

NEWTON-COTES INTEGRATION FOR APPROXIMATING STIELTJES (GENERALIZED EULER) CONSTANTS

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ABSTRACT. In the Laurent expansion

$$\zeta(s, a) = \frac{1}{s-1} + \sum_{k=0}^{\infty} \frac{(-1)^k \gamma_k(a)}{k!} (s-1)^k, \quad 0 < a \leq 1,$$

of the Riemann-Hurwitz zeta function, the coefficients $\gamma_k(a)$ are known as Stieltjes, or generalized Euler, constants. [When $a = 1$, $\zeta(s, 1) = \zeta(s)$ (the Riemann zeta function), and $\gamma_k(1) = \gamma_k$.] We present a new approach to high-precision approximation of $\gamma_k(a)$. Plots of our results reveal much structure in the growth of the generalized Euler constants. Our results when $1 \leq k \leq 3200$ for γ_k , and when $1 \leq k \leq 600$ for $\gamma_k(a)$ (for a such as $53/100$, $1/2$, etc.) suggest that published bounds on the growth of the Stieltjes constants can be much improved, and lead to several conjectures. Defining $g(k) = \sup_{0 < a \leq 1} |\gamma_k(a) - \frac{\log^k a}{a}|$, we conjecture that g is attained: for any given k , $g(k) = |\gamma_k(a) - \frac{\log^k a}{a}|$ for some a (and similarly that, given ϵ and a , $g(k)$ is within ϵ of $|\gamma_k(a) - \frac{\log^k a}{a}|$ for infinitely many k). In addition we conjecture that g satisfies $[\log(g(k))]/k < \log(\log(k))$ for $k > 1$. We also conjecture that $\lim_{k \rightarrow \infty} (\gamma_k(1/2) + \gamma_k)/\gamma_k = 0$, a special case of a more general conjecture relating the values of $\gamma_k(a)$ and $\gamma_k(a + \frac{1}{2})$ for $0 < a \leq \frac{1}{2}$. Finally, it is known that $\gamma_k = \lim_{n \rightarrow \infty} \{\sum_{j=2}^n \frac{\log^k j}{j} - \frac{\log^{k+1} n}{k+1}\}$ for $k = 1, 2, \dots$. Using this to define γ_r for all real $r > 0$, we conjecture that for nonintegral r , γ_r is precisely $(-1)^r$ times the r -th (Weyl) fractional derivative at $s = 1$ of the entire function $\zeta(s) - 1/(s-1) - 1$. We also conjecture that g , now defined for all real arguments $r > 0$, is smooth. Our numerical method uses Newton-Cotes integration formulae for very high-degree interpolating polynomials; it differs in implementation from, but compares in error bounding to, Euler-Maclaurin summation based methods.

1. INTRODUCTION AND CONJECTURES

The Riemann-Hurwitz zeta function, *a priori* defined by $\zeta(s, a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}$ for $\operatorname{Re}(s) > 1$ and $0 < a \leq 1$, yields the following Laurent series upon analytic continuation:

$$(1) \quad \zeta(s, a) = \frac{1}{s-1} + \sum_{k=0}^{\infty} \frac{(-1)^k \gamma_k(a)}{k!} (s-1)^k, \quad s \neq 1,$$

Received by the editor April 8, 1999 and, in revised form, January 14, 2000.
 2000 *Mathematics Subject Classification*. Primary 11M06, 11M35, 11Y60; Secondary 65D32.

for some constants $\gamma_k(a)$. Note that $\zeta(s, 1) = \zeta(s)$. By convention, γ_k denotes $\gamma_k(1)$; hence

$$\zeta(s) = \frac{1}{s-1} + \sum_{k=0}^{\infty} \frac{(-1)^k \gamma_k}{k!} (s-1)^k.$$

Stieltjes ([13]) pointed out that the constants¹ γ_k can be expressed as

$$(2) \quad \gamma_k = \lim_{n \rightarrow \infty} \left\{ \sum_{j=1}^n \frac{\log^k j}{j} - \frac{\log^{k+1} n}{k+1} \right\}$$

for $k = 1, 2, \dots$, while $\gamma_0 = \gamma$ (Euler's gamma constant). Berndt ([1]) showed that

$$(3) \quad \gamma_k(a) = \lim_{n \rightarrow \infty} \left\{ \sum_{j=0}^n \frac{\log^k(j+a)}{j+a} - \frac{\log^{k+1}(n+a)}{k+1} \right\},$$

which is equivalent to (2) when $a = 1$.

In this paper we express γ_k and $\gamma_k(a)$ as a limit of a more rapidly convergent sequence than in (2), yielding approximation methods which can readily be implemented on a personal computer—provided it is capable of very precise evaluation of logarithms (supplied by, e.g., software such as *Mathematica* or Maple). Most computations were performed on a Pentium 199Mhz processor with 32 megabytes of RAM, implementing our algorithm in *Mathematica* 2.2.1; more recent work was performed using an AMD-K6-2/500Mhz processor with 128 megabytes of RAM, implementing the algorithm in *Mathematica* 3.0 and 4.0. Beginning with $k \gtrsim 25$, we believe that our method produces high-precision estimates of γ_k more quickly, for larger values of k , and to more digits of accuracy than has been attained to date. Our numerical results naturally lead to several conjectures, which are the focus of this paper.

Published work on numerical values of these constants includes the following. Numerical values for $\gamma_1, \gamma_2, \dots, \gamma_{20}$, accurate to 20 decimal digits, were reported in [2]. Several years later, using a quite different approach, [6] reported values accurate to 85 decimal digits for $\gamma_1, \gamma_2, \dots, \gamma_{10}$ as well as γ_{20}, γ_{50} , and γ_{100} , and 80 digits were reported for γ_{150} ; these seem to be the most accurate values in the literature to date. In addition, the commercial software packages MapleV and *Mathematica* 3.0 and 4.0 have built-in functions (“gamma” and “StieltjesGamma”, respectively) for the γ_k —but not for $\gamma_k(a)$, nor for related coefficients for nonintegral k , nor for coefficients based on $\zeta(s, a)$ centered at $s \neq 1$. By contrast, our methods require the same amount of time to compute γ_k as to compute $\gamma_k(a)$ (independent of a), and regardless of whether k is integral or not. A table of γ_k values for some k between 1 and 3200, as well as some values for $\gamma_k(a)$ (for such generic a as $a = 3/4, 53/100$, and $1/2$) appears in sections 2 and 3.

Our numerical computations provide evidence that published bounds for γ_k and $\gamma_k(a)$ can be significantly improved. Before stating our conjectures, here is a brief summary of relevant published results. The γ_k are not all of one sign; [11] showed that infinitely many of those with even subscript are positive and infinitely many are negative, and the same is true for those with odd subscript. [1] showed that

¹The γ_k are sometimes ([5]) referred to as generalized Euler constants, sometimes ([6]) as Stieltjes constants. The terminology is not quite well-defined; [3] and [5] note that $A_k = \frac{(-1)^k}{k!} \gamma_k$ are usually referred to as the Stieltjes constants, but [3] points out that Stieltjes actually examined the γ_k .

