ROCKY MOUNTAIN
JOURNAL OF MATHEMATICS
Volume 26, Number 2, Spring 1996

A SET OF POLYNOMIALS ASSOCIATED WITH THE HIGHER DERIVATIVES OF $y = x^x$

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ABSTRACT. The expansion

$$(1)\qquad x^{-x} D_x^n x^x = \sum_{k=0}^{n} (-1)^k \binom{n}{k} (1+\log x)^{n-k} F_k(x)$$

is proved, together with the inverse expansion

$$(2)\qquad F_n(x) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} (1+\log x)^{n-k} x^{-x} D_x^k x^x.$$

The recurrence $F_n(x) = -D_x F_{n-1}(x) + ((n-1)/x) F_{n-2}(x)$, $n \geq 2$, with $F_0(x) = 1$ and $F_1(x) = 0$ shows that $G_n(x) = x^n F_n(x)$ is a polynomial in x. The fact that $G_n(x) = \sum_{0 \leq j \leq n/2} A_j^n x^j$ with $A_j^{n+1} = (n-j)A_j^n + nA_{j-1}^{n-1}$, $j \geq 1$, where $A_j^n = 0$ for $j < 0$ or for $j > n/2$, shows that $G_n(x)$ is of exact degree $[n/2]$ in x. Finally, in terms of Stirling numbers of the first kind

$$(3)\quad F_n(x) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \sum_{j=0}^{k} \binom{k}{j} \sum_{i=0}^{j} \frac{i!}{(i-k+j)!} s(j,i) x^{i-k}.$$

Another curious property is that $\sum_{1 \leq k \leq n} A_k^{n+k} = n^n$, $n \geq 1$. In terms of Comtet-Lehmer numbers,

$$(4)\quad x^n F_n(x) = \sum_{0 \leq j \leq n/2} x^j \sum_{k=n-j}^{n} (-1)^k \binom{n}{k} b(k, k-n+j).$$

An elementary calculus problems asks to find $D_x x^x$. The answer is easily found by logarithmic differentiation and is $x^x(1+\log x)$. The

Received by the editors on November 29, 1993, and in revised form on October 10, 1995.

higher derivatives are quite involved and are the motivation of this paper. My study of these polynomials began in 1955 [**2**, Vol. V, pp. 250–253], and the results presented here were obtained at various times between 1955 and 1975.

Let us examine a few higher derivatives. We find

$$\begin{aligned}
x^{-x}D_x^2 x^x &= \frac{1}{x} + (1+\log x)^2;\\
x^{-x}D_x^3 x^x &= -\frac{1}{x^2} + \frac{3}{x}(1+\log x) + (1+\log x)^3;\\
x^{-x}D_x^4 x^x &= \left(\frac{2}{x^3}+\frac{3}{x^2}\right) - \frac{4}{x^2}(1+\log x)\\
&\quad + \frac{6}{x}(1+\log x)^2 + (1+\log x)^4;\\
x^{-x}D_x^5 x^x &= -\left(\frac{6}{x^4}+\frac{10}{x^3}\right) + 5\left(\frac{2}{x^3}+\frac{3}{x^2}\right)(1+\log x)\\
&\quad - \frac{10}{x^2}(1+\log x)^2\\
&\quad + \frac{10}{x}(1+\log x)^3 + (1+\log x)^5.
\end{aligned}$$

It is then easy to conjecture that there exists a sequence of rational functions $\{F_n(x)\}$, $n = 0, 1, 2, \dots$, such that

$$(1) \qquad x^{-x}D_x^n x^x = \sum_{k=0}^{n} (-1)^k \binom{n}{k} (1+\log x)^{n-k} F_k(x), \qquad n \geq 0.$$

In fact, (1) is easily proved by mathematical induction based on the recurrence relation

$$(2) \qquad F_n(x) = -D_x F_{n-1}(x) + \frac{n-1}{x} F_{n-2}(x), \qquad n \geq 2,$$

with $F_0(x) = 1$ and $F_1(x) = 0$.

The recurrence relation (2) recursively defines $F_n(x)$ to be a rational function. Moreover, if we define $G_n(x) = x^n F_n(x)$, then $G_n(x)$ is a polynomial in x. This is proved by translating the recurrence relation (2) over into the corresponding form:

$$(3) \qquad G_{n+1}(x) = (n - xD_x)G_n(x) + nxG_{n-1}(x), \quad \text{for } n \geq 1,$$

with $G_0(x) = 1$, $G_1(x) = 0$.

