MATHEMATICS OF COMPUTATION
Volume 00, Number 0, Pages 000–000
S 0025-5718(XX)0000-0

A BOUND FOR THE ERROR TERM IN THE BRENT-MCMILLAN ALGORITHM

RICHARD P. BRENT AND FREDRIK JOHANSSON

Abstract. The Brent-McMillan algorithm B3 (1980), when implemented with binary splitting, is the fastest known algorithm for high-precision computation of Euler's constant. However, no rigorous error bound for the algorithm has ever been published. We provide such a bound and justify the empirical observations of Brent and McMillan. We also give bounds on the error in the asymptotic expansions of functions related to the Bessel functions $I_0(x)$ and $K_0(x)$ for positive real x.

1. Introduction

Brent and McMillan [3, 5] observed that Euler's constant

$$\gamma = \lim_{n\to\infty} (H_n - \ln(n)) \approx 0.5772156649, \quad H_n = \sum_{k=1}^{n} \frac{1}{k},$$

can be computed rapidly to high accuracy using the formula

$$\gamma = \frac{S_0(2n) - K_0(2n)}{I_0(2n)} - \ln(n), \tag{1.1}$$

where $n > 0$ is a free parameter (understood to be an integer), $K_0(x)$ and $I_0(x)$ denote the usual Bessel functions, and

$$S_0(x) = \sum_{k=0}^{\infty} \frac{H_k}{(k!)^2} \left(\frac{x}{2}\right)^{2k}.$$

The idea is to choose n optimally so that an asymptotic series can be used to compute $K_0(2n)$, while $S_0(2n)$ and $I_0(2n)$ are computed using Taylor series.

When all series are evaluated using the *binary splitting* technique (see [4, §4.9]), the first d digits of γ can be computed in essentially optimal time $O(d^{1+\varepsilon})$. This approach has been used for all recent record calculations of γ, including the current world record of 29,844,489,545 digits set by A. Yee and R. Chan in 2009 [9].

2010 *Mathematics Subject Classification.* 33C10, 11Y60 (Primary) 65G99, 65Y20, 68Q25, 68W40 (Secondary).

The first author was supported by Australian Research Council grant DP140101417.
The second author was supported by the Austrian Science Fund (FWF) grant Y464-N18.

Brent and McMillan gave three algorithms (B1, B2 and B3) to compute γ via (1.1). The most efficient, B3, approximates $K_0(2n)$ using the asymptotic expansion

$$2xI_0(x)K_0(x) = \sum_{k=0}^{m/2-1} \frac{b_k}{x^{2k}} + T_m(x)\,, \quad b_k = \frac{[(2k)!]^3}{(k!)^4 8^{2k}}\,, \tag{1.2}$$

where one should take $m \approx 4n$. The expansion (1.2) appears as formula 9.7.5 in Abramowitz and Stegun [1], and 10.40.6 in the Digital Library of Mathematical Functions [7]. Unfortunately, neither work gives a proof or reference, and no bound for the error term $T_m(x)$ is provided. Brent and McMillan observed empirically that $T_{4n}(2n) = O(e^{-4n})$, which would give a final error of $O(e^{-8n})$ for γ, but left this as a conjecture.

Brent [2] recently noted that the error term can be bounded rigorously, starting from the individual asymptotic expansions of $I_0(x)$ and $K_0(x)$. However, he did not present an explicit bound at that time. In this paper, we calculate an explicit error bound, allowing the fastest version of the Brent-McMillan algorithm (B3) to be used for provably correct evaluation of γ.

To bound the error in the Brent-McMillan algorithm we must bound the errors in evaluating the transcendental functions $I_0(2n)$, $K_0(2n)$ and $S_0(2n)$ occurring in (1.1) (we ignore the error in evaluating $\ln(n)$ since this is well-understood).

The most difficult task is to bound the error associated with $K_0(2n)$. For reasons of efficiency, the algorithm approximates $I_0(2n)K_0(2n)$ using the asymptotic expansion (1.2), and then the term $K_0(2n)/I_0(2n)$ in (1.1) is computed from $I_0(2n)K_0(2n)/I_0(2n)^2$.