$|\gamma_k| < 4 \frac{(k-1)!}{\pi^k}$ if k is even, while $|\gamma_k| < 2 \frac{(k-1)!}{\pi^k}$ for odd k , and more generally showed that

$$|\gamma_n(a) - \frac{\log^n a}{a}| \leq \frac{(3 + (-1)^n)(n-1)!}{\pi^n},$$

which was improved in [14] to

$$|\gamma_n(a) - \frac{\log^n a}{a}| \leq \frac{(3 + (-1)^n)(2n)!}{n^{n+1}(2\pi)^n} \quad \text{for } n \geq 1,$$

while [12] showed that

$$\frac{\log |\gamma_n|}{n} < \log(\log n) - \frac{4 \log(10)}{n} \quad \text{for } n \geq 10.$$

Based on our numerical results (presented in sections 2-4), we conjecture that these bounds can be considerably strengthened, and we also make other conjectures:

Conjectures (I): Growth of $\gamma_n(a)$. *Let g be defined by*

$$g(n) = \sup_{0 < a \leq 1} |\gamma_n(a) - \frac{\log^n a}{a}|.$$

We conjecture that:

- (a) $[\log(g(n))]/n < \log(\log(n))$, for $n > 1$;
- (b) *this upper bound can be replaced by $\log(\log n) - 4 \log(10)/n$ for $n \geq 10$;*
- (c) *for any a ($0 < a \leq 1$) and any positive ϵ ,*

$$|\left(\gamma_n(a) - \frac{\log^n a}{a}\right) \pm g(n)| < \epsilon$$

for infinitely many values of n ;

- (d) *g is attained, i.e., for each n , $g(n) = |\gamma_n(a) - \frac{\log^n a}{a}|$ for some a ; and*
- (e) *g is increasing for $n \geq 13$, and decreasing for $1 \leq n \leq 13$.*

Conjectures (II): Relationship of $\gamma_k(a)$ to $\gamma_k(a + 1/2)$. (a) *We conjecture that $\gamma_k(1/2) \approx -\gamma_k$ holds for sufficiently large k , and in fact that $\frac{\gamma_k(1/2) + \gamma_k}{\gamma_k} \rightarrow 0$ as $k \rightarrow \infty$ when $\gamma_k \neq 0$.*

(b) *Using the shorthand notation of [14], let $C_k(a) = \gamma_k(a) - \frac{\log^k a}{a}$. Generalizing the case $a = 1/2$ above, we conjecture that for $0 < a \leq 1/2$,*

$$\frac{C_k(a) + C_k(a + 1/2)}{C_k(a)} \rightarrow 0$$

as $k \rightarrow \infty$ for $C_k(a) \neq 0$.

Conjectures (III): Meaning of $\gamma_r(a)$ and $C_r(a)$ for nonintegral r . *For non-integral $r > 0$, extend (3) so as to define $C_r(a)$ and $\gamma_r(a)$:*

$$C_r(a) = \lim_{n \rightarrow \infty} \left\{ \sum_{j=1}^n \frac{\log^r(j+a)}{j+a} - \frac{\log^{r+1}(n+a)}{r+1} \right\}$$

and

$$\gamma_r(a) = C_r(a) + \frac{\log^r(a)}{a},$$

for $0 < a \leq 1$.

(a) Define $h_a(s) = \zeta(s, a) - 1/(s-1) - 1/a^s$ for $s \neq 1$; note that for each a , h_a extends to an entire function. Let $r > 0$ be nonintegral. We conjecture that $C_r(a) = (-1)^r h_a^{(r)}(1)$, where $f^{(r)}(x)$ denotes the r -th (Weyl) fractional derivative of f at x .

(b) This extension of $\gamma_r(a)$ to nonintegral r allows g from Conjectures (I) to be extended to all real $r > 0$. We conjecture that g is smooth, and has an absolute minimum somewhere near $r = 13$.

Numerical support for these conjectures appears in sections 2-4; sections 5-6 supply the details of our method. Briefly, we estimate γ_k in terms of partial sums of the sum in (2), along with correction terms. What is new is that our correction terms arise from weights coming from Newton-Cotes numerical integration methods.

2. NUMERICAL RESULTS FOR γ_k

All tabulated values are *exact to all digits displayed* (not rounded). Values tabulated and plotted below were computed using (13) from section 6. In addition, γ_k values for $k = 2001$ to 8300 (given to over 200 significant digits) and for $k = 1$ to 2000 (given to hundreds of digits) may be downloaded from a web site we maintain, upon request.

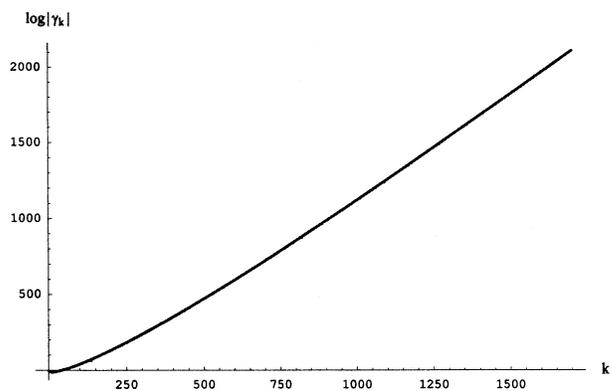
See Figure 1a for growth in $\log |\gamma_k|$ for all k from 1 to 1700, and Figures 1b-c for local behavior of $\log |\gamma_k|$ and $\log(\gamma_k)$. (We plot both $\log(\gamma_k)$ and $\log |\gamma_k|$ to illustrate the sign changes in γ_k .) Plots of local and asymptotic behavior of $\log(|\gamma_k|)/k$ appear in Figures 2a-d.

As noted earlier, [12] showed that

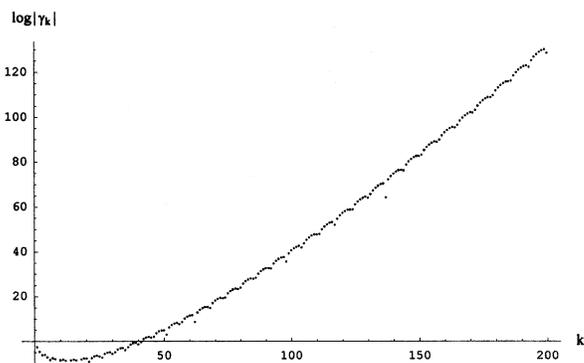
$$\frac{\log |\gamma_k|}{k} < \log(\log k) - \frac{4 \log(10)}{k}$$

for $k \geq 10$. Our data suggest that even this bound can be improved, as indicated in Figure 3.

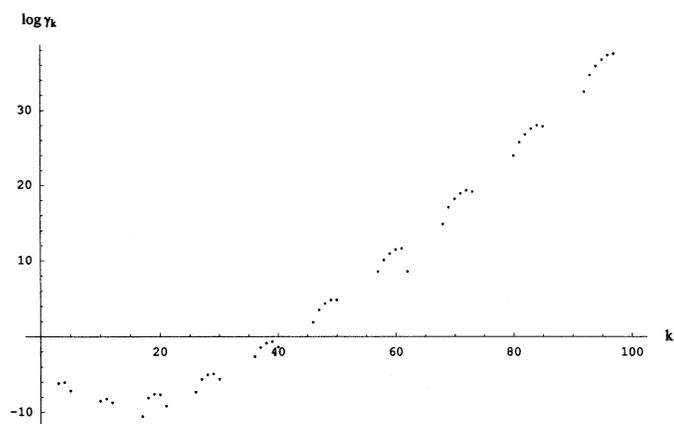
Empirically, γ_k regularly alternates in sign; for instance, for k from 1 to 1000, $\gamma_k > 0$ for exactly 499 values of k . Figures 4a-b provide plots of $\text{sign}(\gamma_k)$ versus k for two ranges of k . The plots indicate that the first two values (i.e., γ_1 and γ_2) are negative, then the next three (γ_3 through γ_5) are positive, and so on. Thus, the γ_k begin with a negative “run” of length two, followed by a positive “run” of length three. Run-size results for the signs of the γ_k are depicted in Figure 4c, extended through γ_{1691} . The signs of γ_k behave in a strikingly regular way; the run sizes of consecutive signs in γ_k grow almost monotonically, and the run sizes appear to be $O(\sqrt{\text{run number}})$. Figures 1b-c and 2b-d seem to indicate that $\log(\gamma_k)/k$ has a significant periodic component. However, the fact that run sizes are by-and-large increasing implies that $\log(\gamma_k)/k$ does not have a true periodic component to its growth; i.e., the bumps apparent in Figures 1b-c and 2b-d are gradually widening.



a



b



c

FIGURE 1. Figure 1a shows a plot of $\log|\gamma_k|$ versus k for $k = 1$ to 1700; 1b shows the plot of $\log|\gamma_k|$ versus k for $k = 1$ to 200; and 1c shows the plot of only the positive γ_k , in the form of $\log(\gamma_k)$, versus k for $k = 1$ to 100.

