Algorithmic Variations on Linear Differential Equations

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MBM’2014
Computer Algebra

• Systems with millions of users

• A scientific area: effective mathematics and their complexity

• 30 years of progress in mathematical algorithms

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

1. Equations as a data-structure
2. Guess & Prove combinatorial walks
3. Proofs of identities
4. Sums and Integrals
5. Numerical evaluation via the Taylor series
6. Chebyshev expansions
I. Equations as a data-structure

erf := (y'' + 2xy' = 0, ini. cond.)

basis of the gfun package
Dynamic Dictionary of Mathematical Functions

- User need
- Recent algorithmic progress
- Maths on the web

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

Heavy work by F. Chyzak
Demonstration
II. Guess & Prove
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 (MBM & Mishna);
- long history of special cases;
- Gessel's was left;
- conjectured not soln of LDE.

**Thm. [Bostan-Kauers 2010]**

G is algebraic!

Computer-driven discovery & 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 million coeffs!
- check for sanity (bit size, more coeffs, Fuchsian, \( p \)-curvature);
- oh!
- conjecture polynomials (deg \( \leq (45, 25, 25) \), 25 digit coeffs);
- **Proof** by (big) resultants.
The 79 cases: finite and infinite groups

79 step sets

23 admit a finite group

[Mishna’07]

4 are algebraic

(3 Kreheras-type + Gessel)

[BMM’10] + [B.-Kauers’10]

56 have an infinite group

[Boosquet-Mélou-Mishna’10]

[Melczer-Mishna’13] for 5 singular cases

all are holonomic

19 transcendental

[Gessel-Zeilberger’92]

[Bousquet-Mélou’02]

all non-holonomic

• [Mishna-Rechnitzer’07] and

• [Kurkoya-Raschel’13] and

[B.-Raschel-Salvy’13] for all others

[Slide borrowed from A. Bostan]
Proving no LDE exists

- \( \log(n) \), \( n^a \ (a \notin \mathbb{Z}) \), \( p_n \), \( e^{\sqrt{n}} \), \( \Gamma(n\sqrt{2}) \), ... by their asymptotic behavior, or that of their generating function (with P. Flajolet & S. Gerhold).

- walks in the \( 1/4 \)-plane (with A. Bostan & K. Raschel)

\[
\chi := \sum_{(i,j) \in S} x^i y^j \\
\]

\[
c := \frac{\partial^2 \chi}{\partial x \partial y} \cdot \frac{\partial^2 \chi}{\partial y^2} (x_0, y_0) \\
arccos(c)/\pi \notin \mathbb{Q}
\]
III. Proofs of Identities
Proof technique

\[ \text{series}(\sin(x)^2 + \cos(x)^2 - 1, x, 4); \]

\[ O(x^4) \]

Why is this a proof?

1. \( \sin \) and \( \cos \) satisfy a 2nd order LDE: \( y'' + y = 0 \);
2. their squares and their sum satisfy a 3rd order LDE;
3. the constant \(-1\) satisfies \( y' = 0 \);
4. thus \( \sin^2 + \cos^2 - 1 \) satisfies a LDE of order at most 4;
5. Cauchy’s theorem concludes.

Proofs of non-linear identities by linear algebra!
Example: Mehler’s identity for Hermite polynomials

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

1. Definition of Hermite polynomials: 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

\[
\frac{H_n(x)H_n(y)}{n!}, \quad \frac{H_{n+1}(x)H_n(y)}{n!}, \quad \frac{H_n(x)H_{n+1}(y)}{n!}, \quad \frac{H_{n+1}(x)H_{n+1}(y)}{n!}
\]

→ recurrence of order at most 4;

3. Translate into differential equation.
Guess & prove continued fractions
(with S. Maulat)

1. Differential equation produces first terms (easy):

\[
\arctan x = \frac{x}{1 + \frac{1}{3}x^2 + \frac{4}{15}x^2 + \frac{9}{35}x^2 + \cdots}
\]

2. Guess a formula (easy):

\[
a_n = \frac{n^2}{4n^2 - 1}
\]

3. Prove that the CF with these \(a_n\) satisfies the differential equation.

No human intervention needed.
Automatic Proof of the guessed CF

\[
\text{arctan} x \triangleq \frac{x}{1 + \frac{n^2 x^2}{4n^2 - 1} + \cdots}
\]

- **Aim**: RHS satisfies \((x^2 + 1)y' - 1 = 0\);
- Convergents \(P_n/Q_n\) where \(P_n\) and \(Q_n\) satisfy a LRE (and \(Q_n(0) \neq 0\));
- Define \(H_n := (Q_n)^2 ((x^2 + 1)(P_n/Q_n)' - 1)\);
- \(H_n\) is a polynomial in \(P_n, Q_n\) and their derivatives;
- therefore, it satisfies a LRE that can be computed;
- from it, \(H_n = O(x^n)\) visible, ie \(\lim P_n/Q_n\) soln;
- conclude \(P_n/Q_n \rightarrow \text{arctan}\) (check initial cond.).

