Rational Chebyshev Approximations for the Bickley Functions $Ki_n(x)$

By J. M. Blair, C. A. Edwards and J. H. Johnson

Abstract. This report presents near-minimax rational approximations for the Bickley functions $Ki_1(x)$ for $x \geq 0$, $Ki_2(x)$ and $Ki_3(x)$ for $0 \leq x \leq 6$, and $Ki_8(x)$, $Ki_9(x)$ and $Ki_{10}(x)$ for $x \geq 6$, with relative errors ranging down to 10^{-23} . The approximations, combined with the recurrence relation, yield a stable method of computing $Ki_n(x)$, $n = 1, 2, \dots, 10$, for the complete range of the argument.

1. Introduction. The Bessel function integrals defined by

$$(1) \quad Ki_n(x) = \int_x^\infty Ki_{n-1}(t) dt, \quad n = 1, 2, 3, \dots,$$

with $Ki_0(x) = K_0(x)$, were first introduced by Bickley [1] in connection with the solution of heat convection problems. They arise in neutron transport calculations, and are widely used in nuclear reactor computer codes.

Taylor series and asymptotic expansions for $Ki_n(x)$ are developed in [2], [3] and [4], and [4] contains a discussion of the numerical stability of the four-term recurrence relation.

Chebyshev series and rational approximations to the $Ki_n(x)$ have been published in a number of reports. [5] gives 7S rational approximations to Ki_3 and Ki_4 ; [6] gives 5S, 7S and 8S rational approximations to Ki_1 , Ki_2 and Ki_3 , respectively; [7] gives 7S rational approximations to Ki_1 ; [8] gives 6S rational approximations to $Ki_1 - Ki_5$; [9] gives 20D Chebyshev series approximations to Ki_1 ; and [4] gives 12S rational approximations to Ki_1 , Ki_2 and Ki_3 for $0 \leq x \leq 7$, and to Ki_{13} , Ki_{14} and Ki_{15} for $x \geq 7$. A number of the approximations in [5]–[9] suffer from significant digit cancellation.

This report gives rational minimax approximations to $Ki_1(x)$ for $x \geq 0$, to Ki_1 , Ki_2 and Ki_3 for $0 \leq x \leq 6$, and to Ki_8 , Ki_9 and Ki_{10} for $x \geq 6$, with relative errors ranging down to 10^{-23} . The approximations, combined with the recurrence relation, yield a stable method of computing $Ki_n(x)$, $n = 1, 2, \dots, 10$, for the complete range of the argument. The results in [4] may be used to determine the accuracy of the Ki_n when the recurrence relation is extended to higher orders.

2. Functional Properties. Most of the results of this section are given in more general terms in [3].

Alternative definitions of $Ki_n(x)$ are

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$$(2) \quad Ki_n(x) = \int_0^\infty \frac{e^{-x \cosh t}}{\cosh^n t} dt$$

$$(3) \quad = \int_1^\infty \frac{e^{-xu}}{u^n(u^2 - 1)^{1/2}} du$$

$$(4) \quad = \int_0^{\pi/2} e^{-x \sec v} \cos^{n-1} v dv.$$

The derivative of Ki_n is given by

$$Ki'_n(x) = -Ki_{n-1}(x),$$

and higher derivatives may be computed recursively from the formulae

$$(5) \quad \begin{aligned} Ki_n^{(k)}(x) &= -Ki_{n-1}^{(k-1)}(x), \quad k = 1, 2, 3, \dots, n = 0, 1, 2, \dots, \\ Ki_{-1}^{(k)}(x) &= -\frac{k}{x} Ki_{-1}^{(k-1)}(x) - Ki_0^{(k-1)}(x) \\ &\quad - \frac{k-1}{x} Ki_0^{(k-2)}(x), \quad k = 1, 2, 3, \dots \end{aligned}$$

The latter equation is obtained by repeated differentiation of the formula

$$K_1'(x) = -\frac{1}{x} K_1(x) - K_0(x),$$

where K_0 and K_1 are the modified Bessel functions, and $Ki_0 \equiv K_0$, $Ki_{-1} \equiv K_1$.

