Examples of Computer Proofs: From Elementary to Recent Ones

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Honours Seminar

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Outline

Example 1

Problem

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$$1^2 + 2^2 + \cdots + n^2 = \sum_{k=1}^{n} k^2 = \frac{1}{6} n(n+1)(2n+1). \qquad (*)$$

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$$1^2 + 2^2 + \cdots + n^2 = \sum_{k=1}^{n} k^2 = ?$$

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$$n^3 = 3\sum_{k=1}^{n} k^2 - 3\sum_{k=1}^{n} k + n = 3\sum_{k=1}^{n} k^2 - \frac{3n(n+1)}{2} + n.$$

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create telescoping

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3. *Proof.*

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   - $n = 1$: $LHS(1) = 1 = RHS(1)$;

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   - $n = 1$: $LHS(1) = 1 = RHS(1)$;
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Theorem

For any positive integer n,

$$f(n) = 1^2 + 2^2 + \cdots + n^2$$

is a polynomial in variable n, of degree 3.

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$$1^2 + 2^2 + \cdots + n^2 = \sum_{k=1}^{n} k^2 = ?\text{a closed form} \qquad (*')$$

$$\begin{cases} \alpha + \beta + \gamma + \delta & = 1 \\ 8\alpha + 4\beta + 2\gamma + \delta & = 5 \\ 27\alpha + 9\beta + 3\gamma + \delta & = 14 \\ 64\alpha + 16\beta + 4\gamma + \delta & = 30 \end{cases} \Rightarrow \begin{cases} \alpha = 1/3 \\ \beta = 1/6 \\ \gamma = 1/2 \\ \delta = 0 \end{cases}$$

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Proof of the Theorem.

$$n^3 = 3\sum_{k=1}^{n} k^2 - 3\sum_{k=1}^{n} k + n.$$

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For any positive integers d and n,

$$Q(n) := 1^d + 2^d + \cdots + n^d = \sum_{k=1}^{n} k^d$$

is a polynomial in variable n of degree $d + 1$.

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Theorem

Let $P_d(x)$ be a polynomial of degree d. Define

$$Q(n) := P_d(1) + P_d(2) + \cdots + P_d(n) = \sum_{k=1}^{n} P_d(k).$$

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$$1 + 2 + \cdots + n = \frac{n(n+1)}{2}$$

$$1^3 + 2^3 + \cdots + n^3 = \left(\frac{n(n+1)}{2}\right)^2$$

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$$\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n}. \qquad (**) \qquad\qquad \binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

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$$LHS = \sum_{k=0}^{n} \binom{n}{k} \binom{n}{n-k}.$$

We shall choose n balls from n red balls and n blue balls.

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

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$$\sum_{k=0}^{n}\binom{n}{k}^2=\binom{2n}{n}. \qquad (**) \qquad \binom{n}{k}=\frac{n!}{k!(n-k)!}.$$

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Consider the term of $j = n$ (the coefficients of x^n on both sides)

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$$\sum_{k=0}^{n} \frac{\binom{n}{k}^2}{\binom{2n}{n}} = 1$$

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Step 1.

$$\sum_{k=0}^{n} \frac{\binom{n}{k}^2}{\binom{2n}{n}} = 1 = \sum_{k\in\mathbb{Z}} \frac{\binom{n}{k}^2}{\binom{2n}{n}}.$$

Example 2

$$\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n}. \qquad (**)$$

Step 1.

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$$F(n,k) = \binom{n}{k}^2 \Big/ \binom{2n}{n} \qquad \text{and} \qquad f(n) = \sum_{k\in\mathbb{Z}} F(n,k).$$

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$$R(n,k) = \frac{(2k-3n-3)\,k^2}{2(n+1-k)^2(2n+1)} \Rightarrow G(n,k) := F(n,k)R(n,k)$$

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Claim:

$$F(n+1,k) - F(n,k) = G(n,k+1) - G(n,k)$$

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$$f(n) = \sum_{k=0}^{n} \frac{\binom{n}{k}^2}{\binom{2n}{n}} = f(0) = 1.$$