More generally: this guess-and-proof approach applies to CF for solutions of (q-)Ricatti equations \(\rightarrow\) all explicit C-fractions in Cuyt et alii.
IV. Sums and Integrals
Creative telescoping

\[ l(x) = \int f(x, t) \, dt =? \quad \text{or} \quad S(n) = \sum_{k} u(n, k) =? \]

**Input**: equations
(differential for \( f \) or recurrence for \( u \)).

**Output**: equations for the sum or the integral.

**Method**: integration (summation) by parts and differentiation (difference) under the integral (sum) sign

Example (with Pascal’s triangle):

\[ u(n, k) = \binom{n}{k} \text{ def. by } \left\{ \begin{array}{l} \binom{n+1}{k} = \frac{n+1}{n+1-k} \binom{n}{k}, \\
\binom{n}{k+1} = \frac{n-k}{k+1} \binom{n}{k} \end{array} \right. \]

\[ S(n+1) = \sum_{k} \binom{n+1}{k} = \sum_{k} \left( \binom{n+1}{k} - \binom{n+1}{k+1} \right) + \left( \binom{n}{k+1} - \binom{n}{k} + 2 \binom{n}{k} \right) = 2S(n). \]

**Algorithms**: reduce the search space.
Telescoping Ideal

$$T_t(f) := \left( \text{Ann } f + \partial_t \mathbb{Q}(x, t) \langle \partial_x, \partial_t \rangle \right) \cap \mathbb{Q}(x) \langle \partial_x \rangle \ .$$

- hypergeometric summation: dim=1 + param. Gosper. [Zeilberger]
- holonomy: restrict int. by parts to $\mathbb{Q}(x) \langle \partial_x, \partial_t \rangle$ and Gröbner bases. [Wilf-Zeilberger]
- finite dim, Ore algebras & GB (with F. Chyzak)
- infinite dim & GB (with F. Chyzak & M. Kauers)
- rational $f$ and restrict to $\mathbb{Q}(x)[t, 1/\text{den } f] \langle \partial_x, \partial_t \rangle$ in very good complexity (with A. Bostan & P. Lairez)
Multiple binomial sums
(with A. Bostan & P. Lairez)

Def. Combination of binomial coefficients, geometric sequences, $\oplus$, $\times$, multiplication by scalars, affine changes of indices and $\sum$.

Thm. The generating series is the integral of a rational function that can be constructed automatically.

$\rightarrow$ whence an efficient summation algorithm using the previous algo.

Ex. (Apéry) $A(n) = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k} \rightarrow \int \frac{dt_1 \wedge dt_2 \wedge dt_3}{t_1 t_2 t_3 (1 - t_1 t_2 - t_1 t_2 t_3) - (1 + t_1)(1 + t_2)(1 + t_3)z}$

$\rightarrow$ LDE $\rightarrow (n + 1)^3 A(n) + (\cdots) A(n + 1) + (n + 2)^2 A(n + 2) = 0.$

More at Pierre’s PhD defense on Nov. 12.
V. Numerical evaluation via the Taylor series

From large integers to precise numerical values
Numerical evaluation of solutions of LDEs

**Principle:**  
\[ f(x) = \sum_{n=0}^{N} a_n x^n + \sum_{n=N+1}^{\infty} a_n x^n \]

- fast evaluation
- good bounds

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

1. linear recurrence in \( N \) for the first sum (easy);
2. tight bounds on the tail (e.g., work with M. Mezzarobba);
3. no numerical roundoff errors.

