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Automatic summation using Zeilberger-Wilf theory

Het vinden van een expliciete uitdrukking voor een som van de vorm

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

was tot voor kort alleen mogelijk met behulp van behoorlijk wat menselijke slimheid en inventiviteit. Echter, computers kunnen dergelijke uitdrukkingen nu ook vinden; het probleem wanneer een hypergeometrische som is uit te drukken in gesloten vorm is geheel opgelost. Andries Brouwer beschrijft het proces van de zogenaamde automatische sommering. Het is gebaseerd op theorieën van Zeilberger en Wilf.

The problem of discovering whether or not a given hypergeometric sum is expressible in a simple closed form, and if so, finding that form, and if not, proving that the sum is not expressible in a closed form, has now been completely automated. There is no ingenuity or mathematician required: a computer algebra package can do it all.

In his treatise [2], Exercise 1.2.6.63, Knuth asks: *Develop computer programs for simplifying sums that involve binomial coefficients*, and rates this exercise M50, the same difficulty as assigned to Fermat's last Theorem!

Here is the recipe for finding $f(n) = \sum_k F(n,k)$:

i. Go to `http://www.cis.upenn.edu/~wilf/progs.html` and download `EKHAD`. (While you are there you might as well also take `hyper`, `WZ` and `gosper.m`.)
ii. Start Maple (some might prefer Mathematica, but that has a serious flaw: whenever you really need it, it turns out that your license has expired, or the password of your computer has changed because you exchanged your ethernet card, and it may well take a while before it is usable again).
iii. Read `EKHAD`.
iv. Define the summand $F(n,k)$.
v. Call `zeil(F(n,k),k,n,N)`.
vi. Your problem is solved.

For example, look at the sum $\sum_{k=0}^{m}(-1)^k\binom{m}{k}^3$. For odd m this vanishes since the terms for k and $m-k$ cancel, so take $m=2n$. Here are the relevant snippets of the maple session, after reading in EKHAD.

```
> F := (n,k) -> (-1)^k * binomial(2*n,k)^3;

                                k                3
          F := (n,k) -> (-1)  binomial(2 n, k)

> z := zeil(F(n,k),k,n,N);
```

Hypergeometric sums

Informally, a hypergeometric sum has the shape

$$f(n) = \sum_k F(n,k),$$

where $F(n,k)$ involves factorials and binomial coefficients as in

$$F(n,k) = (-1)^k \binom{n}{k}^3.$$

A precise definition is given in formula (2). Sums and series with such summands occur in the field of special functions, viz. hypergeometric functions.

Maple returns two expressions:

$$-6(3n+2)(3n+1) - 2(n+1)^2 N,$$

and a fraction with numerator

$$k^3(784n - 207k - 48k^3 + 2084n^2 - 1113nk + 147k^2 - 2214n^2k + 594nk^2 + 2728n^3 + 6k^4 + 448n^5 + 1760n^4 + 116 - 1932n^3k - 624n^4k + 792n^2k^2 + 348n^3k^2 - 132nk^3 - 90n^2k^3 + 9k^4n)$$

and denominator

$$(2n-k+1)^3(2n+2-k)^3.$$

What is it that we found? The function `zeil` will find recurrences of the form

$$\sum_{j=0}^{J} a_j(n)F(n+j,k) = G(n,k+1) - G(n,k) \tag{1}$$

given the function $F(n,k)$. Once we have such a recurrence, summing over k will yield

$$\sum_{j=0}^{J} a_j(n) f(n+j) = 0$$

where $f(n) = \sum_k F(n,k)$, a recurrence relation for the sum that we wanted to find. In the maple call, N is the forward shift operator, which action is given by $(Nf)(n) = f(n+1)$.The first part of the answer says that

