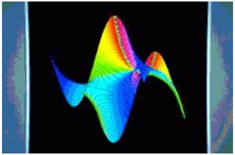
Computational Variations on Linear Differential Equations

Bruno Salvy
Bruno.Salvy@inria.fr

Algorithms Project, Inria



IHES, October 19, 2011

Computer Algebra

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

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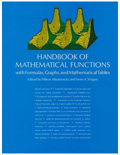
Thesis in this talk: *linear differential equations are a good data-structure*.

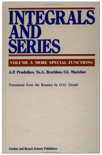
Menu dégustation

- 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



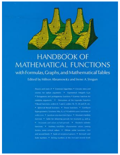


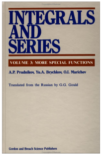
1. In the beginning, there were handbooks of identities.

   Among the most cited documents in the scientific literature.

   Thousands of useful mathematical formulas,
   computed, compiled and edited by hand.

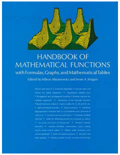
Dynamic Dictionary of Mathematical Functions

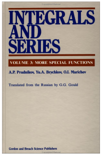


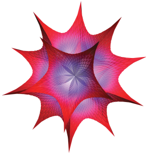


1. In the beginning, there were handbooks of identities.
2. Then, came computer algebra. Computation with exact mathematical objects.
   Several million users.
   30 years of algorithmic progress in effective mathematics.

Dynamic Dictionary of Mathematical Functions







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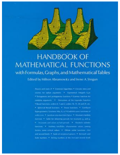
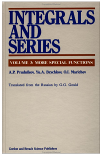
3. Last, came the Web. New kinds of interaction with documents.

Dynamic Dictionary of Mathematical Functions





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DDMF = Mathematical Handbooks + Computer Algebra + Web

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

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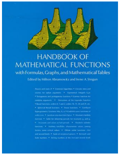

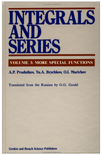

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Heavy work by F. Chyzak

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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, Schroeppel, Chudnovsky^2):

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- $n!$ by divide-and-conquer:

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

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;
- 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 package NumGfun; his defense next Thursday at École polytechnique.

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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- S satisfies a LDE of order $\leq D$ (Abel, Cockle, Harley, Tannery);
  Algorithm:
  1. invert P_Y mod 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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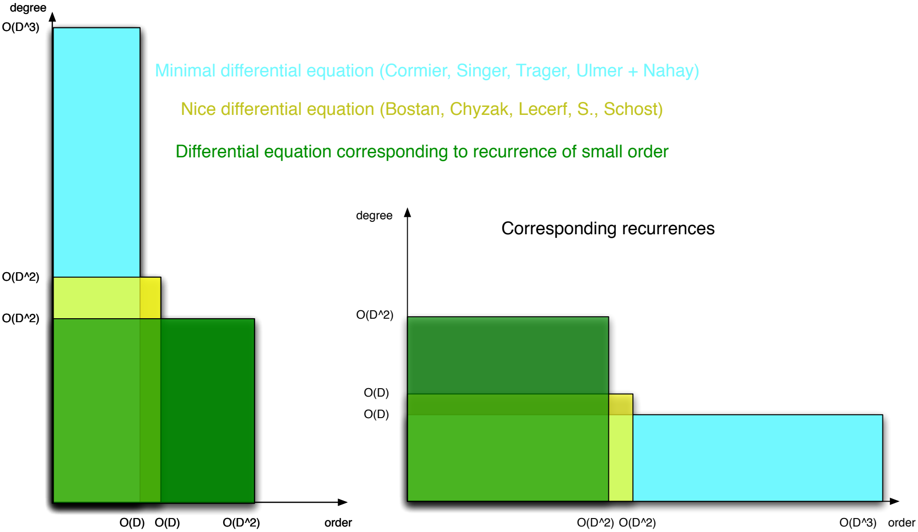
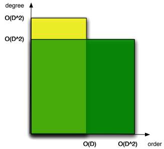
Minimality has a cost



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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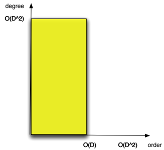

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Bounds by counting dimensions

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

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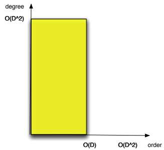

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Taking $i \leq N_z$, $j+k \leq N_\partial$,

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

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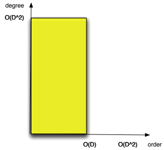

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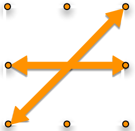
Taking $i \leq N_z$, $j + k \leq N_\partial$, $N_z = 4D^2$, $N_\partial = 4D$,

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

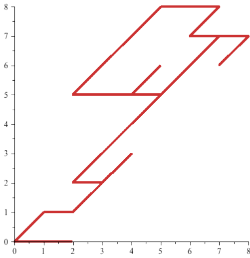
IV Combinatorial Walks

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

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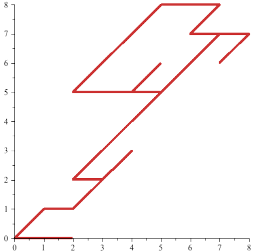

- Compute G up to t^{1000};
- conjecture LDE with 1.5 billion coeffs!;
- check for sanity (bit size, more coeffs, Fuchsian, p-curvature);
- Oho!
- conjecture polynomials (deg $\leq (45, 45, 25)$, 25 digit coeffs);
- Proof by (big) resultants.

