A Proof of a Conjecture of Knuth

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Abstract

From numerical experiments, D. E. Knuth conjectured that $0 < D_{n+4} < D_n$ for a combinatorial sequence (D_n) defined as the difference $D_n = R_n - L_n$ of two definite hypergeometric sums. The conjecture implies an identity of type $L_n = \lfloor R_n \rfloor$, involving the floor function. We prove Knuth's conjecture by applying Zeilberger's algorithm as well as classical hypergeometric machinery.

1 The Conjecture

In a combinatorial study, D. E. Knuth [8] was led to consider a nonterminating hypergeometric series representation of the numbers

$$L_n := \sum_{k=0}^{n} \binom{2k}{k} \quad (n \geq 0).$$

The (ordinary) generating function of $(\binom{2k}{k})_{k\geq 0}$ is $1/\sqrt{1-4z}$, a special instance of the binomial series, and thus $\sum_{n=0}^{\infty} L_n z^n = 1/((1-z)\sqrt{1-4z})$. Expanding $1/(1-z)$ as a series in powers of $(1-4z)$ and equating like coefficients results in

$$L_n = \sum_{k=0}^{\infty} \frac{4}{3}(-\frac{1}{3})^k \binom{k-1/2}{n}(-4)^n. \tag{1}$$

Let $r_{n,k}$ denote the summand expression, and recall a bit of hypergeometric notation, for instance, from [6]. The rising factorials are defined as $x^{\bar{k}} = x(x+1)\dots(x+k-1)$ for $k \geq 1$, $x^{\bar{0}} = 1$, and the general hypergeometric series as

$$ {}_pF_q\left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix}; z\right) = \sum_{k\geq 0} \frac{a_1^{\bar{k}} \dots a_p^{\bar{k}}}{b_1^{\bar{k}} \dots a_q^{\bar{k}}} \frac{z^k}{k!}. $$

Now, if the series representation of L_n is rewritten in hypergeometric form,

$$ L_n = \sum_{k\geq 0} r_{n,k} = \frac{4}{3}\binom{2n}{n} {}_2F_1\left(\begin{matrix} 1/2, 1 \\ -n+1/2 \end{matrix}; -\frac{1}{3}\right), $$

the essential asymptotic information about L_n for $n \to \infty$ becomes explicit. But Knuth observed a good deal more. Assuming n as fixed, we quote from his letter [8]: "First the terms $r_{n,k}$ decrease rapidly, until $k = \lfloor \frac{3}{4}n + \frac{1}{2} \rfloor$, after which they increase and begin to oscillate wildly — so they look like they're diverging for sure. But then after $k = \lfloor \frac{3}{2}n + \frac{1}{2} \rfloor$ they begin to settle down and soon are converging like $(-\frac{1}{3})^k$". He added some numerical evaluations; for instance, for $n = 10$ the partial sum

$$ \sum_{k=0}^{\lfloor \frac{3}{4}10 + \frac{1}{2} \rfloor} r_{10,k} = 250953.29 $$

is quite close to the exact value of $L_{10} = 250953$. From those experiments he became convinced of the "curious" identity

$$ \sum_{k=0}^{n} \binom{2k}{k} = \left\lfloor \sum_{k=0}^{\lfloor (3n+2)/4 \rfloor} \frac{4}{3}(-\frac{1}{3})^k \binom{k-1/2}{n} (-4)^n \right\rfloor. \tag{2} $$

More generally, if R_n denotes the sum inside the floor brackets on the right hand side of (2), Knuth conjectured

Conjecture 1 (Knuth) *For $D_n := R_n - L_n$,*

$$ 0 < D_{n+4} < D_n \quad \textit{for all } n \geq 0. \tag{3} $$

Indeed, this implies (2), because the four initial values are less than 1, i.e., $(D_0, D_1, D_2, D_3, \ldots) = (1/3, 5/9, 7/9, 1/27, \ldots)$, and,

$$0 = \lfloor D_n \rfloor = \lfloor R_n - L_n \rfloor = \lfloor R_n \rfloor - L_n.$$

In view of the derivation above one could guess that there are many more identities involving the floor function like (2). But up to now identities of this type have not been discussed in the literature, and no standard tools are available for their treatment. The object of this note is to show that the key for the proof of Knuth's conjecture consists in applying methods belonging to different, sometimes even considered as opposite, paradigms, the Zeilberger algorithm and the classical hypergeometric machinery. For an introduction to both theories see, for instance, [6].