Sections 2–3 contain bounds on the size of various error terms that are needed for the main result. For example, Lemma 2.1 bounds the error in the asymptotic expansion for $I_0(x)$, which is nontrivial as the terms do not have alternating signs.

The asymptotic expansion (1.2) can be obtained formally by multiplying the asymptotic expansions (see (2.1)–(2.2) below) for K_0 and I_0. To obtain m terms in the asymptotic expansion, we multiply the polynomials $P_m(-1/z)$ and $P_m(1/z)$ occurring in (2.1)–(2.2), then discard half the terms (here $z = 1/x$ is small when $x \approx 2n$ is large, so we discard the terms involving high powers of z). To bound the error, we show in Lemma 3.1 that the discarded terms are sufficiently small, and also take into account the error terms R_m and Q_m in the asymptotic expansions for K_0 and I_0.

The main result, Theorem 4.1, is given in Section 4. Provided the parameter N (the number of terms used to approximate $S_0(2n)$ and $I_0(2n)$) is sufficiently large, the error is bounded by $24e^{-8n}$. Corollary 4.3 shows that it is sufficient to take $N \approx 4.971n$.

2. Bounds for the individual Bessel functions

Asymptotic expansions for $I_0(x)$ and $K_0(x)$ are given by Olver [8, pp. 266–269] and can be found in [7, §10.40]. They can be written as

$$K_0(x) = e^{-x}\left(\frac{\pi}{2x}\right)^{1/2}(P_m(-x) + R_m(x)) \tag{2.1}$$

and

$$I_0(x) = \frac{e^x}{(2\pi x)^{1/2}} \left(P_m(x) + Q_m(x)\right), \tag{2.2}$$

where $R_m(x)$ and $Q_m(x)$ denote error terms,

$$P_m(x) = \sum_{k=0}^{m-1} a_k x^{-k}, \quad \text{and} \quad a_k = \frac{[(2k)!]^2}{(k!)^3 32^k} \cdot \tag{2.3}$$

For $n \geq 1$,

$$\sqrt{2\pi} n^{n+1/2} e^{-n} \leq n! \leq e n^{n+1/2} e^{-n}, \tag{2.4}$$

so the coefficients a_k in (2.3) satisfy

$$a_k \leq \frac{e^2}{\pi^{3/2} 2^{1/2}} \frac{1}{k^{1/2}} \left(\frac{k}{2e}\right)^k < \frac{1}{k^{1/2}} \left(\frac{k}{2e}\right)^k \tag{2.5}$$

for $k \geq 1$ (the first term is $a_0 = 1$).

For $x > 0$, we also have the global bounds

$$0 < K_0(x) < e^{-x} \left(\frac{\pi}{2x}\right)^{1/2} \tag{2.6}$$

and

$$I_0(x) > \frac{e^x}{(2\pi x)^{1/2}} \cdot \tag{2.7}$$

Observe that the bound on $K_0(x)$ and equation (2.1) imply that

$$|P_m(-x) + R_m(x)| < 1. \tag{2.8}$$

For $x > 0$, the series (2.1) for $K_0(x)$ is alternating, and the remainder satisfies

$$|R_m(x)| \leq \frac{a_m}{x^m} < \frac{1}{m^{1/2}} \left(\frac{m}{2e}\right)^m \frac{1}{x^m} \cdot \tag{2.9}$$

The series (2.2) for $I_0(x)$ is not alternating. The following lemma bounds the error $Q_m(x)$.

Lemma 2.1. *Let $Q_m(x)$ be defined by (2.2). Then for $m \geq 1$ and real $x \geq 2$ we have*

$$|Q_m(x)| \leq 4 \left(\frac{m}{2ex}\right)^m + e^{-2x}.$$

Proof. The identity $I_0(x) = i(K_0(xe^{\pi i}) - K_0(x))/\pi$ (see [7, 10.34.5]) gives

$$Q_m(x) = R_m(xe^{\pi i}) - \frac{i}{\pi} \frac{(2\pi x)^{1/2}}{e^x} K_0(x).$$

According to Olver [8, p. 269],

$$|R_m(xe^{\pi i})| \leq 2\chi(m) \exp(\tfrac{1}{8}\pi x^{-1}) a_m x^{-m},$$

where

$$\chi(m) = \pi^{1/2} \frac{\Gamma(m/2+1)}{\Gamma(m/2+1/2)} \leq \frac{\pi}{2} m^{1/2}$$

(the bound on $\chi(m)$ follows as $\chi(m)/m^{1/2}$ is monotonic decreasing for $m \geq 1$).

