JOURNAL OF RESEARCH of the National Bureau of Standards—Mathematical Sciences
Vol. 76B, Nos. 3 and 4, July–December 1972

# The Stieltjes Constants*

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(July 31, 1972)

The Stieltjes Constants are the coefficients in the Laurent expansion of the Riemann Zeta function $\xi(z)$ about its simple pole at $z=1$. They can be represented as the limit of the difference between the sum of the first $n$ terms of a series and the integral of its $n$-th term.

The first 20 coefficients have been computed to 15 $D$ using the Euler-Maclaurin method. As a by-product the sums of the series

$$\tau_n=\sum_2^\infty (-1)^k(\log k)^n/k$$

have been obtained to 15 $D$ for $n=1(1)20$.

Key words: Bernoulli numbers; Euler-Maclaurin method; Euler transform; Euler's constant; multiple precision package; Riemann zeta function.

## 1. Introduction.

The Riemann $\zeta$-function defined by

$$\zeta(z)=\sum_0^\infty n^{-z} \tag{1.0}$$

is regular if $x=\mathscr{R}z>1$; a continuation into the half plane $\mathscr{R}z>0$ is given by

$$(2^{1-z}-1)\zeta(z)=\sum_1^\infty (-1)^n n^{-z}. \tag{1.0$'$}$$

We can avoid the introduction of the idea of continuation by defining $\zeta(z)$ in $\mathscr{R}z>0$, except at $z=1$, by (1.0′). Uniform convergence in $\mathscr{R}z>0$ follows since $\Sigma(-1)^n n^{-x}$ is convergent as an alternating series for $x>0$. (Cf. Knopp. [10, p. 441][1].) The fact that

$$(z-1)\zeta(z)\rightarrow 1$$

as $z\rightarrow 1$ then follows since $\sum\limits_1^\infty (-1)^n n^{-1}=-\log 2$ and since the exponential series gives

$$\begin{aligned}(2^{1-z}-1)&=e^{(1-z)\log 2}-1\\ &=-(z-1)\log 2\left[1+\frac{(z-1)\log 2}{2!}+\dots\right].\end{aligned}$$

This function has a Laurent expansion about the simple pole at $z=1$:

$$\zeta(z)=\frac{1}{z-1}+A_0+A_1(z-1)+A_2(z-1)^2+A_3(z-1)^3+\dots \tag{1.1}$$

AMS Subject classification: Primary 10H05, Secondary 65B10, 65B15.
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[1] Figures in brackets indicate the literature references at the end of this paper.

where the coefficients are given by

$$A_n = (-1)^n \gamma_n / n!$$

where

$$\gamma_n = \lim_{m\to\infty} \left\{ \sum_{k=1}^{m} \frac{(\log k)^n}{k} - \frac{(\log m)^{n+1}}{n+1} \right\}, \; n=0, 1, 2, \ldots \tag{1.2}$$

(We have changed the notation of Stieltjes and Jensen to agree with that of Hardy and Briggs and Chowla.)

It is clear that $\gamma_0 = \gamma$, Euler's constant. Stieltjes proposed [3, I, Letter 77] the computation of (the first five of) these constants and gave [3, I, Letter 71] the value

$$-A_1 = \gamma_1 = -0.07281\ 5520$$

and estimated

$$A_2 \doteqdot -0.0047$$

Hermite [3, I, Letter 74] wrote that, during a session of the Academy of Sciences, he found some objections to Stieltjes' proof of (1.2) and that he had obtained a more correct proof. Stieltjes [3, I, Letter 75] gave a detailed proof of (1.2). This result was also obtained by Jensen ([9] and [3, II, p. 451]) and stated by Hardy [8] and by Ramanujan [12]. Two proofs have been given recently by Briggs and Chowla [2]—we reproduce one of these in section 4.

We note that tables of the $A$'s have been prepared by Jensen [9], who gives $A_i$, $i = 1\,(1)\,9$ to $9D$, and by Gram [7], who gives $A_i, i = 1(1)\ 16$ to $16D$. In section 9 we describe Gram's method of computation. In each table the later coefficients are zero to the number of decimals given. We shall see that these results appear to be correct. It is interesting to note that one of the reasons for calculating these constants was the determination of the small complex zeros of $\zeta(s)$. (See also Lammel [21].) The apparently irregular behavior of these coefficients has been investigated analytically by Briggs [1].