2 The Proof

Because of the floor function arising in the upper summation bound of R_n, we consider the problem separately for each congruence class mod 4. First, for $n = 4m$, $m \geq 0$, let $l_m = L_{4m}$, $r_m = R_{4m}$, and $d_m = D_{4m}$ The proof of (3) splits into the monotonicity part, $d_{m+1} < d_m$, and the positivity part, $0 < d_m$.

2.1 The Monotonicity Part

The Mathematica implementation [10] of Zeilberger's algorithm is able to treat also definite hypergeometric sums where the summation bounds are integer linear in the recurrence parameter. The package is available via anonymous ftp from `ftp.risc.uni-linz.ac.at` in the directory `/pub/combinatorics/mathematica/PauleSchorn`. Applying the program to $l_m = \sum_{k=0}^{4m} \binom{2k}{k}$ and $r_m = \sum_{k=0}^{3m} r_{4m,k}$ delivers the simple inhomogeneous recurrences

$$l_{m+1} - l_m = a(m) \quad \text{and} \quad r_{m+1} - r_m = a(m) - b(m), \tag{4}$$

where

$$a(m) = 16\,(680m^3 + 1302m^2 + 784m + 147)\frac{(8m+1)!}{(4m)!\,(4m+4)!} \tag{5}$$

and

$$b(m) = \frac{4}{27}\,(8m+7)\,(\frac{1}{3})^{3m}\,\frac{(2m+1)!\,(6m+1)!}{(m+1)!\,(3m)!\,(4m+3)!}. \tag{6}$$

The proof of the computer result is human-verifiable and is also delivered by the program.

Combining the recurrences by subtraction yields

$$d_m - d_{m+1} = b(m), \tag{7}$$

which, because of $b(m) > 0$, proves the monotonicity part of (3) for $n = 4m$.

The other cases work analogously; see (11).

2.2 The Positivity Part

Applying the computer program from [10] monotonicity turned out to be surprisingly simple to prove. In this section we demonstrate that recursion (7), derived with help of the computer, also provides the key for the proof of positivity, i.e., of $0 < d_m$ for all $m \geq 0$. But to this end we have to make extensive use of classical hypergeometric machinery. Nevertheless, the Mathematica package `hyp.m` developed by C. Krattenthaler [9] greatly facilitates the work. It can be obtained via anonymous ftp from `pap.univie.ac.at`.

From (7) and $d_0 = 1/3$, for all $M \geq 0$ we have that

$$d_M = d_0 + \sum_{m=0}^{M-1}(d_{m+1} - d_m) = d_0 - \sum_{m=0}^{M-1} b(m) > \frac{1}{3} - \sum_{m=0}^{\infty} b(m).$$

Hence positivity is proven once we can show that

$$\sum_{m=0}^{\infty} b(m) = \frac{1}{3}. \tag{8}$$

The convergence of this series is extremely slow, and all computer algebra systems the author has access to failed on its evaluation.

The hypergeometric evaluation proceeds as follows. First one rewrites the series as a hypergeometric ${}_5F_4$, and, because no standard summation formula can be found, one — in view of top entry 1 and bottom entry 2 — applies contiguous relation `C16` of Krattenthaler's package,

$$\sum_{m=0}^{\infty} b(m) = \frac{14}{81} {}_5F_4\left(\begin{matrix} 1/2, 5/6, 7/6, 15/8, 1 \\ 7/8, 5/4, 7/4, 2 \end{matrix}; 1\right) = \frac{1}{3} - \frac{1}{3} {}_4F_3\left(\begin{matrix} -1/2, -1/6, 1/6, 7/8 \\ -1/8, 1/4, 3/4 \end{matrix}; 1\right).$$