Table 1 gives some values of $G_n(x)$. Examination of these yields the conjecture that $G_n(x)$ is of exact degree $[n/2]$. To prove this, let

$$G_n(x) = \sum_{0 \le j \le n/2} A_j^n x^j. \tag{4}$$

This may be proved by induction using (3) and the recurrence

$$A_j^{n+1} = (n-j)A_j^n + nA_{j-1}^{n-1}, \qquad j \ge 1 \tag{5}$$

with $A_j^n = 0$ for $j < 0$ or for $j > n/2$. Indeed, assuming (4) we have

$$\begin{aligned}(n - xD_x)G_n(x) &= (n - xD_x) \sum_{0 \le j \le n/2} A_j^n x^j \\ &= \sum_{0 \le j \le n/2} \{nA_j^n - jA_j^n\} x^j \\ &= \sum_{0 \le j \le n/2} (n-j) A_j^n x^j\end{aligned} \tag{6}$$

and

$$\begin{aligned}nxG_{n-1}(x) &= \sum_{0 \le j \le (n-1)/2} nA_j^{n-1} x^{j+1} \\ &= \sum_{1 \le j \le (n+1)/2} nA_{j-1}^{n-1} x^j.\end{aligned} \tag{7}$$

Adding (6) and (7), then in virtue of (3) we have

$$\begin{aligned}G_{n+1}(x) &= \sum_{0 \le j \le (n+1)/2} \{(n-j)A_j^n + nA_{j-1}^{n-1}\} x^j \\ &= \sum_{0 \le j \le (n+1)/2} A_j^{n+1} x^j\end{aligned}$$

provided we assume recurrence (5).

Examination of Table 1 yields another conjecture:

$$\sum_{k=1}^{n} A_k^{n+k} = n^n, \qquad n \ge 1. \tag{8}$$

TABLE 1.

n	$G_n(x) = x^n F_n(x) = \sum_{0\le j\le n/2} A_j^n x^j$
0	1
1	0
2	x
3	x
4	$2x + 3x^2$
5	$6x + 10x^2$
6	$24x + 40x^2 + 15x^3$
7	$120x + 196x^2 + 105x^3$
8	$720x + 1148x^2 + 700x^3 + 105x^4$
9	$5040x + 7848x^2 + 5068x^3 + 1260x^4$
10	$40320x + 61416x^2 + 40740x^3 + 12600x^4 + 945x^5$

Examples.

$$A_1^2 = 1; \qquad A_1^3 + A_2^4 = 1 + 3 = 4 = 2^2;$$
$$A_1^4 + A_2^5 + A_3^6 = 2 + 10 + 15 = 27 = 3^3$$
$$A_1^5 + A_2^6 + A_3^7 + A_4^8 = 6 + 40 + 105 + 105 = 256 = 4^4.$$

This interesting fact may be proved by introducing the change of notation

$$T(n,k) = A_k^{n+k}. \tag{9}$$

Then relation (8) becomes

$$\sum_{k=0}^{n} T(n,k) = n^n, \qquad n \ge 1 \tag{10}$$

and recurrence (5) becomes

$$T(n+1,k) = nT(n,k) + (n+k)T(n,k-1), \tag{11}$$

with $T(0,0) = 1$ and $T(0,k) = T(n,0)$ for $n,k \ge 1$. The proof of (10) (with notation $S(n,k)$ for $T(n,k)$) was the subject of a problem posed by Peter Shor [**7**]. Two proofs were given, by Shor and by Otto Ruehr. There was no indication there that the array had anything to do with the derivatives of x^x.

A somewhat different perspective on the higher derivatives of x^x has been given by Comtet [**1**, pp. 139–140] in 1974 who obtained the expansion

$$x^{-x} D_x^n x^x = \sum_{j=0}^{n} (\log x)^j \binom{n}{j} \sum_{k=0}^{n-j} b(n-j, n-1-j) x^{-k}, \qquad n \geq 0, \tag{12}$$

where the array of integers $\{b(n,k)\}$ is defined by the expansion

$$\sum_{n=1}^{\infty} b(n,k) \frac{x^n}{n!} = \frac{1}{k!} \{(1+x)\log(1+x)\}^k. \tag{13}$$

As Lehmer notes [**3**, p. 469] Comtet gave the relation

$$b(n,k) = \sum_{j=k}^{n} \binom{j}{k} k^{j-k} s(n,j) \tag{14}$$

where the $s(n,j)$ are the Stirling numbers of the first kind in Riordan's notation [**4, 5**]:

$$\begin{aligned} x(x-1)\cdots(x-n+1) &= n!\binom{x}{n} \\ &= \sum_{j=0}^{n} s(n,j) x^j, \qquad n \geq 0. \end{aligned} \tag{15}$$

Lehmer works with the equivalent generating function expansion

$$\{\log(1+x)\}^k = k! \sum_{n=1}^{\infty} s(n,k) \frac{x^n}{n!}, \qquad k \geq 0. \tag{16}$$

Lehmer develops many interesting relations involving $b(n,k)$, its inverse $B(n,k)$, Stirling numbers of the first kind $s(n,k)$, and their inverse the Stirling numbers of second kind $S(n,k)$.

