CR06: Modern Algorithms for Symbolic Summation and Integration

Lecture 12:
Definite summation by creative telescoping

Examples

$$\sum_{k=0}^{2n} (-1)^k \binom{2n}{k}^3 = (-1)^n \frac{(3n)!}{n!^3}$$ Dixon

$$\sum_{i=0}^{n} \sum_{j=0}^{n} \binom{i+j}{i}^2 \binom{4n-2i-2j}{2n-2i} = (2n+1)\binom{2n}{n}^2$$ Andrews-Paule

$$\sum_{j,k} (-1)^{j+k} \binom{j+k}{k+l}\binom{r}{j}\binom{n}{k}\binom{s+n-j-k}{m-j} = (-1)^l \binom{n+r}{n+l}\binom{s-r}{m-n-l}$$ Graham-Knuth-Patashnik

$$\sum_{r_1\geq 0, r_2\geq 0, r_3\geq 0} \frac{(r_2+1)(r_3+1)(r_2+r_3+2)}{(n+1)(n+2)} \binom{n+2}{r_1}\binom{n+2}{r_1+r_2+1}\binom{n+2}{r_1+r_2+r_3+2} = 2^{n-1}\binom{2n+1}{n}$$ Essam-Guttmann

Aims:
1. Prove them automatically
2. Find the rhs given the lhs

Note: at least one free variable

First, find a linear recurrence

Why is this a solution?

With a linear recurrence, it is easy to:

- find hypergeometric closed-forms (Petkovšek's algo.); next lecture
- compute efficiently the first n terms, the nth term;
- (less easy) study the asymptotic behavior;
- build other sequences by closure properties;
- prove identities.

This is what summing means in symbolic computation

Hypergeometric Sequences - Definitions

Def. $(u_n) \in \mathbb{K}^{\mathbb{N}}$ is hypergeometric if there exists $R(n) \in \mathbb{K}(n)$ s.t.

$$\frac{u_{n+1}}{u_n} = R(n), \qquad n \in \mathbb{N}.$$

$\mathbb{K}$ a field of char. 0

Note: writing $R(n) = P(n)/Q(n)$, 1st order recurrence solves as

$$u_n = u_0 \frac{\mathrm{lc}(P)^n}{\mathrm{lc}(Q)^n} \frac{\prod_{P(\alpha)=0} (-\alpha)_n}{\prod_{Q(\beta)=0} (-\beta)_n}.$$

lc: leading coefficient

Def. $(u_{n,k}) \in \mathbb{K}^{\mathbb{N}\times\mathbb{N}}$ is hypergeometric if there exists $a(n,k)$ and $b(n,k)$ in $\mathbb{K}(n,k)$ s.t.

$$\frac{u_{n+1,k}}{u_{n,k}} = a(n,k), \quad \frac{u_{n,k+1}}{u_{n,k}} = b(n,k), \qquad (n,k) \in \mathbb{N}^2.$$

Creative Telescoping for Sums

$$U_n = \sum_k u_{n,k} = ?$$

hypergeometric today

Wanted: linear recurrence for the sum.

Notation
$S_n : u_n \mapsto u_{n+1}$
$\Delta_k : v_k \mapsto v_{k+1} - v_k$

IF one knows $A(n, S_n)$ and $B(n, k, S_n, S_k)$ such that

$$(A(n, S_n) + \Delta_k B(n, k, S_n, S_k)) \cdot u_{n,k} = 0$$

telescoper

certificate

then the sum often telescopes, leading to $A(n, S_n) \cdot U_n = 0$.

When $u_{n,k}$ is hypergeometric, the certificate reduces:

$$B(n, k, S_n, S_k) \cdot u_{n,k} = G(n, k) u_{n,k}$$

rational function

I. Gosper’s Algorithm for Indefinite Summation

Indefinite Summation

Def. (v_n) is an indefinite sum of (u_n) when

$$v_{n+1} - v_n = u_n, \quad n \in \mathbb{N}\,.$$

Discrete analogue of primitive function

Ex.: $u_n = \dfrac{3n+1}{n+1}\dbinom{2n}{n}, \quad v_n = \dbinom{2n}{n} \qquad \displaystyle\sum_{k=0}^{n} u_n = \binom{2n+2}{n+1} - 1.$

Lemma. (v_n) hypergeometric, indefinite sum of (u_n), then

1. (u_n) hypergeometric;
2. $v_n = R(n)u_n$ for some $R(n) \in \mathbb{K}(n)$.