This reduces the original problem to showing that the ${}_4F_3$ evaluates to zero. Again no standard summation formula can found. But, observing that top entry 7/8 and bottom entry $-1/8$ differ exactly by 1, a further reduction is possible by applying contiguous relation `C30` of Krattenthaler's package,

$${}_4F_3\left(\begin{matrix} -1/2, -1/6, 1/6, 7/8 \\ -1/8, 1/4, 3/4 \end{matrix}; 1\right) = {}_3F_2\left(\begin{matrix} -1/6, 1/6, 1/2 \\ 1/4, 3/4 \end{matrix}; 1\right) - \frac{4}{9} {}_3F_2\left(\begin{matrix} 1/2, 5/6, 7/6 \\ 5/4, 7/4 \end{matrix}; 1\right). \tag{9}$$

Now the decisive step consists in using an important but less known cubic transformation of W. N. Bailey ([4], (4.06)), which the author found in a paper by I. Gessel and D. Stanton ([5], (5.6)), namely

$${}_3F_2\left(\begin{matrix} a, a+1/3, a+2/3 \\ b+1/2, 3a-b+1 \end{matrix}; \frac{27x^2}{4(1-x)^3}\right) = (1-x)^{3a} {}_3F_2\left(\begin{matrix} 3a, b, 3a-b+1/2 \\ 2b, 6a-2b+1 \end{matrix}; 4x\right). \tag{10}$$

The two ${}_3F_2$ from (9) correspond to the left hand side of (10) with $x = 1/4$ and $(a, b) = (-1/6, -1/4)$ or $(1/2, 3/4)$, respectively. In both cases we have $3a = 2b$. This means that applying (10) reduces each of the two ${}_3F_2$ from (9) to a ${}_2F_1$ with argument 1, which can be evaluated in closed form by using well-known Gauss summation

$${}_2F_1(\alpha, \beta; \gamma; 1) = \frac{\Gamma(\gamma-\alpha-\beta)\Gamma(\gamma)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}.$$

For the latter see, for instance, [6]. From the closed form evaluations it is easily verified that the difference on the right hand side of (9) indeed is zero, which completes the proof of the positivity part of (3) for $n = 4m$. The other cases work analogously as made explicit in the following section.

2.3 Summary

In order to give a complete picture of the situation, let $d_m^{(i)} := D_{4m+i}$. The general version of the monotonicity result, including (7), is

Proposition 1 (Monotonicity) *For* $i \in \{0, 1, 2, 3\}$*:*

$$d_m^{(i)} - d_{m+1}^{(i)} = b^{(i)}(m) \quad (m \geq 0), \tag{11}$$

where $b^{(0)}(m) = b(m)$ *and*

$$\begin{aligned}
b^{(1)}(m) &= \frac{16}{81}\,(168m^2 + 343m + 170)\,(\frac{1}{3})^{3m}\,\frac{(2m+1)!\,(6m+1)!}{m!\,(3m)!\,(4m+5)!},\\
b^{(2)}(m) &= \frac{4}{243}\,(40m + 47)\,(\frac{1}{3})^{3m}\,\frac{(2m)!\,(6m+5)!}{m!\,(3m+2)!\,(4m+5)!},\\
b^{(3)}(m) &= \frac{8}{243}\,(8m + 7)(2m + 3)\,(\frac{1}{3})^{3m}\,\frac{(2m+1)!\,(6m+5)!}{m!\,(3m+2)!\,(4m+7)!}.
\end{aligned}$$

This settles monotonicity, i.e., $D_{n+4} < D_n$, for all $n \geq 0$; the proof is analogous to that of (7).

The proof of positivity, i.e., of $0 < D_n$ $(= d_m^{(i)}$ if $n = 4m + i)$, follows analogously to that of case $i = 0$ using

Proposition 2 (Positivity) *For* $i \in \{0, 1, 2, 3\}$*:*

$$\sum_{m=0}^{\infty} b^{(i)}(m) = d_0^{(i)}. \tag{12}$$

These evaluations can be obtained by following essentially the same steps as made in the derivation of the corresponding result (8) for $i = 0$. For the reader who is interested in the underlying hypergeometric structure, we spell out a more conceptual proof of (12) in Section 3. It is based on one-parameter generalizations of the crucial cubic Bailey transform evaluation; it also explains a slight subtlety that arises in the case $i = 1$.

