

Computational Variations on Linear Differential Equations

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Computer Algebra

- Effective mathematics (what can we compute?);
- their complexity (how fast?).

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Thesis in this talk: *linear differential equations are a good data-structure.*

Menu dégustation

- Dynamic Dictionary of Mathematical Functions
- Fast numerical evaluation
- Algebraic series and matters of size
- Combinatorial walks
- Automatic proofs of identities

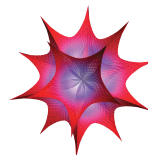
I Dynamic Dictionary of Mathematical Functions

Dynamic Dictionary of Mathematical Functions



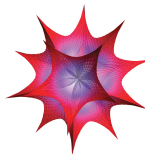
- ① In the beginning, there were **handbooks** of identities.
 Among the most cited documents in the scientific literature.
 Thousands of **useful** mathematical formulas,
 computed, compiled and edited by hand.

Dynamic Dictionary of Mathematical Functions



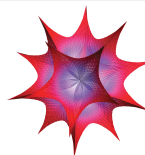
- ① In the beginning, there were **handbooks** of identities.
- ② Then, came **computer algebra**. Computation with exact mathematical objects.
Several million users.
30 years of **algorithmic progress** in effective mathematics.

Dynamic Dictionary of Mathematical Functions



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- ② Then, came **computer algebra**.
- ③ Last, came **the Web**. **New kinds of interaction** with documents.

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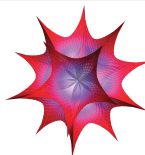
Aim of the project

DDMF = Mathematical Handbooks + Computer Algebra + Web

- ① Develop and use computer algebra algorithms to **generate** the formulas;
- ② Provide web-like interaction with the document **and the computation**.

<http://ddmf.msr-inria.inria.fr/>

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Heavy work
by F. Chyzak

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II Fast Numerical Evaluation

Fast Arithmetic

Fast Fourier Transform (Gauss, Cooley-Tuckey, Schönhage-Strassen)

Two integers of n digits can be multiplied with $O(n \log n \log \log n)$ bit operations.

Applications (in the 70's & 80's) (Brent, Schroepel, Chudnovsky²):

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$$n! = \underbrace{n \times \cdots \times \lceil n/2 \rceil}_{\text{size } O(n \log n)} \times \underbrace{\lfloor n/2 \rfloor \times \cdots \times 1}_{\text{size } O(n \log n)}$$

Cost: $O(n \log^3 n \log \log n)$

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- any linear recurrence of order 1 (coeffs in $\mathbb{Q}(n)$): idem;

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- any linear recurrence of order 1 (coeffs in $\mathbb{Q}(n)$): idem;
- arbitrary order: same idea, same cost (matrix factorial).

Numerical Evaluation of Solutions of LDEs

Principle:

$$f(x) = \underbrace{\sum_{n=0}^N a_n x^n}_{\text{fast evaluation}} + \underbrace{\sum_{n=N+1}^{\infty} a_n x^n}_{\text{good bounds}}.$$

f solution of a LDE with coefficients in $\mathbb{Q}(x)$ (our data-structure!)

- linear recurrence in N for the first sum (easy);
- tight bounds on the tail (technical);
- no numerical roundoff errors.

The technique used for recent records of π :

$$\frac{1}{\pi} = \frac{12}{C^{3/2}} \sum_{n=0}^{\infty} \frac{(-1)^n (6n)! (A + nB)}{(3n)! n!^3 C^{3n}}$$

with $A = 13591409$, $B = 545140134$, $C = 640320$.

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Analytic Continuation: compute $f(x), f'(x), \dots, f^{(d)}(x)$ as new initial conditions and handle propagation of errors.

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Ad.: Marc Mezzarobba's papers and package NumGfun.

III Algebraic Series and Matters of Size

Algebraic Series can be Computed Fast

$P(X, Y) \in \mathbb{Q}[X, Y]$ irreducible, $\deg P = D$, $S \in \mathbb{Q}[[X]]$,

$$P(X, S) = 0.$$

Wanted: first N coefficients of S , for large N .

Application: combinatorics (context-free languages).

Idea:

- S satisfies a LDE of order $\leq D$ (Abel, Cockle, Harley, Tannery);
- translate into a linear recurrence;
- unroll the recurrence $\rightarrow O(N)$ operations.