By integrating (4) by parts we can derive the recurrence relation

$$(6) \quad (n-1)Ki_n(x) = x[Ki_{n-3}(x) - Ki_{n-1}(x)] + (n-2)Ki_{n-2}(x).$$

From (4) and (6) it follows that

$$(7) \quad Ki_n(0) = \begin{cases} \pi/2, & n = 1, \\ 1, & n = 2, \\ \frac{n-2}{n-1} Ki_{n-2}(0), & n \geq 3. \end{cases}$$

Ascending series for the Ki_n can be developed by repeated integration of the ascending series for $K_0(x)$. The resulting formula is

$$(8) \quad \begin{aligned} Ki_n(x) &= P_n(x) + (-1)^n \left[\frac{x^n}{n!} \left(1 + \frac{1}{2} + \dots + \frac{1}{n} - \gamma - \ln \frac{x}{2} \right) \right. \\ &\quad + \sum_{k=1}^{\infty} \frac{2^n (x/2)^{2k+n}}{(k!)^2 \prod_{j=1}^n (2k+j)} \left(1 + \frac{1}{2} + \dots + \frac{1}{k} + \frac{1}{2k+1} \right. \\ &\quad \left. \left. + \dots + \frac{1}{2k+n} - \gamma - \ln \frac{x}{2} \right) \right], \end{aligned}$$

where γ is Euler's constant, and $P_n(x)$ is defined recursively, starting with $P_0(x) = 0$, by

$$P_n(x) = Ki_n(0) - \int_0^x P_{n-1}(t) dt, \quad n = 1, 2, 3, \dots$$

Asymptotic expansions for large arguments can be developed by writing (3) in the form

$$(9) \quad \frac{e^{-x}}{(2x)^{1/2}} \int_0^\infty \frac{e^{-u}}{u^{1/2}} \left(1 + \frac{u}{x}\right)^{-n} \left(1 + \frac{u}{2x}\right)^{-1/2} du$$

and expanding the integrand binomially. The resulting asymptotic formula is

$$(10) \quad Ki_n(x) \sim e^{-x} \left(\frac{\pi}{2x}\right)^{1/2} \sum_{m=0}^{\infty} (-1)^m a_m x^{-m}, \quad x \rightarrow \infty,$$

where

$$(11) \quad a_m = \begin{cases} 1, & m = 0, \\ \frac{1 \cdot 3 \cdot 5 \cdots (2m-1)}{2^m (n-1)!} \sum_{k=0}^m \frac{(2k)!(n+m-k-1)!}{8^k (k!)^2 (m-k)!}, & m = 1, 2, 3, \dots \end{cases}$$

The alternative formula

$$(12) \quad 2(m+1)a_{m+1} = (m + \frac{1}{2})\{(3m + \frac{1}{2} + 2n)a_m - (m - \frac{1}{2})(m - \frac{1}{2} + n)a_{m-1}\}$$

is derived in [4].

The change of variable $u = v^2$ in (9) gives the formula

$$(13) \quad Ki_n(x) = (2/x)^{1/2} e^{-x} \int_0^\infty e^{-v^2} \left(1 + \frac{v^2}{x}\right)^{-n} \left(1 + \frac{v^2}{2x}\right)^{-1/2} dv,$$

which proves to be useful for computations.

3. Stability of Recurrence Relation. If (6) is used for forward recursion, the growth of the absolute error in $Ki_n(x)$ is determined by the factor $x/(n-1)$. Since Ki_n is a slowly decreasing function of n , the relative error is comparable to the absolute error, and forward recursion over a short range is stable provided $x/(n-1)$ is not large.

As a check of this result, $Ki_4, Ki_5, \dots, Ki_{10}$ were computed by forward recursion on Ki_1, Ki_2 and Ki_3 for $x = 0(0.01)6.0$. The greatest loss of accuracy noted was one digit, which occurred near $x = 6$. In general, the accuracy loss was less than one digit.

If (6) is used for backward recursion, the main factor determining the growth of the absolute error is $(n-1)/x$. Since the relative error grows more slowly than the absolute error, backward recursion is stable provided $(n-1)/x$ is not large.

A numerical test consisted of computing $Ki_7, Ki_6, \dots, Ki_1$ by backward recursion on Ki_8, Ki_9 and Ki_{10} , for $x \geq 6$. The greatest loss of accuracy noted was less than one digit, and occurred near $x = 6$. In general, the accuracy loss was very small.

[4] contains a more detailed discussion of the stability of the recurrence relation, and tables of values of the relative error from forward recursion for $n \leq 50$ and $x \leq 600$.

4. Generation of Approximations. Rational minimax approximations to $Ki_n(x)$ were computed in 29 decimal arithmetic on a CDC 6600 using a version of the second algorithm of Remes due to Ralston [10]. The relative error of the approximations was levelled to three digits.