Example 2

$$F(n,k) = \frac{(n!)^4}{(k!)^2\,((n-k)!)^2\,(2n)!} \quad \text{and} \quad R(n,k) = \frac{(2k-3n-3)\,k^2}{2(n+1-k)^2(2n+1)}$$

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- $$F(n+1,k) - F(n,k)$$

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- $$\begin{aligned} & F(n+1,k) - F(n,k) \\ = \quad & \frac{((n+1)!)^4}{(k!)^2\,((n+1-k)!)^2\,(2n+2)!} - \frac{(n!)^4}{(k!)^2\,((n-k)!)^2\,(2n)!} \end{aligned}$$

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$$\begin{aligned}
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\end{aligned}$$

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$$F(n,k)=\frac{(n!)^4}{(k!)^2\left((n-k)!\right)^2(2n)!}\quad \text{and} \quad R(n,k)=\frac{(2k-3n-3)\,k^2}{2(n+1-k)^2(2n+1)}$$

▶

$$\begin{aligned}
& F(n+1,k)-F(n,k) \\
= \quad & \frac{((n+1)!)^4}{(k!)^2\left((n+1-k)!\right)^2(2n+2)!}-\frac{(n!)^4}{(k!)^2\left((n-k)!\right)^2(2n)!} \\
= \quad & \frac{(n!)^4}{(k!)^2\left((n-k)!\right)^2(2n)!}\left[\frac{(n+1)^4}{(n+1-k)^2(2n+2)(2n+1)}-1\right] \\
= \quad & F(n,k)\frac{3n^3+(7-8k)\,n^2+\left(2k^2+5\right)n+2k^2-4k+1}{2\,(n+1-k)^2\,(2n+2)}
\end{aligned}$$

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= \;& \frac{(n!)^4}{(k!)^2\left((n-k)!\right)^2(2n)!}\left[\frac{(n+1)^4}{(n+1-k)^2(2n+2)(2n+1)}-1\right] \\
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= \;& G(n,k+1)-G(n,k)
\end{aligned}$$

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Find/Show

$$f(n) = \sum_{k=0}^{n} F(n, k)$$

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Summing k *from* 0 *to* n*, we see*

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Remark. It will be great that if $F(n,k) = 0$ when $k > n$ (and $k < 0$).

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$$f(n+1)-f(n)=G(n,n+2)-G(n,0).$$

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we can sum over $k \in \mathbb{Z}.\Rightarrow f(n+1) = f(n) = f(1).$

Example 2

Example 2

Recall in Example 1

$$k^2 = \left[\frac{(k+1)^3 - \frac{3}{2}(k+1)^2 + \frac{k+1}{2}}{3} \right] - \left[\underbrace{\frac{k^3 - \frac{3}{2}k^2 + \frac{k}{2}}{3}}_{G(k)} \right]$$

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$$\sum_{k=1}^{n} k^2 = \underbrace{\frac{(n+1)^3 - \frac{3}{2}(n+1)^2 + \frac{n+1}{2}}{3}}_{G(n+1)} - \underbrace{\frac{1 - \frac{3}{2} + \frac{1}{2}}{3}}_{G(1)}$$

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$$F(n,k) = \frac{\binom{n}{k}^2}{\binom{2n}{n}} \quad \text{and} \quad R(n,k) = \frac{(2k-3n-3)\,k^2}{2(n+1-k)^2(2n+1)}$$

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$$F(n,k) = \frac{\binom{n}{k}^2}{\binom{2n}{n}} \quad \text{and} \quad R(n,k) = \frac{(2k-3n-3)\,k^2}{2(n+1-k)^2(2n+1)}$$

$R(n,k)$ is called WZ proof certificate

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$R(n,k)$ is called WZ proof certificate (Wilf–Zeilberger)

Example 2

$$\left.\begin{aligned} \frac{F(n+1,k)}{F(n,k)} = \frac{(n+1)^4}{(n+1-k)^2\,(2n+2)\,(2n+1)} \\ \frac{F(n,k+1)}{F(n,k)} = \frac{(n-k)^2}{(k+1)^2} \end{aligned}\right\} \text{rational in } n \ \& \ k.$$

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6.3 How the algorithm works

The creative telescoping algorithm is for the fast discovery of the recurrence for a proper hypergeometric term, in the telescoped form (6.1.3). The algorithmic implementation makes strong use of the existence, but not of the method of proof used in the existence theorem.