Blackboard proof

Indefinite Hypergeometric Summation

Input: $r(n)$ s.t. $u_{n+1} = r(n)u_n$

Specification of a hypergeometric sequence

Output: $R(n)$ s.t. $v_n = R(n)u_n$ is a hypergeometric sum of u_n

if such a R exists

$$\frac{v_{n+1} - v_n}{u_n} = R(n+1)r(n) - R(n) = 1$$

$R(n)$ rational solution of a linear recurrence of order 1

General algorithm (by Abramov, 1989): next lecture.

Specialized efficient algorithm: Gosper (1978).

Gosper-Petkovšek Decomposition

Recall: $\mathbb{K}$ field of char. 0

Prop. Every rational function $R(n) \in \mathbb{K}(n)$ can be written

$$R(n) = Z\frac{A(n)}{B(n)}\frac{C(n+1)}{C(n)}, \text{ with}$$

Also useful for Petkovšek's algorithm (next lecture)

$Z \in \mathbb{K},\ A, B, C$ monic in $\mathbb{K}[n]$,

$\gcd(A(n), C(n)) = \gcd(B(n), C(n+1)) = 1,$

$\gcd(A(n), B(n+i)) = 1$ for $i \in \mathbb{N}$.

C gathers the roots of the numerator/denominator that differ by a positive integer

Ex.: $$\frac{2(n+5)^2}{n^2(n+3)} = 2\frac{1}{n}\frac{(n+1)(n+2)(n+3)(n+4)^2(n+5)^2}{n(n+1)(n+2)(n+3)^2(n+4)^2}.$$

Constructive Proof

Input: P, Q in $\mathbb{K}[n]$, with $\gcd(P, Q) = 1$ and $R = P/Q$

Output: Z, A, B, C giving the decomposition of R

1. $A := P/\mathrm{lc}(P); B := Q/\mathrm{lc}(Q); Z := \mathrm{lc}(P)/\mathrm{lc}(Q); C := 1$
2. $r(h) := \mathrm{Res}_n(A(n), B(n+h)) \in \mathbb{K}[h]$
3. $1 \leq h_1 < h_2 < \cdots < h_m$ its roots in $\mathbb{N}$
4. For $i = 1, \ldots, m$ do

   $g(n) := \gcd(A(n), B(n+h_i));$

   $A(n) := A(n)/g(n); B(n) := B(n)/g(n-h_i);$

   $C(n) := C(n)g(n-h_i)\cdots g(n-1)$
5. Return Z, A, B, C .

Loop invariants

$R(n) = ZA(n)C(n+1)/(B(n)C(n)),$

$A(n) \mid P(n), B(n) \mid Q(n)$

$\gcd(A(n), C(n)) = \gcd(B(n), C(n+1)) = 1$

Loop variant

$\gcd(A(n), B(n+h)) = 1$

for $h < h_{i+1}$ in $\mathbb{N}$

Blackboard proof

Application to Hypergeometric Summation

(E) $\qquad R(n+1)r(n) - R(n) = 1 \qquad R(n)$ unknown

Write $r(n) = Z\dfrac{A(n)}{B(n)}\dfrac{C(n+1)}{C(n)}, \quad R(n) = \dfrac{B(n-1)}{C(n)}X(n)$

Gosper-Petkovšek → C $\qquad$ new unknown → $X(n)$

Prop. [Gosper] If (E) has a rational solution $R(n)$, then $X(n)$ is a polynomial solution of

$$ZA(n)X(n+1) - B(n-1)X(n) = C(n)\,.$$

Blackboard proof

Gosper's Algorithm

Input: $r(n)$ in $\mathbb{K}(n)$ s.t. $u_{n+1}/u_n = r(n)$

Output: $R(n) \in \mathbb{K}(n)$ s.t. $R(n)u_n$ is an indefinite sum of u_n
FAIL if the sum is not hypergeometric

1. Compute the Gosper-Petkovšek decomposition

$$r(n) = Z\frac{A(n)}{B(n)}\frac{C(n+1)}{C(n)}$$

2. Find polynomial solutions of

$$ZA(n)X(n+1) - B(n-1)X(n) = C(n)$$

3. Return FAIL if none, $B(n-1)X(n)/C(n)$ otherwise.

Exercise: $\sum_k \frac{1}{k!}$ is *not* hypergeometric.