Since $x \geq 2$, applying (2.5) gives

$$|R_m(xe^{\pi i})| \leq \pi e^{\pi/16} \left(\frac{m}{2e}\right)^m \frac{1}{x^m} < 4 \left(\frac{m}{2ex}\right)^m.$$

Combined with the global bound (2.6) for $K_0(x)$, we obtain

$$|Q_m(x)| \le |R_m(xe^{\pi i})| + \frac{1}{\pi}\frac{(2\pi x)^{1/2}}{e^x}K_0(x) \le 4\left(\frac{m}{2ex}\right)^m + e^{-2x}. \tag{2.10}$$

□

Corollary 2.2. *For $x \ge 2$, we have $0 < I_0(x)K_0(x) < 1/x$.*

Proof. The first inequality is obvious, since both $I_0(x)$ and $K_0(x)$ are positive. Also, using (2.2) and (2.10) with $m = 1$ gives

$$I_0(x) \le \frac{e^x}{(2\pi x)^{1/2}}(1 + e^{-1} + e^{-4}),$$

so from (2.6) we have

$$I_0(x)K_0(x) \le \frac{1 + e^{-1} + e^{-4}}{2x} < \frac{1}{x}\,.$$

□

Lemma 2.3. *If $R_m(x)$ and $Q_m(x)$ are defined by* (2.1) *and* (2.2) *respectively, then*

$$|R_{4n}(2n)| \le \frac{e^{-4n}}{2n^{1/2}} \quad \text{and} \quad |Q_{4n}(2n)| \le 5e^{-4n}. \tag{2.11}$$

Proof. Taking $x = 2n$ and $m = 4n$, the inequality (2.9) gives the first inequality, and Lemma 2.1 gives the second inequality. □

We also need the following lemma.

Lemma 2.4. *If $P_m(x)$ is defined by* (2.3)*, then*

$$|P_{4n}(2n)| < 2 \quad \text{and} \quad |P_{4n}(-2n)| < 1. \tag{2.12}$$

Proof. Using (2.3) and (2.5), we have

$$\begin{aligned} P_{4n}(2n) &= 1 + \sum_{k=1}^{4n-1} \frac{a_k}{(2n)^k} \\ &\le 1 + \sum_{k=1}^{4n-1} k^{-1/2}\left(\frac{k}{4en}\right)^k \\ &\le 1 + \sum_{k=1}^{4n-1} e^{-k} < \frac{e}{e-1} < 2. \end{aligned}$$

The right inequality in (2.12) can be proved in a similar manner, taking the sign alternations into account. □

3. Bounds for the product

We wish to bound the error term $T_m(x)$ in (1.2) when evaluated at $x = 2n$, $m = 4n$. The result is given by the following lemma.

Lemma 3.1. *If $T_m(x)$ is defined by* (1.2)*, then $T_{4n}(2n) < 7e^{-4n}$.*

Proof. In terms of the expansions for $I_0(x)$ and $K_0(x)$, we have

$$\begin{aligned} 2xI_0(x)K_0(x) &= (P_m(-x)+R_m(x))(P_m(x)+Q_m(x)) \\ &= P_m(x)P_m(-x) + \left[(P_m(-x)+R_m(x))Q_m(x) + P_m(x)R_m(x)\right]. \end{aligned} \tag{3.1}$$

It follows from (2.8), (2.11) and (2.12) that the expression $[\cdots]$ in (3.1), evaluated at $x = 2n$, $m = 4n$, is bounded in absolute value by

$$5e^{-4n} + e^{-4n}/n^{1/2} \le 6e^{-4n}. \tag{3.2}$$

Next, we rewrite

$$P_m(x)P_m(-x) = \sum_{i=0}^{m-1}\sum_{j=0}^{m-1} (-1)^i a_i a_j x^{-(i+j)}$$

as $L + U$, where

$$L = \sum_{k=0}^{m-1}\left(\sum_{j=0}^{k}(-1)^j a_j a_{k-j}\right) x^{-k} \tag{3.3}$$

and

$$U = \sum_{k=m}^{2m-2}\left(\sum_{j=k-(m-1)}^{m-1}(-1)^j a_j a_{k-j}\right) x^{-k}. \tag{3.4}$$