Our first calculations were based on extensions by Hardy [8] of a result of Vacca [15] which leads to expressions for the $\gamma$'s in terms of elementary constants and the series

$$\tau_n = \sum_{k=2}^{\infty} (-1)^k \frac{(\log k)^n}{k}, \qquad n = 0,1,2, \ldots.$$

For instance, Hardy gave

$$\tau_0 = 1 - \log 2 = 1 - 0.69314\ 718 = 0.30685\ 282$$

$$\tau_1 = -\frac{1}{2} (\log 2)^2 + \gamma \log 2 = 0.15986\ 890$$

$$\tau_2 = -\frac{1}{3} (\log 2)^3 + \gamma\ (\log 2)^2 + 2\gamma_1 \log 2 = 0.06537\ 259.$$

(We have corrected errors of sign in Hardy's expressions for $\tau_1$, $\tau_2$.) The general form of the relations connecting the $\tau$'s and $\gamma$'s has been given by Briggs and Chowla and is discussed in section 3. We calculated the $\tau$'s by use of a delayed Euler transform and then obtained the $\gamma$'s by solving the triangular system of linear equations. However (see sec. 5) this method proved unsatisfactory and we made direct calculations of the $\gamma$'s using the Euler-Maclaurin series. This is a natural extension of the calculations made by Knuth [11] in which he obtained $\gamma$ to 1271 $D$. Error estimates are easier to obtain in the Euler-Maclaurin computation, but these computations are more lengthy than the direct ones.

We have only given error estimates for the cases of $\gamma_1$, $\gamma_2$ but representative computations for the later $\gamma$'s suggest that our values of $\gamma$ are secure. We have therefore to regard the $\gamma$'s as our primary results and the $\tau$'s as derived from them.

Our interest in the present problem was aroused by an entry (giving $\gamma_1$) in the tables of Wheelon [6] which we used for exercises in courses dealing with the Euler transforms.

Professor H. Zassenhaus has called our attention to rapidly convergent series for $\gamma$ obtained by Jacobstahl [24] (see also Addison [25]) which might lead to alternative attacks on the higher $\gamma$'s.

## 2. The $\gamma$'s

The limits by which the $\gamma$'s are defined clearly exist, e.g., in view of a supplement to the integral test (Knopp, [10, p. 295]), since

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

is ultimately decreasing because

$$f_k'(x)=\frac{(\log x)^{k-1}}{x^2}[k-\log x],$$

which is negative for $x>e^k$. The sequences $\gamma_k^{(1)}, \gamma_k^{(2)}, \gamma_k^{(3)}, \ldots$ where

$$\gamma_k^{(n)}=\sum_{\nu=1}^{n}\frac{(\log \nu)^k}{\nu}-\frac{1}{k+1}(\log n)^{k+1}-\gamma_k$$

are ultimately monotone decreasing since

$$\begin{aligned}\gamma_k^{(n)}-\gamma_k^{(n+1)}&=\frac{1}{k+1}(\log (n+1))^{k+1}-\frac{1}{k+1}(\log n)^{k+1}-\frac{(\log (n+1))^k}{n+1}\\&=\int_n^{n+1} f_k(t)\,dt-f_k(n+1)\qquad\qquad(2.1)\\&>0 \text{ if } f_k(t) \text{ is decreasing for } t\geqslant n, \text{ i.e., if } n\geqslant e^k.\end{aligned}$$

We shall now investigate the size of $\gamma_k^{(n)}$, i.e., the speed of convergence of

$$\sum_{\nu=1}^{n}\frac{(\log \nu)^k}{\nu}-\frac{1}{k+1}(\log n)^{k+1}$$

to its limit $\gamma_k$. It will appear that

$$\gamma_k^{(n)}=\frac{1}{2}\frac{(\log n)^k}{n}+0(n^{-2+\epsilon})\qquad(2.2)$$

which means that direct computation of $\gamma_k$ does not come in question. We follow the analysis given in the case $k=0$ by Francis and Littlewood [5, (Question B7, p. 2, 19)].