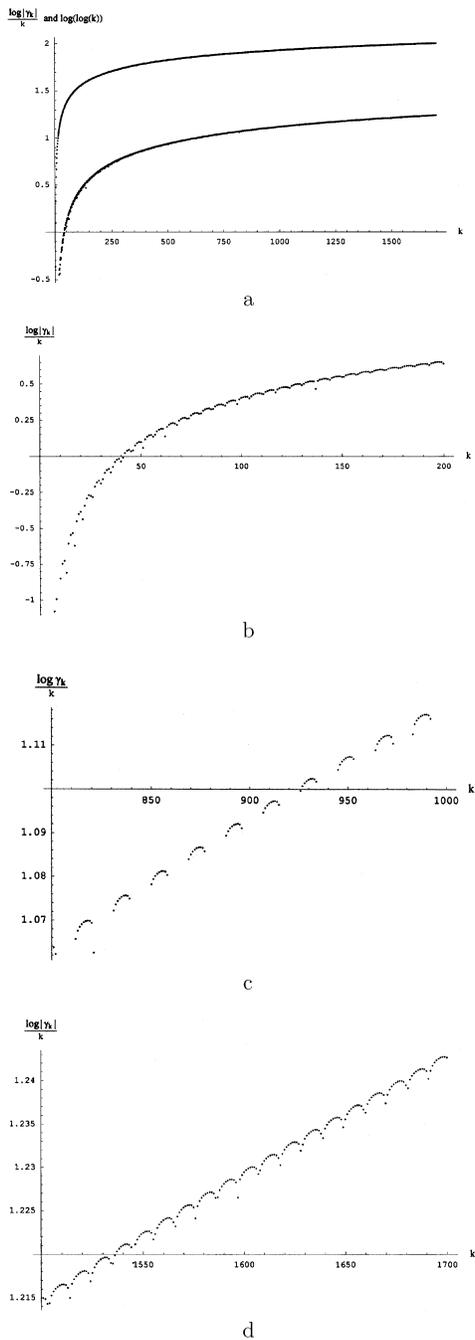


FIGURE 2. Figure 2a shows a plot of $(\log |\gamma_k|)/k$ (lower curve) and $\log(\log k)$ (upper curve), $1 \leq k \leq 1700$; 2b shows a blow-up of part of 2a showing the plot of $(\log |\gamma_k|)/k$ for $1 \leq k \leq 200$; 2c shows a blow-up of 2a of only positive γ_k , in the form of $(\log \gamma_k)/k$, $801 \leq k \leq 1000$; and 2d shows a blow-up of $(\log |\gamma_k|)/k$ for $1501 \leq k \leq 1700$.

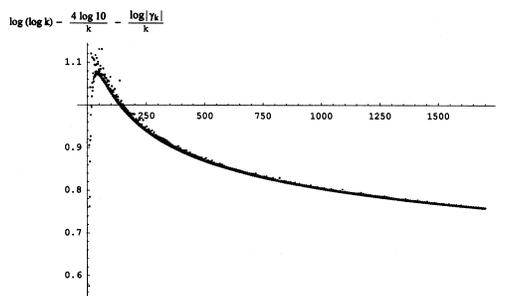


FIGURE 3. The largest value is 1.13061... attained when $k = 62$; the smallest value is .758287... attained when $k = 1688$.

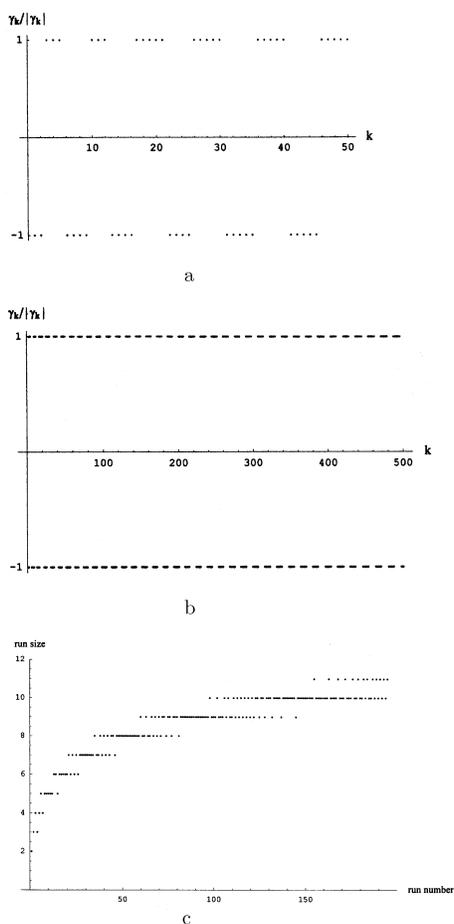


FIGURE 4. Figure 4a shows a plot of the signs of γ_k versus k , for $k = 1$ to 50; 4b shows a plot of the signs of γ_k versus k , for $k = 1$ to 500; 4c shows a plot of the lengths of the runs in the values of $\text{sign}(\gamma_k)$, in order, for the first 195 runs (accounting for the signs of γ_k from γ_1 to γ_{1691}).

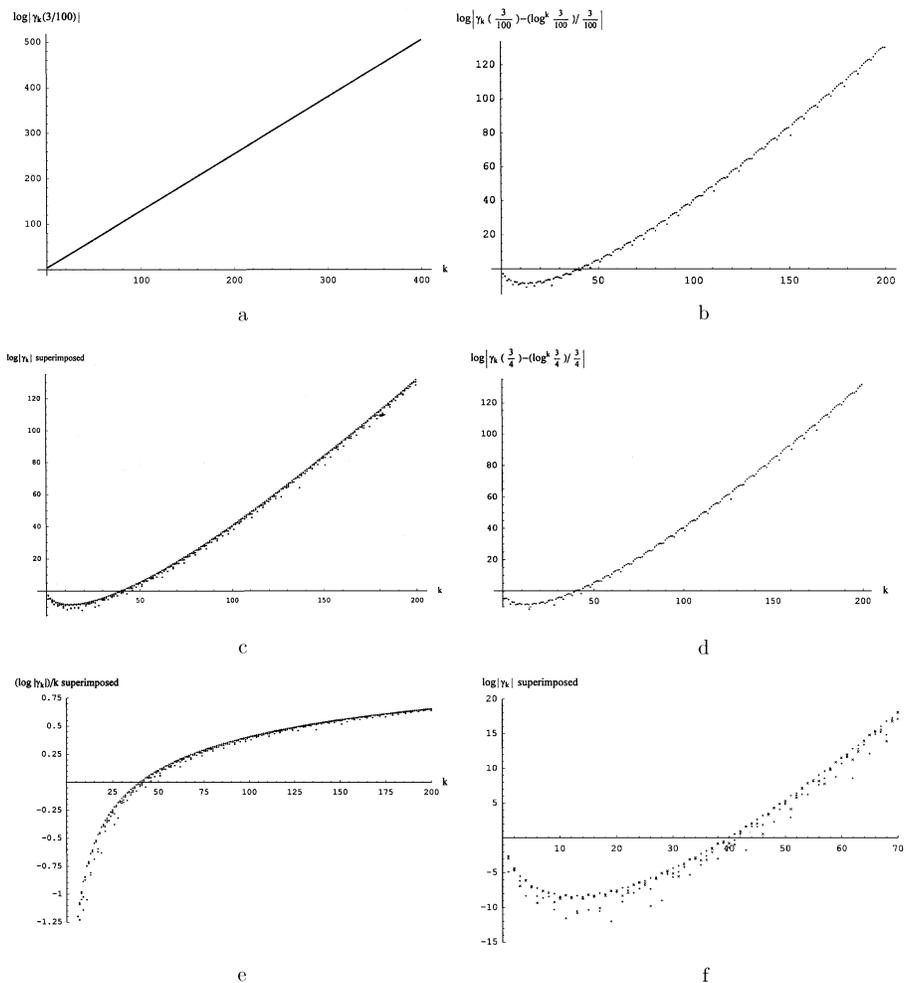


FIGURE 5. $\log |\gamma_k|$ versus k , superimposed with Figures 5b and 5c, is depicted in 5d, and again in 5e (where the largest dots show $\log |\gamma_k|$, then $\log |C_k(3/4)|$, and the smallest are $\log |C_k(3/100)|$). Figure 5f superimposes $(\log |\gamma_k|)/k$ with $(\log |C_k(3/4)|)/k$ and $(\log |C_k(3/100)|)/k$