The "lower" sum L is precisely $\sum_{k=0}^{m/2-1} b_k x^{-2k}$. Replacing k by $2k$ in (3.3) (as the odd terms vanish by symmetry), we have to prove

$$\sum_{j=0}^{2k} \frac{(-1)^j[(2j)!]^2[(4k-2j)!]^2}{(j!)^3[(2k-j)!]^3 32^{2k}} = \frac{[(2k)!]^3}{(k!)^4 8^{2k}}. \tag{3.5}$$

This can be done algorithmically using the creative telescoping approach of Wilf and Zeilberger. For example, the implementation in the Mathematica package `HolonomicFunctions` by Koutschan [6] can be used. The command

```
a = ((2j)!)^2 / ((j!)^3 32^j);
CreativeTelescoping[(-1)^j a (a /. j -> 2k-j),
    {S[j]-1}, S[k]]
```

outputs the recurrence equation

$$(8+8k)b_{k+1} - \left(1+6k+12k^2+8k^3\right) b_k = 0$$

matching the right-hand side of (3.5), together with a telescoping certificate. Since the summand in (3.5) vanishes for $j < 0$ and $j > 2k$, no boundary conditions enter into the telescoping relation, and checking the initial value ($k = 0$) suffices to prove the identity.[1]

It remains to bound the "upper" sum U given by (3.4). The coefficients of $U = \sum_{k=m}^{2m-2} c_k x^{-k}$ can be written as

$$c_k = \sum_{j=1}^{2m-k-1} (-1)^{j+k+m} a_{k-m+j} a_{m-j}.$$

[1]Curiously, the built-in `Sum` function in Mathematica 9.0.1 computes a closed form for the sum (3.5), but returns an answer that is wrong by a factor 2 if the factor $[(4k-2j)!]^2$ in the summand is input as $[(2(2k-j))!]^2$.

By symmetry, this sum is zero when k is odd, so we only need to consider the case of k even. We first note that, if $1 \le i < j$, then $a_i a_j \ge a_{i+1} a_{j-1}$. This can be seen by observing that the ratio satisfies

$$\frac{a_i a_j}{a_{i+1} a_{j-1}} = \frac{(i+1)(2j-1)^2}{j(2i+1)^2} \ge 1.$$

Thus, after adding the duplicated terms, c_k can be written as an alternating sum in which the terms decrease in magnitude, e.g. for $m = 10$ we have

$$\begin{aligned}
c_{10} &= -2a_1a_9 + 2a_2a_8 - 2a_3a_7 + 2a_4a_6 - a_5a_5,\\
c_{12} &= -2a_3a_9 + 2a_4a_8 - 2a_5a_7 + a_6a_6,\\
c_{14} &= -2a_5a_9 + 2a_6a_8 - a_7a_7,\\
c_{16} &= -2a_7a_9 + a_8a_8,\\
c_{18} &= -a_9a_9.
\end{aligned}$$

Hence $|c_k|$ is bounded by $2a_{1+k-m}a_{m-1}$, giving

$$\left|\sum_{k=m}^{2m-2} \frac{c_k}{x^k}\right| \le \sum_{k=m}^{2m-2} t_k, \quad t_k = \frac{2a_{1+k-m}a_{m-1}}{x^k}\,.$$

Evaluating at $x = 2n, m = 4n$ as usual, the term ratio

$$\frac{t_{k+1}}{t_k} = \frac{(3+2k-8n)^2}{16n(2+k-4n)}$$

is bounded by 1 when $4n \le k \le 8n-2$. Therefore, using (2.5),

$$\sum_{k=m}^{2m-2} t_k \le (m-1)t_m \le e^{-4n}\frac{(4n-1)^{4n-1/2}}{2^{8n-1}n^{4n}} < e^{-4n}. \tag{3.6}$$

Adding (3.2) and (3.6), we find that $|T_{4n}(2n)| < 7e^{-4n}$. □

4. A complete error bound

We are now equipped to justify Algorithm B3. The algorithm computes an approximation $\widetilde{\gamma}$ to γ. Theorem 4.1 bounds the error $|\widetilde{\gamma} - \gamma|$ in the algorithm, excluding rounding errors and any error in the evaluation of $\ln n$. The finite sums S and I approximate $S_0(2n)$ and $I_0(2n)$ respectively, while T approximates $I_0(2n)K_0(2n)$.