II. Zeilberger's Algorithm for Hypergeometric Summation

Example: Apéry's sequence

from his proof that $\zeta(3) \notin \mathbb{Q}$

$$U_n := \sum_{k=0}^{n} \underbrace{\binom{n}{k}^2 \binom{n+k}{k}^2}_{\text{hypergeometric } u_{n,k}}$$

1. Zeilberger's algorithm finds a telescoping relation

$$(n+2)^3 u_{n+2,k} - (17n^2 + 51n + 39) u_{n+1,k} + (n+1)^3 u_{n,k} = g_{n,k+1} - g_{n,k}$$

with $\quad g_{n,k} = \dfrac{\mathrm{Pol}(n,k)}{(n+1-k)^2(n+2-k)^2} u_{n,k}$

Starting point: $g_{n,k}$ is an indefinite sum wrt k of the lhs

2. Sum over k and telescope (with care)

$$(n+2)^3 U_{n+2} + \cdots + (n+1)^3 U_n = 0$$

Definite Hypergeometric Summation

To be tried for increasing values of m

Input: $r(n,k), s(n,k)$ s.t. $u_{n+1,k} = r(n,k)u_{n,k}$, $u_{n,k+1} = s(n,k)u_{n,k}$

Output: $a_0(n), \ldots, a_m(n)$ rational, $G(n,k)$ hypergeometric s.t.

(T) $G(n,k+1) - G(n,k) = a_m(n)u_{n+m,k} + \cdots + a_0(n)u_{n,k}$ — if such a_i, G exist

Two approaches:

1. Set $G(n,k) = R(n,k)u_{n,k}$, divide (T) by $u_{n,k}$ and look for a rational solution $R \in \mathbb{K}(k)$, with $\mathbb{K} = \mathbb{L}(n)$ of this inhomogeneous LRE with parameterized right-hand side. — Next lecture?

2. Apply Gosper's algorithm directly on $A(n, S_n) \cdot u_{n,k}$ — Zeilberger's algorithm (1992)

Termination

Thm. (Wilf-Zeilberger) If $u_{n,k}$ is proper hypergeometric, ie,

$$u_{n,k} = P(n,k)Z^k \prod_{\ell=1}^{L} (a_\ell n + b_\ell k + c_\ell)!^{e_\ell},$$

a_ℓ, b_ℓ, e_ℓ in $\mathbb{Z}$
$P \in \mathbb{K}(n,k)$
$Z \in \mathbb{K}$,

then Zeilberger's algorithm terminates.

General case clarified algorithmically by Abramov (2003).

Proof in the proper hypergeometric case

$$\frac{u_{n+i,k+j}}{u_{n,k}} = \frac{P(n+i,k+j)}{P(n,k)} Z^j \prod_{\ell=1}^{L} \left(\frac{(a_\ell n + b_\ell k + c_\ell + a_\ell i + b_\ell j)!}{(a_\ell n + b_\ell k + c_\ell)!} \right)^{e_\ell}$$

For r, s in $\mathbb{N}$, $\sigma_\ell = |a_\ell e_\ell| r + |b_\ell e_\ell| s$, $\exists Q(n,k)$ pol. of deg $\leq \sum_\ell \sigma_\ell$ s.t.

$$\left.\begin{matrix} 0 \leq i \leq r \\ 0 \leq j \leq s \end{matrix}\right\} \Rightarrow P(n,k)Q(n,k)\frac{u_{n+i,k+j}}{u_{n,k}} \in \mathbb{K}(n)[k] \text{ of deg} \leq \delta := \deg_k P + 2\sum_\ell \sigma_\ell .$$