More precisely, what we do is this. We now *know* that a recurrence (6.1.3) exists. On the left side of the recurrence there are unknown coefficients $a_0, \ldots, a_J$; on the right side there is an unknown function G; and the order J of the recurrence is unknown, except that bounds for it were established in the Fundamental Theorem (Theorem 4.4.1 on page 65).

We begin by fixing the assumed order J of the recurrence. We will then look for a recurrence of that order, and if none exists, we'll look for one of the next higher order.

For that fixed J, let's denote the left side of (6.1.3) by t_k, so that

$$t_k = a_0F(n,k) + a_1F(n+1,k) + \cdots + a_JF(n+J,k). \qquad (6.3.1)$$

Example 2

Then we have for the term ratio

$$\frac{t_{k+1}}{t_k} = \frac{\sum_{j=0}^{J} a_j F(n+j,k+1)/F(n,k+1)}{\sum_{j=0}^{J} a_j F(n+j,k)/F(n,k)} \frac{F(n,k+1)}{F(n,k)}. \tag{6.3.2}$$

The second member on the right is a rational function of n, k, say

$$\frac{F(n,k+1)}{F(n,k)} = \frac{r_1(n,k)}{r_2(n,k)},$$

where the r's are polynomials, and also

$$\frac{F(n,k)}{F(n-1,k)} = \frac{s_1(n,k)}{s_2(n,k)},$$

say, where the s's are polynomials. Then

$$\frac{F(n+j,k)}{F(n,k)} = \prod_{i=0}^{j-1} \frac{F(n+j-i,k)}{F(n+j-i-1,k)} = \prod_{i=0}^{j-1} \frac{s_1(n+j-i,k)}{s_2(n+j-i,k)}. \tag{6.3.3}$$

It follows that

$$\begin{aligned} \frac{t_{k+1}}{t_k} &= \frac{\sum_{j=0}^{J} a_j \left\{\prod_{i=0}^{j-1} \frac{s_1(n+j-i,k+1)}{s_2(n+j-i,k+1)}\right\}}{\sum_{j=0}^{J} a_j \left\{\prod_{i=0}^{j-1} \frac{s_1(n+j-i,k)}{s_2(n+j-i,k)}\right\}} \frac{r_1(n,k)}{r_2(n,k)} \\ &= \frac{\sum_{j=0}^{J} a_j \left\{\prod_{i=0}^{j-1} s_1(n+j-i,k+1) \prod_{r=j+1}^{J} s_2(n+r,k+1)\right\}}{\sum_{j=0}^{J} a_j \left\{\prod_{i=0}^{j-1} s_1(n+j-i,k) \prod_{r=j+1}^{J} s_2(n+r,k)\right\}} \\ &\quad \times \frac{r_1(n,k)}{r_2(n,k)} \frac{\prod_{r=1}^{J} s_2(n+r,k)}{\prod_{r=1}^{J} s_2(n+r,k+1)}. \end{aligned} \tag{6.3.4}$$

Thus we have

$$\frac{t_{k+1}}{t_k} = \frac{p_0(k+1)}{p_0(k)} \frac{r(k)}{s(k)}, \tag{6.3.5}$$

where

$$p_0(k) = \sum_{j=0}^{J} a_j \left\{ \prod_{i=0}^{j-1} s_1(n+j-i,k) \prod_{r=j+1}^{J} s_2(n+r,k) \right\}, \tag{6.3.6}$$

and

$$r(k) = r_1(n,k) \prod_{r=1}^{J} s_2(n+r,k), \tag{6.3.7}$$

$$s(k) = r_2(n,k) \prod_{r=1}^{J} s_2(n+r,k+1). \tag{6.3.8}$$

Note that *the assumed coefficients* a_j *do not appear in* $r(k)$ *or in* $s(k)$, but only in $p_0(k)$.