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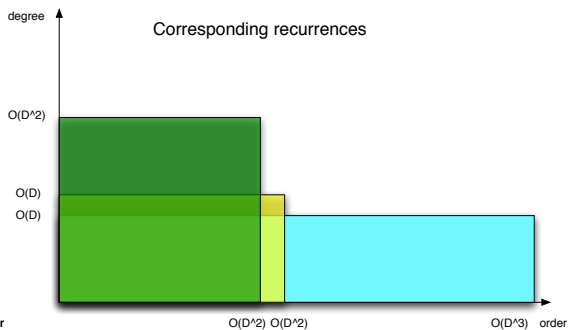
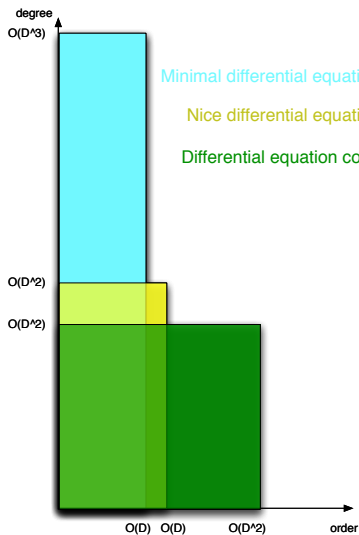
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Algorithm:

- ① invert $P_Y \bmod P$ in $\mathbb{Q}(X)[Y]$;
 - ② $S' = -P_Y^{-1}(S)P_X(S) = Q_1(S)$ with $\deg_Y Q_1 < \deg_Y P$;
 - ③ obtain $S^{(i)} = Q_i(S)$ for $i = 2, \dots, d$, with $\deg_Y Q_i < \deg_Y P$;
 - ④ linear algebra to eliminate S^2, \dots, S^{d-1} .
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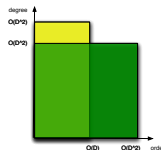
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Minimality has a cost



Bounds by Creative Telescoping

$$S(z) = \frac{1}{2\pi i} \oint \underbrace{\frac{yP_y(z, y)}{P(z, y)}}_{F(z, y)} dy.$$

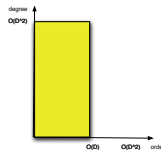


Creative telescoping: an algorithm for differentiation under \int and integration by parts.

- 1 Find $\Lambda = A(z, \partial_z) + \partial_y B(z, \partial_z, y, \partial_y)$ s.t. $\Lambda \cdot F = 0$;
- 2 return A .

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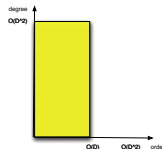
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Bounds by counting dimensions

$$z^i \partial_z^j \partial_y^k \cdot F = \frac{Q}{p_{j+k+1}}, \quad \deg Q \leq i + (j + k + 1)D.$$

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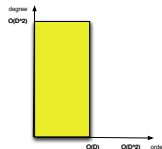
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Taking $i \leq N_z, j + k \leq N_\partial$,

$$\dim(\text{lhs}) = (N_z + 1) \binom{N_\partial + 2}{2}, \quad \dim(\text{rhs}) = \binom{(N_\partial + 1)D + N_z + 2}{2}.$$

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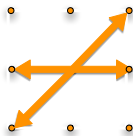
Taking $i \leq N_z$, $j + k \leq N_\partial$, $N_z = 4D^2$, $N_\partial = 4D$,

$$\dim(\text{lhs}) = (N_z + 1) \binom{N_\partial + 2}{2} > \dim(\text{rhs}) = \binom{(N_\partial + 1)D + N_z + 2}{2}.$$

IV Combinatorial Walks

Gessel's Walks in the 1/4 plane

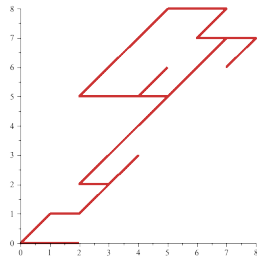
$$G(x, y, t) := \sum_{n \geq 0} \sum_{i, j} f_{i, j; n} x^i y^j t^n$$



- 79 inequivalent step sets;
- long history of special cases;
- Gessel's was left;
- conjectured **not** soln of LDE.

Bostan-Kauers 2010

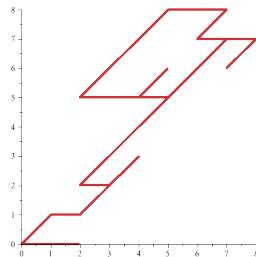
G is algebraic!