$$-6(3n+2)(3n+1)f(n) - 2(n+1)^2 f(n+1) = 0,$$

that is, $f(n+1) = -3(3n+1)(3n+2)f(n)/(n+1)^2$. Since $f(0) = 1$ we find that

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

How can we verify that this really is true? The second part of the answer is the *certificate*, a rational function $R(n,k)$ that makes it possible to verify all claims by straightforward checking. It defines the G of (1) by $G(n,k) = R(n,k)F(n,k)$. Now dividing both sides of (1) by $F(n,k)$ yields a claimed equality of two rational functions in n and k, multiplying by the denominators yields a claimed equality between polynomials, and this is true by inspection.

```
> R := (an,ak) -> subs(n=an,k=ak,z[2]):
> simplify(expand(- 6*(3*n + 2)*(3*n + 1)
> - 2*(n+1)^2*F(n+1,k)/F(n,k)
> - R(n,k+1)*F(n,k+1)/F(n,k) + R(n,k)));

                              0
```

The final 0 is what we wanted (and we could have done it by hand, if necessary). This proves our result.

The mathematics behind automatic summation

When precisely does this work? As we saw before, the heart of the matter is to find suitable recurrence relations. Before we formulate the two results stating the existence of such recurrence relations in a convenient form, we describe the exact shape of the term $F(n,k)$ in $f(n) = \sum_k F(n,k)$ for which the results hold.

Recurrence relations

Suitable recurrence relations for the $F(n,k)$ and, subsequently, the $f(n) = \sum_k F(n,k)$ are the key to producing closed forms. Solving an appropriate system of equations, one can come up with a recurrence relation like

$$a(n)F(n,k) + b(n)F(n+1,k) + c(n)F(n,k+1) + d(n)F(n+1,k+1) = 0.$$

(In a given case, possibly more terms are needed in a recurrence relation.) For example, with $F(n,k) = 2^k\binom{n}{k}$, solving

$$a(n) + b(n)\frac{n+1}{n+1-k} + c(n)\frac{2n-2k}{k+1} + d(n)\frac{2n+2}{k+1} = 0$$

for $a(n)$, $b(n)$, $c(n)$ and $d(n)$ leads to $F(n+1,k+1) = 2F(n,k) + F(n,k+1)$. Summing over k then gives the recurrence $f(n+1) = 3f(n)$ for $f(n)$. It is in this step that the dependence of $a(n), b(n), c(n), d(n)$ on n only (in our simple example just constants) is crucial. Of course, $f(n) = 3^n$.

Definition. A function $F(n,k)$ is said to be a *proper hypergeometric term* if it can be written in the form

$$F(n,k) = P(n,k)\frac{\prod_{r=1}^{s}(a_r n + b_r k + c_r)!}{\prod_{r=1}^{t}(u_r n + v_r k + w_r)!} x^k \tag{2}$$

in which x is an indeterminate, P a polynomial, the a_r, b_r, u_r, v_r are specific integers (i.e., do not contain additional parameters) and s, t are finite, nonnegative, specific integers. (The c_r and w_r are allowed to be arbitrary parameters that take complex values. Also the coefficients of the polynomial P may contain additional parameters.)

The following theorem was already discovered in the fourties.

Theorem [Mary Celine Fasenmyer]. *If $F(n,k)$ is a proper hypergeometric term, then it satisfies a recurrence relation*

$$\sum_{i=0}^{I}\sum_{j=0}^{J} a_{ij}(n)F(n-j,k-i) = 0 \tag{3}$$

where the $a_{ij}(n)$ are polynomials in n, not all zero, and the equation holds for all n, k for which $F(n,k) \neq 0$ and all occurring $F(n-j,k-i)$ are defined. Furthermore, there is such a recurrence with $(I,J) = (I_0,J_0)$, where $J_0 = \sum_r |b_r| + \sum_r |v_r|$ and $I_0 = 1 + \deg(P) + J_0(\sum_r |a_r| + \sum_r |u_r| - 1)$.