Next, by Theorem 5.3.1, we can write $r(k)/s(k)$ in the canonical form

$$\frac{r(k)}{s(k)} = \frac{p_1(k+1)}{p_1(k)} \frac{p_2(k)}{p_3(k)}, \tag{6.3.9}$$

in which the numerator and denominator on the right are coprime, and

$$\gcd(p_2(k), p_3(k+j)) = 1 \quad (j = 0, 1, 2, \dots).$$

Hence if we put $p(k) = p_0(k)p_1(k)$ then from eqs. (6.3.5) and (6.3.9), we obtain

$$\frac{t_{k+1}}{t_k} = \frac{p(k+1)}{p(k)} \frac{p_2(k)}{p_3(k)}. \tag{6.3.10}$$

This is now a standard setup for Gosper's algorithm (compare it with the discussion on page 76), and we see that t_k will be an indefinitely summable hypergeometric term if and only if the recurrence (compare eq. (5.2.6))

$$p_2(k)b(k+1) - p_3(k-1)b(k) = p(k) \tag{6.3.11}$$

has a polynomial solution $b(k)$.

The remarkable feature of this equation (6.3.11) is that *the coefficients* $p_2(k)$ *and* $p_3(k)$ *are independent of the unknowns* $\{a_j\}_{j=0}^{J}$, *and the right side* $p(k)$ *depends on them linearly.* Now watch what happens as a result. We look for a polynomial solution to (6.3.11) by first, as in Gosper's algorithm, finding an upper bound on the degree, say Δ, of such a solution. Next we assume $b(k)$ as a general polynomial of that degree, say

$$b(k) = \sum_{l=0}^{\Delta} \beta_l k^l,$$

with all of its coefficients to be determined. We substitute this expression for $b(k)$ in (6.3.11), and we find a system of simultaneous *linear* equations in the $\Delta + J + 2$ unknowns

$$a_0, a_1, \dots, a_J, \beta_0, \dots, \beta_\Delta.$$

The linearity of this system is directly traceable to the italicized remark above.

We then solve the system, if possible, for the a_j's and the β_l's. If no solution exists, then there is no recurrence of telescoped form (6.1.3) and of the assumed order J. In such a case we would next seek such a recurrence of order $J+1$. If on the other

Example 2

hand a polynomial solution $b(k)$ of equation (6.3.11) does exist, then we will have found all of the a_j's of our assumed recurrence (6.1.3), and, by eq. (5.2.5) we will also have found the $G(n,k)$ on the right hand side, as

$$G(n,k) = \frac{p_3(k-1)}{p(k)} b(k) t_k. \tag{6.3.12}$$

See Koornwinder [Koor93] for further discussion and a q-analogue.

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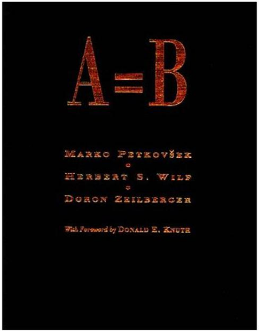

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6.4 Examples **109**

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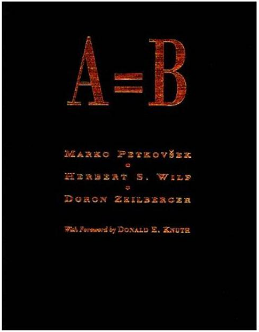

https://www.math.upenn.edu /~wilf/AeqB.html

Example 3

J. Math. Anal. Appl. 420 (2014) 1154–1166

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The unimodality of a polynomial coming from a rational integral. Back to the original proof

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with

$$d_\ell(m) = 2^{-2m} \sum_{k=\ell}^{m} 2^k \binom{2m-2k}{m-k} \binom{m+k}{m} \binom{k}{\ell} \tag{1.2}$$

made its appearance in [1] in the evaluation of the quartic integral

$$\int_0^\infty \frac{dx}{(x^4 + 2ax^2 + 1)^{m+1}} = \frac{\pi}{2^{m+3/2}(a+1)^{m+1/2}} P_m(a). \tag{1.3}$$

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- The sequence

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$$d_0(m) \leq d_1(m) \leq \cdots \leq d_j(m)$$