We require the following lemma which is a simple case of the Euler-Maclaurin formula. (See Hardy [22, p. 300, Ex. 4]).



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LEMMA. *If* g *is three times differentiable in* $[0, 1]$ *then*

$$g(1) = g(0) + \frac{1}{2}[g'(0) + g'(1)] - \frac{1}{12}g'''(\theta)$$

*where* $0 < \theta < 1$.
PROOF. Consider

$$G(x) = g(x) - g(0) - \frac{1}{2}x[g'(0) + g'(x)] - x^3\left[g(1) - g(0) - \frac{1}{2}\{g'(0) + g'(1)\}\right].$$

We have

$$G'(x) = g'(x) - \frac{1}{2}[g'(0) + g'(x)] - \frac{1}{2}xg''(x) - 3x^2\left[g(1) - g(0) - \frac{1}{2}\{g'(0) + g'(1)\}\right]$$

and

$$G''(x) = -\frac{1}{2}xg'''(x) - 6x\left[g(1) - g(0) - \frac{1}{2}\{g'(0) + g'(1)\}\right].$$

We note that $G(0) = G(1) = 0$ and so $G'(\theta_0) = 0$ for some $\theta_0$, $0 < \theta_0 < 1$. Also $G'(0) = 0$. Hence $G''(\theta) = 0$ for some $\theta$, $0 < \theta < \theta_1$. Since $\theta \neq 0$ we have

$$g'''(\theta) = -12\left[g(1) - g(0) - \frac{1}{2}\{g'(0) + g'(1)\}\right]$$

which is the result required.

Applying the lemma in the case

$$g(x) \equiv (\log(x + n))^{k+1}/(k+1),$$

gives (cf. (2.1)):

$$\begin{aligned}\frac{(\log(n+1))^{k+1}}{k+1} - \frac{(\log n)^{k+1}}{k+1} - \frac{(\log(n+1))^k}{n+1} &= \gamma_k^{(n)} - \gamma_k^{(n+1)} \\ &= \frac{1}{2}[f_k(n) - f_k(n+1)] + e(n,k)\end{aligned} \tag{2.3}$$

where

$$e(n,k) = O((\log n)^k/n^3).$$

Summing (2.3) for $n=m$ to $m=M-1$ gives for a suitable $K$,

$$\gamma_k^{(m)} - \gamma_k^{(M)} \geqslant \frac{1}{2}[f_k(m) - f_k(M)] - K\sum_{n=m}^{M-1}(\log n)^k/n^3$$

and

$$\gamma_k^{(m)} - \gamma_k^{(M)} \leqslant \frac{1}{2}[f_k(m) - f_k(M)] + K\sum_{n=m}^{M-1}(\log n)^k/n^3.$$

Letting $M \to \infty$ gives, for any $\epsilon > 0$,

$$\gamma_k^{(m)} = \frac{1}{2} f_k(m) + O(m^{-2+\epsilon})$$

which is the result (2.2) announced.

## 3. Derivation of the $\tau$–$\gamma$ Relations

We have seen that as $n \to \infty$:

$$\sum_{\nu=1}^{n} \frac{(\log \nu)^k}{\nu} = \frac{(\log n)^{k+1}}{k+1} + \gamma_k + o(1). \tag{3.1}$$

Hence

$$\sum_{\nu=1}^{2n} \frac{(\log \nu)^k}{\nu} = \frac{(\log 2n)^{k+1}}{k+1} + \gamma_k + o(1). \tag{3.2}$$

The binomial series for $(\log 2\nu)^k = (\log 2 + \log \nu)^k$ gives

$$\begin{aligned} 2\sum_{\nu=1}^{n} \frac{(\log 2\nu)^k}{2\nu} &= \sum_{\nu=1}^{n} \frac{1}{\nu}\left\{\sum_{t=0}^{k} \tbinom{k}{t}(\log 2)^{k-t}(\log \nu)^t\right\} \\ &= \sum_{t=0}^{k} \binom{k}{t} (\log 2)^{k-t} \sum_{\nu=1}^{n} \frac{(\log \nu)^t}{\nu} \\ &= \sum_{t=0}^{k} \binom{k}{t} (\log 2)^{k-t}\left[\frac{(\log n)^{t+1}}{t+1} + \gamma_t + o(1)\right] \end{aligned} \tag{3.3}$$

where we have used (3.1) in the last stage.

