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500. ON COEFFICIENTS FOR NUMERICAL DIFFERENTIATION AND INTEGRATION*

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The literature surces containing the tables of coefficients $a_{n,k}$ of formulas for numerical differentiation and integration of

$$\left(h\frac{\mathrm{d}}{\mathrm{d}x}\right)^n f(x)=\sum_{k=1}^{+\infty} a_{n,k}\,\Delta^{n+k-1}f(x),$$

$$\frac{1}{h}\int_x^{x+h} f(t)\,\mathrm{d}t=\sum_{k=1}^{+\infty} a_{-1,k}\,\Delta^{k-1}f(x)$$

are briefly surveyed. The difference equation

$$(n+k-1)\,a_{n,k}=(2-n-k)\,a_{n,k-1}+n\,a_{n-1,k}$$

is solved. The formula

$$a_{n,k}=0\ (k<1),\ a_{n,1}=1,\ \sum_{m=1}^{k}(-1)^m\frac{kn-mn-m+1}{k-m+1}\,a_{n,m}=0\qquad(k>1)$$

is derived and $a_{n,k}$ for $k\leq 7$ is calculated. The computer program for calculating $a_{n,k}$ is developed. An example of its application to regression is proposed.

A. ANDOYER [1] has calculated $a_{n,k}$ for $n=-2(1)7$, $k=1(1)8-n$; T. N. THIELE [2] for $n=-5(1)5$, $k=1(1)8$; W. F. SHEPPARD [3] for $n=1(1)8$, $k=1(1)9-n$; K. PEARSON and M. V. PEARSON [4] for $n=2$, $k=1(1)13$; W. G. BICKLEY and J. C. P. MILLER [5] for $n=1(1)12$, $k=1(1)13-n$; A. N. LOWAN, H. E. SALZER and A. HILLMAN [6] for $n=1(1)20$, $k=1(1)21-n$. See also [7, pp. 105–108].

The most complete table of coefficients for numerical differentiation was given by D. S. MITRINOVIĆ, R. S. MITRINOVIĆ and S. S. TURAJLIĆ [8]. Coefficients $A_{r,m}$, defined by

$$\prod_{j=1}^{m}(x+m-j)=\sum_{r=1}^{m}\frac{m!}{r!}\,A_{r,m}\,x^r,$$

were calculated for $m\leq 30$ by means of the formula $A_{r,m}=\frac{r!}{m!}\,S_m^r$ and by the tables of STIRLING's numbers of the first order S_m^r which were formerly published by D. S. MITRINOVIĆ and R. S. MITRINOVIĆ. Using the previous notation, we can say that the paper [8] contains coefficients $a_{n,k}$ for $n=1(1)29$, $k=2(1)31-n$. In [8] we also find $A_{m,m}=1$, i. e., $a_{n,1}=1$.

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If GREGORY interpolation formula

$$f(x+hs)=\sum_{m=0}^{+\infty}\binom{s}{m}\Delta^m f(x)$$

(see for example [9, p. 56]) is differentiated n times with respect to s and provided that $s\to 0$, we get

$$a_{n,k}=\lim_{s\to 0}\left(\frac{\mathrm{d}}{\mathrm{d}s}\right)^n\binom{s}{n+k-1}\qquad (n\geqq 0,\ k>0),$$

[compare **10**, p. 98].

The recurrent formula

$$\frac{\mathrm{d}^m}{\mathrm{d}p^m}({}_pC_{r+1})\Big|_{p=0}=\left[-r\frac{\mathrm{d}^m}{\mathrm{d}p^m}({}_pC_r)\Big|_{p=0}+m\frac{\mathrm{d}^{m-1}}{\mathrm{d}p^{m-1}}({}_pC_r)\Big|_{p=0}\right]/(r+1),$$

[see **11**, p. 74], is equivalent with

$$mA_{r,m}=(m-1)A_{r,m-1}+rA_{r-1,m-1},$$

[see **8**, p. 115], as well as with

$$(1)\qquad (n+k-1)\,a_{n,k}=(2-n-k)\,a_{n,k-1}+na_{n-1,k}$$

because

$$a_{n,k}=(-1)^{k+1}A_{n,n+k-1},\quad A_{n,m}=(-1)^{m-n}a_{n,m-n+1}$$

are valid.