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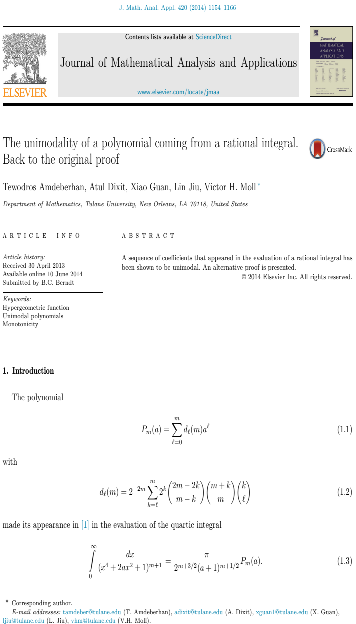

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- The last step requires the sequence

$$T_n := \sum_{k=2}^{n+1} \binom{2k}{k}\binom{n+1}{k} \frac{k-1}{2^k \binom{4n}{k}}$$

to be monotonic increasing.

Example 3

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$$\begin{aligned} a_n =& 7195230 + 87693273n + 448856568n^2 + 1263033897n^3 + 2147597568n^4 \\ &+ 2279791176n^5 + 1502157312n^6 + 586779648n^7 + 121208832n^8 + 9732096n^9 \end{aligned}$$

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With some discussion, and the great help of the recurrence, the

Example 4

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Calculation and Properties of Zonal Polynomials

Lin Jiu · Christoph Koutschan

Received: 1 November 2018 / Accepted: 15 December 2019 / Published online: 11 February 2020

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Keywords Zonal polynomial · Symmetric function · Integer partition · Laplace–Beltrami operator · Wishart matrix · Hypergeometric function of a matrix argument

Mathematics Subject Classification Primary 05E05; Secondary 33C20 · 33C70 · 15B52 · 65C60

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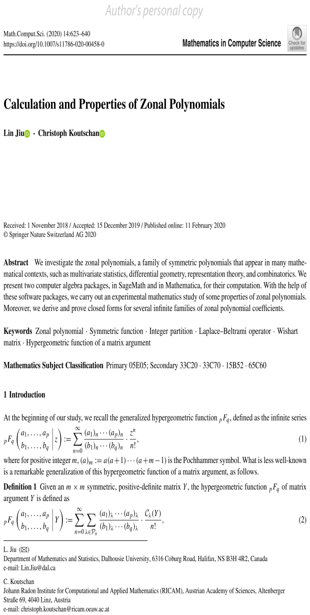
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for some partition $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_k)$ of a positive integer n, i.e.,

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- In particular, we want to give the formula of some coefficients

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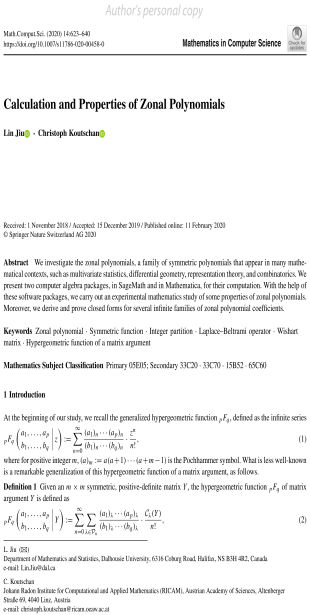

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Mathematics in Computer Science

Calculation and Properties of Zonal Polynomials

Lin Jiu · Christoph Koutschan

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Abstract We investigate the zonal polynomials, a family of symmetric polynomials that appear in many mathematical contexts, such as multivariate statistics, differential geometry, representation theory, and combinatorics. We present two computer algebra packages, in SageMath and in Mathematica, for their computation. With the help of these software packages, we carry out an experimental mathematics study of some properties of zonal polynomials. Moreover, we derive and prove closed forms for several infinite families of zonal polynomial coefficients.