Integrating (with respect to $\beta$) the binomial expansion of $(a+\beta)^k$ from 0 to $b$, or otherwise, we find

$$\sum_{t=0}^{k} \binom{k}{t} a^{k-t} \frac{b^{t+1}}{t+1} = \left[\frac{(a+\beta)^{k+1}}{k+1}\right]_0^b = \frac{(a+b)^{k+1}}{k+1} - \frac{a^{k+1}}{k+1}.$$

We use this with

$$a = \log 2, \qquad b = \log n$$

to get

$$\sum_{t=0}^{k} \binom{k}{t} (\log 2)^{k-t} \frac{(\log n)^{t+1}}{t+1} = \frac{(\log 2n)^{k+1}}{k+1} - \frac{(\log 2)^{k+1}}{k+1}. \tag{3.4}$$

Substituting from (3.4) in (3.3) we get

$$2\sum_{\nu=1}^{n} \frac{(\log 2\nu)^k}{2\nu} = \frac{(\log 2n)^{k+1}}{k+1} - \frac{(\log 2)^{k+1}}{k+1} + \sum_{t=0}^{k} \binom{k}{t} (\log 2)^{k-t}\gamma_t + o(1) \tag{3.5}$$

and then subtracting (3.5) from (3.2) gives

$$-\sum_{\nu=1}^{2n} \frac{(-1)^{\nu-1}(\log \nu)^k}{\nu} = -\frac{(\log 2)^{k+1}}{k+1} + \sum_{t=0}^{k-1} \binom{k}{t} (\log 2)^{k-t}\gamma_t + o(1),$$

the last term ($t=k$) in the summation with respect to $t$ cancelling the $\gamma_k$ on the right of (3.2). We now let $n\rightarrow\infty$ and find

$$\tau_k=-\frac{(\log 2)^{k+1}}{k+1}+\sum_{t=0}^{k-1}\binom{k}{t}(\log 2)^{k-t}\gamma_t. \tag{3.6}$$

For $k=1, 2, \ldots$ we find

$$\tau_1=-\frac{1}{2}(\log 2)^2+\gamma\log 2$$

$$\tau_2=-\frac{1}{3}(\log 2)^3+\gamma(\log 2)^2+2\gamma_1\log 2$$

$$\tau_3=-\frac{1}{4}(\log 2)^4+\gamma(\log 2)^3+3\gamma_1(\log 2)^2+3\gamma_2\log 2.$$

The result for $k=0$ is, trivially,

$$\tau_0=\left(\frac{1}{2}-\frac{1}{3}+\frac{1}{4}\ldots\right)=1-\left(1-\frac{1}{2}+\frac{1}{3}-\ldots\right)=-\log 2+1.$$

## 4. Proof of Representation

If we differentiate the relation

$$g(z)\equiv(2^{1-z}-1)\zeta(s)=\sum_{n=1}^{\infty}(-1)^n n^{-z}$$

$k$ times with respect to $z$ we get

$$g^{(k)}(z)=(-1)^k\sum_{n=1}^{\infty}(-1)^n(\log n)^k/n^z$$

and, in particular,

$$g^{(k)}(1)=(-1)^k\tau_k. \tag{4.1}$$

We have

$$(2^{1-z}-1)=e^{-(z-1)\log 2}-1=\sum_{n=1}^{\infty}\frac{(-1)^n(\log 2)^n}{n!}(z-1)^n$$

and multiplying this by

$$\zeta(s)=(z-1)^{-1}+\sum_{0}^{\infty}A_n(z-1)^n$$

we get

$$g(z)=\sum_{k=0}^{\infty}\sum_{t=1}^{k+1}\frac{(-1)^t(\log 2)^t}{t!}A_{k-t}(z-1)^k$$