Combining monotonicity (11) and the positivity result (12) Knuth's conjecture (3) is proved for all $n \geq 0$.

We conclude this section by a corollary.

Corollary 1 *For the differences* $d_M^{(i)} = R_{4M+i} - L_{4M+i}$ *with* $i \in \{0, 1, 2, 3\}$*:*

$$d_M^{(i)} = \sum_{m=M}^{\infty} b^{(i)}(m) \quad (M \geq 0). \tag{13}$$

Proof: The monotonicity part (11) establishes (13) up to a constant; the positivity part (12) establishes (13) for $M = 0$.

3 Generalizations

In Section 2.2, we evaluated $\sum_{m\geq 0} b^{(0)}(m)$ $(= 1/3)$ by using Bailey's transform (10). In this section we state one-parameter generalizations (16) and (17) that, in certain combinations, specialize to evaluations of $\sum_{m\geq 0} b^{(i)}(m)$ for all residues i. Additional light on the underlying hypergeometric structure is shed by the two-parameter generalization (21).

For base case evaluation we need the following lemma.

Lemma 1 *If* $3a + 1 = 2b$ *then*

$${}_3F_2\left(\begin{matrix} a, a+1/3, a+2/3 \\ b+1/2, 3a-b+2 \end{matrix}; 1\right) = \frac{(3/2)^{3a}}{a+1}. \tag{14}$$

Proof: By contiguous relation `C34` from Krattenthaler's package the left hand side of (14) equals

$$\begin{aligned} &\frac{3a-b+1}{2a-b+1}\, {}_3F_2\left(\begin{matrix} a, a+1/3, a+2/3 \\ b+1/2, 3a-b+1 \end{matrix}; 1\right) - \\ &\frac{a}{2a-b+1}\, {}_3F_2\left(\begin{matrix} a+1/3, a+2/3, a+1 \\ b+1/2, 3(a+1/3)-b+1 \end{matrix}; 1\right). \end{aligned} \tag{15}$$

Now on each of the ${}_3F_2$'s Bailey's transform (10) can be applied and the lemma follows by

$$\frac{\Gamma(1/2)\Gamma(2b)}{\Gamma(b)\Gamma(b+1/2)} = 2^{2b-1},$$

which is a consequence of the factorial duplication formula, e.g., [6] (Exercise 5.22).

For $\delta \in \{1,2\}$ let

$$K_\delta(a,b,c) := {}_5F_4\left(\begin{array}{c} a, a+1/3, a+2/3, c+1, 1 \\ b+1/2, 3a-b+\delta, c, 2 \end{array}; 1\right).$$

Then the generalizations involving the extra parameter c read as follows:

Proposition 3 *(i) If $3a = 2b$ then*

$$K_1(a,b,c) = -\frac{(3/2)^2}{a-1}\frac{b(c-1)}{(b-1)c} + \frac{(3/2)^{2b}}{c}\left(1 + \frac{c-1}{(a-1)(b-1)}\right). \tag{16}$$

(ii) If $3a+1 = 2b$ then

$$K_2(a,b,c) = \tag{17}$$
$$-\frac{(3/2)^2}{a-1}\frac{(b-1/2)b(c-1)}{(b-3/2)(b-1)c} + \frac{(3/2)^{2b}}{(a-1)c}\left(\frac{a-c}{b+1} + \frac{a(c-1)}{(a-2/3)(b-1)}\right).$$

Proof: The evaluations can be derived by following the same steps as made in Section 2.2; in the situation of (17) one needs the above lemma for base case evaluation.

Now positivity can be derived as follows; note that because of (11) it suffices to prove (13) for $M = 0$.