Solving the equation (1) leads to the following result:

Equation (1) can be solved to within a single multiplicative constant. For $n+k=1$ it follows from (1) $a_{n,-n}=n\,a_{n-1,1-n}$, wherefrom $a_{-n,n}=a_{-1,1}/\Gamma(n)\,(n>0)$, and

$$(2)\qquad a_{n,-n}=0\qquad (n\geqq 0).$$

For $n+k=2$, from (1) it follows that: $a_{n,2-n}=n\,a_{n-1,2-n}$.

For $n=0$, from (1) it follows that $(k-1)\,a_{0,k}=(2-k)\,a_{0,k-1}$, wherefrom

$$(3)\qquad a_{0,k}=0\qquad (k\neq 1).$$

From (1), (2), (3) are also have $a_{n,k}=0\ (0\leqq n\leqq -k)$ while the other coefficients cannot be obtained from (1).

The following complete set of implications expresses the possibility of calculating the values of coefficients $a_{n,k}$, only by means of formula (1):

$$\begin{array}{lll}
a_{0,1} & & \Rightarrow a_{1,k}\ (k>0),\\
a_{n,1} & (0<n\leqq N) & \Rightarrow a_{n,k}\ (0<n<N,\ k\geqq 1-n),\\
a_{n,1} & (0<n\leqq N) & \Rightarrow a_{N,k}\ (k>1-N),\\
a_{-1,k} & (2\leqq k<K) & \Rightarrow a_{n,k}\ (-k<n<0,\ 2<k\leqq K),\\
a_{n,1} & (-N\leqq n\leqq -1) & \Rightarrow a_{n,k}\ (-1\leqq n\leqq -N,\ n-N<k\leqq n),\\
a_{n,-n} & (1<n\leqq N) & \Rightarrow a_{n,k}\ (k\leqq -n).
\end{array}$$

Other complete sets of implications are also possible. However, if all values of $a_{n,k}$ were known, except $a_{-1,2}$ the value of the last item cvuld be obtained only from (1):

$$a_{n,k}\ \left((n+1)^2+(k-2)^2\neq 0\right) \not\Rightarrow a_{-1,2}.$$

From (1) the following implication ensues:

(4) $$a_{n,1}=1 \Rightarrow a_{n,k}=0 \qquad (k<1).$$

On the basis of the definition of the generalized BERNOULLI's numbers

$$\left(\frac{1}{t}\log(1+t)\right)^n=\sum_{p=0}^{+\infty}\frac{n}{n+p}B_p^{(n+p)}\frac{t^p}{p!},$$

[see for example **7**, p. 69], and using the definition of the cofficients $a_{n,k}$

$$(\log(1+\Delta))^n f(x)=\left(\sum_{k=1}^{+\infty}a_{n,k}\,\Delta^{n+k-1}\right)f(x)$$

we get

$$a_{n,k}=\frac{n}{(k-1)!\,(n+k-1)}B_{k-1}^{(n+k-1)},\ \text{i.e.,}\ B_p^{(m)}=\frac{p!\,m}{m-p}a_{m-p,\,p-1}.$$

In [**7**, p. 103] we find $B_p^{(m)}$ for $p=0\,(1)\,3$.

N. E. NÖRLUND [**12**, p. 459] has calculated $B_p^{(m)}$ for $p=0\,(1)\,12$.

L. G. KELLY [**13**, p. 51] quotes the results equvalent to $a_{1,k}$ and $a_{n,k}$ $(k=1, 2, 3)$.

F. B. HILDEBRAND [**14**, p. 182] gives the results equivalent to $a_{1,k}$ and $a_{n,k}\,(k=1, 2, 3, 4)$.

Three centuries ago J. GREGORY had given the formula

$$\frac{1}{h}\int_x^{x+nh}f(t)\,dt=\sum_{m=0}^{n}f(m)-\sum_{k=0}^{+\infty}C_{k+2}\left(\Delta^k f(0)+(-1)^k\Delta^k f(n-k)\right)$$

equivalent to EULER—MACLAURIN formula

$$\frac{1}{h}\int_x^{x+nh}f(t)\,dt=\sum_{m=0}^{n}f(m)-\frac{f(0)+f(n)}{2}-\sum_{k=1}^{+\infty}\frac{h^{2k-1}B_{2k}}{(2k)!}\left(f^{(2k-1)}(n)-f^{(2k-1)}(0)\right),$$