where $A_{-1}=1$. Hence

$$g^{(k)}(1)=k!\sum_{t=1}^{k+1}\frac{(-1)^t(\log 2)^t}{t!}A_{k-t}. \tag{4.2}$$

We now use the representation (3.6) for $\tau_k$ to find from (4.1) and (4.2)

$$(-1)^k\left[-\frac{(\log 2)^{k+1}}{k+1}+\sum_{t=0}^{k-1}\binom{k}{t}(\log 2)^{k-t}\gamma_t\right]=k!\sum_{t=1}^{k+1}\frac{(-1)^t(\log 2)^t}{t!}A_{k-t}. \tag{4.3}$$

If we use this relation for $k=1, 2, 3$ respectively we find

$$\gamma=\gamma_0=A_0,$$

$$\gamma_1=-A_1,$$

$$\gamma_2=2!A_2.$$

These suggest the general solution

$$\gamma_n=(-1)^n n!\,A_n$$

which is readily verified. The term outside the summation on the left in (4.3),

$$(-1)^{k+1}(\log 2)^{k+1}/(k+1),$$

is the same as the term for $t=k+1$ in the summation as the right. Then the $t$-th term on the left, for $t=0, 1, \ldots, k-1$, can be identified with the $(k-t)$-th term on the right.

## 5. Calculation of the $\tau$'s by Euler Transforms

Knowing the efficiency of the Euler transform in handling the logarithmic series, it is natural to apply this to calculate the $\tau$'s.

Specifically, the Euler transform of $\Sigma(-1)^n/n$, when there is a delay of $r$, is

$$1-\frac{1}{2}+\frac{1}{3}-\ldots+(-1)^{r-1}\frac{1}{r}+(-1)^r\frac{1}{r+1}\left[\frac{1}{2}+\frac{1}{4}\cdot\frac{1}{r+2}+\frac{1}{8}\cdot\frac{1\cdot 2}{r+2\cdot r+3}+\ldots\right].$$

Since the sequence $\{n^{-1}\}$ is completely monotone, all the terms in the tail of the transform are of one sign and we can readily estimate the error. When we take $n$ terms in the tail this error is

$$\log 2-(s(r)+c(r,n))=(-1)^r\frac{1}{r+1}\left[\frac{1}{2^{n+1}}\cdot\frac{1\cdot 2\cdot\cdots\cdot n}{r+2\cdot r+3\cdot\cdots\cdot(r+n+1)}+\ldots\right]$$

and is less in absolute value than

$$((r+1)2^{n+1})^{-1}.$$

Various hypotheses lead to various optimal choices of $r,n$. But these are not critical. It has also been pointed out that the optimal choice of $r,n$ did not seem to depend critically on the (alternating) series being summed (see, e.g. Todd, [14]).

The Euler transform is, of course, convergent if the original series is, but improvement in the speed of convergence of $\Sigma(-1)^n u_n$ has only been established in case the sequence $\{u_n\}$ is completely monotone and if $(u_{n+1}/u_n)\geqslant k>\frac{1}{2}$ (see, e.g., Knopp [10, p. 253]).

When $u_n$ is completely monotone the terms in the remainder are all of one sign and error estimates are easy to obtain. However the terms in $\tau_k$ are not even monotone: since

$$\frac{d}{dx}\left[\frac{(\log x)^k}{x}\right]=\frac{(\log x)^{k-1}}{x^2}[k-\log x]$$

we expect the terms in $\tau_k$ to increase up to about the $[e^k]$ -th and then to decrease. Continuing we see that

$$\frac{d^2}{dx^2}\left[\frac{(\log x)^k}{x}\right]=\frac{(\log x)^{k-2}}{x^3}[2(\log x)^2-3k\log x+k(k-1)]$$

which vanishes for

$$\log x=\frac{3}{4}k\pm\frac{1}{4}\sqrt{k^2+8}$$

so that the second difference may be expected to decrease, become negative and then increase to positive values.

We have not obtained useful error bounds for the Euler transforms of the $\tau_k\,(k>1)$.

We shall discuss these matters in some detail elsewhere.