3. SAMPLE NUMERICAL RESULTS FOR $\gamma_k(a)$

Recall the notation $C_k(a) = \gamma_k(a) - \frac{\log^k a}{a}$. The graphs in Figure 5 depict an apparent universality in the growth not of the $\gamma_k(a)$, but rather of the $C_k(a)$. Such plots support the statements labeled Conjectures (I) in section 1, which involve the function $g(n) = \sup_{0 < a \leq 1} |\gamma_n(a) - \frac{\log^n a}{a}| (= \sup_{0 < a \leq 1} |C_n(a)|)$. Evidence that g is in some sense a universal curve, which all the functions $|C_n(a)|$ for $0 < a \leq 1$ approach within any arbitrary amount, and which is itself quite smooth, is most clearly apparent in Figures 5d-e. We consider the function g to be one of the most intriguing finds in our empirical studies.

TABLE I.

k	γ_k
200	$-6.97464971947882286862433306942681458447463309083796965410651256959874542147151868516329155259383 \cdot 10^{55}$
400	$-1.76164218667592614688327394016006297062306156164871264021403038343199209574026683399457363218748 \cdot 10^{152}$
600	$3.5627462868188804049170046684345765169069476039754550000949652101075496437088562838543634195696507 \cdot 10^{257}$
800	$4.9135405617183059420222476712064847339402719362442113026262039583988755867359438843536710158276178 \cdot 10^{369}$
1000	$-1.57095384420474493454940234251208252423802995545703429980593511612582940990371998542062540960084 \cdot 10^{486}$
1200	$8.684029915258273732365295242603914497049915740171534878614560878033837219649037144277085892120418 \cdot 10^{605}$
1400	$-4.09728733423435323949823194614198060836475179557710250104197849823734021001495058902441286319991 \cdot 10^{728}$
1600	$-2.05745363325152193936446719112695548704092973450069944568788616971004408742860823153915430019591 \cdot 10^{854}$
1800	$3.315312480255275238485257832628014604412693521955068471455113042275598848452876518074180850700459 \cdot 10^{981}$
2000	$2.680424678918000809504929834609356277409099264836410829548331346701687949728089727686622380790342 \cdot 10^{1109}$
2200	$-1.22286968059290784555088133767387031683960863518230592897701857949354195118561847798487103653917 \cdot 10^{1241}$
2400	$-1.10170195316296433765205377955346812193237450968035906769260654203913611687955057955880561646664 \cdot 10^{1373}$
2600	$-1.74978067036140255245203722980524710947418537680995790400249691619541927376484114232757764295566 \cdot 10^{1506}$
2800	$-2.5739785400684507054745368034212942364346800690192801742804905228803874403276103494616652917341 \cdot 10^{1640}$
3000	$6.461281430618359954840322389860361543135682033560427625320333049395288889181477851444797014340317 \cdot 10^{1775}$
3200	$1.369181256156237620168729200741538372420863775398034969587991415128021236536477106328552841560036 \cdot 10^{1912}$

TABLE II.

k	$\gamma_k \equiv \gamma_k(1) \equiv C_k(1)$	$C_k(53/100)$	$C_k(1/2)$	$C_k(3/100)$	$\gamma_k(3/100)$
10	$2.0533281 \cdot 10^{-4}$	$-1.599283612 \cdot 10^{-4}$	$-2.040689386 \cdot 10^{-4}$	$1.617124536 \cdot 10^{-4}$	$9.3689060 \cdot 10^6$
20	$4.6634356 \cdot 10^{-4}$	$-5.342524477 \cdot 10^{-4}$	$-4.664213305 \cdot 10^{-4}$	$5.341470909 \cdot 10^{-4}$	$2.6332920 \cdot 10^{12}$
30	$3.5577288 \cdot 10^{-3}$	$-5.929465853 \cdot 10^{-3}$	$-3.557620478 \cdot 10^{-3}$	$5.929552018 \cdot 10^{-3}$	$7.4013197 \cdot 10^{17}$
40	$2.4872155 \cdot 10^{-1}$	$-4.533352374 \cdot 10^{-1}$	$-2.487212081 \cdot 10^{-1}$	$4.533357285 \cdot 10^{-1}$	$2.0802680 \cdot 10^{23}$
50	$1.2682360 \cdot 10^2$	$-1.644843411 \cdot 10^2$	$-1.268236037 \cdot 10^2$	$1.644843432 \cdot 10^2$	$5.8469508 \cdot 10^{28}$
100	$-4.2534015 \cdot 10^{17}$	$3.697293639 \cdot 10^{17}$	$4.253401571 \cdot 10^{17}$	$-3.697293639 \cdot 10^{17}$	$1.0256050 \cdot 10^{56}$
150	$8.0288537 \cdot 10^{35}$	$-1.329856627 \cdot 10^{36}$	$-8.028853731 \cdot 10^{35}$	$1.329856627 \cdot 10^{36}$	$1.7989986 \cdot 10^{83}$
200	$-6.9746497 \cdot 10^{55}$	$4.564416715 \cdot 10^{56}$	$6.974649719 \cdot 10^{55}$	$-4.564416715 \cdot 10^{56}$	$3.1555970 \cdot 10^{110}$
250	$3.0592128 \cdot 10^{79}$	$-3.479950592 \cdot 10^{79}$	$-3.059212855 \cdot 10^{79}$	$3.479950592 \cdot 10^{79}$	$5.5351863 \cdot 10^{137}$
300	$-5.5567282 \cdot 10^{102}$	$3.984976277 \cdot 10^{102}$	$5.556728220 \cdot 10^{102}$	$-3.984976277 \cdot 10^{102}$	$9.7091887 \cdot 10^{164}$
400	$-1.7616421 \cdot 10^{152}$	$1.818358278 \cdot 10^{152}$	$1.761642186 \cdot 10^{152}$	$-1.818358278 \cdot 10^{152}$	$2.9873378 \cdot 10^{219}$
500	$-1.1655052 \cdot 10^{204}$	$1.084835733 \cdot 10^{204}$	$1.165505272 \cdot 10^{204}$	$-1.084835733 \cdot 10^{204}$	$9.1914862 \cdot 10^{273}$
600	$3.5627462 \cdot 10^{257}$	$-4.657182402 \cdot 10^{257}$	$-3.562746286 \cdot 10^{257}$	$4.657182402 \cdot 10^{257}$	$2.8280503 \cdot 10^{328}$
700	$-3.5494521 \cdot 10^{312}$	$6.349887759 \cdot 10^{312}$	$3.549452184 \cdot 10^{312}$	$-6.349887759 \cdot 10^{312}$	$8.7013881 \cdot 10^{382}$
800	$4.9135405 \cdot 10^{369}$	$-5.779001856 \cdot 10^{369}$	$-4.913540561 \cdot 10^{369}$	$5.779001856 \cdot 10^{369}$	$2.6772562 \cdot 10^{437}$

Next we examine evidence for Conjectures (II). Again, tabulated values are accurate to all digits displayed (i.e., no rounding). For convenience we repeat some of the values of γ_k from Table I.