[see for example **9**, p. 129]. Coefficients $C_k\,(=a_{-1,k})$ were calculated by T. CLAUSEN for $k=2\,(1)\,13$; K. PEARSON for $k=1\,(1)\,14$; R. A. FISHER and F. YATES for $k=1\,(1)\,17$; A. N. LOWAN and H. SALZER for $k=1\,(1)\,20$. [See **7**, p. 108].

G. BOOLE [**15**, p. 61] quoted the results equivalent to

$$a_{-1,k}=\int_0^1\binom{s}{k-1}ds \qquad (k>0).$$

L. G. KELLY [**13**, p. 57] quoted the result:

$$C_1=1,\ C_2=\frac{1}{2},\ C_{k+1}=\frac{C_k}{2}-\frac{C_{k-1}}{3}+\frac{C_{k-2}}{4}-\cdots+(-1)^{k+1}\frac{C_1}{k+1},$$

equivalent to recurrent formula

$$(5)\qquad a_{-1,1}=1,\ \sum_{m=1}^{k}\frac{(-1)^m}{k-m+1}a_{-1,m}=0\qquad (k>1).$$

We shall give the generalization of the recurrent formula (5) for arbitrarily fixed n. Starting from the known formula

$$\left(\sum_{n=0}^{+\infty}E_n z^n\right)^p=\sum_{m=0}^{+\infty}D_m z^m \Rightarrow$$

$$D_0=E_0^p,\ D_m=\frac{1}{mE_0}\sum_{k=1}^{m}(kp+k-m)E_k D_{m-k}\qquad (m\geqq 1),$$

[see for example **16**, p. 28], and

$$\left(h\frac{\mathrm{d}}{\mathrm{d}x}\right)f(x)=\big(\log(1+\Delta)\big)f(x)$$

[see for example **12**, p. 25], for coefficients $a_{n,k}$ of the development

$$h\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n f(x)=\left(\sum_{k=0}^{+\infty}a_{n,k}\,\Delta^{n-1+k}\right)f(x)$$

the following result is obtained

$$(6)\qquad a_{n,k}=0\,(k<1),\ a_{n,1}=1,\ \sum_{m=1}^{k}(-1)^m\frac{kn-mn-m+1}{k-m+1}a_{n,m}=0\qquad (k>1).$$

(5) follows from (6) for $n=-1$.

From (5) it follows that $a_{n,k}\,(k>0)$ is a polynomial with respect to n

$$a_{n,1}=1,\qquad a_{n,2}=-\frac{1}{2}n,\qquad a_{n,3}=\frac{1}{24}(3n^2+5n),$$

$$a_{n,4}=-\frac{1}{48}(n^3+5n^2+6n),\qquad a_{n,5}=\frac{1}{5760}(15n^4+150n^3+485n^2+502n),$$

$$a_{n,6}=-\frac{1}{11520}(3n^5+50n^4+305n^3+802n^2+760n),$$

$$a_{n,7}=\frac{1}{2903040}(63n^6+1575n^5+15435n^4+73801n^3+171150n^2+152696n),$$

and a transcendent function with respect to k

$$(7)\qquad a_{n,k}=\sum_{m=0}^{k-1}\frac{P_m(k)}{\Gamma(k-m)}\left(\frac{n}{2}\right)^{k-1-m},$$

where $P_m(k)$ is a polynomial with respect to k of order m

$$P_0(k)=1,\ P_1(k)=\frac{5}{12}(k-2),\ P_2(k)=\frac{1}{288}(k-3)(25k-28),$$

$$P_3(k)=\frac{1}{51840}(k-4)(625k^2-1475k+786),\ \ldots$$

while $s\mapsto\Gamma(s)$ Euler gamma function. Observe that

$$P_{k-1}(k)=0\quad (k>1).$$

Formula (6) is suitable for computer calculations, because the implication

$$a_{n,1}=1 \Rightarrow a_{n,k} \quad (k>1).$$

follows from it.