## 6. Calculation of the $\gamma$'s from the $\tau$'s

In section 3 we have derived the relations:

$$\tau_n=-(\log 2)^{n+1}/(n+1)+\sum_{r=0}^{n-1}\binom{n}{r}(\log 2)^{n-r}\gamma_r,\ n=1,2,3,\ldots, \tag{3.6}$$

which we have used to compute the $\tau$'s from the $\gamma$'s. From this triangular system of linear equations it is also trivial to obtain the $\gamma$'s, given the $\tau$'s. Although the solution of a triangular system is a numerically stable process (see, e.g., Wilkinson [17, 247]) we have obtained the exact inverse of the $20\times 20$ matrix

$$A=[a_{ij}],\ a_{ij}=\begin{cases}\binom{i}{j} & j=0,1,2,\ldots,i-1\\ 0 & j>i\end{cases}\qquad i=1,2,\ldots$$

so that the $\gamma$'s can be obtained with less rounding from the $\tau$'s.

$$\begin{bmatrix}\gamma_0\\ \gamma_1/\log 2\\ \cdots\\ \gamma_{n-1}/(\log 2)^{n-1}\end{bmatrix}=A^{-1}\times\begin{bmatrix}\frac{1}{2}\log 2+\tau_1/\log 2\\ \frac{1}{3}\log 2+\tau_2/(\log 2)^2\\ \cdots\\ \frac{1}{n+1}\log 2+\tau_n/(\log 2)^n\end{bmatrix}$$

It is easy to find $A^{-1}$ when $n=10$, e.g., by inverting $A$ and identifying the appropriate rational entries in $A^{-1}$. Specifically, we find

$$A^{-1}=\begin{bmatrix} 1 &&&&&&&&& \\ -\frac{1}{2} & \frac{1}{2} &&&&&&&& \\ \frac{1}{6} & -\frac{1}{2} & \frac{1}{3} &&&&&&& \\ 0 & \frac{1}{4} & -\frac{1}{2} & \frac{1}{4} &&&&&& \\ -\frac{1}{30} & 0 & \frac{1}{3} & -\frac{1}{2} & \frac{1}{5} &&&&& \\ 0 & -\frac{1}{12} & 0 & \frac{5}{12} & -\frac{1}{2} & \frac{1}{6} &&&& \\ \frac{1}{42} & 0 & -\frac{1}{6} & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{7} &&& \\ 0 & \frac{1}{12} & 0 & -\frac{7}{24} & 0 & \frac{7}{12} & -\frac{1}{2} & \frac{1}{8} && \\ -\frac{1}{30} & 0 & \frac{2}{9} & 0 & -\frac{7}{15} & 0 & \frac{2}{3} & -\frac{1}{2} & \frac{1}{9} & \\ 0 & -\frac{3}{20} & 0 & \frac{1}{2} & 0 & -\frac{7}{10} & 0 & \frac{3}{4} & -\frac{1}{2} & \frac{1}{10} \end{bmatrix}$$

This naive approach will not work to find $A^{-1}$ in the $20\times 20$ case, owing to the condition of $A$. We are indebted to Morris Newman for providing us with the inverse in the general case:

$$[A^{-1}]_{ij}=\begin{cases} 0 \text{ if } i<j \\ \binom{i}{j}\frac{B_{i-j}}{i}, \; i\geqslant j \end{cases} \qquad i=1,2,\ldots$$

where the $B_k$'s are the Bernoulli numbers ($B_0=1$, $B_1=-\frac{1}{2}$, $B_2=\frac{1}{6}$, $B_3=0$, etc.)which are readily available as rational fractions or as decimals. Incidentally the characteristic vectors of $A$ can be expressed as Stirling numbers of the second kind.