Proof. The idea is to rewrite (3), for suitable I and J, as a system of equations with more unknowns than equations.
Define (for integral nonnegative x) $\mathrm{rf}(x,y) := \prod_{j=1}^{x}(y+j)$ and $\mathrm{ff}(x,y) := \prod_{j=0}^{x-1}(y-j)$. Extend ff for integral negative x by $\mathrm{ff}(-x,y) := \mathrm{rf}(x,y)^{-1}$. (The abbreviations should suggest raising resp. falling factorial.) Then, if $H(n,k) = (an+bk+c)!$, we

have

$$\frac{H(n-j,k-i)}{H(n,k)} = \frac{1}{\mathrm{ff}(aj+bi, an+bk+c)}.$$

Thus $x^i \frac{F(n-j,k-i)}{F(n,k)}$ is a rational function in n, k, say $\frac{\nu_{ij}(n,k)}{\delta_{ij}(n,k)}$, and

$$\delta_{ij}(n,k) = P(n,k) \prod_{a_r j + b_r i \geq 0} \mathrm{ff}(a_r j + b_r i, a_r n + b_r k + c_r)$$
$$\prod_{u_r j + v_r i < 0} \mathrm{rf}(-u_r j - v_r i, u_r n + v_r k + w_r).$$

We now try to solve (3) for the coefficients $a_{ij}(n)$. Place the expressions over a single common denominator, collect the numerator as a polynomial in k, and equate the coefficient of each power of k to zero. This will work when the number of unknowns is larger than the number of equations. Put $x^+ := \max(x, 0)$. Then

$$\max\{aj+bi \mid aj+bi \geq 0,\ 0 \leq i \leq I,\ 0 \leq j \leq J\} = a^+J + b^+I,$$

$$\max\{-aj-bi \mid aj+bi < 0,\ 0 \leq i \leq I,\ 0 \leq j \leq J\}$$
$$= (-a)^+J + (-b)^+I.$$

The least common multiple of all $\delta_{ij}(n,k)$ divides

$$\Delta := P(n,k) \prod_r \mathrm{ff}(a_r^+ J + b_r^+ I, a_r n + b_r k + c_r)$$
$$\prod_r \mathrm{rf}((-u_r)^+ J + (-v_r)^+ I, u_r n + v_r k + w_r).$$

After multiplying by $x^I \Delta$, we have to find the $a_{ij}(n)$ from the polynomial equation

$$\sum_{i=0}^{I} \sum_{j=0}^{J} a_{ij}(n) \nu_{ij}(n,k) \frac{\Delta}{\delta_{ij}(n,k)} x^{I-i} = 0.$$

The number of unknowns a_{ij} equals $(I+1)(J+1)$. The number of different powers of k occurring is at most

$$1 + \deg(P) + (\sum |a_r| + \sum |u_r|)J + (\sum |b_r| + \sum |v_r|)I.$$

For sufficiently large I, J, e.g. for the I_0, J_0 given in the theorem, there are more unknowns than equations, and we find a solution where a_{ij} equals x^i times a polynomial in n. □

Telescoped recurrences

So, we found, in a constructive way, a recurrence satisfied by $F(n,k)$. But it is not in a form convenient for summation.

Theorem [Doron Zeilberger]. *If $F(n,k)$ is a proper hypergeometric term, then it satisfies a nontrivial recurrence relation of the form*

$$\sum_{j=0}^{J} a_j(n) F(n+j,k) = G(n,k+1) - G(n,k)$$

in which $G(n,k)/F(n,k)$ is a rational function of n and k.

Proof. Let N, K be the forward shift operators in n and k. Then a recurrence $\sum_{i=0}^{I} \sum_{j=0}^{J} a_{ij}(n) F(n+j,k+i) = 0$ can be written as $p(n,N,K)F(n,k) = 0$ for a certain polynomial p with coefficients in $\mathbf{Z}[x]$. Take such a p that has minimal degree in K. Write

$$p(n,N,K) = p(n,N,1) + (1-K)q(n,N,K).$$

Then

$$p(n,N,1)F(n,k) = (K-1)q(n,N,K)F(n,k)$$
$$= G(n,k+1) - G(n,k),$$

where $G(n,k) = q(n,N,K)F(n,k)$. This proves the claim, since shift operators multiply $F(n,k)$ by a rational function. But could $p(n,N,1)$ be identically zero? Then $G(n,k)$ does not depend on k and hence is a hypergeometric term in the single variable n and satisfies some recurrence (of order 1) $r(n,N)G(n,k) = 0$. Now $r(n,N)q(n,N,K)F(n,k) = 0$, a recurrence of lower degree in K than the one we started with. □