Keywords Zonal polynomial · Symmetric function · Integer partition · Laplace–Beltrami operator · Wishart matrix · Hypergeometric function of a matrix argument

Mathematics Subject Classification Primary 05E05; Secondary 33C20 · 33C70 · 15B52 · 65C60

1 Introduction

At the beginning of our study, we recall the generalized hypergeometric function ${}_pF_q$, defined as the infinite series

$$ {}_pF_q\left(\begin{matrix} a_1,\dots,a_p \\ b_1,\dots,b_q \end{matrix}\middle| z\right) := \sum_{n=0}^{\infty} \frac{(a_1)_n\cdots(a_p)_n}{(b_1)_n\cdots(b_q)_n}\cdot\frac{z^n}{n!}, \quad (1)$$

where for positive integer m, $(a)_m := a(a+1)\cdots(a+m-1)$ is the Pochhammer symbol. What is less well-known is a remarkable generalization of this hypergeometric function of a matrix argument, as follows.

Definition 1 Given an $m\times m$ symmetric, positive-definite matrix Y, the hypergeometric function ${}_pF_q$ of matrix argument Y is defined as

$$ {}_pF_q\left(\begin{matrix} a_1,\dots,a_p \\ b_1,\dots,b_q \end{matrix}\middle| Y\right) := \sum_{n=0}^{\infty}\sum_{\lambda\in\mathcal{P}_n} \frac{(a_1)_\lambda\cdots(a_p)_\lambda}{(b_1)_\lambda\cdots(b_q)_\lambda}\cdot\frac{\mathcal{C}_\lambda(Y)}{n!}, \quad (2)$$

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- The Zonal polynomials

$$C_\lambda(y_1,\dots,y_m)$$

for some partition $\lambda=(\lambda_1,\lambda_2,\dots,\lambda_k)$ of a positive integer n, i.e.,

$$\lambda_1\ge\cdots\ge\lambda_k\ge 1 \text{ and } \lambda_1+\cdots+\lambda_k=n.$$

- In particular, we want to give the formula of some coefficients

$$c_{(a,a-b),(a-d,a-b+d)} = \frac{(2a-b)!\left(b+\frac{1}{2}\right)\left(\frac{1}{2}\right)_d}{d!(a-b)!(b-d)!\left(b-d+\frac{1}{2}\right)_{a-b+d+1}}$$

In general, coefficients are denoted by $c_{\kappa,\lambda}$ for partitions κ,λ of the same number n.

Example 4

Using special-purpose computer algebra packages, such as the HolonomicFunctions package [10], we find that expression in the sum, denote it by $f(j)$, is Gosper-summable. More precisely, we find a function

$$g(j) = \frac{j\,(2b-2j+1)}{b-2j}\cdot f(j) = \binom{b}{j}\frac{j\,(2b-2j+1)\left(\frac{1}{2}\right)_j}{d\,(2b-2d+1)\left(b-j+\frac{1}{2}\right)_j}$$

with the property $g(j+1)-g(j) = f(j)$ (the latter can be easily verified). By telescoping, and by noting t $g(0)=0$, we obtain the value of the right-hand side of (18):

$$g(d) = \binom{b}{d}\cdot\frac{\left(\frac{1}{2}\right)_d}{\left(b-d+\frac{1}{2}\right)_d},$$

which matches exactly the left-hand side of (18).

Theorem 25 *Let $a, b, d \in \mathbb{N}$ with $0 \le b < a$ and $0 \le d \le b/2$. Then we have*

$$c_{(a,a-b),(a-d,a-b+d)} = \frac{(2a-b)!\left(b+\frac{1}{2}\right)\left(\frac{1}{2}\right)_d}{d!\,(a-b)!\,(b-d)!\left(b-d+\frac{1}{2}\right)_{a-b+d+1}}.$$