Minimal polynomial $\approx$ 30 Gb (but unnecessary).

V Automatic Proofs of Identities

Examples of Identities

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

$$\int_0^{+\infty} xJ_1(ax)I_1(ax)Y_0(x)K_0(x)\,dx=-\frac{\ln(1-a^4)}{2\pi a^2} \quad \text{[GlMo94]}$$

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

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

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

More Identities

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

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

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

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

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

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

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: recent 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 (gcrd, lclm).
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

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

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

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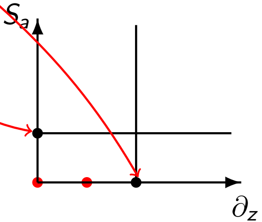

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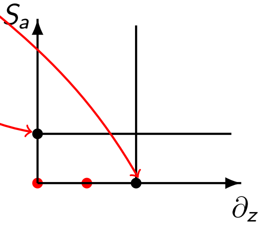
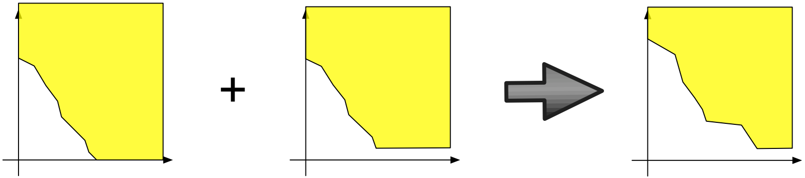
Gauss 1812: contiguity relation.
dim=2 $\Rightarrow$ S_a^2F, S_aF, F linearly dependent:
(Coordinates in $\mathbb{Q}(a,b,c,z)$.)



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

Closure Properties



Proposition

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

Algorithms by linear algebra

simple definitions $\to$ 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

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

$\rightarrow$ recurrence of order at most 4;

3. Translate into differential equation.

Creative Telescoping (Zeilberger 90)

Creative telescoping= "differentiation" under integral+ "integration" by parts

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

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

$$I''(z) + I(z) = \underbrace{\left[\sqrt{1-t^2}\frac{\sin zt}{z}\right]_0^1}_{0} + \int_0^1 \frac{t}{\sqrt{1-t^2}}\frac{\sin zt}{z}\,dt = -\frac{I'(z)}{z}.$$

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$$\operatorname{ann}\frac{\cos zt}{\sqrt{1-t^2}}\ni\underbrace{A(z,\partial_z)}_{\text{no }t,\partial_t}-\partial_t\underbrace{\frac{t^2-1}{t}\partial_z}_{\text{anything}}$$

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Creative Telescoping

Input: generators of (a subideal of) ann f;
Output: A, B such that $A - \partial_t B \in \operatorname{ann} f$, 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

$$0 \neq (\mathcal{I} + \partial_t \mathbb{Q}(z)\langle\partial_z,\partial_t\rangle) \cap \mathbb{Q}(z)\langle\partial_z\rangle.$$

Example: Discovering Pascal's Triangle Automatically

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

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

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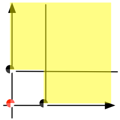
Reduce all monomials of degree $\le s = 2$:



$$1 \to 1,\quad S_n \to \frac{n+1}{n+1-k}1,\quad S_k \to \frac{n-k}{k+1}1$$

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

$D_2, D_2S_n, D_2S_k, D_2S_n^2, D_2S_k^2, D_2S_nS_k$ confined in

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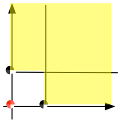

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This has to happen for some degree: $\deg D_s = O(s)$.

Polynomial Growth

Definition (Polynomial Growth p)

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

Theorem (ChyzakKauersSalvy2009)

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

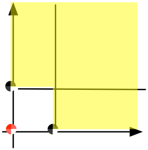
- In degree s, dim $O(s^q)$ below stairs.
- Number of monomials in $\partial_t, \partial_{i_1}, \dots, \partial_{i_q}$: $O(s^{q+1})$;

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

This proof gives an algorithm. Also, bounds available.

Examples (all with $p = 1$)

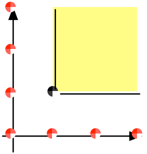
- Proper hypergeometric [Wilf & Zeilberger 1992]:



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

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:



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

  - Abel type: dim $= 2 \to$ 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

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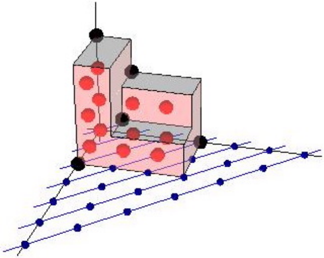
- Summary:
  - Linear differential/recurrence equations as a data structure;
  - Confinement in vector spaces + creative telescoping $\rightarrow$ identities.
- Also:
  - *q*-analogues;
  - Fast algorithms: Zeilberger 1990 (hypergeom); Chyzak 2000 (D-finite) Us 2009 (non-D-finite).
  - Bounds $\rightarrow$ identities;
  - Fast algorithms for special classes;
  - Efficient numerical evaluation.



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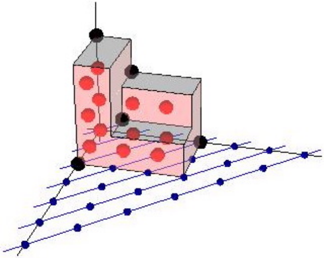

THE END