It is possible to translate (1) into (12) and conversely; however, the compelling reason for my having worked with expansion (1) is that it lends itself more easily to finding $D_x^n x^x|_{x=1}$ which can be found by direct substitution of $x = 1$ in (1) but would have to be found by taking limits in Comtet's expansion (12). In the present terminology, of course,

$$(17) \qquad D_x^n x^x \Big|_{x=1} = \sum_{k=0}^{n} (-1)^k \binom{n}{k} F_k(1), \qquad n \geq 0,$$

so that we have only to evaluate $F_n(1)$ to find these higher derivatives. Table 2 gives some values for $F_n(1)$ as well as the derivatives.

TABLE 2.

n	$D_x^n x^x\|_{x=1}$	$F_n(1)$
0	1	1
1	1	0
2	2	1
3	3	1
4	8	5
5	10	16
6	54	79
7	-42	421
8	944	2673
9	-5112	19216
10	47160	156021

It is interesting to note that the derivative values are identical to the numbers σ_n which are found in a different context by Lehmer [**3**, pp. 467–468], who obtains σ_n as the coefficient of $x^n/n!$ in the expansion of $(1+x)^{1-x}$ in powers of x. He gives a table of values for $n = 0, 1, \ldots, 14$ which agree with the values we give in Table 2.

Lehmer defines $\sigma_n = \sigma_n(1)$ with $\sigma_n(t)$ defined by

$$\sigma_n(t) = \sum_{k=0}^{n} b(n,k)t^n, \qquad n \geq 0, \tag{18}$$

where $b(n,k)$ is the array defined by Comtet in expansion (13) above.

We now return to the further study of expansion (1). First we find that the expansion inverts to give

$$F_n(x) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} (1+\log x)^{n-k} x^{-x} D_x^k x^x, \qquad n \geq 0. \tag{19}$$

The proof follows from the well-known (e.g., see Riordan [**4**]) binomial series inversion pair

$$A_n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} B_k, \qquad n \geq 0,$$

if and only if

$$B_n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} A_k, \qquad n \geq 0,$$

by setting

$$A_n = F_n(x)(1+\log x)^{-n}$$

and

$$B_n = x^{-x} D_x^n x^x (1+\log x)^{-n}.$$

But expansion (19) is not an explicit formula for $F_n(x)$ unless we already know the higher derivatives of x^x.

We come to our first major result.

Theorem. *The rational functions $F_n(x)$ are given explicitly by*

$$F_n(x) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \sum_{j=0}^{k} \binom{k}{j} \sum_{i=0}^{j} \frac{i!}{(i-k+j)!} s(j,i) x^{i-k}, \qquad n \geq 0. \tag{20}$$

Proof. Apply the binomial theorem to $(1+\log x)^{n-k}$ in (1), and we find

$$x^{-x} D_x^n x^x = \sum_{i=0}^{n} (\log x)^i \sum_{k=i}^{n} (-1)^{n-k} \binom{n}{k} \binom{k}{i} F_{n-k}(x). \tag{21}$$

On the other hand, we have

$$\begin{aligned} D_x^n x^x &= D_x^n \exp(x \log x) \\ &= D_x^n \sum_{k=0}^{\infty} \frac{x^k}{k!} (\log x)^k \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{j=0}^{n} \binom{n}{j} D_x^{n-j} x^k D_x^j (\log x)^k \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{j=0}^{n} \binom{n}{j} \frac{k!}{(k-n+j)!} x^{k-n+j} \frac{k!}{x^j} \sum_{i=0}^{k} \frac{(\log x)^i}{i!} s(j, k-i) \end{aligned}$$

so that

$$D_x^n x^x = \sum_{i=0}^{\infty} \frac{(\log x)^i}{i!} \sum_{k=i}^{\infty} \sum_{j=0}^{n} \binom{n}{j} \frac{k!}{(k-n+j)!} x^{k-n} s(j, k-i). \tag{22}$$

Now, however,

$$x^{-x} = \exp(-x \log x) = \sum_{i=0}^{\infty} (-1)^i x^i \frac{(\log x)^i}{i!}, \tag{23}$$

so that, multiplying (22) and (23) together as formal power series in the variable $z = \log x$ and simplifying, we get

$$\begin{aligned} x^{-x} D_x^n x^x = \sum_{s=0}^{\infty} \frac{(\log x)^s}{s!} \sum_{i=0}^{\infty} (-1)^{s-i} x^{s-i} \\ \sum_{k=i}^{\infty} \sum_{j=0}^{n} \binom{n}{j} \frac{k!}{(k-n+j)!} x^{k-n} s(j, k-i) \end{aligned} \tag{24}$$

