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 $x > 0$, $Ki_2(x)$ and $Ki_3(x)$ for $0 < x < 6$, and $Ki_8(x)$, $Ki_9(x)$ and $Ki_{10}(x)$ for $x > 6$, with relative errors ranging down to $10^{-23}$. The approximations, combined with the recurrence relation, yield a stable method of computing $Ki_n(x)$, $n = 1, 2, \ldots, 10$, for the complete range of the argument.

1. Introduction. The Bessel function integrals defined by

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

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 $0 < x < 7$, and to $Ki_{13}$, $Ki_{14}$ and $Ki_{15}$ for $x > 7$. A number of the approximations in [5]–[9] suffer from significant digit cancellation.

This report gives rational minimax approximations to $Ki_n(x)$ for $x > 0$, to $Ki_1$, $Ki_2$ and $Ki_3$ for $0 < x < 6$, and to $Ki_8$, $Ki_9$ and $Ki_{10}$ for $x > 6$, with relative errors ranging down to $10^{-23}$. The approximations, combined with the recurrence relation, yield a stable method of computing $Ki_n(x)$, $n = 1, 2, \ldots, 10$, 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
CHEBYSHEV APPROXIMATIONS FOR THE BICKLEY FUNCTIONS

\[ K_{i_n}(x) = \int_0^\infty \frac{e^{-x \cosh t}}{\cosh^n t} \, dt \]

(2)

\[ = \int_1^\infty \frac{e^{-x u}}{u^n(u^2 - 1)^{1/2}} \, du \]

(3)

\[ = \int_0^{\pi/2} e^{-x \sec \nu} \cos^{n-1} \nu \, d\nu \]

(4)

The derivative of \( K_{i_n} \) is given by

\[ K_{i_n}'(x) = -K_{i_{n-1}}(x), \]

and higher derivatives may be computed recursively from the formulae

\[ K_{i_n}^{(k)}(x) = -K_{i_{n-1}}^{(k-1)}(x), \quad k = 1, 2, 3, \ldots, n = 0, 1, 2, \ldots, \]

(5)

\[ K_{i_n}^{(k)}(x) = \frac{k}{x} K_{i_n-1}^{(k-1)}(x) - K_{i_n}^{(k-1)}(x) + \frac{k-1}{x} K_{i_n-2}^{(k-1)}(x), \quad k = 1, 2, 3, \ldots. \]

The latter equation is obtained by repeated differentiation of the formula

\[ K_{i_n}'(x) = -\frac{1}{x} K_{i_n}(x) - K_{i_0}(x), \]

where \( K_0 \) and \( K_1 \) are the modified Bessel functions, and \( K_{i_0} \equiv K_0, K_{i_{-1}} \equiv K_1 \).

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

\[ (n - 1)K_{i_n}(x) = x [K_{i_{n-3}}(x) - K_{i_{n-1}}(x)] + (n - 2)K_{i_{n-2}}(x). \]

(6)

From (4) and (6) it follows that

\[ K_{i_n}(0) = \begin{cases} \pi/2, & n = 1, \\ 1, & n = 2, \\ \frac{n-2}{n-1} K_{i_{n-2}}(0), & n \geq 3. \end{cases} \]

(7)

Ascending series for the \( K_{i_n} \) can be developed by repeated integration of the ascending series for \( K_0(x) \). The resulting formula is

\[ K_{i_n}(x) = P_n(x) + (-1)^n \left[ \frac{x^n}{n!} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{n} - \gamma - \ln \frac{x}{2} \right) \right. \]

\[ + \sum_{k=1}^{\infty} \frac{2^n(x/2)^{2k+n}}{(k!)^2 \prod_{j=1}^{n} (2k+j)} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{k} + \frac{1}{2k+1} \right. \]

\[ \left. \left. \cdots + \frac{1}{2k+n} - \gamma - \ln \frac{x}{2} \right) \right], \]

(8)

where \( \gamma \) is Euler's constant, and \( P_n(x) \) is defined recursively, starting with \( P_0(x) = 0 \), by
Asymptotic expansions for large arguments can be developed by writing (3) in the form

\[ P_n(x) = K_i n(0) - \int_0^x P_{n-1}(t) \, dt, \quad n = 1, 2, 3, \ldots. \]

and expanding the integrand binomially. The resulting asymptotic formula is

\[ K_i n(x) \sim e^{-x} \left( \frac{\pi}{2x} \right)^{\frac{1}{2}} \sum_{m=0}^{\infty} (-1)^m a_m x^{-m}, \quad x \to \infty, \]

where

\[ a_m = \begin{cases} 1, & m = 0, \\ \frac{1 \cdot 3 \cdot 5 \cdots (2m - 1)}{2^m (n - 1)!} \sum_{k=0}^{m} \frac{(2k)! (n + m - k - 1)!}{8^k (k!)^2 (m - k)!}, & m = 1, 2, 3, \ldots. \end{cases} \]

The alternative formula

\[ 2(n + 1) a_{m+1} = (m + \frac{1}{2}) [(3m + \frac{1}{2} + 2n)a_m - (m - \frac{1}{2})(m - \frac{1}{2} + n)a_m - 1] \]

is derived in [4].