Theorem 4.1. *Given an integer $n \ge 1$, let $N \ge 4n$ be an integer such that*

$$\frac{2n^{2N}H_N}{(N!)^2} < \varepsilon_0, \tag{4.1}$$

where

$$\varepsilon_0 = \frac{e^{-6n}}{(4\pi n)^{1/2}(1+H_N)}\,. \tag{4.2}$$

Let

$$S = \sum_{k=0}^{N-1} \frac{H_k n^{2k}}{(k!)^2}\,, \quad I = \sum_{k=0}^{N-1} \frac{n^{2k}}{(k!)^2}\,, \quad T = \frac{1}{4n}\sum_{k=0}^{2n-1} \frac{[(2k)!]^3}{(k!)^4 8^{2k}(2n)^{2k}}\,,$$

and

$$\widetilde{\gamma} = \frac{S}{I} - \frac{T}{I^2} - \ln n\,.$$

Then

$$|\widetilde{\gamma} - \gamma| < 24e^{-8n}. \tag{4.3}$$

Proof. Let

$$\varepsilon_1 = S_0(2n) - S = \sum_{k=N}^{\infty} \frac{H_k n^{2k}}{(k!)^2}\,,$$
$$\varepsilon_2 = I_0(2n) - I = \sum_{k=N}^{\infty} \frac{n^{2k}}{(k!)^2}\,\cdot$$

Inspection of the term ratios for $k \ge N$ shows that ε_1 and ε_2 are bounded by the left side of (4.1). Using (2.7) to bound $1/I_0(2n)$, it follows that

$$\begin{aligned}
\left|\frac{S+\varepsilon_1}{I+\varepsilon_2} - \frac{S}{I}\right| &= \left|\frac{\varepsilon_1 I - \varepsilon_2 S}{(I+\varepsilon_2)I}\right| \\
&\le \frac{\varepsilon_0(I+S)}{(I+\varepsilon_2)I} \\
&= \varepsilon_0\left(\frac{1}{I_0(2n)}\right)\left(1+\frac{S}{I}\right) \\
&< \frac{e^{-6n}}{(4\pi n)^{1/2}(1+H_N)}\left(\frac{(4\pi n)^{1/2}}{e^{2n}}\right)(1+H_N) \\
&= e^{-8n}.
\end{aligned}$$

We have $T+\varepsilon_3 = I_0(2n)K_0(2n)$ where, from Lemma 3.1, $|\varepsilon_3| < 7e^{-4n}/(4n)$. Thus, from Corollary 2.2,

$$T \le \frac{1}{2n} + \frac{7e^{-4n}}{4n} < \frac{1}{n}\,\cdot$$

Therefore, using (2.7) again,

$$\begin{aligned}
\left|\frac{T+\varepsilon_3}{(I+\varepsilon_2)^2} - \frac{T}{I^2}\right| &= \left|\frac{\varepsilon_3 I^2 - T\varepsilon_2(2I+\varepsilon_2)}{(I+\varepsilon_2)^2 I^2}\right| \\
&\le \frac{|\varepsilon_3|}{(I+\varepsilon_2)^2} + T\varepsilon_2\frac{(2I+\varepsilon_2)}{(I+\varepsilon_2)^2 I^2} \\
&\le \frac{|\varepsilon_3|}{I_0(2n)^2} + T\varepsilon_2\frac{3}{I_0(2n)^3} \\
&< 7\pi e^{-8n} + e^{-8n} \\
&< 23e^{-8n}.
\end{aligned}$$

Thus, the total error $|\widetilde{\gamma} - \gamma|$ is bounded by $e^{-8n} + 23e^{-8n} = 24e^{-8n}$. □

Remark 4.2. We did not try to obtain the best possible constant in (4.3). A more detailed analysis shows that we can reduce the constant 24 by a factor greater than two if n is large. See also Remark 4.5.