The approximation forms and intervals are

$$\begin{aligned} Ki_n(x) &\simeq R_{lm}(x) + x^n \ln x S_{lm}(x^2), & 0 \leq x \leq 1, n = 1, 2, 3, \\ &\simeq x^{-1/2} e^{-x} R_{lm}(1/x), & x \geq 1, n = 1, \\ &\simeq x^{-1/2} e^{-x} R_{lm}(1/x), & 1 \leq x \leq 6, n = 1, 2, 3, \\ &\simeq x^{-1/2} e^{-x} R_{lm}(1/x), & x \geq 6, n = 8, 9, 10, \end{aligned}$$

where $R_{lm}(x)$ and $S_{lm}(x)$ are rational functions of degree l in the numerator and m in the denominator.

For the range $0 \leq x \leq 1$, R_{lm} is positive for $n = 1, 2, 3$, while S_{lm} is positive for $n = 1, 3$ and negative for $n = 2$, and so a loss of accuracy occurs for $n = 1, 3$ by subtraction. However, the amount of cancellation is small, being less than 1 bit for $n = 1$, and considerably less for $n = 3$.

The master routine for the range $0 \leq x \leq 1$ uses the power series expansions in (8). For sufficiently large values of x , for which terms in the asymptotic series in (10) become less than 10^{-30} in magnitude, the master routine uses the series in (10). For the intermediate range $Ki_n(x)$ is computed by a local Taylor series expansion of the form

$$(14) \quad Ki_n(x_0 + h) = Ki_n(x_0) + \sum_{m=1}^N \frac{h^m}{m!} Ki_n^{(m)}(x_0),$$

where $Ki_n(x_0)$ is the closest of a set of reference values, and where the derivatives $Ki_n^{(m)}(x_0)$ are computed by (5). The table of reference values is constructed by using (10) at an appropriate large value, and then using (14) repeatedly with negative values of h .

As a check of the master routine, the results of (8) and (14) were compared for a range of values of x between 0.6 and 1 and for $n = 0, 1, 2, \dots, 10$. The relative difference was less than 5×10^{-27} in every case. The values of $Ki_0(x)$ were compared to those in [11], and showed agreement to at least 26 digits. An independent check is provided by (13), which was evaluated by a 136-point Gauss-Hermite integration formula. Agreement to 26 digits was obtained for $n = 1, 2, \dots, 10$, and $x > x_n$, where x_n increases slowly with n . Typical values of x_n are $x_1 = 4$ and $x_{10} = 8$. The quadrature formula becomes progressively less accurate as x decreases.

As a result of the tests, we conclude that the master routine is accurate to at least 26 digits.

5. Results. The details of the approximations are given in Tables 1–245, in a format similar to that used in [12]. Tables 1–13 summarize the best approximations in the L_∞ Walsh arrays of the functions, and Tables 14–245 give the coefficients of selected approximations. Tables 14–245 are included in the microfiche section of this issue.

TABLE 1

$$Ki_1(x) \approx P_\ell(x)/Q_m(x) + x \ln x S(x^2)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[0,1]	1.49	1	0	14
	2.43	1	1	15
	3.83	3	0	16
	5.59	1	3	17
	6.55	3	2	18
	7.89	3	3	19
	10.09	1	6	20
	11.06	5	3	21
	12.99	7	2	22
	14.44	7	3	23
	16.43	9	2	24
	17.94	9	3	25
	20.02	9	4	26
	21.59	9	5	27
	23.77	11	4	28

TABLE 2

$$Ki_1(x) \approx R(x) + x \ln x P_\ell(x^2)/Q_m(x^2)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[0,1]	1.38	0	0	29
	3.41	1	0	30
	5.77	1	1	31
	8.44	2	1	32
	11.24	3	1	33
	14.17	4	1	34
	17.25	4	2	35
	20.47	5	2	36
	23.76	6	2	37

TABLE 3

$$Ki_2(x) \approx P_\ell(x)/Q_m(x) + x^2 \ln x S(x^2)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[0,1]	1.04	0	1	38
	2.25	2	0	39
	3.26	2	1	40
	4.83	4	0	41
	6.75	2	3	42
	8.24	2	4	43
	9.56	3	4	44
	11.49	4	4	45
	13.38	2	7	46
	14.41	8	2	47
	15.89	8	3	48
	17.91	10	2	49
	19.45	10	3	50
	21.61	10	4	51
	23.21	10	5	52

TABLE 4

$$Ki_2(x) \approx R(x) + x^2 \ln x P_\ell(x^2)/Q_m(x^2)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[0,1]	1.68	0	0	53
	4.05	0	1	54
	7.35	0	2	55
	9.21	2	1	56
	12.07	3	1	57
	15.13	0	5	58
	18.23	4	2	59
	21.48	5	2	60
	24.76	5	3	61