Proof of Proposition 2: The cases $i = 2$ and $i = 3$ are immediate from the following representations which can be verified easily:

$$\sum_{m=0}^{\infty} b^{(2)}(m) = \frac{2\cdot 3\cdot 47}{3^5\cdot 5}K_1(\frac{5}{6},\frac{5}{4},\frac{47}{40}) + \frac{2^2\cdot 47}{3^5\cdot 5}K_2(\frac{1}{2},\frac{5}{4},\frac{47}{40}), \tag{18}$$

and

$$\sum_{m=0}^{\infty} b^{(3)}(m) = \frac{2}{3^5}K_1(\frac{7}{6},\frac{7}{4},\frac{7}{8}). \tag{19}$$

The $i = 1$ evaluation is more delicate, because $b^{(1)}(m)$ involves the polynomial factor $168m^2 + 343m + 170$ which turns out to be irreducible over the rational number field. Nevertheless, a suitable representation can be found *automatically* by using the package [10]. Calling the procedure `Gosper[F, m, order]` with `order` $= 2$ and `F` $= F(m) = b^{(1)}(m)/(168m^2 + 343m + 170)$

one finds a quadratic-polynomial multiple $f(m)$ of $F(m)$, namely $f(m) = (72m^2+139m+65)\cdot F(m)$, such that

$$\sum_{m=0}^{\infty} b^{(1)}(m) = \frac{2\cdot 7}{3^4} K_1(\frac{1}{2}, \frac{3}{4}, \frac{7}{8}) + \sum_{m=0}^{\infty} f(m), \tag{20}$$

and

$$f(m) = g(m+1) - g(m) \quad \text{where } g(m) = -9(m+1)(4m+3)(4m+5)\cdot F(m).$$

Hence $\sum_{m=0}^{\infty} f(m)$ telescopes and reduces to $-g(0) = 2/9$. Finally, evaluating $2\cdot 7/3^4\, K_1(1/2, 3/4, 7/8) + 2/9 = 5/9 = d_0^{(1)}$ completes the proof.

Remark: Case $i = 1$ can be put in a somehow more natural hypergeometric context if one climbs up the "hypergeometric hierarchy" as follows. Let

$$L_2(a,b,c,d) := {}_6F_5\left(\begin{matrix} a, a+1/3, a+2/3, c+1, d+1, 1 \\ b+1/2, 3a-b+2, c, d, 2 \end{matrix} ; 1 \right),$$

then one can prove (the details are left to the reader):
If $3a+1 = 2b$ *then*

$$L_2(a,b,c,d) = -\frac{(3/2)^2}{a-1} \frac{(b-1/2)b(c-1)(d-1)}{(b-3/2)(b-1)c\,d} + \frac{(3/2)^{2b}}{c\,d} r(a,b,c,d), \tag{21}$$

where

$$r(a,b,c,d) = \\ \frac{2}{3}\frac{(b-1/2)b(c-1)(d-1)}{(a-1)(b-3/2)(b-1)} - \frac{4b}{3}\frac{(a-c)(a-d)}{(a-1)(a+1)} + 3a\frac{(b-c)(b-d)}{(b-1)(b+1)}. \tag{22}$$

One easily checks that $L_2(a,b,c,\infty) = K_2(a,b,c)$. For the $i = 0$ case we have

$$\sum_{m=0}^{\infty} b^{(1)}(m) = \frac{2^4\cdot 7\cdot c\cdot d}{3^4\cdot 5} L_2(\frac{1}{2}, \frac{5}{4}, c, d), \tag{23}$$

where

$$c = (343 - \sqrt{3409})/336 \quad \text{and} \quad d = (343 + \sqrt{3409})/336.$$

We also get an alternative and more simple representation for the $i = 2$ case, namely

$$\sum_{m=0}^{\infty} b^{(2)}(m) = \frac{2 \cdot 47}{3^5} L_2(\frac{1}{2}, \frac{5}{4}, \frac{47}{40}, \frac{5}{6}). \tag{24}$$