## 7. Calculation of the $\gamma$'s by Euler-Maclaurin

The Euler-Maclaurin summation formula can be written as

$$\sum_{j=p}^{q} f(j)-\int_p^q f(t)dt=\frac{1}{2}\{f(p)+f(q)\}+\sum_{j=1}^{k}\frac{B_{2j}}{(2j)!}\{f^{(2j-1)}(q)-f^{(2j-1)}(p)\}+R_k(p,q), \tag{7.0}$$

where the $B_k$'s are the Bernoulli numbers, $B_2=\frac{1}{6}$, $B_4=\frac{-1}{30}$, $B_6=\frac{1}{42}$, . . .. We give expressions for the remainder:

$$R_k(p,q)=\frac{1}{(2k+1)!}\int_p^q P_{2k+1}(t)\, f^{(2k+1)}(t)\, dt, \tag{7.1a}$$

where

$$P_{2k+1}(t)=\sum_{\nu=1}^{\infty}\frac{2\sin 2\nu\pi t}{(2\pi\nu)^{2k+1}};$$

$$R_k(p,q)=\frac{-1}{(2k)!}\int_0^1 B_{2k}(t)\left[\sum_{\nu=p}^{q-1}f^{(2k)}(\nu+t)\right]dt, \tag{7.1b}$$

where $B_{2k}(t)$ is the Bernoulli polynomial. For up-to-date discussions of these results see Ostrowski [19].

We use (7.0) in the following way. We first take $p=1$, $q=n$:

$$\mathscr{E}(n)\equiv\sum_{j=1}^{n}f(j)-\int_1^n f(t)dt=\frac{1}{2}[f(n)+f(1)]+\sum_{j=1}^{k}\frac{B_{2j}}{(2j)!}\{f^{(2j-1)}(n)-f^{(2j-1)}(1)\}+R_k(1,n). \tag{7.2a}$$

We next assume $f$ is such that $f^{(\mu)}(t)\to 0$ for all relevant $\mu$ and that $R_k(1,\infty)$ exists. Letting $n\to\infty$ gives

$$\lim\left[\sum_{j=1}^{n}f(j)-\int_1^n f(t)dt\right]=\frac{1}{2}f(1)+\sum_{j=1}^{k}\frac{B_{2j}}{(2j)!}\{-f^{(2j-1)}(1)\}+R_k(1,\infty). \tag{7.2b}$$

If we now subtract (7.2a) from (7.2b) we get

$$\lim_{m\to\infty}\mathscr{E}(m)=\mathscr{E}_n-\frac{1}{2}f(n)-\sum_{j=1}^{k}\frac{B_{2j}}{(2j)!}f^{(2j-1)}(n)+R_k(n,\infty). \tag{7.3}$$

This is the formula which is used to calculate the $\gamma$'s. We have to choose $n$, $k$ so that $R_k(n,\infty)$ is appropriately small. In the cases with which we are concerned, the series

$$\sum t_j\equiv\sum_{j=1}^{\infty}\frac{B_{2j}}{(2j)!}f^{(2j-1)}(n)$$

is easily seen to be divergent using the well known (Knopp, [10, p. 237]) estimates for $B_{2j+2}/B_{2j}$ and the form of $f^{(2j-1)}(t)$ when $f(t)=(\log t)^k/t$. Indeed, using the expression for $f^{(r)}(t)$ given below (7.11), we find

$$\left|\frac{t_{j+1}}{t_j}\right|=\left|\frac{B_{2j+2}}{B_{2j}}\right|\times\frac{1}{(2j+1)(2j+2)}\times\frac{f^{(2j+1)}(n)}{f^{(2j-1)}(n)}$$

$$\approx\frac{(2j+1)(2j+2)}{4\pi^2}\times\frac{1}{(2j+1)(2j+2)}\times\frac{(2j+1)(2j+2)}{n^2}$$

which tends to infinity with $j$, $n$ and $k$ being fixed.

We shall discuss the behavior of $R_k(n,\infty)$ in the case of $\gamma_1$, $\gamma_2$ using Ostrowski's estimate for (7.1b). We shall begin with an examination of $\gamma$ using (7.1a) which is a convenient way of finding an estimate which we require.