From Table II, we first note how $C_k(1/2) \approx -\gamma_k$ for some k ; and since, for large k , $C_k(1/2)$ is well-approximated by $\gamma_k(1/2)$, we have that $\gamma_k(1/2) \approx -\gamma_k$. This result, specified as Conjecture (IIa) in section 1, has more numerical support than is displayed in the table above.² To a certain extent, Figure 5e displays how the phase of the (almost-periodic) “bumps” seen in Figures 5b-c compare with the “bumps” in Figure 1. Figures 6a-b indicate this phase difference in a more striking way. Fixing $k = 100$ and varying a yields the plots in Figures 6c-d, giving yet another perspective on how the phase of the $C_k(a)$ values varies with a . Comparing these latter two figures, it again appears that the values of $C_k(a)$ and $C_k(a + 1/2)$ are virtually negatives of one another, for $0 < a \leq 1/2$, lending further support to Conjecture (IIb).

As one possible step in proving Conjectures (II), note that

$$(5) \quad \zeta(s, a + \frac{1}{2}) + \zeta(s, a) = 2^s \zeta(s, 2a),$$

as shown by simple algebraic manipulations, *a priori* valid for $Re(s) > 1$, as follows:

$$\begin{aligned} \zeta(s, a + 1/2) &= \sum_{n=0}^{\infty} \frac{1}{(n + a + \frac{1}{2})^s} \\ &= 2^s \sum_{n=0}^{\infty} \frac{1}{(2n + 2a + 1)^s} \\ &= 2^s (\zeta(s, 2a) - \frac{1}{2^s} \zeta(s, a)), \end{aligned}$$

where the last equality follows since

$$\begin{aligned} \zeta(s, A) &= \sum_{n=0}^{\infty} \frac{1}{(2n + 1 + A)^s} + \sum_{n=0}^{\infty} \frac{1}{(2n + A)^s} \\ &= \sum_{n=0}^{\infty} \frac{1}{(2n + 1 + A)^s} + \frac{1}{2^s} \sum_{n=0}^{\infty} \frac{1}{(n + \frac{A}{2})^s}. \end{aligned}$$

It remains to use this result to extract information about the Stieltjes constants. Multiplying both sides of (5) by $(s - 1)$, then expressing each side in a power series using (1), taking the n th derivative of each side, and finally taking the limit as $s \rightarrow 1^+$ yields a relation between $\gamma_n(a) + \gamma_n(a + 1/2)$ and $\gamma_k(2a)$ for $0 \leq k \leq n$, namely

$$(6) \quad \begin{aligned} &(-1)^{(n-1)} n ((\gamma_{n-1}(a + \frac{1}{2}) + \gamma_{n-1}(a)) \\ &= 2(\log 2)^n + \sum_{j=1}^n \binom{n}{j} 2(\log 2)^{n-j} (-1)^{j-1} j \gamma_{j-1}(2a). \end{aligned}$$

While it is possible that this relation can be part of a proof of Conjecture (IIa) above, we used (6) as a nontrivial consistency check for our values of $\gamma_n(1/2)$ and

²For example, $C_{300}(1/2)$ (which matches $\gamma_{300}(1/2)$ to over 32 significant digits) matches $-\gamma_{300}$ to precisely 29 significant digits. Similarly, γ_{600} agrees with $-\gamma_{600}(1/2)$ to exactly 51 significant digits, and γ_{800} agrees with $-\gamma_{800}(1/2)$ to exactly 64 significant digits.

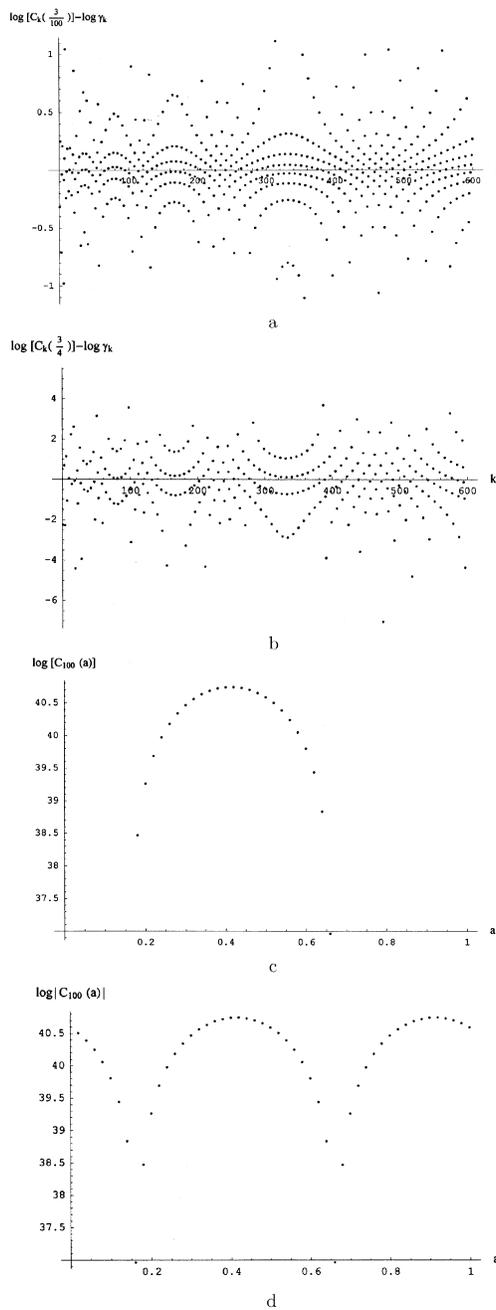


FIGURE 6. Figure 6a shows a plot of $\log[\gamma_k(3/100) - (\log^k(3/100)/(3/100))] - \log \gamma_k$, $1 \leq k \leq 600$; 6b shows a plot of $\log[\gamma_k(3/4) - (\log^k(3/4)/(3/4))] - \log \gamma_k$, $1 \leq k \leq 600$; 6c shows a plot of $\log[\gamma_{100}(a) - (\log^{100} a)/a]$, for $0 < a \leq 1$ ($a = n/50$ for $n = 1$ to 50); and 6d shows a plot of $\log |\gamma_{100}(a) - (\log^{100} a)/a|$, for $0 < a \leq 1$ ($a = n/50$ for $n = 1$ to 50).

γ_k , and for other $\gamma_k(a)$, as follows. Note that when $a = 1/2$, (5) implies that $\zeta(s, 1/2) + \zeta(s) = 2^s \zeta(s)$, so (6) yields

$$(-1)^{n-1} n (\gamma_{n-1} + \gamma_{n-1}(1/2)) = 2(\log 2)^n + \sum_{j=1}^n \binom{n}{j} 2(\log 2)^{n-j} (-1)^{j-1} j \gamma_{j-1}.$$

Hence the choice of $a = 1/2$ in (6) constitutes a nontrivial consistency check of the values³ of $\gamma_k(1/2)$ and γ_k .

4. NUMERICAL RESULTS FOR TAYLOR SERIES COEFFICIENTS FOR $s \neq 1$
AND $\gamma_k(a)$ FOR NONINTEGRAL k

Our method of computing the Laurent coefficients of $\zeta(s, a)$ centered at $s = 1$ can be adapted to compute the Taylor coefficients for $\zeta(s, a)$ centered at $s \neq 1$, e.g., at $s = 1 + \epsilon$. The function $h(s) = \zeta(s) - \frac{1}{s-1}$ is (when extended to $s = 1$) entire, so by analogy with (1) the Taylor expansion of h is

$$h(s) = \zeta(s) - \frac{1}{s-1} = \sum_{k=0}^{\infty} \frac{(-1)^k \gamma_k^{(s=s_0)}}{k!} (s - s_0)^k$$

for constants $\gamma_k^{(s=s_0)} = (-1)^k h^{(k)}(s_0)$. Our computational methods can extend to numerically estimate $\gamma_k^{(s=s_0)}$ for integral k to high precision. However, our real interest in examining the case $s \neq 1$ stems from numerical exploration of nonintegral derivatives of h , evaluated for $s \gtrsim 1$, as follows.

