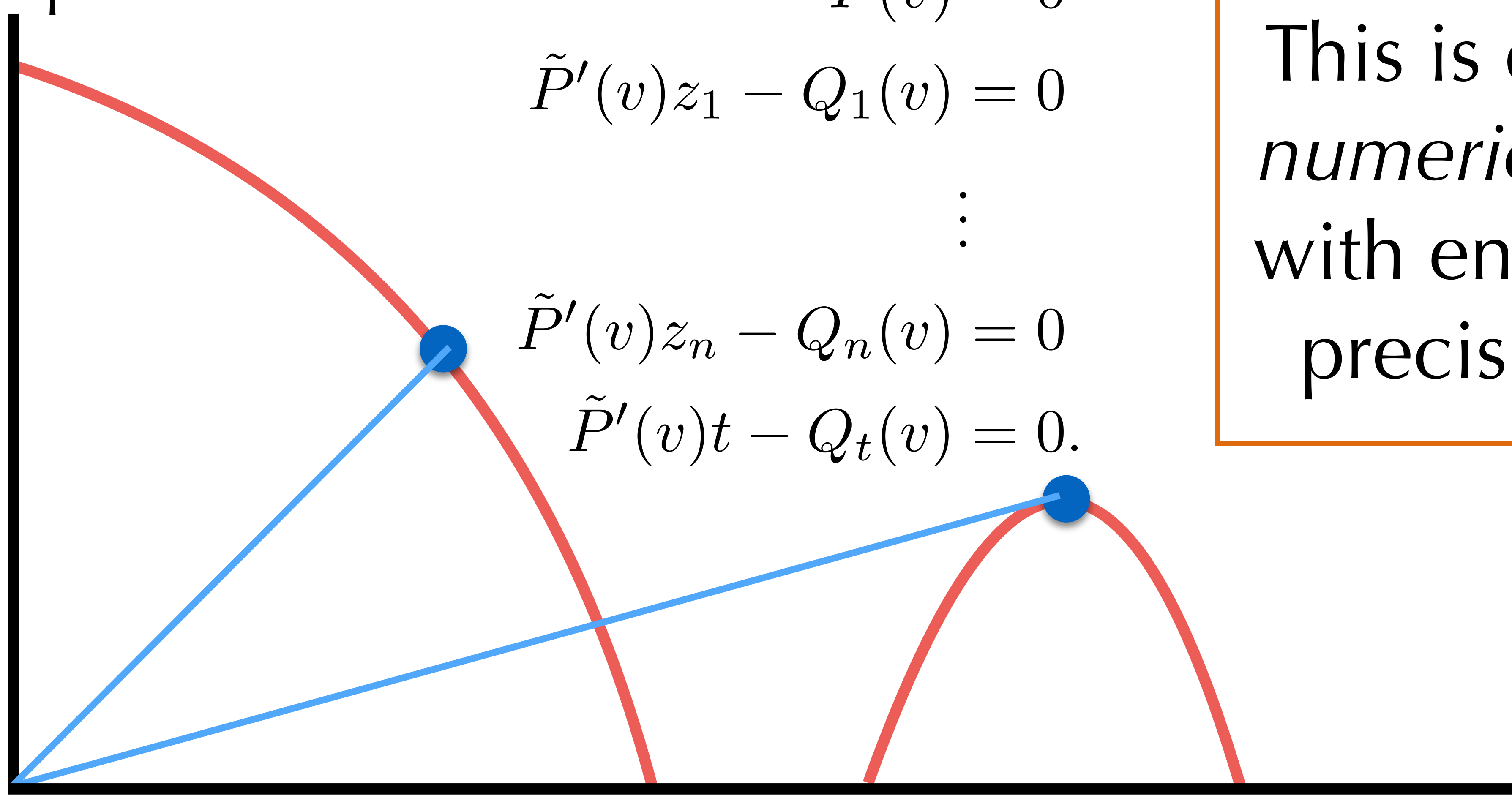
Def. $F(z_1,\ldots,z_n)$ is **combinatorial** if every coefficient is ≥ 0.