An example

As an example of the above theorems, we prove Boersma's identity. This identity was found in 1961 by Boersma, and later shown to Askey. Askey forgot, and many years later rediscovered and published it (with the same proof Boersma had given). The final version of the paper [1] contains an acknowledgement to Boersma. Define the *up-down factorial* $\mathrm{ud}(x,y)$ by

$$\mathrm{ud}(x,y) := \frac{(x+1)(x+3)...(x+2y-1)}{x(x+2)(x+4)...(x+2y)}.$$

Theorem [Boersma, 1961]. *Let a, b, c be nonnegative integers such that $a+b+c$ is odd, and $c \leq a+b$. Then*

$$\sum_{k=0}^{\min(b,c)} \frac{\binom{2b-2k}{b-k}\binom{2c-2k}{c-k}\binom{2k}{k}}{\binom{2b+2c-2k}{b+c-k}} \cdot \frac{(b+c-2k+\frac{1}{2})}{(b+c-k+\frac{1}{2})} \times$$
$$\times \frac{1}{(a-b-c+2k)(a+b+c+1-2k)}$$
$$= \mathrm{ud}(a-b-c,c) \cdot \mathrm{ud}(a+b+1-c,c).$$

Note that the left-hand side is symmetric in b and c. But so is the right-hand side: if $c > b$, then the zigzags from $a-b-c$ to $a-b+c$ and from $a+b+1-c$ to $a+b+1+c$ overlap, and we see that $\mathrm{ud}(a-b-c,c).\mathrm{ud}(a+b+1-c,c) = \mathrm{ud}(a-b-c,b).\mathrm{ud}(a+c+1-b,b)$.

```
> F := (a,b,c,k) -> binomial(2*(b-k),b-k)*
>   binomial(2*(c-k),c-k)*binomial(2*k,k)*
>   (b+c-2*k+1/2) / (binomial(2*(b+c-k),b+c-k)*
>   (b+c-k+1/2)*(a-b-c+2*k)*(a+b+c+1-2*k)):
> T := (c,k) -> F(a,b,c,k):
> z := zeil(T(c,k),k,c,C);
bytes used=245350904, alloc=3276200, time=181.68
z :=

     (c+2)(c+1)(a-b+c+1)(a-b-c-1)(a+b+c+2)(a+b-c)

     -(c+2)(c+1)(a+b+c+3)(a+b-c-1)(a-b+c+2)

                   2
     (a-b-c-2)C ,
...
```

Thus, after 3 minutes on a Pentium with Linux (it was 7 minutes on a Sparcstation with SunOS) we find a recurrence relation for the sum $S(a,b,c) = \sum F(a,b,c,k)$ of the left-hand side. Here C is the shift operator in c. It says

$$\begin{aligned}&(c+2)(c+1)(a+b+c+3)(a+b-c-1)\\&(a-b+c+2)(a-b-c-2)S(a,b,c+2) =\\&(c+2)(c+1)(a-b+c+1)(a-b-c-1)\\&(a+b+c+2)(a+b-c)S(a,b,c).\end{aligned}$$

This recurrence is valid for all integers b and c, and for arbitrary complex a different from the integers $b+c$, $b+c-2$, ..., $b-c$, $-b-c-1$, $-b-c+1$, ..., $-b+c-1$ (for $c \le b$). We need integers b and c to make sure that only finitely many summands are nonzero. For negative c the sum vanishes, for nonnegative c it is interesting, and the factor $(c+2)(c+1)$ in the relation makes sure we cannot continue the recurrence down past $c = 0$. Clearly, $\mathrm{ud}(a-b-c,c).\mathrm{ud}(a+b+1-c,c)$ satisfies this same recurrence (for $c \ge 0$). It remains to compute $S(a,b,0) = F(a,b,0,0) = 1/(a-b)(a+b+1)$ and, as desired

$$\begin{aligned}&S(a,b,1) = F(a,b,1,0) + F(a,b,1,1)\\&= (a-b)(a+b+1)/(a+b)(a-b+1)(a+b+2)(a-b-1)\end{aligned}$$

Note that we proved a slightly more general result — the integrality of a (and that $a+b+c$ is odd) does not play a role, we only need a to be a complex number distinct from a handful of given integers.