The α th Weyl fractional derivative ([10], [4]) of a function f is defined by

$$\frac{(-1)^{j-\alpha}}{\Gamma(j-\alpha)} \frac{d^j}{dx^j} \int_x^{\infty} (t-x)^{j-\alpha-1} f(t) dt \quad \text{for } 0 < \alpha,$$

where j is the smallest integer greater than α . The α th derivative of a decreasing exponential function $f(s) = e^{-as}$ satisfies $(D^\alpha f)(s) = (-1)^{-\alpha} a^\alpha e^{-as}$. Thus, for real $s_0 > 1$, the derivative $\zeta^{(\alpha)}(s_0)$ for real $\alpha > 0$ is

$$(-1)^{-\alpha} \sum_{n=1}^{\infty} \frac{(\log n)^\alpha}{n^{s_0}}.$$

The α th Weyl derivative of $p(s) = \frac{1}{s-1}$ may also be computed: for $0 < \alpha < 1$,

$$(D^\alpha p)(s) = \frac{(-1)^{-\alpha} \alpha \pi \csc(\alpha \pi)}{\Gamma(1-\alpha) (s-1)^{\alpha+1}}$$

(which can be extended for $\alpha > 1$ by ordinary differentiation). Combining these results for ζ and p , we can numerically compute $h^{(\alpha)}(s_0)$ for real $\alpha > 0$, for $s_0 > 1$. We set $\tilde{h}^{(\alpha)}(s_0) = (-1)^\alpha h^{(\alpha)}(s_0)$. Letting $s_0 = 1 + 10^{-6}$ and $1 + 10^{-9}$, to mimic $s_0 \rightarrow 1$, we arrive at the data in the third and fourth columns of Table III below

³For $1 \leq k \leq 200$, we computed $\gamma_k(a)$ values to 90 digit accuracy for $a=1/10, 2/10, 5/10, 6/10$ and $10/10$. However, since the right side summation in (6) at times involves large coefficients, a loss of significant digits routinely occurs. E.g., for some large values of k near 200, only 70 significant digits can be computed for the right side in (6) despite using 90-digit values for $\gamma_k(2a)$. Taking this into account, our values confirmed that the left side of (6) precisely matched the right side to *all* significant digits, for all $1 \leq k \leq 200$, for the cases $a=1/10$ and $5/10$.

TABLE III.

r	γ_r	$\tilde{h}^{(r)}(1 + 10^{-6})$	$\tilde{h}^{(r)}(1 + 10^{-9})$
183/17	$2.71689990440551 \cdot 10^{-4}$	$2.71689787110 \cdot 10^{-4}$	$2.71689990237221 \cdot 10^{-4}$
127/3	-3.47361949369674824	-3.473613390820989	-3.47361948759386890
r	$\tilde{h}^{(r)}(1 + 10^{-9}) - \gamma_r$	γ_{r+1}	
183/17	$-2.0333009378476 \cdot 10^{-13}$	$2.0333009379535 \cdot 10^{-4}$	
127/3	$6.1028793372495 \cdot 10^{-9}$	-6.1028793408313	

(for two presumably generic values of r). For the other columns, as in Conjecture (IIIa) we *define*

$$\gamma_r = \gamma_r(1) = \lim_{k \rightarrow \infty} \left\{ \sum_{j=2}^k \frac{\log^r(j)}{j} - \frac{\log^{r+1}(k)}{r+1} \right\}$$

for real $r > 0$.

The top four columns in Table III support Conjecture (IIIa), namely that for γ_r as we define it, $\gamma_r = \tilde{h}^{(r)}(1)$. Further evidence comes from the mean value theorem: since $h^{(r)}(1 + \epsilon) - h^{(r)}(1) = \epsilon h^{(r+1)}(c_\epsilon)$ for $1 < c_\epsilon < 1 + \epsilon$, multiplication by $(-1)^r$ and the conjecture imply $\tilde{h}^{(r)}(1 + \epsilon) - \gamma_r \approx -\epsilon \gamma_{r+1}$. The last two columns on the bottom row thus provide further support for the conjecture. Note that these computations require precise numerical estimates at $s \neq 1$ for derivatives of the zeta function, which the Newton-Cotes integration method can provide (as seen below).

5. DETAILS ABOUT THE METHOD FOR ESTIMATING γ_k (I):

NEWTON-COTES INTEGRATION AND SUMS OF FINITELY MANY TERMS

The heart of our approach to estimating $\gamma_k(a)$ is high-precision estimation of the sums in (2) and (3), using Newton-Cotes integration formulae. We first set notation. (Closed-form) Newton-Cotes integration weights $w_{q,m}$ are chosen so that the following equation is valid for all polynomials of degree at most $2m + 1$:

$$(7) \quad \int_{-m}^m p(x) dx = \sum_{q=-m}^m p(q) w_{q,m}.$$

While the weights $w_{q,m}$ are well-known for small m , we are not aware of their being tabulated (or studied in detail) for large m . The $w_{q,m}$ may be obtained by first noting that (7) will immediately hold for all $p(x)$ of the form x^l if l is odd, provided $w_{-q,m} = w_{q,m}$. Upon inserting x^l for $p(x)$, for $l = 0, 2, 4, \dots, 2m$, into (7), one has $m + 1$ linear equations for the remaining $m + 1$ unknowns. (For example, if $m = 1$ we have $w_{-1,1} = w_{1,1}$, $2 = w_{-1,1} + w_{0,1} + w_{1,1}$, and $2/3 = w_{-1,1} + w_{1,1}$, yielding $w_{-1,1} = 1/3, w_{0,1} = 4/3, w_{1,1} = 1/3$, i.e., the familiar weights of Simpson's rule.) For implementation on a personal computer, this approach to computing the weights can be improved, as suggested by a referee: Define

$$p_q(x) = \prod_{-m \leq j \leq m, j \neq q} (x - j).$$

p_q has degree $2m$, so (7) implies

$$(8) \quad w_{q,m} p_q(q) = \int_{-m}^m p_q(x) dx.$$

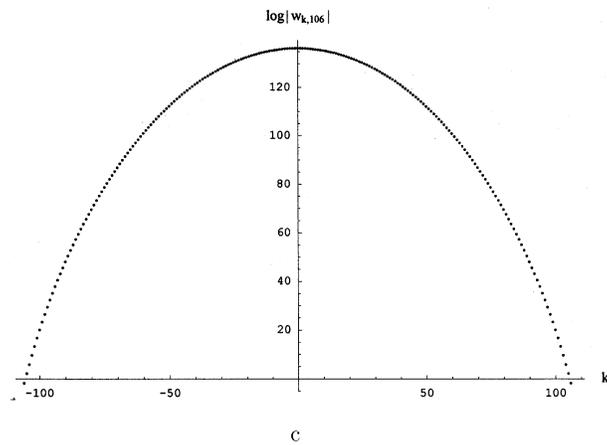
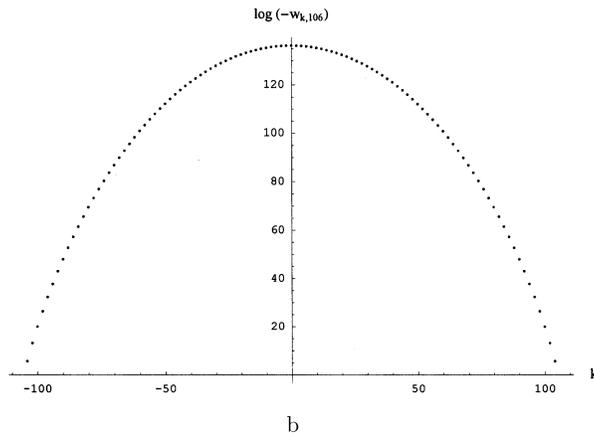
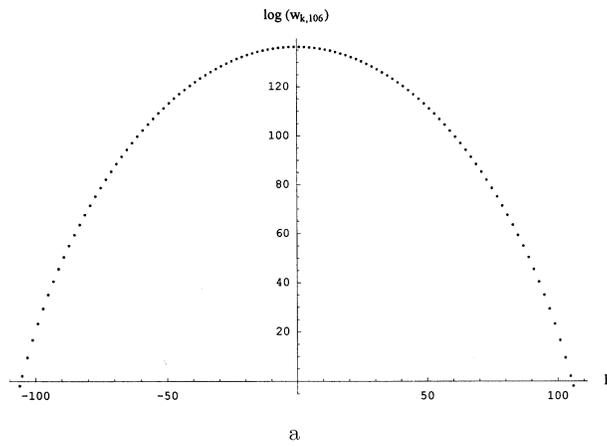


FIGURE 7. Figure 7a shows a plot of the logarithm of (only the positive) weights, i.e., $\log(w_{k,106})$; 7b shows a plot of the logarithm of (only the negative) weights, i.e., $\log(-w_{k,106})$; and 7c shows a plot of the logarithm of the absolute value of all weights, i.e., $\log|w_{k,106}|$.