The technique used for fast evaluation of constants like

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

with \( A = 13591409, \)  
\( B = 545140134, \)  
\( C = 640320. \)

Code available: [NumGfun][Mezzarobba 2010]
Binary Splitting for linear recurrences (70’s and 80’s)

- \( n! \) by divide-and-conquer:
  \[
  n! = \underbrace{n \times \cdots \times \lceil n/2 \rceil}_{\text{size } O(n \log n)} \times \underbrace{\lceil n/2 \rceil \times \cdots \times 1}_{\text{size } O(n \log n)}
  \]
  
  Cost: \( O(n \log^3 n \log \log n) \) using FFT

- linear recurrences of order 1 reduce to
  \[
  p!(n) := (p(n) \times \cdots \times p(\lceil n/2 \rceil)) \times (p(\lceil n/2 \rceil) \times \cdots \times p(1))
  \]

- arbitrary order: same idea, same cost (matrix factorial):

  **ex:** \( e_n := \sum_{k=0}^{n} \frac{1}{k!} \) satisfies a 2nd order rec, computed via

  \[
  \begin{pmatrix} e_n \\ e_{n-1} \end{pmatrix} = \frac{1}{n} \begin{pmatrix} n+1 & -1 \\ n & 0 \end{pmatrix} \begin{pmatrix} e_{n-1} \\ e_{n-2} \end{pmatrix} = \frac{1}{n!} A!(n) \begin{pmatrix} 1 \\ 0 \end{pmatrix}.
  \]
Analytic continuation

Compute $f(x), f'(x), \ldots, f^{(d-1)}(x)$ as new initial conditions and handle error propagation:

Ex: \(\text{erf}(\pi)\) with 15 digits:

\[
0 \xrightarrow{200 \text{ terms}} 3.1416 \xrightarrow{18 \text{ terms}} 3.1415927 \xrightarrow{6 \text{ terms}} 3.14159265358979
\]

Again: computation on integers. No roundoff errors.
VI Chebyshev expansions

Taylor

Chebyshev
From equations to operators

\[
d/dx \leftrightarrow D \\
mult \text{ by } x \leftrightarrow x \\
\text{composition} \leftrightarrow \text{product} \\
Dx = xD + 1
\]

\[
(n \mapsto n+1) \leftrightarrow S \\
mult \text{ by } n \leftrightarrow n \\
\text{composition} \leftrightarrow \text{product} \\
S^n = (n+1)S
\]

Taylor morphism: \( D \mapsto (n+1)S; \ x \mapsto S^{-1} \)
produces linear recurrence from LDE

erf:
\[
D^2 + 2xD \mapsto (n + 1)S(n + 1)S + 2S^{-1}(n + 1)S = (n + 1)(n + 2)S^2 + 2n
\]

Ore (1933): general framework for these non-commutative polynomials.

Main property: \( \text{deg } AB = \text{deg } A + \text{deg } B \).

Consequence 1: (non-commutative) Euclidean division

Consequence 2: (non-commutative) Euclidean algorithm.
Ore fractions ($Q^{-1}P$ with P&Q operators)

**Thm.** (Ore 1933) Sums and products reduce to that form.

Application: extend Taylor morphism to Chebyshev expansions

Taylor

$\frac{x^{n+1}}{x^n} = x \cdot x^n, \quad (x^n)' = nx^{n-1}$

$\leftrightarrow \quad X := S^{-1}, \quad D := (n+1)S$

Chebyshev

\[
2xT_n(x) = T_{n+1}(x) + T_{n-1}(x),
\]

\[
2(1-x^2)T_n'(x) = -nT_{n+1}(x) + nT_{n-1}(x)
\]

$\leftrightarrow \quad X := (S+S^{-1})/2,$

$D := (1-X^2)^{-1} n(S-S^{-1})/2 = 2(S^{-1}-S)^{-1} n.$

erf:

\[
D^2 + 2xD \leftrightarrow (2(S^{-1} - S)^{-1} n)^2 + 2 \frac{S + S^{-1}}{2} 2(S^{-1} - S)^{-1} n
\]

\[= \text{pol}(n, S)^{-1} (2(n+1)(n+4)S^4 - 4(n+2)^3S^2 + 2n(n+3))
\]

**Prop.** [with A. Benoit] If $y$ is a solution of $L(x, d/dx)$, then its Chebyshev coefficients annihilate the **numerator** of $L(X, D)$.

Next steps: FastRelax (starting this Fall)

\[ y'' + 2xy' = 0 + \text{ini. cond.} \]

Computer Algebra

Formal proofs

\[ \text{double erf(double x) \{\ldots\}} \]

Computer Arithmetic

5 teams, 4 years
Conclusion

• Linear differential equations and recurrences are a great data-structure;
• Numerous algorithms have been developed in computer algebra;
• Efficient code is available;
• More is true (creative telescoping, diagonals,…);
• More to come for Mireille and her followers.

Bravo Mireille!