The number of such sequences is $(r+1)(s+1) \gg \delta$ for large r, s

$\Rightarrow$ there exists $U(n, S_n, S_k)$ such that $U(n, S_n, S_k) \cdot u_{n,k} = 0$

$$U(n, S_n, S_k) = (S_k - 1)B(n, S_n, S_k) + A(n, S_n).$$

If $A(n, S_n) = 0$, use $k(S_k - 1) = (S_k - 1)(k-1) - 1.$

III. Multiple Binomial Sums

An identity of Andrews & Paule

$$\sum_{i=0}^{n}\sum_{j=0}^{n}\underbrace{\binom{i+j}{i}^2\binom{4n-2i-2j}{2n-2i}}_{f_{i,j,n}} = (2n+1)\binom{2n}{n}^2$$

WANTED: $\sum a_k(n) f_{i,j,n+k} = (g_{i+1,j,n} - g_{i,j,n}) + (h_{i,j+1,n} - h_{i,j,n})$

. Andrews & Paule (93): two proofs with human insight;

. Wegschaider (97): via a generalization of Sister Celine's technique;

. Koutschan's code (2010):

$$f_{i,j,n} = (g_{i+1,j,n} - g_{i,j,n}) + (h_{i,j+1,n} - h_{i,j,n})$$

more work → result

g, h are

$$\frac{\mathrm{pol}(i,j,n)}{(i+1)(j+1)(i+j-2n)} f_{i,j,n}$$

Generating Function Method

$$\sum_{n\geq 0} \underbrace{\sum ()()\cdots()}_{u_n} z^n$$

today →

$$\oint\!\!\!\int \frac{()\cdots()}{()\cdots()}$$

↓ last week

$$y^{(m)}(z) + \cdots + (\ldots)y(z) = 0$$

⟵

$$u_{n+p} + \cdots + (\ldots)u_n = 0$$

An identity of Andrews & Paule

(via generating functions)

$$\sum_{i=0}^{n}\sum_{j=0}^{n}\underbrace{\binom{i+j}{i}^2\binom{4n-2i-2j}{2n-2i}}_{f_{i,j,n}} = (2n+1)\binom{2n}{n}^2$$

$$F(z) := \sum_{n=0}^{\infty}\sum_{i=0}^{n}\sum_{j=0}^{n} f_{i,j,n} z^n$$

next pages

$$= \frac{1}{(2\pi i)^2}\oint \frac{u_2(1+u_2)^2\,du_1du_2}{(u_2^2 - z(1+u_2)^4)(u_1(u_2^2+2u_2-u_1) - z(1+u_1)(1+u_2)^4)}$$

$$F^{(6)}(z) + \ldots + (\ldots)F(z) = 0$$

last week's algorithm

$S_{n+4} + \cdots + (\ldots)S_n = 0$ plus initial conditions

→ (Petkovšek's algorithm) $F_n = (2n+1)\binom{2n}{n}^2$

next lecture

No human help. Total time < 2sec.

Constant Terms of Rational Functions

Notation:

$[x^k]f(x)$ $(k \in \mathbb{Z})$: coefficient of x^k in expansion of $f(x)$ at $x = 0$

$[x_1^{k_1}x_2^{k_2}\cdots x_r^{k_r}]f(\underline{x}) = [x_2^{k_2}\cdots x_r^{k_r}][x_1^{k_1}]f(\underline{x})$, $[1]f(\underline{x}) := [x_1^0\cdots x_r^0]f(\underline{x})$.

Exs. $[1_{x,y}]\dfrac{x}{x+y} = [1_{x,y}]\dfrac{x/y}{1+\frac{x}{y}} = 0, \quad [1_{x,y}]\dfrac{y}{x+y} = [1_{x,y}]\dfrac{1}{1+\frac{x}{y}} = 1.$

Order matters

Def. Constant term: $u_{\underline{n}} = [1]R_0R_1^{n_1}\cdots R_d^{n_d}$, with $R_i \in \mathbb{K}(x_1,\ldots,x_r)$; $\underline{n} \in \mathbb{Z}^d$.

Exs.

1. $d = r, R_i = 1/x_i \ (i = 1,\ldots,r) \to [x_1^{n_1}\cdots x_r^{n_r}]R_0$;
2. $d = 1, R_1 = 1/(x_1\cdots x_r) \to \mathrm{Diag}(R_0)$.