Fig. 1 represents the DIFF program, based on (6), generalizing

$$A(K)=a_{N,K} \qquad (K=1\,(1)\,L).$$

The DIFF program verifies the accuracy of the table in [8].

```
      SUBROUTINE DIFF(N,L,A)
      DIMENSION A(1)
      A(1)=1.
      DO 2 K=2,L
      B=0.
      I=K*N+1
      JJ=K-1
      DO 1 J=1,JJ
      I=I-N-1
      C=K-J+1
    1 B=I*A(J)/C+B
    2 A(K)=B/JJ
      DO 3 K=2,L,2
    3 A(K)=-A(K)
      RETURN
      END
```

Fig. 1

n	c_n
-1	1.00000 00000 00000 000
0	0.57721 56649 01532 861
1	0.07281 58454 83676 725
2	-0.00484 51815 96436 159
3	-0.00034 23057 36717 224
4	0.00009 68904 19394 471
5	-0.00000 66110 31810 842
6	-0.00000 03316 24090 875
7	0.00000 01046 20945 845
8	-0.00000 00087 33218 100
9	0.00000 00000 94782 778
10	0.00000 00000 56584 219
11	-0.00000 00000 06768 690
12	0 00000 00000 00349 212
13	0.00000 00000 00004 410
14	-0.00000 00000 00002 400
15	0.00000 00000 00000 217
16	-0.00000 00000 00000 010

Table 1

EXAMPLE. From D. S. MITRINOVIĆ's correspondence, I am familiar with RIEMANN's zeta function

$$\zeta(s)=\sum_{n=1}^{+\infty}\frac{1}{n^s} \qquad (\operatorname{Re} s>1)$$

for $s=1.01\,(0.01)\,21.31$ with thirty decimals, calculated by R. E. SHAFER [17]. Using the values $\zeta(s)$ from these tables, the values of the function

$$g(s)=\zeta(s)-\frac{1}{s-1} \qquad (s\neq 1)$$

con easily be calculated. Function $s\mapsto g(s)$ is analytical and has only an apparent singularity for $s=1$ in the finite complex plane. That is why we should adopt:

$$g(1)=\lim_{s\to 1} g(s)=C,$$

where $C=0.5772156649\ldots$ is EULER's constant, [compare **20**, p. 1088].

Forming the differences $\Delta^k g(s)$ $(k=1\,(1)\,13)$, by the application of the quoted program, the tables of coefficients c_n of LAURENT's series of RIEMANN's zeta function

$$\zeta(s)=\sum_{n=-1}^{+\infty} c_n (s-1)^n \tag{8}$$

is obtained.

According to J. P. Gram [**18**, p. 317], the table of coefficients c_n with 9 decimals was calculated by J. L. W. V. Jensen [**19**] and with 16 decimals by J. P. Gram [**20**]. Coefficients c_n may also obtained by means of

$$c_n=\frac{(-1)^n}{n!}\lim_{m\to+\infty}\left(\sum_{k=1}^{m}\frac{(\log k)^n}{k}-\frac{(\log m)^{n+1}}{n+1}\right).$$

[compare **21**, p. 807]. By Table 1 it is possible to calculate the value $\zeta(s)$ with over 15 decimals on the disc $|s-1|\leqq 1$. For $\operatorname{Re} s\leqq 1$ the value of the analytically extended function $\zeta(s)$ is obtained, by means of formula

$$\zeta(s)=-\Gamma(1-s)+\sum_{k=1}^{+\infty}\left(\frac{1}{n^s}-\frac{\Gamma(n+1-s)}{\Gamma(n+1)}\right) \qquad (\operatorname{Re} s>0),$$

[see **22**, p. 56]. The paper by J. P. Gram [**18**] contains the table of the function $\zeta(s)$ for $s=-24\,(0.1)\,24$ with ten decimals. The values of this table for $s=-1.5\,(0.1)\,3.5$ are verified up to the row (8).

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