Proof We first show that the asserted expression is compatible with the result of Proposition 24: indeed, by comput the quotient

$$\frac{c_{(a,a-b),(a-d,a-b+d)}}{c_{(a,a-b),(a,a-b)}} = \frac{(2a-b)!\left(b+\frac{1}{2}\right)\left(\frac{1}{2}\right)_d\cdot(a-b)!\,b!\left(b+\frac{1}{2}\right)_{a-b+1}}{d!\,(a-b)!\,(b-d)!\left(b-d+\frac{1}{2}\right)_{a-b+d+1}\cdot(2a-b)!\left(b+\frac{1}{2}\right)}$$
$$= \frac{b!\left(\frac{1}{2}\right)_d\left(b+\frac{1}{2}\right)_{a-b+1}}{d!\,(b-d)!\left(b-d+\frac{1}{2}\right)_{a-b+d+1}} = \binom{b}{d}\frac{\left(\frac{1}{2}\right)_d}{\left(b-d+\frac{1}{2}\right)_d},$$

we see that this is the case. It remains to prove that the asserted expression is correct in the case $d=0$, i.e., wl $\kappa=\lambda$. For this purpose, we employ the recursion (12), specialized to partitions with two parts:

$$\sum_{d=0}^{a-b} c_{(a+d,a-b-d),(a,a-b)} = \binom{2a-b}{a}. \qquad ($$

By dividing both sides with the binomial coefficient of the right-hand side, and by inserting the asserted clo form (after the change of variables $a \to a+d$ and $b \to b+2d$), we are left with the summation identity

$$\sum_{d=0}^{a-b}\frac{a!\,(a-b)!\left(b+2d+\frac{1}{2}\right)\left(\frac{1}{2}\right)_d}{d!\,(a-b-d)!\,(b+d)!\left(b+d+\frac{1}{2}\right)_{a-b+1}} = 1. \qquad ($$

Taking into account the recursive definition of the coefficients $c_{\kappa,\lambda}$, the (inductive) proof is completed by veri ing (20). For this purpose, we denote by $f(a,b,d)$ the expression inside the sum (20) and construct two WZ pa i.e., two functions

$$g_1(d) = \frac{-2d(b+d)}{(a-b-d+1)(2b+4d+1)}\cdot f(a,b,d)$$
$$= -\frac{a!\,(a-b)!\left(\frac{1}{2}\right)_d}{(d-1)!\,(b+d-1)!\,(a-b-d+1)!\left(b+d+\frac{1}{2}\right)_{a-b+1}},$$
$$g_2(d) = \frac{d(2a+2d+1)}{(a-b)(2b+4d+1)}\cdot f(a,b,d)$$
$$= \frac{a!\,(a-b-1)!\left(\frac{1}{2}\right)_d}{(d-1)!\,(b+d)!\,(a-b-d)!\left(b+d+\frac{1}{2}\right)_{a-b}},$$

such that the following identities hold (they can be verified by routine calculations):

$$f(a+1,b,d) - f(a,b,d) = g_1(d+1) - g_1(d), \qquad (21)$$
$$f(a,b+1,d) - f(a,b,d) = g_2(d+1) - g_2(d). \qquad (22)$$

Now we sum (21) for $d = 0,\dots,a-b$ and obtain

$$\sum_{d=0}^{a-b}\big(f(a+1,b,d) - f(a,b,d)\big) = g_1(a-b+1) - g_1(a,0),$$

or equivalently,

$$\sum_{d=0}^{a-b+1} f(a+1,b,d) - \sum_{d=0}^{a-b} f(a,b,d) = g_1(a-b+1) - g_1(a,0) + f(a+1,b,a-b+1).$$

A straightforward calculation shows that the left-hand side equals 0, thereby showing that the sum $\sum_{d=0}^{a-b} f(a,b,d)$ is independent of a. Summing over (22), followed by a similar calculation, shows that the sum does not depend on b either. Therefore, the sum in (20) is constant, and by setting $a=b=0$, one immediately sees that this constant is 1. □

Remark 26 By setting $b=a$ in Theorem 25 and by interpreting $(a,0)$ as the partition (a), we recover Theorem 21:

$$c_{(a),(a-d,d)} = \frac{(a)!\left(a+\frac{1}{2}\right)\left(\frac{1}{2}\right)_d}{d!\,(a-d)!\left(a-d+\frac{1}{2}\right)_{d+1}} = \binom{a}{d}\frac{\left(\frac{1}{2}\right)_d}{\left(a-d+\frac{1}{2}\right)_d}.$$

7 Partitions with Three and Four Parts

We have seen that the coefficients of the zonal polynomial $\mathcal{C}_\kappa(Y)$ are given by the row indexed by κ in the $c_{\kappa,\lambda}$-matrix. Using (11) we can express all coefficients $c_{\kappa,\lambda}$ in the κ-th row as constant multiples of the diagonal coefficient $c_{\kappa,\kappa}$. Unfortunately, the latter one is harder to obtain: to apply (12) we need to know all $c_{\kappa,\lambda}$ in the λ-th column, which in turn are obtained by (11) and so on. Hence, in the worst case, we need to compute the whole triangle above the position (κ,κ).