In this the coefficient of $(\log x)^0$ is

$$\sum_{k=0}^{\infty} \sum_{j=0}^{n} \binom{n}{j} \frac{k!}{(k-n+j)!} x^{k-n} s(j, k). \tag{25}$$

But in (21) the coefficient of $(\log x)^0$ is

$$\sum_{k=0}^{n}(-1)^{n-k}\binom{n}{k}F_{n-k}(x) = \sum_{k=0}^{n}(-1)^k\binom{n}{k}F_k(x). \tag{26}$$

Equating (25) and (26), we have then

$$\begin{aligned}\sum_{k=0}^{n}(-1)^k\binom{n}{k}F_k(x) &= \sum_{k=0}^{\infty}\sum_{j=0}^{n}\binom{n}{j}\frac{k!}{(k-n+j)!}x^{k-n}s(j,k)\\ &= \sum_{j=0}^{n}\sum_{k=0}^{\infty}\binom{n}{j}\frac{k!}{(k-n+j)!}x^{k-n}s(j,k)\\ &= \sum_{j=0}^{n}\sum_{k=0}^{j}\binom{n}{j}\frac{k!}{(k-n+j)!}x^{k-n}s(j,k),\end{aligned}$$

since $s(j,k) = 0$ whenever $k > j$. Therefore, we have proved that

$$\sum_{k=0}^{n}(-1)^k\binom{n}{k}F_k(x) = \sum_{j=0}^{n}\sum_{k=0}^{j}\binom{n}{j}\frac{k!}{(k-n+j)!}x^{k-n}s(j,k), \quad n \geq 0. \tag{27}$$

By appealing to the binomial inversion pair we used earlier we find

$$F_n(x) = \sum_{k=0}^{n}(-1)^k\binom{n}{k}\sum_{j=0}^{k}\sum_{i=0}^{j}\binom{k}{j}\frac{i!}{(i-k+j)!}x^{i-k}s(j,i), \qquad n \geq 0,$$

which proves formula (20). □

In the language of the calculus of finite differences,

$$\sum_{k=0}^{n}(-1)^{n-k}\binom{n}{k}f(z+kh) = h^n\Delta_z^n f(z), \qquad n \geq 0, \tag{28}$$

where $\Delta_{z,h}f(x) = (f(z+h)-f(z))/h$, so that the relation (27) is $(-1)^n$ times the nth difference of $F_z(x)$ with respect to z and increment $h = 1$, evaluated at $z = 0$.

To see how $F_n(x)$ is related to Comtet's array $\{b(n,k)\}$, we find the coefficient of $(\log x)^0$ in (12) above and recall (26). We have proved then that

$$\sum_{k=0}^{n}(-1)^k\binom{n}{k}F_k(x)=\sum_{k=0}^{n}b(n,n-k)x^{-k}. \tag{29}$$

Again by simple binomial inversion we find the simple and elegant formula

$$F_n(x)=\sum_{k=0}^{n}\frac{1}{x^j}\sum_{k=j}^{n}\binom{n}{k}b(k,k-j), \qquad n\geq 0. \tag{30}$$

However, there are some zero terms in this expansion. Indeed, recall that we showed that $G_n(x)=x^nF_n(x)$ is a polynomial of exact degree $[n/2]$ in x. It follows easily then that

$$G_n(x)=\sum_{0\leq j\leq n/2}x^j\sum_{k=n-j}^{n}(-1)^k\binom{n}{k}b(k,k-n+j). \tag{31}$$

Another way of saying this is that

$$A_j^n=\sum_{k=n-j}^{n}(-1)^k\binom{n}{k}b(k,k-n+j). \tag{32}$$

Since $b(n,k)$ is given in terms of $s(n,k)$ by (14), then (31) says that
(33)

$$G_n(x)=\sum_{0\leq j\leq n/2}x^j\sum_{k=n-j}^{n}(-1)^k\binom{n}{k}\sum_{i=k-n+j}^{k}\binom{i}{k-n+j}s(k,j).$$

Comparing (33) with our (20) we see that each requires a triple iterated summation of Stirling numbers of the first kind to express the form of $F_n(x)$ explicitly. I have not been able to reduce the number of summations needed. My first result years ago required five summations, but then I found (20) using three. I am reminded of the 20 years spent by Ludwig Schläfli [**6**] in his search for a way to represent the Stirling numbers of the first kind using as few summations as possible. He went from five to two, but never realized that Schlömilch and others had already done this in a slightly different form. The Comtet numbers and their inverse counterparts, as Lehmer shows, have many interesting properties and so, by using them, we are able in formula (31) to require only two summations involving them instead of the three we need in formula (20) when we use Stirling numbers. Lehmer's paper is also valuable in giving an extensive table of the $b(n,k)$ and the inverse set $B(n,k)$ which he defines and studies.

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