It is evident that there are several further families of hypergeometric series evaluations which could be found along similar lines. For instance, as pointed out by one of the referees, Lemma 1 can be generalized to

$$ {}_3F_2 \left(\begin{matrix} a, a+1/3, a+2/3 \\ b+1/2, 3a-b+2 \end{matrix} ; w \right) = \tag{25}$$

$$\frac{3a+1}{a+1} \left(\frac{1-x}{y} \right)^{3a} - \frac{2a}{a+1} \left(\frac{1-x}{y} \right)^{3a+1}$$

where again $3a + 1 = 2b$, but with $w = 27/4 \cdot x^2/(1-x)^3$ and $y = (1 + \sqrt{1-4x})/2$. The proof is almost the same as that of Lemma 1 which has $x = 1/4$; the only difference is that instead of Gauss summation one uses

$$ {}_2F_1 \left(\begin{matrix} \alpha, \alpha+1/2 \\ 2\alpha+1 \end{matrix} ; z \right) = \left(\frac{1+\sqrt{1-z}}{2} \right)^{-2\alpha} \tag{26}$$

for evaluating the resulting ${}_2F_1$'s. This summation formula follows directly from Gauss' quadratic transformation (eq. (5.110) in [6]).

The same referee also indicated that analogously explicit formulae for

$$ {}_3F_2 \left(\begin{matrix} a, a+1/3, a+2/3 \\ (3a+n)/2, (3a+n+1)/2 \end{matrix} ; w \right) \qquad (n \text{ integer})$$

and for an x-generalization of Proposition 3 can be found. For instance, Proposition 3 generalizes as follows:

For $\delta \in \{1, 2\}$ and $w = 27/4 \cdot x^2/(1-x)^3$ let

$$K_\delta(a, b, c; w) := {}_5F_4 \left(\begin{matrix} a, a+1/3, a+2/3, c+1, 1 \\ b+1/2, 3a-b+\delta, c, 2 \end{matrix} ; w \right);$$

(i) if $3a = 2b$ and $y = (1 + \sqrt{1-4x})/2$ then

$$K_1(a, b, c; w) = -\frac{1}{w} \frac{(3/2)^2}{a-1} \frac{b(c-1)}{(b-1)c} + \tag{27}$$

$$\frac{1}{w} \frac{(3/2)^2}{a-1} \frac{b(c-1)}{(b-1)c} \left(\frac{1-x}{y} \right)^{2b-2} + \frac{a-c}{(a-1)c} \left(\frac{1-x}{y} \right)^{2b},$$

(ii) if $3a+1=2b$ and y as above then

$$K_2(a,b,c) = -\frac{1}{w}\frac{(3/2)^2}{a-1}\frac{(b-1/2)b(c-1)}{(b-3/2)(b-1)c} + \frac{1}{w}\frac{(3/2)^2}{a-1}\times \tag{28}$$
$$\frac{(b-1/2)(c-1)}{(b-3/2)(b-1)c}\left[3(b-1)\left(\frac{1-x}{y}\right)^{2b-3} - 2(b-\frac{3}{2})\left(\frac{1-x}{y}\right)^{2b-2}\right] +$$
$$\frac{a-c}{(a-1)(b+1)c}\left[3b\left(\frac{1-x}{y}\right)^{2b-1} - 2(b-\frac{1}{2})\left(\frac{1-x}{y}\right)^{2b}\right].$$

Again, the proof is almost the same as that of Proposition 3 which has $x=1/4$; the only difference is using (26) for evaluating the resulting ${}_2F_1$'s.

We also want to note that independently P. W. Karlsson [7] derived some evaluations of type ${}_3F_2(a_1,a_2,a_3;b_1,b_2;z)$ at $z=1/4$ from transformations related to Bailey's other cubic transformation ([4], (4.05), listed also in [5], (5.3)). There the results are based on a limit formula ([7], (1)), but contiguous relations are used in an analogous manner.

4 Conclusion

In his letter D.E. Knuth asked whether his conjecture can be proved with "mechanical summation methods". With respect to this question the presented solution succeeds only partially . Despite the fact that Krattenthaler's package was significantly helpful, it has to be viewed as a collection of manipulation rules that provides computer assistance in classical hypergeometric work. Hence, not only concerning the ${}_5F_4$ arising in (8) and (12), but also in general, the problem of mechanical evaluation of (nonterminating) hypergeometric series seems to be quite far from being solved. One possible approach is to make algorithmic use of contiguous relations. With respect to terminating cases this has been suggested by G. E. Andrews in connection with his recent work on "Pfaff's method" [1], [2] and [3]. A first interesting attempt has been made by N. Takayama [11].

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