MATHEMATICS OF COMPUTATION, VOLUME 27, NUMBER 121, JANUARY, 1973

Chebyshev Approximations for the Psi Function*

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Abstract. Rational Chebyshev approximations to the psi (digamma) function are presented for $.5 \leqq x \leqq 3.0$, and $3.0 \leqq x$. Maximum relative errors range down to the order of 10^{-20}.

1. Introduction. The principal mathematical properties of the psi (digamma) function

$$\psi(z) = d[\ln \Gamma(z)]/dz = \Gamma'(z)/\Gamma(z) \tag{1}$$

are summarized by Davis [2] and Luke [3]. For real arguments, the function is traditionally computed using either the classical power series expansion

$$\psi(1 + z) = -\gamma + \sum_{n=2}^{\infty} (-1)^n \zeta(n) z^{n-1}, \qquad |z| < 1, \tag{2}$$

or the asymptotic expansion

$$\psi(z) \sim \ln(z) - \frac{1}{2z} - \sum_{n=1}^{\infty} \frac{B_{2n}}{2nz^{2n}}, \tag{3}$$

with the recurrence relation

$$\psi(z + 1) = \psi(z) + 1/z. \tag{4}$$

The reflection formula

$$\psi(1 - z) = \psi(z) + \pi \cot(\pi z) \tag{5}$$

allows computation for negative arguments. (For complex arguments, see Luke [4].)

Recently, Luke [3] presented an expansion of $\psi(x + 3)$, $0 \leqq x \leqq 1$, in Chebyshev polynomials, 17 coefficients being required to compute the function with an absolute error on the order of 10^{-20}. For computations outside of the primary range, it is still necessary to use one or more of the relations (3), (4) and (5) in addition to Luke's expansion. In this note, we present rational Chebyshev approximations which allow direct computation of $\psi(x)$ for any $x \geqq .5$ with various choices of maximum *relative* error, including some of the order of 10^{-20}. For $x < .5$, either (4) or (5) is still required in conjunction with our approximations.

Received June 12, 1972.

AMS (MOS) subject classifications (1969). Primary 3315, 6520.

Key words and phrases. Psi function, digamma function, rational Chebyshev approximation.

* Work performed under the auspices of the U.S. Atomic Energy Commission.

TABLE I

$$\varepsilon_{jk} = -100 \log_{10} \max \left| \frac{\psi(x) - \psi_{jk}(x)}{\psi(x)} \right|$$

.5 < x < 3.

k \ j	1	2	3	4	5	6	7	8
0	67	107	146	184	222	260	298	335
1	214*	289	359	426	491			
2	332	435*	528	617	702			
3	425	560	674*	781	884			
4	508	668	807	930*	1047			
5	588	768	926	1068	1199*			
6						1480*		
7							1771*	
8								2071*

3. < x

k \ j	1	2	3	4	5	6	7	8
0	513	706	868	1011	1140	1257	1366	1467
1	717*	898	1054	1194	1322			
2	878	1060*	1212	1349	1475			
3	1018	1201	1353*	1488	1613			
4	1145	1328	1481	1617*	1740			
5	1261	1444	1598	1735	1860*			
6						2088*		

*Coefficients for these approximations only are given in Tables II and III.

2. Generation of the Approximations. The approximation forms used are

$$\psi_{jk}(x) = (x - x_0)R_{jk}(x), \qquad .5 \leqq x \leqq 3.0,$$

and

$$\psi_{jk}(x) = \ln(x) - 1/2x + R_{jk}(1/x^2), \qquad 3.0 \leqq x,$$

where x_0 is the positive zero of $\psi(x)$,

$$x_0 = 1.46163\ 21449\ 68362\ 34126\ 26595\ 42325\ 72132\ 5 \cdots,$$

and the R_{jk} are rational functions of degree j in the numerator and k in the denominator. Our value of x_0, determined in 40S arithmetic by applying the secant method to a Taylor series expansion of $\psi(x)$ about $x = 1.5$, agrees with the 33D value given by Wrench [5].