TABLE 5

$$Ki_3(x) \approx P_\ell(x)/Q_m(x) + x^3 \ln x S(x^2)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[0,1]	1.13	1	0	62
	1.76	1	1	63
	3.40	3	0	64
	4.47	3	1	65
	6.23	3	2	66
	8.55	3	3	67
	9.89	4	3	68
	11.31	4	4	69
	12.69	7	2	70
	14.84	3	7	71
	16.16	4	7	72
	17.63	9	3	73
	19.71	9	4	74
	21.28	9	5	75
	23.46	11	4	76

TABLE 6

$$Ki_3(x) \approx R(x) + x^3 \ln x P_\ell(x^2)/Q_m(x^2)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[0,1]	1.90	0	0	77
	4.64	0	1	78
	7.33	0	2	79
	9.83	2	1	80
	12.97	0	4	81
	15.84	3	2	82
	19.06	4	2	83
	22.35	5	2	84
	24.78	8	0	85

TABLE 7

$$Ki_1(x) \approx x^{-1/2} e^{-x} P_\ell(z)/Q_m(z), \quad z = 1/x$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[0,1] _z	1.84	0	1	86
	2.81	1	1	87
	3.75	1	2	88
	4.65	2	2	89
	5.53	2	3	90
	6.38	3	3	91
	7.22	3	4	92
	8.05	4	4	93
	8.86	4	5	94
	9.66	5	5	95
	10.45	5	6	96
	11.24	6	6	97
	12.01	6	7	98
	12.78	7	7	99
	13.54	7	8	100
	14.29	8	8	101
	15.04	8	9	102
	15.78	9	9	103
	16.51	9	10	104
	17.24	10	10	105
	17.97	10	11	106
	18.69	11	11	107
	19.41	11	12	108
	20.12	12	12	109
	20.83	12	13	110
	21.53	13	13	111
	22.18	13	14	112

TABLE 8

$$Ki_1(x) \approx x^{-1/2} e^{-x} P_\ell(1/x)/Q_m(1/x)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[1,6]	2.13	0	1	113
	3.28	1	1	114
	4.41	1	2	115
	5.52	2	2	116
	6.62	2	3	117
	7.70	3	3	118
	8.78	3	4	119
	9.85	4	4	120
	10.91	4	5	121
	11.96	5	5	122
	13.01	5	6	123
	14.06	6	6	124
	15.10	6	7	125
	16.14	7	7	126
	17.17	7	8	127
	18.21	8	8	128
	19.23	8	9	129
	20.26	9	9	130
	21.29	9	10	131
	22.31	10	10	132
	23.33	10	11	133

TABLE 9

$$Ki_2(x) \approx x^{-1/2} e^{-x} P_\ell(1/x)/Q_m(1/x)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[1, 6]	1.93	0	1	134
	3.04	1	1	135
	4.15	1	2	136
	5.23	2	2	137
	6.31	2	3	138
	7.38	3	3	139
	8.44	3	4	140
	9.50	4	4	141
	10.55	4	5	142
	11.59	5	5	143
	12.63	5	6	144
	13.67	6	6	145
	14.71	6	7	146
	15.74	7	7	147
	16.77	7	8	148
	17.79	8	8	149
	18.82	8	9	150
	19.84	9	9	151
	20.86	9	10	152
	21.88	10	10	153
	22.90	10	11	154

TABLE 10

$$Ki_3(x) \approx x^{-1/2} e^{-x} P_\ell(1/x)/Q_m(1/x)$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
[1, 6]	1.81	0	1	155
	2.91	1	1	156
	3.99	1	2	157
	5.07	2	2	158
	6.13	2	3	159
	7.19	3	3	160
	8.24	3	4	161
	9.29	4	4	162
	10.33	4	5	163
	11.37	5	5	164
	12.40	5	6	165
	13.43	6	6	166
	14.46	6	7	167
	15.49	7	7	168
	16.51	7	8	169
	17.53	8	8	170
	18.55	8	9	171
	19.57	9	9	172
	20.59	9	10	173
	21.60	10	10	174
	22.62	10	11	175
	23.63	11	11	176