Computer-driven discovery and proof

Computation

$$G(x, y, t) := \sum_{n \geq 0} \sum_{i, j} f_{i, j; n} x^i y^j t^n$$



- Compute G up to t^{1000} ;
- conjecture LDE with 1.5 billion coeffs!;
- check for sanity (bit size, more coeffs, Fuchsian, p -curvature);
- Oho!
- conjecture polynomials ($\deg \leq (45, 45, 25)$, 25 digit coeffs);
- **Proof** by (big) resultants.

Minimal polynomial ≈ 30 Gb (but unnecessary).

V Automatic Proofs of Identities

Examples of Identities

$$\sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{k}^2 = \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k} \sum_{j=0}^k \binom{k}{j}^3 \quad [\text{Strehl92}]$$

$$\int_0^{+\infty} x J_1(ax) I_1(ax) Y_0(x) K_0(x) dx = -\frac{\ln(1-a^4)}{2\pi a^2} \quad [\text{GIMo94}]$$

$$\frac{1}{2\pi i} \oint \frac{(1+2xy+4y^2) \exp\left(\frac{4x^2y^2}{1+4y^2}\right)}{y^{n+1}(1+4y^2)^{\frac{3}{2}}} dy = \frac{H_n(x)}{[n/2]!} \quad [\text{Doetsch30}]$$

$$\sum_{k=0}^n \frac{q^{k^2}}{(q; q)_k (q; q)_{n-k}} = \sum_{k=-n}^n \frac{(-1)^k q^{(5k^2-k)/2}}{(q; q)_{n-k} (q; q)_{n+k}} \quad [\text{Andrews74}]$$

$$\sum_{j=0}^n \sum_{i=0}^{n-j} \frac{q^{(i+j)^2+j^2}}{(q; q)_{n-i-j} (q; q)_i (q; q)_j} = \sum_{k=-n}^n \frac{(-1)^k q^{7/2k^2+1/2k}}{(q; q)_{n+k} (q; q)_{n-k}} \quad [\text{Paule85}].$$

More Identities

$$\sum_{k=0}^n \binom{n}{k} i(k+i)^{k-1} (n-k+j)^{n-k} = (n+i+j)^n \quad [\text{Abel1826}]$$

$$\sum_{k=0}^n (-1)^{m-k} k! \binom{n-k}{m-k} \left\{ \begin{matrix} n+1 \\ k+1 \end{matrix} \right\} = \left\langle \begin{matrix} n \\ m \end{matrix} \right\rangle, \quad [\text{Frobenius1910}]$$

$$\sum_{k=0}^m \binom{m}{k} B_{n+k} = (-1)^{m+n} \sum_{k=0}^n \binom{n}{k} B_{m+k}, \quad [\text{Gessel03}]$$

$$\int_0^\infty x^{k-1} \zeta(n, \alpha + \beta x) dx = \beta^{-k} B(k, n-k) \zeta(n-k, \alpha),$$

$$\int_0^\infty x^{\alpha-1} \text{Li}_n(-xy) dx = \frac{\pi(-\alpha)^n y^{-\alpha}}{\sin(\alpha\pi)},$$

$$\int_0^\infty x^{s-1} \exp(xy) \Gamma(a, xy) dx = \frac{\pi y^{-s}}{\sin((a+s)\pi)} \frac{\Gamma(s)}{\Gamma(1-a)}$$

Computer Algebra Algorithms

Aim

- Prove these identities automatically (fast?);
- Compute the rhs given the lhs;
- Explain why these identities exist.

Examples:

- 1st slide: Zeilberger's algorithm and variants;
- 2nd slide (1st 3): Majewicz, Kauers, Chen & Sun;
- last 3: generalization of previous ones (with Chyzak & Kauers).

Ideas

Confinement in finite dimension + Creative telescoping.

Framework: Ore polynomials

$$(fg)' = f'g + fg', \quad \Delta_n(f_n g_n) = f_{n+1} \Delta_n(g_n) + \Delta_n(f_n) g_n,$$

q -analogues of these and many more

are captured by $\mathbb{A}\langle\partial\rangle$ (\mathbb{A} integral domain) with commutation

$$\partial a = \sigma(a)\partial + \delta(a),$$

σ ring morphism, δ σ -derivation ($\delta(ab) = \sigma(a)\delta(b) + \delta(a)b$).

Main property

$P, Q \in \mathbb{A}\langle\partial\rangle$, then $\deg PQ = \deg P + \deg Q$.

Consequences:

- ① In one variable:
 - Euclidean division;
 - Euclidean algorithm (gcd, lcm).
- ② In several variables (allow for mixed diff-diff):
 - Gröbner bases.