Note that $p_q(q) = (-1)^{m-q}(m - q)!(m + q)!$. It remains to evaluate the integral on the right in (8). Define $p(x) = \prod_{-m \leq j \leq m} (x - j)$. On the one hand, p is $(x + m)^{(2m+1)}$, adopting notation from the calculus of finite differences, namely p is a shifted version of a falling factorial. As such, $p(x) = \sum_{i=1}^{2m+1} a_i x^i$, where

$$a_i = \sum_{j=i}^{2m+1} s_j^{2m+1} \binom{j}{i} m^{j-i}$$

(here s_i^k denotes a Stirling number of the first kind). Now

$$p_q(x) = \frac{p(x) - p(q)}{x - q} = \sum_{i=1}^{2m+1} a_i (x^i - q^i) / (x - q);$$

expanding the fraction in the summation as a finite geometric series, the integral of $p_q(x)$ can be computed, and so (8) leads to

$$(9) \quad w_{q,m} = \frac{(-1)^{m-q}}{(m - q)!(m + q)!} \left[\sum_{i=1}^{2m+1} a_i 2 \left(\sum_{j=1, j \text{ odd}}^{j=i} \frac{m^j}{j} q^{i-j} \right) \right].$$

Using (9), we computed the weights for $m = 325$ in less than 2 hours on the AMD-K6-2 processor (a vast improvement to solving the related system of equations described above).⁴ We henceforth assume that the $w_{q,m}$ values for some fixed m have been computed and stored for further use, and proceed to describe how these are used to approximate γ_k .

In order to estimate $\sum_{j=1}^n \frac{\log^k j}{j}$ in (2), we use (7) to more generally estimate $\sum_{j=n_1}^{n_2} f(j)$ for large $n_2 > n_1$. The algebra is more tractable when n_2 is $n_1 + N(2m) - 1$ for some integer N . So we first consider $\sum_{j=n_1}^{n_1+N(2m)-1} p(j)$, as follows. Let s_j denote the partial sum of the first j weights, i.e., $s_j = \sum_{n=-m}^{-m+j-1} w_{n,m}$, and let S denote the sum of all the weights, i.e., $S = s_{2m+1}$. (Of course, S is just $\int_{-m}^m 1 dx$, i.e., $S = 2m$, a simplification we will make later.) Next, we use (7) to produce a total of $2Nm$ equations, i.e., one for each term in $\sum_{j=n_1}^{n_1+N(2m)-1} p(j)$, wherein the intervals of integration are “staggered”, each of width $2m$. The equations are

$$\sum_{j=n_1}^{n_1+2m} p(j) w_{j-n_1-m,m} = \int_{n_1}^{n_1+2m} p(x) dx,$$

⁴ In computing γ_k , weights based on 8 different values of m from $m = 60$ through 360 were used, for timing comparisons as well as for consistency checks. The weights themselves are of interest; see Figure 7 for plots of $w_{q,106}$. Note the extremely large values of (most of) the weights, the curiosity that they precisely alternate in sign (excepting $w_{106,106}$ and $w_{-106,106}$), and the remarkable regularity in their values. Also, the absolute values of the weights are well-described by a Gaussian function, i.e., by $Ce^{-k(q-a)^2}$, where C , k and a are constants depending on m . These experimental observations concerning the behavior of Newton-Cotes weights for large m may be anticipated from the following result of [9]: rewriting 6.2.4 from p. 86 of [9] in our notation, we get

$$w_{q,m} = \frac{(-1)^{q+m-1}}{2m(m^2 - q^2) \ln^2 2m} \binom{2m}{m+q} \left[1 + O\left(\frac{1}{\ln 2m}\right) \right]$$

for $|q| \leq m - 1$. The presence of the $(-1)^{q+m-1}$ term explains the sign alternation in $w_{q,m}$, and the normal approximation to the binomial distribution explains the Gaussian distribution of the weights.

$$\begin{aligned}
 & \sum_{j=n_1+1}^{n_1+2m+1} p(j)w_{j-n_1-m-1,m} = \int_{n_1+1}^{n_1+2m+1} p(x) dx, \dots, \\
 (10) \quad & \sum_{j=n_1+2Nm-1}^{n_1+2Nm+2m-1} p(j)w_{j-n_1-2Nm-m+1,m} = \int_{n_1+2Nm-1}^{n_1+2Nm+2m-1} p(x) dx.
 \end{aligned}$$

Upon adding the equations, combining the integrals, and algebraic manipulation (including adding some terms such as $(S - s_1)p(n_1)$, $(S - s_2)p(n_1 + 1)$, etc., and subtracting other terms such as $(S - s_1)p(n_2 + 1)$) we obtain the following result:

$$\begin{aligned}
 S \left(\sum_{j=n_1}^{n_1+2Nm-1} p(j) \right) &= \int_{n_1}^{n_1+2Nm} p(x) dx + \int_{n_1+1}^{n_1+2Nm+1} p(x) dx \\
 &+ \int_{n_1+2}^{n_1+2Nm+2} p(x) dx + \dots + \int_{n_1+2m-1}^{n_1+2Nm+2m-1} p(x) dx \\
 &+ (S - s_1)p(n_1) + (S - s_2)p(n_1 + 1) + (S - s_3)p(n_1 + 2) \\
 &+ \dots + (S - s_{2m})p(n_1 + 2m - 1) \\
 &- ((S - s_1)p(n_1 + 2Nm) + (S - s_2)p(n_1 + 2Nm + 1) \\
 &+ (S - s_3)p(n_1 + 2Nm + 2) \\
 &+ \dots + (S - s_{2m})p(n_1 + 2Nm + 2m - 1)).
 \end{aligned}$$

If we replace p , any polynomial of degree less than or equal to $2m + 1$, by a function f – the function we will use first is $f(x) = \frac{\log^k x}{x}$ – and recall that $S = 2m$, we now have

$$\begin{aligned}
 & \sum_{j=n_1}^{n_1+2Nm-1} f(j) \\
 & \approx \frac{\int_{n_1}^{n_1+2Nm} f(x) dx}{2m} \\
 & + \frac{\int_{n_1+1}^{n_1+2Nm+1} f(x) dx + \int_{n_1+2}^{n_1+2Nm+2} f(x) dx + \dots + \int_{n_1+2m-1}^{n_1+2Nm+2m-1} f(x) dx}{2m} \\
 & + ((S - s_1)(f(n_1) - f(n_1 + 2Nm)) + (S - s_2)(f(n_1 + 1) - f(n_1 + 2Nm + 1)) \\
 & + (S - s_3)(f(n_1 + 2) - f(n_1 + 2Nm + 2)) \\
 (11) \quad & + \dots + (S - s_{2m})(f(n_1 + 2m - 1) - f(n_1 + 2Nm + 2m - 1)))/2m,
 \end{aligned}$$

where the error incurred comes from replacing the polynomial p by a more general f in each of the $2Nm$ equations (such as those in (10)).