TABLE 11

$$Ki_8(x) \approx x^{-1/2} e^{-x} P_8(z)/Q_8(z), \quad z = 1/x$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
$[0, 1/6]_z$	1.90	0	1	177
	3.04	1	1	178
	4.12	1	2	179
	5.20	2	2	180
	6.26	2	3	181
	7.29	3	3	182
	8.32	3	4	183
	9.33	4	4	184
	10.33	4	5	185
	11.31	5	5	186
	12.29	5	6	187
	13.26	6	6	188
	14.22	6	7	189
	15.17	7	7	190
	16.12	7	8	191
	17.05	8	8	192
	17.98	8	9	193
	18.91	9	9	194
	19.83	9	10	195
	20.74	10	10	196
	21.65	10	11	197
	22.55	11	11	198
	23.45	11	12	199

TABLE 12

$$Ki_9(x) \approx x^{-1/2} e^{-x} P_9(z)/Q_9(z), \quad z = 1/x$$

RANGE	PRECISION	ℓ	m	TABLE OF COEFFICIENTS
$[0, 1/6]_z$	1.84	0	1	200
	2.96	1	1	201
	4.04	1	2	202
	5.09	2	2	203
	6.14	2	3	204
	7.16	3	3	205
	8.17	3	4	206
	9.17	4	4	207
	10.16	4	5	208
	11.14	5	5	209
	12.11	5	6	210
	13.07	6	6	211
	14.02	6	7	212
	14.96	7	7	213
	15.90	7	8	214
	16.83	8	8	215
	17.75	8	9	216
	18.67	9	9	217
	19.59	9	10	218
	20.49	10	10	219
	21.39	10	11	220
	22.29	11	11	221
	23.18	11	12	222

TABLE 13

$$Ki_{10}(x) \approx x^{-1/2} e^{-x} P_\ell(z)/Q_m(z), \quad z = 1/x$$

RANGE	PRECISION	TABLE OF COEFFICIENTS		
		ℓ	m	
$[0, 1/6]_z$	1.79	0	1	223
	2.90	1	1	224
	3.96	1	2	225
	5.00	2	2	226
	6.03	2	3	227
	7.04	3	3	228
	8.04	3	4	229
	9.03	4	4	230
	10.01	4	5	231
	10.98	5	5	232
	11.94	5	6	233
	12.89	6	6	234
	13.84	6	7	235
	14.77	7	7	236
	15.70	7	8	237
	16.63	8	8	238
	17.55	8	9	239
	18.46	9	9	240
	19.36	9	10	241
	20.26	10	10	242
	21.16	10	11	243
	22.05	11	11	244
	22.94	11	12	245

The precision is defined as

$$-\log_{10} \max_x \left| \frac{f(x) - R_{lm}(x)}{f(x)} \right|,$$

where $f(x)$ is the function being approximated and the maximum is taken over the appropriate interval.

For the range $0 \leq x \leq 1$ the first auxiliary function $R_{lm}(x)$ is ill-conditioned, and loses up to two significant digits by cancellation. To eliminate the cancellation the numerator and denominator were converted to minimal Newton form [13], and the resulting coefficients rounded off by an algorithm similar to that described in [12].

For the range $0 \leq x \leq 1$ the first auxiliary function $R_{1,2}$ for $Ki_2(x)$ is almost degenerate, and the rational function could only be found by Cody's method of artificial poles [14].

The approximations in Tables 14–245 were verified by comparing them with the master routine for 5000 pseudorandom values of the argument in each interval.

6. Use of Coefficients. The coefficients may be used to construct a subroutine to compute $Ki_n(x)$ for $n = 1, 2, \dots, 10$, and for all values of x . For $x \leq 6$, approximations to Ki_1 , Ki_2 and Ki_3 , obtained from Tables 14–85 and 113–176, may be extended to Ki_4 , Ki_5 , $\dots$, Ki_{10} by forward recursion in (6) with the loss of at most one digit of accuracy. For $x \geq 6$, Tables 177–245 give Ki_8 , Ki_9 and Ki_{10} , and these may be extended to Ki_7 , Ki_6 , $\dots$, Ki_1 by backward recursion in (6) with less than one digit loss of accuracy.

Full range approximations to $Ki_1(x)$ are given in Tables 14–37 and 86–112, since it is the most commonly occurring function.

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Atomic Energy of Canada Limited
Chalk River Nuclear Laboratories
Mathematics and Computation Branch
Chalk River, Ontario K0J 1J0, Canada

Atomic Energy of Canada Limited
Chalk River Nuclear Laboratories
Mathematics and Computation Branch
Chalk River, Ontario K0J 1J0, Canada

Statistics Canada
Business Survey Methods Division
Coats Building
Tunney's Pasture
Ottawa, Ontario K1A 0T6, Canada

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