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

\[ K_i n(x) = (2/x)^{\frac{1}{2}} e^{-x} \int_0^\infty e^{-u^2} \left( 1 + \frac{v^2}{x} \right)^{-n} \left( 1 + \frac{u^2}{2x} \right)^{-\frac{1}{2}} \, du, \]

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 \( K_i n(x) \) is determined by the factor \( x/n - 1 \). Since \( K_i n \) 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, \( K_i 4, K_i 5, \ldots, K_i 10 \) were computed by forward recursion on \( K_i 1, K_i 2 \) and \( K_i 3 \) 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 \( K_i 7, K_i 6, \ldots, K_i 1 \) by backward recursion on \( K_i 8, K_i 9 \) and \( K_i 10 \), 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 $K_i(x)$ 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

\[
K_i(x) \approx R_{lm}(x) + x^n \ln x S_{lm}(x^2), \quad 0 \leq x \leq 1, \quad n = 1, 2, 3,
\]
\[
\approx x^{-\frac{1}{2} e^{-x} R_{lm}(1/x),} \quad x \geq 1, \quad n = 1,
\]
\[
\approx x^{-\frac{1}{2} e^{-x} R_{lm}(1/x),} \quad 1 \leq x \leq 6, \quad n = 1, 2, 3,
\]
\[
\approx x^{-\frac{1}{2} e^{-x} R_{lm}(1/x),} \quad x \geq 6, \quad n = 8, 9, 10,
\]

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 $K_i(x)$ is computed by a local Taylor series expansion of the form

\[
K_i(x_0 + h) = K_i(x_0) + \sum_{m=1}^{N} \frac{h^m}{m!} K_i^{(m)}(x_0),
\]

where $K_i(x_0)$ is the closest of a set of reference values, and where the derivatives $K_i^{(m)}(x_0)$ 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 $n = 0, 1, 2, \ldots, 10$. The relative difference was less than $5 \times 10^{-27}$ in every case. The values of $K_i(0)$ 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 $n = 1, 2, \ldots, 10$, 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 $L_\infty$ 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

\[ K_i^1(x) \approx \frac{P_n(x)}{Q_m(x)} + x \ln x S(x^2) \]

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Table 2

\[ K_i^2(x) \approx R(x) + x \ln x \frac{P_n(x)}{Q_m(x^2)} \]

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Table 3

\[ K_i^3(x) \approx P_n(x) + x^2 \ln x S(x^2) \]

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Table 4

\[ K_i^2(x) \approx R(x) + x^2 \ln x \times P_\ell(x^2)/Q_m(x^2) \]

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Table 5

\[ K_i^3(x) \approx P_\ell(x)/Q_m(x) + x^3 \ln x \times S(x^2) \]

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Table 6

\[ K_i^3(x) \approx R(x) + x^3 \ln x \times P_\ell(x^2)/Q_m(x^2) \]

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Table 7

\[ K_{i_1}(x) \approx x^{-h} e^{-x} P_{\ell}(z)/Q_{m}(z), \; z = 1/x \]

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CHEBYSHEV APPROXIMATIONS FOR THE BICKLEY FUNCTIONS

Table 9

\[ K_{i_2}(x) \approx x^{-\frac{i}{2}} e^{-x} \frac{P_i(1/x)}{Q_m(1/x)} \]

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Table 10

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\[ K_{1g}(x) \approx x^{-1} e^{-x} p_{1}(z)/Q_{m}(z), \quad z = 1/x \]

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Table 12

\[ K_{1g}(x) \approx x^{-1} e^{-x} p_{1}(z)/Q_{m}(z), \quad z = 1/x \]

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Table 13

Ki₁₀(x) \approx x^{-\frac{1}{6}} e^{-x} Pₗ(z)/Qₓ(z), \quad z = 1/x

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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 < x < 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 < x < 1 the first auxiliary function R_{1,2} for Ki₂(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 Kiᵣ(x) for n = 1, 2, ..., 10, and for all values of x. For x ≤ 6, approximations to Ki₁, Ki₂ and Ki₃, obtained from Tables 14–85 and 113–176, may be extended to Ki₄, Ki₅, ..., Ki₉₀ by forward recursion in (6) with the loss of at most one digit of accuracy. For x ≥ 6, Tables 177–245 give Ki₈, Ki₉ and Ki₁₀, and these may be extended to Ki₇, Ki₆, ..., Ki₁ by backward recursion in (6) with less than one digit loss of accuracy.
Full range approximations to $K_i(x)$ are given in Tables 14–37 and 86–112, since it is the most commonly occurring function.

7. Acknowledgement. We wish to thank the referee for a suggestion which reduced the size of the tables.

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11. B. S. BERGER & H. McALLISTER, "A table of the modified Bessel functions $K_n(x)$ and $I_n(x)$ to at least 60S for $n = 0, 1$ and $x = 1, 2, \ldots, 40$," Math. Comp., v. 24, 1970, p. 488, RMT 34.