Multiple Binomial Sums

3 basic examples: $\delta_n = [1]x^n$, $\binom{n}{k} = [1]\frac{(1+x)^n}{x^k}$, $C^n = [1]C^n$.

Closure properties: with $u_{\underline{n}} = [1]R_0(\underline{x})\underline{R}(\underline{x})^{\underline{n}}$, $v_{\underline{n}} = [1]S_0(\underline{y})\underline{S}(\underline{y})^{\underline{n}}$

1. $u_{\underline{n}}v_{\underline{n}} = [1_{\underline{x},\underline{y}}](R_0S_0)(R_1S_1)^{n_1}\cdots(R_dS_d)^{n_d}$
2. $u_{\lambda(\underline{n})} = [1]R_0R_1^{\lambda_1(\underline{n})}\cdots R_d^{\lambda_d(\underline{n})}$, $\quad \lambda : \mathbb{Z}^d \to \mathbb{Z}^e$ affine
3. $\sum_{n_d=0}^{m} u_{\underline{n}} = [1]R_0R_1^{n_1}\cdots R_{d-1}^{n_{d-1}}\frac{1-R_d^{m+1}}{1-R_d}$.

These properties give an algorithm

Def. Multiple binomial sums form the smallest subspace of sequences containing these 3 examples and closed under these 3 properties.

Example: Delannoy numbers

$$u_n = \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k}$$

1. $\binom{n}{k} = [1]\dfrac{(1+x)^n}{x^k}$
2. $\binom{n+k}{k} = [1](1+x)^n \left(\dfrac{1+x}{x}\right)^k$
3. $\binom{n}{k}\binom{n+k}{k} = [1_{x,y}]\big((1+x)(1+y)\big)^n \left(\dfrac{1+y}{xy}\right)^k$
4. $u_n = [1]\dfrac{((1+x)(1+y))^n}{1-\frac{1+y}{xy}} - [1]\dfrac{1+y}{xy-1-y}\left(\dfrac{(1+x)(1+y)^2}{xy}\right)^n$

Generating Functions

If $u_{\underline{n}} = [1_{\underline{x}}]R_0(\underline{x})R_1^{n_1}(\underline{x})\cdots R_d^{n_d}(\underline{x}),\ (\underline{n} \in \mathbb{Z}^d)$

then $$\sum_{\underline{n}\in\mathbb{N}^d} u_{\underline{n}} t^{\underline{n}} = \sum_{\underline{n}\in\mathbb{N}^d} [1_{\underline{x}}]R_0(\underline{x})(R_1(\underline{x})t_1)^{n_1}\cdots(R_d(\underline{x})t_d)^{n_d},$$

$$= [1_{\underline{x}}]\frac{R_0}{(1-t_1R_1)\cdots(1-t_dR_d)}$$

$$= \left(\frac{1}{2\pi i}\right)^r \oint \frac{R_0}{(1-t_1R_1)\cdots(1-t_dR_d)}\frac{dx_1\cdots dx_r}{x_1\cdots x_r}.$$

last week's algorithm applies

$(t_1, \ldots, t_d) \ll |x_r| \ll \cdots \ll |x_1| \ll 1$

Optimizations possible

Example: Apéry's sequence

$$U_n := \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 \qquad U(z) := \sum_{n\geq 0} U_n z^n$$

↓

$$U(z) = \frac{1}{(2\pi i)^3} \oint \frac{dt_1 dt_2 dt_3}{t_1t_2t_3(1 - t_1t_2 - t_1t_2t_3) - (1+t_1)(1+t_2)(1+t_3)z}$$

↓

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

↓

$$(n+2)^3 U_{n+2} - (2n+3)(17n^2 + 51n + 39)U_{n+1} + (n+1)^3 U_n = 0$$

Relation to Diagonals

Thm. The sequence $(u_n)_{n\in\mathbb{N}}$ is a multiple binomial sum **iff** its generating function is the diagonal of a rational series.