Another example

Aart Blokhuis asked for the value of $\sum_{j=0}^{k} \binom{-a}{j}\binom{b}{k-j}\binom{c+j}{r}$ for $b = k+a-1$ and $b = k+a-2$, where a, b are nonnegative integers. This one is much easier than the previous example. Within two seconds we find a recurrence relation.

But let us first worry a little about the meaning of $\binom{x}{m}$ for possibly negative m. For nonnegative m we have the definition $\binom{x}{m} = \frac{x(x-1)\dots(x-m+1)}{m!} = \mathrm{ff}(x,m)/\mathrm{rf}(0,m)$, valid for all x. Below we shall use the convention $\binom{x}{m} = 0$ for $m < 0$. Then $\binom{x+1}{m} = \binom{x}{m} + \binom{x}{m-1}$ for all integers m.

[Note however, that this is not Maple's convention. Indeed, Maple says for negative m that $\binom{x}{m} = \mathrm{ff}(0,-m)/\mathrm{rf}(x,-m)$ and this is zero, unless x is an integer with $m \le x \le -1$, in which case $\binom{x}{m} = \mathrm{ff}(x,x-m)/\mathrm{rf}(0,x-m) = \binom{x}{x-m}$. Thus, with this convention we have $\binom{n}{m} = \binom{n}{n-m}$ for all integers m, n.]

Proposition. *Let a, b be nonnegative integers.*
(i) If $b = k+a-1$, we have

$$\sum_{j=0}^{k} \binom{-a}{j}\binom{b}{k-j}\binom{c+j}{r} = (-1)^k \binom{b}{k}\binom{c}{r-k}.$$

(ii) If $b = k+a-2$, we have

$$\sum_{j=0}^{k} \binom{-a}{j}\binom{b}{k-j}\binom{c+j}{r}$$
$$= (-1)^k \left(\binom{b}{k}\binom{c}{r-k} + \binom{b}{k-1}\binom{c+1}{r+1-k}\right)$$

Proof. If the sum is $S(k)$, then in the first case we find (regarding a, c, r as constants) the recurrence $(k-r)(k+a)S(k) = (k+1)(k-r+c+1)S(k+1)$ and $S(0) = \binom{c}{r}$. The certificate is $(c+j-r)j(k+a)/(k+1-j)$.
In the second case we find the recurrence

$$\begin{aligned}&(k-r-1)(k+a-1)(kc-ka+ar+2k-r+c+1)S(k) =\\&(k+1)(k-r+c+1)(kc-ka+ar+2k-r+a-1)S(k+1).\end{aligned}$$

This means that with $T(k) := S(k)/(kc-ka+ar+2k-r+a-1)$ we have $T(k+1) = \frac{(k-r-1)(k+a-1)}{(k+1)(k-r+c+1)}T(k)$ (essentially the same recurrence as before), so that

$$\sum_{j=0}^{k} \binom{-a}{j}\binom{b}{k-j}\binom{c+j}{r}$$
$$= (-1)^k \binom{b}{k}\binom{c+1}{r+1-k} \cdot \frac{k(c+1)+(a-1)(r+1-k)}{(a-1)(c+1)}. \qquad \square$$

Generalization and a Maple proof

Inspired by the above we conjecture that

$$(-1)^k \sum_j \binom{k-b-e-1}{j}\binom{b}{k-j}\binom{c+j}{r} = \sum_j \binom{e}{j}\binom{b}{k-j}\binom{c+j}{r-k+j}.$$

We shall give both a Maple and a traditional proof. It suffices to prove the identity in case $c = 0$ (see below for the argument), so we assume this, since it greatly simplifies the recurrences obtained.