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

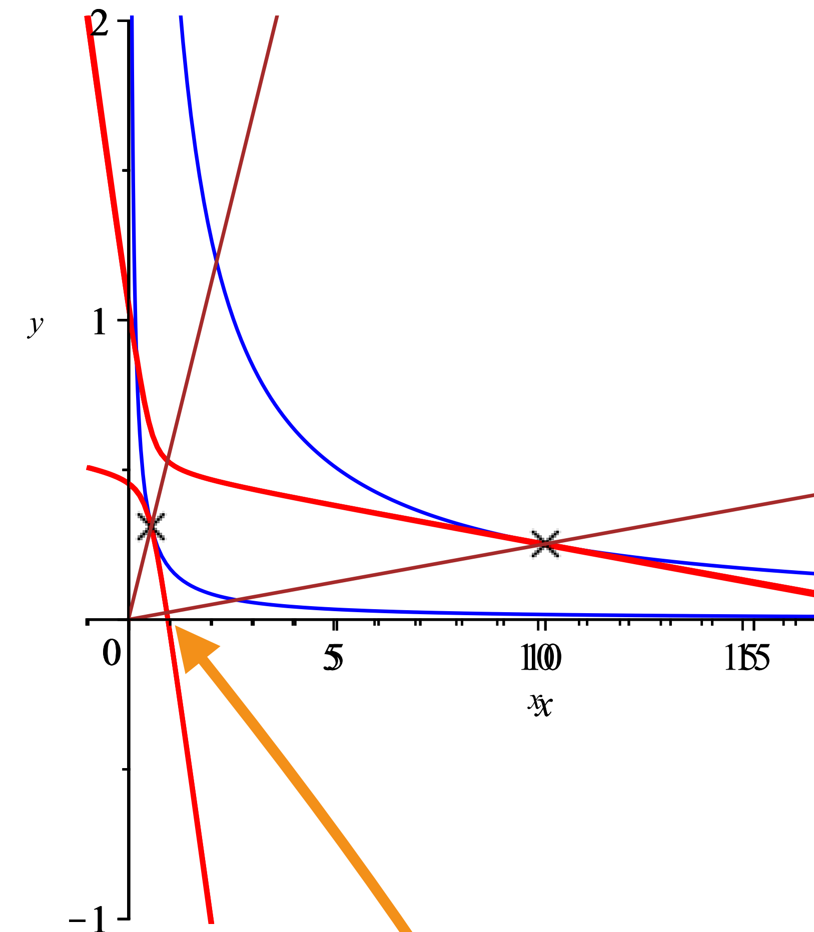
Thus, we add the equation $H(tz_1,\ldots,tz_n) = 0$ for a new variable t and select the positive real point(s) $\mathbf{z}$ with no $t \in (0,1)$ from a new Kronecker representation:

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

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.

explicit algebraic number

This result covers the easiest cases.
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:

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

$$x = \frac{2u - 1006}{P'(u)}, \quad y = z = -\frac{320}{P'(u)}, \quad t = -\frac{164u + 7108}{P'(u)}$$

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)));
```

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

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;
```

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

```
> 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:

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

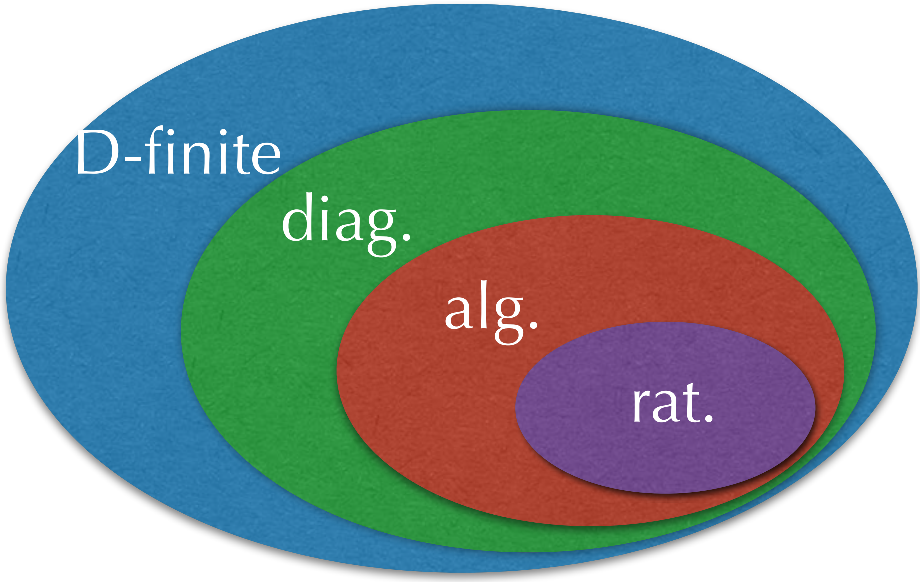
$$H(\underline{u}) = 0 \qquad |u_1|^2 = t|z_1|^2, \ldots, |u_n|^2 = t|z_n|^2$$

+ 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.
- Complexity issues become clearer.

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

The End