Proof not difficult

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

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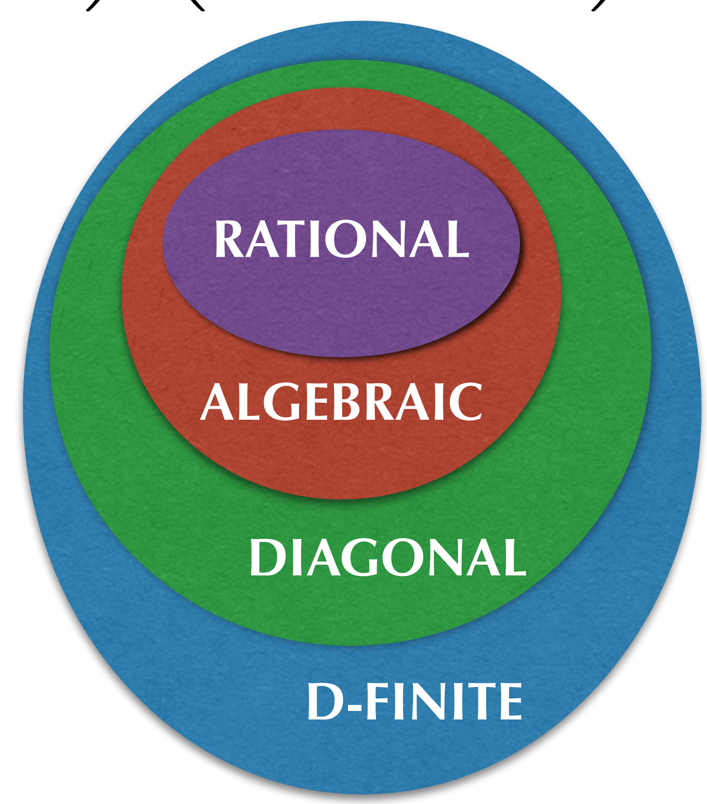
$$\frac{1}{1-t(1+u_1)(1+u_2)(1-u_1u_3)(1-u_2u_3)}$$

has for diagonal the generating function of C_n

→LDE→LRE → fast eval, asymptotics, proofs of identities,…

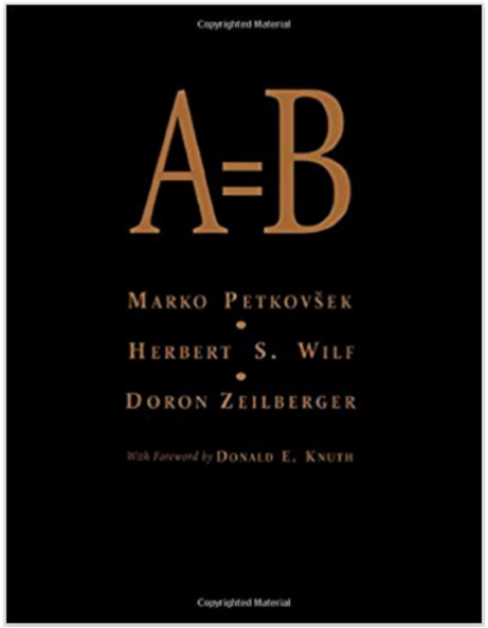


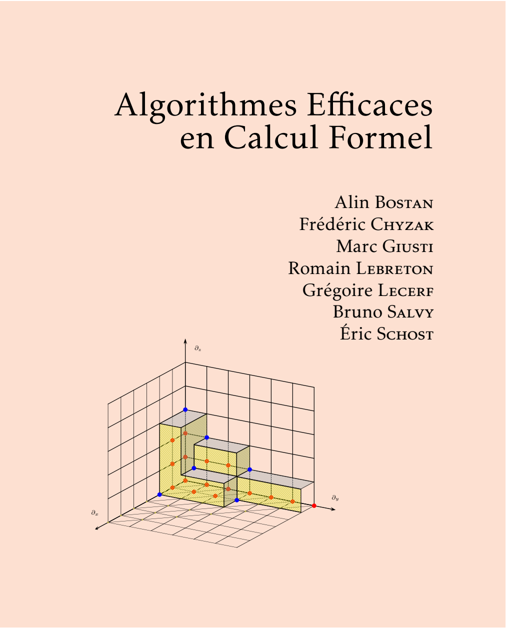
Comparison with Zeilberger's Algorithm

This method

1. avoids discussions about summing the certificate;
2. deals with multiple sums very easily;
3. keeps size & complexity under control;
4. is restricted to a specific (but common) class of sums;
5. deserves a good implementation, generalizations…

References for this lecture





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