The approximations were generated with standard versions of the Remes algorithm [1] in 25S arithmetic on a CDC 3600 computer, using values computed from variations of the methods described in Section 1. A Taylor series expansion about x_0 was used to compute $\psi(x)/(x - x_0)$ for arguments close to x_0. For other small arguments, the computation was based upon Eq. (2), using the form

$$\psi(1 + z) = -\gamma - \sum_{n=2}^{\infty} (\zeta(n) - 1)(-z)^{n-1} + z/(1 + z), \qquad |z| \leqq \tfrac{1}{2},$$

TABLE II

$$\psi(x) = (x-x_0)\sum_{j=0}^{n} p_j x^j \Big/ \sum_{j=0}^{n} q_j x^j, \qquad .5 \le x \le 3.0$$

n	j	p_j		q_j	
1	0	1.2456	(00)	1.6946	(-01)
	1	2.2307	(-01)	1.0000	(00)
2	0	1.70157 6	(00)	2.68787 0	(-02)
	1	2.36517 9	(00)	2.29160 7	(00)
	2	8.24324 7	(-02)	1.00000 0	(00)
3	0	4.91896 925	(00)	3.93688 191	(-03)
	1	1.09639 225	(01)	7.15251 612	(00)
	2	3.18318 480	(00)	7.12335 364	(00)
	3	3.94931 823	(-02)	1.00000 000	(00)
4	0	2.33423 60610 5	(01)	5.23146 54092 7	(-04)
	1	6.21604 79005 7	(01)	3.41119 27163 6	(01)
	2	3.36117 99693 8	(01)	4.78528 74758 8	(01)
	3	3.81936 31179 6	(00)	1.53695 89516 1	(01)
	4	2.20215 83467 8	(-02)	1.00000 00000 0	(00)
5	0	1.54115 78977 980	(02)	6.30179 76261 473	(-05)
	1	4.54652 99037 301	(02)	2.25259 74317 882	(02)
	2	3.32425 06881 581	(02)	3.80401 14183 590	(02)
	3	7.54568 96431 969	(01)	1.82176 02814 266	(02)
	4	4.33875 92564 704	(00)	2.77171 52851 731	(01)
	5	1.35594 74028 651	(-02)	1.00000 00000 000	(00)
6	0	1.30560 26982 78969 4	(03)	6.91091 68271 45328 9	(-06)
	1	4.13810 16126 90130 0	(03)	1.90831 07659 63000 2	(03)
	2	3.63351 84680 64987 2	(03)	3.64127 34907 93806 0	(03)
	3	1.18645 20071 34252 3	(03)	2.21000 79924 78297 5	(03)
	4	1.42441 58508 40285 0	(02)	5.20752 77146 71618 4	(02)
	5	4.77762 82804 26274 0	(00)	4.48452 57342 98264 0	(01)
	6	8.95385 02298 19699 9	(-03)	1.00000 00000 00000 0	(00)
7	0	1.35249 99667 72634 6383	(04)	6.93891 11753 76344 4376	(-07)
	1	4.52856 01699 54728 9655	(04)	1.97685 74263 04673 6421	(04)
	2	4.51351 68469 73666 2555	(04)	4.12551 60835 35383 2333	(04)
	3	1.85290 11818 58261 0168	(04)	2.93902 87119 93268 1918	(04)
	4	3.32915 25149 40693 5532	(03)	9.08196 66074 85517 0271	(03)
	5	2.40680 32474 35720 1831	(02)	1.24474 77785 67085 6039	(03)
	6	5.15778 92000 13908 4710	(00)	6.74291 29516 37859 3773	(01)
	7	6.22835 06918 98474 5826	(-03)	1.00000 00000 00000 0000	(00)
8	0	1.65856 95029 76102 23207 66	(05)	6.41552 23783 57622 59962 50	(-08)
	1	5.80413 12783 53756 99927 83	(05)	2.42421 85002 01798 52519 81	(05)
	2	6.36069 97788 96445 87965 52	(05)	5.42563 84537 26999 37332 49	(05)
	3	3.06559 76301 98736 56738 04	(05)	4.34878 80712 76832 90368 16	(05)
	4	7.14515 95818 95193 32102 93	(04)	1.62065 66091 53367 16388 42	(05)
	5	7.95254 90849 15199 80654 00	(03)	2.98624 97022 25027 79195 06	(04)
	6	3.76466 93175 92927 68559 71	(02)	2.62877 15790 58119 33301 23	(03)
	7	5.49328 55833 00038 53561 68	(00)	9.61416 54774 22235 85246 14	(01)
	8	4.51046 81245 76293 41596 09	(-03)	1.00000 00000 00000 00000 00	(00)

and upon a Taylor series expansion about 2.5, applying Eq. (4) when necessary. For arguments greater than 15.0, the asymptotic expansion was used.