Gröbner bases as a data-structure to encode special functions

Example: Contiguity of Hypergeometric Series

$$F(a, b; c; z) = \sum_{n=0}^{\infty} \underbrace{\frac{(a)_n(b)_n}{(c)_n n!}}_{u_{a,n}} z^n, \quad (x)_n := x(x+1) \cdots (x+n-1).$$

$$\frac{u_{a,n+1}}{u_{a,n}} = \frac{(a+n)(b+n)}{(c+n)(n+1)} \rightarrow z(1-z)F'' + (c - (a+b+1)z)F' - abF = 0,$$

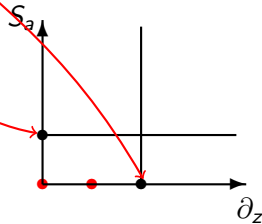
$$\frac{u_{a+1,n}}{u_{a,n}} = \frac{n}{a} + 1 \rightarrow S_a F := F(a+1, b; c; z) = \frac{z}{a}F' + F.$$

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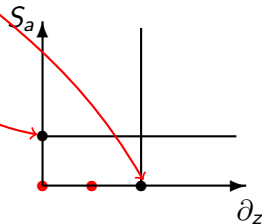
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Gauss 1812: contiguity relation.

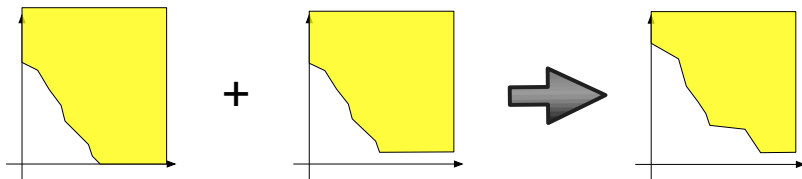
$\dim=2 \Rightarrow S_a^2 F, S_a F, F$ linearly dependent:

(Coordinates in $\mathbb{Q}(a, b, c, z)$.)



$$(a+1)(z-1)S_a^2 F + ((b-a-1)z+2-c+2a)S_a F + (c-a-1)F = 0.$$

Closure Properties



Proposition

$$\begin{aligned}\dim \operatorname{ann}(f + g) &\leq \max(\dim \operatorname{ann} f, \dim \operatorname{ann} g), \\ \dim \operatorname{ann}(fg) &\leq \dim \operatorname{ann} f + \dim \operatorname{ann} g, \\ \dim \operatorname{ann} \partial f &\leq \dim \operatorname{ann} f.\end{aligned}$$

Algorithms by linear algebra
simple definitions \rightarrow data-structures for more complicated functions

Example: Mehler's Identity for Hermite Polynomials

$$\sum_{n=0}^{\infty} H_n(x) H_n(y) \frac{u^n}{n!} = \frac{\exp\left(\frac{4u(xy - u(x^2 + y^2))}{1 - 4u^2}\right)}{\sqrt{1 - 4u^2}}$$

- ① Definition of Hermite polynomials (D-finite over $\mathbb{Q}(x)$):
recurrence of order 2;
- ② Product by linear algebra: $H_{n+k}(x)H_{n+k}(y)/(n+k)!$, $k \in \mathbb{N}$
generated over $\mathbb{Q}(x, n)$ by

$$\frac{H_n(x)H_n(y)}{n!}, \frac{H_{n+1}(x)H_n(y)}{n!}, \frac{H_n(x)H_{n+1}(y)}{n!}, \frac{H_{n+1}(x)H_{n+1}(y)}{n!}$$

→ recurrence of order at most 4;

- ③ Translate into differential equation.



Creative Telescoping (Zeilberger 90)

Creative telescoping = “differentiation” under integral + “integration” by parts

Ex.: $\int_0^1 \frac{\cos zt}{\sqrt{1-t^2}} dt = \frac{\pi}{2} J_0(z), \quad \underbrace{(zJ_0'' + J_0' + zJ_0)}_{A(z, \partial_z) \cdot J_0} = 0, \quad J_0(0) = 1).$

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$$I(z) = \int_0^1 \frac{\cos zt}{\sqrt{1-t^2}} dt, \quad I'(z) = \int_0^1 -t \frac{\sin zt}{\sqrt{1-t^2}} dt,$$

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Creative Telescoping

Input: generators of (a subideal of) $\text{ann } f$;

Output: A, B such that $A - \partial_t B \in \text{ann } f$, A free of t, ∂_t .

Algorithm: sometimes. (Why would they exist?)