We briefly comment about the magnitude of the error. In each of the equations in (10) (that are added to yield (11)), replacing p by f incurs a Newton-Cotes approximate integration error of the form $c_m f^{(2m+2)}(\xi_j)$ (where each ξ_j lies in an interval of the form $[n_1 + k, n_1 + k + 2m]$, and c_m is a constant that can readily be found for any given m). Summing these errors produces a Riemann sum for the integral of $f^{(2m+2)}$; hence the overall error in (11) is bounded by, and behaves like, $f^{(2m+1)}(n_1)$ times a constant for sufficiently large n_1 (e.g., if $|f^{(2m+1)}|$ is decreasing on $[n_1, \infty)$).

6. THE METHOD FOR ESTIMATING γ_k (II):
SUMS WITH INFINITELY MANY TERMS

Equation (11) may be used to estimate series with finitely, as well as infinitely, many terms; for examples with small m , see [7] and [8]. Here we use (11) to obtain our estimates for γ_k . First, rewrite (2) as

$$(12) \quad \gamma_k = \sum_{j=1}^{n_1-1} \frac{\log^k j}{j} - \lim_{N \rightarrow \infty} \left\{ \sum_{j=n_1}^{n_1+2Nm} \frac{\log^k j}{j} - \frac{\log^{k+1}(n_1 + 2Nm)}{k+1} \right\}.$$

Next, the sum in braces is approximated using (11), as follows. The antiderivative of the relevant f is simply $\frac{\log^{k+1} x}{k+1}$. Also note that there are $2m$ integrals in (11); i.e., an average of $2m$ integrals is taken. As $N \rightarrow \infty$, there is a cancellation between the $2m$ integrals' upper limit of integration and the $\log^{k+1}(n_1 + 2Nm)$ term. Thus, combining (11) with (12) yields our algorithm, namely

$$(13) \quad \begin{aligned} \gamma_k = & \sum_{j=1}^{n_1-1} f(j) + (S - s_1)f(n_1) + (S - s_2)f(n_1 + 1) \\ & + \cdots + (S - s_{2m})f(n_1 + 2m - 1) \\ & - \frac{F(n_1) + F(n_1 + 1) + \cdots + F(n_1 + 2m - 1)}{2m} \\ & + O(f^{2m+1}(n_1)), \end{aligned}$$

where

$$f(x) = \frac{\log^k x}{x}$$

and

$$F(x) = \frac{\log^{k+1} x}{k+1},$$

for sufficiently large n_1 . Fewer than 15 lines of *Mathematica* code (available from the author) are used to find the Newton-Cotes weights, then implement (13).

The related variant of (13) for $\gamma_k(a)$ uses

$$f(x) = \frac{\log^k(x+a)}{x+a} \quad \text{and} \quad F(x) = \frac{\log^{k+1}(x+a)}{k+1},$$

and the summation of $f(j)$ in (13) runs from $j = 0$ to $n_1 - 1$ rather than from $j = 1$ to $n_1 - 1$. Similarly, to evaluate the derivative $\zeta^{(\alpha)}(s_0)$ in section 4, (11) is used to estimate the "tail" of the series, where $f(x) = \frac{(\log x)^\alpha}{x^{s_0}}$ and $N \rightarrow \infty$.

7. ERROR CONTROL IN NUMERICAL RESULTS FOR γ_k

Precise error bounds are readily come by if one estimates γ_k using $m = 1$ (i.e., Simpson's rule) or other small m . For high precision estimates of γ_k for small k , or for any estimates at all of γ_k for large k , one must use larger m (otherwise the processor time involved is too great). Unfortunately, using $m \gtrsim 60$ leads to impractical error bounds: crude bounds of the $O(f^{2m+1})$ term in (13) are useless, and tight bounding is problematic since such derivatives generically consist of sums of $(2m + 2)$ terms with large coefficients of varying signs (e.g., the 121st derivative of $f(x) = \log^{150}(x)/x$, as needed in error bounding for the estimate of γ_{150} using

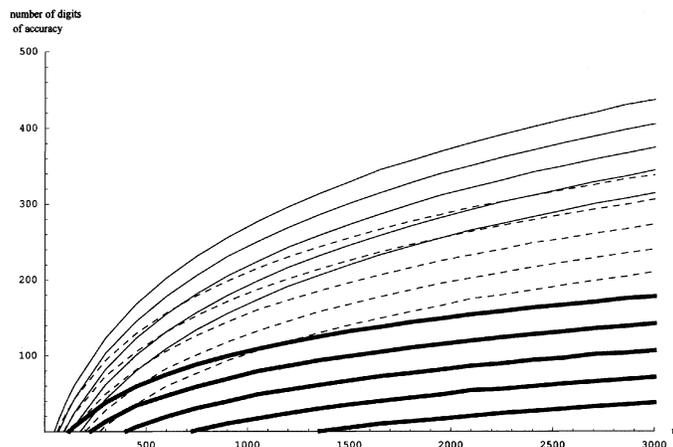


FIGURE 8. Empirical results for a number of digits of accuracy attained while computing γ_k , as a function of n_1 , for various values of k and m . The lowest family of five curves, coded by wide bands, corresponds to $m = 106$; the middle family of five curves, coded by dashed, corresponds to $m = 175$; and the upper family of five curves, coded by solid thin curves, corresponds to $m = 225$. For each m , the curves in the corresponding family represent results for computing γ_k for 400, 500, 600, 700, and 800, from top to bottom, respectively.

$m = 60$, consists of 122 terms, with large coefficients of varying sign). Instead, we propose a heuristic approach to error bounding.

For each m , (13) specifies a different approximation formula, using different weights for the correction terms (since both S and s_j depend on m). We postulate that these different formulas yield errors that are in a practical sense “numerically independent” of one another—not even of the same order of magnitude, in general. Specifically, let v_1 denote the value for the estimate of γ_k using $m = m_1$ (for some n_1) in (13), and v_2 denote the value obtained from using $m = m_2$ (from some different n_1 , denoted n_2), with $m_2 \neq m_1$. Then if v_1 and v_2 agree to N digits, we maintain that we have achieved an estimate of γ_k accurate to (almost) N digits; or, more appropriately, to $N - j$ digits with probability at least $1 - 10^{-j}$ (e.g., to $N - 6$ digits with probability⁵ .999999). In obtaining the values in sections 2-4 of this paper, we implemented (13) using $m = 60, 70, 101, 106, 225, 325, 345$ and 360 to insure accuracy. Moreover, our values are in complete agreement with the independent consistency check described in section 3.

⁵For instance, we postulate that the application of (13) for $m = 60$ (for some value of n_1) yields errors that are “numerically independent” of the application of (13) for, e.g., $m = 106$ (for perhaps some other value of n_1). For both γ_k estimates to agree to N digits, yet produce an erroneous estimate in those N digits, the error term for the first value, essentially $f^{(2m_1+1)}(n_1)$, must have exactly the same order of magnitude as the error term for the second value, essentially $f^{(2m_2+1)}(n_2)$, where $m_1 \neq m_2$ and $n_1 \neq n_2$. We consider such an agreement to be highly unlikely, and so we (nonrigorously) maintain that the only reason digits erroneously agree in two such estimates of γ_k is pure chance. So two estimates agreeing to N digits are accurate to at least $N - j$ digits, with probability at least $1 - 10^{-j}$.

Figure 8 gives some empirical indication of the algorithmic efficiency of (13) in computing γ_k . In that figure, we plot the number of digits of accuracy in γ_k for three values of m , namely $m = 106, 175$ and 225 . For each value of m , five values of k were chosen: $k = 400, 500, 600, 700$ and 800 .

8. REMARK

The difficulty in carefully bounding higher order derivatives of f , and thus obtaining useful error bounds for our estimates of γ_k , is not unique to our method. In fact, Euler-Maclaurin summation methods require accurate estimation of higher order derivative values of f simply to produce an estimate of γ_k , even before attempting to bound the error (which in turn will require bounding yet another derivative of f). We emphasize this crucial distinction between our algorithm and such Euler-Maclaurin methods: our approach does not require precise evaluations of derivatives of f in the estimation process, only in the error bounding. It seems likely that this accounts for at least part of the increased speed of our algorithm compared to other methods that have appeared in the literature.

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