Therefore, it would be highly desirable to have a more direct way to compute the diagonal coefficients $c_{\kappa,\kappa}$. We present formulas for the special cases that κ has three resp. four parts.

Conjecture 27 *Let $\kappa = (a, a-b, a-c)$ with integers $0 \le b \le c \le a$ be a partition of $n = 3a-b-c$ into at most three parts. Then the diagonal coefficient*

$$c_{\kappa,\kappa} = \frac{(c+1)!}{(a+1)!}\cdot\frac{n!}{\delta_1!\,\delta_2!\,\delta_3!\left(\delta_1+\frac{3}{2}\right)_{\delta_2}\left(\delta_2+\frac{3}{2}\right)_{\delta_3}},$$

with $\delta_1 = \kappa_1-\kappa_2 = b$, $\delta_2 = \kappa_2-\kappa_3 = c-b$, and $\delta_3 = \kappa_3-\kappa_4 = a-c$ being the differences between consecutive parts of κ (with the convention $\kappa_4 = 0$).

Conjecture 28 *Let $\kappa = (a, a-b, a-c, a-d)$ with integers $0 \le b \le c \le d \le a$ be a partition of $n = 4a-b-c-d$ into at most four parts. Then the diagonal coefficient $c_{\kappa,\kappa}$ is given by*

Example 5

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Multi-headed lattices and Green functions

Qipin Chen[1], **Shane Chern**[2,3] **and Lin Jiu**[3,4,*]

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Abstract

Lattice geometries and random walks on them are of great interest for their applications in different fields such as physics, chemistry, and computer science. In this work, we focus on multi-headed lattices and study properties of the Green functions for these lattices such as the associated differential equations and the Pólya numbers. In particular, we complete the analysis of three missing cases in dimensions no larger than five. Our results are built upon an automatic machinery of creative telescoping.

Keywords: multi-headed lattice, Green function, Pólya number, differential equation, recurrence, creative telescoping

1. Introduction

Bravais lattices are important objects in crystallography, and they are used to formally model the orderly arrangement of atoms in a crystal [31, section 42]. For example, the crystal structure of NaCl can be illustrated by the face-centered cubic Bravais lattice as shown in figure 1. Visually, a *Bravais lattice* is an arrangement of points in the three-dimensional space such that when viewed from each point the lattice appears exactly the same; from a mathematical perspective, it is a $\mathbb{Z}$-module generated by three linearly independent vectors in $\mathbb{R}^3$. Up to equivalence, there are 14 Bravais lattices in the three-dimensional space [16, p 744].

When it comes to higher-dimensional generalizations, if one insists on the criterion of having the same appearance at each lattice point, which is essential in crystal structures, the formalization is usually restricted and sometimes confusing. According to Guttmann [14, p 15,

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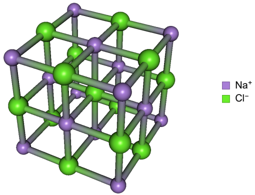

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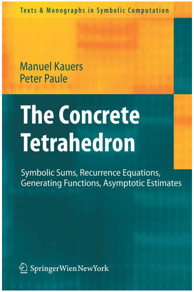

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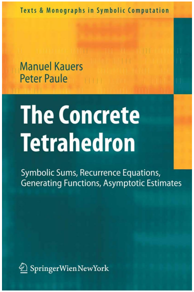

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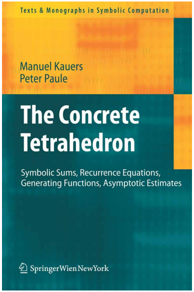

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