Telescoping of \mathcal{I} wrt t :

$$T_t(\mathcal{I}) := (\mathcal{I} + \partial_t \mathbb{Q}(z, t) \langle \partial_z, \partial_t \rangle) \cap \mathbb{Q}(z) \langle \partial_z \rangle.$$

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Note: **holonomy** is a sufficient condition for

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Example: Discovering Pascal's Triangle Automatically

$$(S_n S_k - S_k - 1) \cdot \binom{n}{k} = 0 = (\underbrace{S_n - 2}_{\text{no } k, S_k} + (S_k - 1) \underbrace{(S_n - 1)}_{\text{certificate}}) \cdot \binom{n}{k}.$$

$$\text{Sum over } k \Rightarrow (S_n - 2) \sum_k \binom{n}{k} = 0.$$

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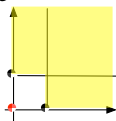
Reduce all monomials of degree $\leq s = 2$:

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Common denominator: $D_2 = (k+1)(k+2)(n+1-k)(n+2-k)$.

$D_2, D_2 S_n, D_2 S_k, D_2 S_n^2, D_2 S_k^2, D_2 S_n S_k$ **confined** in

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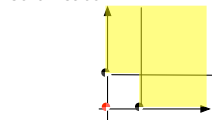


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This **has to happen** for some degree: $\deg D_s = O(s)$.

Polynomial Growth

Definition (Polynomial Growth p)

There exists a sequence of polynomials P_s , s.t. for all (a_1, \dots, a_k) with $a_1 + \dots + a_k \leq s$, $P_s \partial_1^{a_1} \dots \partial_k^{a_k}$ reduces to a combination of elements below the stairs with **polynomial** coefficients of degree $O(s^p)$.

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Proof. Same as above. Set $q := \dim \mathcal{I} + p$.

- In degree s , $\dim O(s^q)$ below stairs.
- Number of monomials in $\partial_t, \partial_{i_1}, \dots, \partial_{i_q}$: $O(s^{q+1})$;

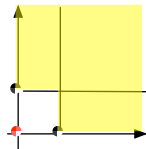
\Rightarrow any q variables linearly dependent $\Rightarrow \dim \leq q - 1$.

This proof gives an algorithm. Also, bounds available.

Examples (all with $p = 1$)

- Proper hypergeometric [Wilf & Zeilberger 1992]:

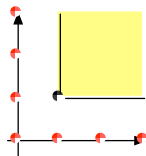
$$Q(n, k) \xi^k \frac{\prod_{i=1}^u (a_i n + b_i k + c_i)!}{\prod_{i=1}^v (u_i n + v_i k + w_i)!},$$



Q polynomial, $\xi \in \mathbb{C}$, a_i, b_i, u_i, v_i **integers**.

- Differential D-finite (definite integration);
- Stirling: ok for $n \geq 3$, e.g., Frobenius:

$$\sum_{k=0}^n (-1)^{m-k} k! \binom{n-k}{m-k} \left\{ \begin{matrix} n+1 \\ k+1 \end{matrix} \right\} = \left\langle \begin{matrix} n \\ m \end{matrix} \right\rangle.$$



- Abel type: $\dim = 2 \rightarrow$ ok for $n \geq 4$, e.g., Abel:

$$\sum_{k=0}^n \binom{n}{k} i(k+i)^{k-1} (n-k+j)^{n-k} = (n+i+j)^n.$$

VI Conclusion

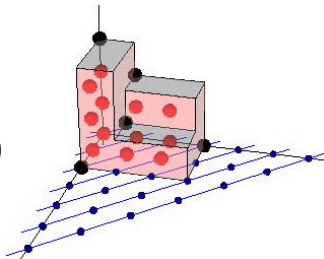
Conclusion

- Summary:

- Linear differential/recurrence equations as a data structure;
- Confinement in vector spaces + creative telescoping \rightarrow identities.

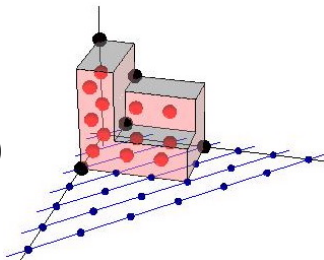
- Also:

- q -analogues;
- Fast algorithms: Zeilberger 1990 (hypergeom); Chyzak 2000 (D-finite) Us 2009 (**non-D-finite**).
- Bounds \rightarrow identities;
- Fast algorithms for special classes;
- Efficient numerical evaluation.



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THE END