3. Results. Table I lists the values of

$$\epsilon_{jk} = -100 \log_{10} \max \left| \frac{\psi(x) - \psi_{jk}(x)}{\psi(x)} \right|,$$

TABLE III

$$\psi(x) = \ln(x) - \frac{1}{2x} + \sum_{j=0}^{n} p_j x^{-2j} \bigg/ \sum_{j=0}^{n} q_j x^{-2j}, \qquad 3.0 \leq x$$

n	j	p_j		q_j	
1	0	-2.71580 1589	(-06)	1.06496 6945	(01)
	1	-8.67212 8684	(-01)	1.00000 0000	(00)
2	0	-2.00288 09639 95	(-09)	1.83393 20868 04	(01)
	1	-1.52827 61729 27	(00)	1.86234 52532 39	(01)
	2	-1.39916 28425 82	(00)	1.00000 00000 00	(00)
3	0	-2.10638 77134 36026	(-12)	1.49604 03955 01592	(01)
	1	-1.24670 03283 19607	(00)	4.85175 82510 26104	(01)
	2	-3.91846 20126 40745	(00)	2.56563 23856 68056	(01)
	3	-1.79307 10243 80592	(00)	1.00000 00000 00000	(00)
4	0	-2.72817 57513 15296 783	(-15)	7.77788 54852 29616 042	(00)
	1	-6.48157 12376 61965 099	(-01)	5.46117 73810 32150 702	(01)
	2	-4.48616 54391 80193 579	(00)	8.92920 70048 18613 702	(01)
	3	-7.01677 22776 67586 642	(00)	3.22703 49379 11433 614	(01)
	4	-2.12940 44513 10105 168	(00)	1.00000 00000 00000 000	(00)
5	0	-4.03243 06017 35749 11804	(-18)	2.95381 67608 14838 86052	(00)
	1	-2.46151 39673 45628 90390	(-01)	3.68983 53845 69604 30939	(01)
	2	-3.05024 76808 03867 49109	(00)	1.28621 37781 52642 53627	(02)
	3	-1.04226 83363 88352 86361	(01)	1.40521 63132 63703 12714	(02)
	4	-1.07724 05634 64792 99398	(01)	3.86804 66083 54867 03234	(01)
	5	-2.43139 31584 34655 50347	(00)	1.00000 00000 00000 00000	(00)
6	0	-6.51353 87732 71817 13058 11	(-21)	8.84275 20398 87348 03422 02	(-01)
	1	-7.36896 00332 39454 99107 26	(-02)	1.74639 65060 67856 99061 23	(01)
	2	-1.44796 14616 89984 29858 77	(00)	1.07425 43875 70227 83259 79	(02)
	3	-8.81009 58828 31221 98214 36	(00)	2.47369 79003 31529 00565 08	(02)
	4	-1.97845 54148 71921 86672 38	(01)	2.02409 55312 67993 11593 17	(02)
	5	-1.51662 71776 89612 13830 24	(01)	4.49927 60373 78936 58461 73	(01)
	6	-2.71032 26277 75783 41916 47	(00)	1.00000 00000 00000 00000 00	(00)

where the maximum is taken over the appropriate interval, for the initial segments of the L_∞ Walsh arrays. Tables II and III present coefficients for the approximations along the main diagonals of these arrays.

All coefficients are given to an accuracy greater than that justified by the maximal errors to allow precise determination of the corresponding octal or hexadecimal representations. Each approximation listed, with the coefficients just as they appear here, was tested against the master function routines with 5000 pseudorandom arguments. In all cases, the maximal error agreed in magnitude and location with the values given by the Remes algorithm.

4. Use of the Coefficients. The rational approximations all appear to be well conditioned. With a little care, they can be used to generate function values close to working machine precisions up to 20S.

To maintain machine precision in $\psi(x)$ for x close to x_0, the computation of $(x - x_0)$ must be carried out in higher than machine precision to preserve the low order bits of x_0. This can be achieved by breaking x_0 into two parts, x_1 and x_2, such that $x_0 \equiv x_1 + x_2$ to the precision desired, and such that the floating-point exponent on x_2 is much less than that on x_1. Then $(x - x_0)$ is computed as $(x - x_0) = (x - x_1) - x_2$. This breakup of x_0 is most easily accomplished by examining the octal or hexadecimal representation

$$x_0 = 1.35426\ 60615\ 26574\ 37556\ 06516\ 21031\ 36024\ 47402_8$$
$$= 1.762D8\ 6356B\ E3F6E\ 1A9C8\ 865E0\ A4F02_{16}.$$

One remaining avoidable source of error is in the use of the reflection formula (5) for negative arguments. We suggest that z be broken into $z = z_i + z_f$, where z_i is the integer part of z, and z_f is the fractional part. Then Eq. (5) should be reformulated as

$$\psi(1 - z) = \psi(z) + \pi \cot(\pi z_f).$$

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