Let $F(r,j)$ and $H(r,j)$ be the summands on the left-hand and right-hand side. Then we have for $j \ge 0$

$$\begin{aligned}&(k-r-e-1)(r+1)F(r+1,j) - (k-r)(k-b-r-e-1)F(r,j)\\&= G(r,j+1) - G(r,j)\end{aligned}$$

and

$$\begin{aligned}&(k-r-e-1)(r+1)H(r+1,j) - (k-r)(k-b-r-e-1)H(r,j)\\&= J(r,j+1) - J(r,j),\end{aligned}$$

where $G(r,j) = (k-b-j)(j-r)F(r,j)$ and $J(r,j) = (k-b-j)(k-r)H(r,j)$, as one easily checks by dividing both sides by $F(r,j)$ resp. $H(r,j)$. (We need not worry about $b = k-j-1$, since both sides are polynomials in b, and if they agree for all nonintegral b, they are identical.)

Sum over $j \ge 0$, and note that $G(r,0) = J(r,0) = 0$. We see that both sums satisfy the same recurrence relation

$$(k-r-e-1)(r+1)S(r+1) = (k-r)(k-b-r-e-1)S(r).$$

Both sums vanish for $r < 0$, and if we check that they agree for $r = 0$ the recurrence wil show that they always agree. (Again, we need not worry about $r = k-e-1$.)

But for $r = 0$ we find (this time taking b integral)

$$(-1)^k \sum_j \binom{k-b-e-1}{j} \binom{b}{k-j} = (-1)^k \binom{k-e-1}{k}$$
$$= \binom{e}{k} = \sum_j \binom{e}{j} \binom{b}{k-j} \binom{j}{k}.$$

This proves the claimed identity.

A traditional proof

Let Δ_x be the forward difference operator in x (acting on the space of polynomials in x), that is, $\Delta_x f(x) := f(x+1) - f(x)$. Then Δ_x decreases the degree of nonzero polynomials by one (if we agree that the zero polynomial has degree -1), and it follows that $f = g$ when $\Delta_x f = \Delta_x g$ and $f(c) = g(c)$ for some c. This operator is useful when manipulating binomial coefficients, since $\Delta_x \binom{x}{m} = \binom{x}{m-1}$.

Lemma. *Let m, n be integers, and $m \geq 0$. Then*

$$\sum_i (-1)^i \binom{m}{i} \binom{x+i}{n} = (-1)^m \binom{x}{n-m}.$$

Proof. Δ_x turns this equation into the same equation with n decreased by 1. Thus, it suffices to check this identity for $x = 0$. Then both sides equal $(-1)^m$ if $n = m$ and 0 otherwise. $\square$

Proposition. *Let k, m, n be integers. Then*

$$\sum_i (-1)^i \binom{x}{i} \binom{x+y-i}{k+m-i} \binom{z+k-i}{n}$$
$$= \sum_i \binom{x}{k-i} \binom{y}{m+i} \binom{z+i}{n-k+i}.$$

Proof. Δ_y and Δ_z decrease m and n, respectively, so it suffices to prove this for a suitable choice of y and z. Pick $y = 0$ and $z = n - k$. We have to show that

$$\sum_i (-1)^i \binom{x}{i} \binom{x-i}{k+m-i} \binom{n-i}{n} = \binom{x}{k+m} \binom{n-k-m}{n-k-m}.$$

But $\binom{x}{i}\binom{x-i}{k+m-i} = \binom{x}{k+m}\binom{k+m}{i}$, so it remains to show that if $p \geq 0$ then

$$\sum_i (-1)^i \binom{p}{i} \binom{n-i}{n} = \binom{n-p}{n-p}.$$

But this is the case $m = p$, $x = -1$ of the above lemma. $\square$

Of course the identity we had is obtained by substituting $b, e, c, 0, r, j$ for x, y, z, m, n, i and interchanging j and $k - j$ on the left.

References

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