Since the condition on N in Theorem 4.1 is rather complicated, we give the following corollary.

Corollary 4.3. *Let $\alpha \approx 4.970625759544$ be the unique positive real solution of $\alpha(\ln\alpha - 1) = 3$. If $n \ge 138$ and $N \ge \alpha n$ are integers, then the conclusion of Theorem* 4.1 *holds.*

Proof. For $138 \le n \le 214$ we can verify by direct computation that conditions (4.1)–(4.2) of Theorem 4.1 hold. Hence, in the following we assume that $n \ge 215$. Since $N \ge \alpha n$, this implies that $N \ge \lceil 215\alpha \rceil = 1069$.

Let $\beta = N/n$. Then $\beta \ge \alpha$, so $\beta(\ln\beta - 1) \ge 3$. Thus $2n(\beta\ln\beta - \beta - 3) \ge 0$. Taking exponentials and using $\beta = N/n$, we obtain

$$N^{2N} \ge e^{2N+6n} n^{2N}. \tag{4.4}$$

Define the real analytic function $h(x) := \ln x + \gamma + 1/(2x)$. The upper bound $H_N \le h(N)$ follows from the Euler-Maclaurin expansion

$$H_N - \ln(N) - \gamma \sim \frac{1}{2N} - \sum_{k=1}^{\infty} \frac{B_{2k}}{2k} N^{-2k},$$

since the terms on the right-hand-side alternate in sign.

Using our assumption that $N \ge 1069$, it is easy to verify that

$$\sqrt{\pi\alpha N} \ge 2h(N)(h(N)+1). \tag{4.5}$$

Since $\beta \ge \alpha$, it follows from (4.5) that

$$\sqrt{\pi\beta N} \ge 2h(N)(h(N)+1). \tag{4.6}$$

Substituting $\beta = N/n$ in (4.6), it follows that

$$\pi N > 2h(N)(h(N)+1)(\pi n)^{1/2}.$$

Using (4.4), this gives

$$\pi N^{2N+1} > 2n^{2N} h(N)(h(N)+1)(\pi n)^{1/2} e^{2N+6n}. \tag{4.7}$$

From the first inequality of (2.4) we have $(N!)^2 \ge 2\pi N^{2N+1} e^{-2N}$. Using this and $h(N) \ge H_N$, we see that (4.7) implies

$$(N!)^2 > 4n^{2N} H_N(1+H_N)(\pi n)^{1/2} e^{6n}. \tag{4.8}$$

However, it is easy to see that (4.8) is equivalent to conditions (4.1)–(4.2) of Theorem 4.1. Hence, the conclusion of Theorem 4.1 holds. □

Remark 4.4. If $0 < n < 138$ then Corollary 4.3 does not apply, but a numerical computation shows that it is always sufficient to take $N \ge \alpha n + 1$.

Remark 4.5. As illustrated in Table 1, the bound in (4.3) is close to optimal for large n. Our bound $24e^{-8n}$ overestimates the true error, but by a factor which is inconsequential for high-precision computation of γ.

n	N	$\lvert\widetilde{\gamma} - \gamma\rvert$	$24e^{-8n}$
10	50	$7.68 \cdot 10^{-38}$	$4.34 \cdot 10^{-34}$
100	498	$5.32 \cdot 10^{-349}$	$8.81 \cdot 10^{-347}$
1000	4971	$1.96 \cdot 10^{-3476}$	$1.06 \cdot 10^{-3473}$
10000	49706	$2.85 \cdot 10^{-34746}$	$6.64 \cdot 10^{-34743}$

Table 1. The error $\lvert\widetilde{\gamma} - \gamma\rvert$ compared to the bound (4.3).

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Mathematical Sciences Institute, Australian National University, Canberra, ACT 0200, Australia
E-mail address: rpb256@rpbrent.com

RISC, Johannes Kepler University, 4040 Linz, Austria
E-mail address: fredrik.johansson@risc.jku.at