Taking $f(x)=x^{-1}$ in (7.3) we have, with the remainder in the form (7.1a),

$$\gamma=1+\frac{1}{2}+\cdot\cdot\cdot+\frac{1}{n}-\log n-\frac{1}{2n}+\int_n^{\infty}P_1(t)\left[\frac{-1}{t^2}\right]dt$$

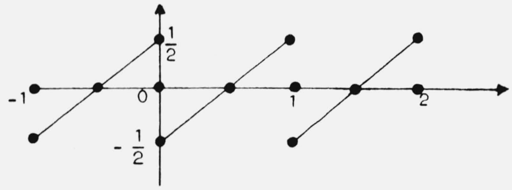
so that

$$1+\frac{1}{2}+\cdot\cdot\cdot+\frac{1}{n}=\log n+\gamma+\frac{1}{2n}+\int_n^\infty P_1(t)t^{-2}dt.$$

By the Second Mean Value Theorem, there is an $\eta \geqslant n$ such that

$$\int_n^\infty P_1(t)t^{-2}dt=n^{-2}\int_n^\eta P_1(t)dt.$$

Now it is known that the graph of $P_1(t)$ has the following form:




It follows that $0 \geqslant \int_n^\eta P_1(t)dt \geqslant -1/8$. Hence

$$\log n+\gamma+\frac{1}{2n}\geqslant 1+\frac{1}{2}+\cdot\cdot\cdot+\frac{1}{n}\geqslant \log n+\gamma+\frac{1}{2n}-\frac{1}{8n^2}\cdot \tag{7.4}$$

We shall use this result presently.

By a similar argument, starting from

$$\gamma_1=\frac{\log 2}{2}+\frac{\log 3}{3}+\cdot\cdot\cdot+\frac{\log n}{n}-\frac{1}{2}(\log n)^2-\frac{\log n}{2n}+\int_n^\infty P_1(t)\frac{[1-\log t]}{t^2}dt$$

we obtain

$$\frac{1}{2}(\log n)^2+\gamma_1+\frac{\log n}{2n}\geqslant\frac{\log 1}{1}+\frac{\log 2}{2}+\ldots+\frac{\log n}{n}$$

$$\geqslant\frac{1}{2}(\log n)^2+\gamma_1+\frac{\log n}{2n}-\frac{1}{8}\left[\frac{1-\log n}{n^2}\right]. \tag{7.5}$$

(Cf. Boas and Wrench [20].)

We now want to discuss the error in (7.3) in the case of $\gamma_1$, i.e., when $f(t)\equiv f_1(t)=(\log t)/t$. We have to find the derivatives of $f_1(t)$.

LEMMA 1. *If* $f_1(x)=(\log x)/x$ *then for* $r\geqslant 0$ *we have*

$$f_1^{(r)}(x)=\frac{(-1)^r(r!)}{x^{r+1}}[\log x-d_r] \tag{7.6}$$

*where* $d_0=1$ *and for* $r>0$

$$d_r=1+\frac{1}{2}+\ldots+\frac{1}{r}.$$

PROOF. Induction.

The error estimate given by Ostrowski is

$$|R_k(n,\infty)| \leqslant \frac{1}{2}\left(1-\frac{1}{2^{2k}}\right)\frac{|B_{2k}|}{(2k)!}|f^{(2k)}(n)| \tag{7.7}$$

and this is valid if $f^{(2k)}(x)$ is monotonic in $(n,\infty)$. In our case we shall examine when $f^{(2k+1)}(x)$ is of one sign in $(n,\infty)$. In view of Lemma 1 we have to determine a value of $x$ for which

$$\log x > d_{2k+1}.$$

Using the estimate (7.4) we see that we require

$$\log x > \log(2k+1)+\gamma+\frac{1}{2(2k+1)}-\frac{1}{8(2k+1)^2}$$

i.e.,

$$x > (2k+1)\, e^{\gamma} \exp\left(\frac{1}{2(2k+1)}-\frac{1}{8(2k+1)^2}\right).$$

For $k=10$ this gives

$$x > 21\times 1.7811\times 1.025 = 38.34.$$

A rough estimate of the error in the case $k=10$, $n=40$ is, from (7.7),

$$\frac{1}{2}\cdot 1\cdot\frac{|B_{20}|}{(20)!}\cdot\frac{(20)!}{40^{21}}\left[\log 40-\left(1+\frac{1}{2}+\ldots+\frac{1}{20}\right)\right]=\frac{1}{2}\cdot\frac{5.2912\times 10^{2}}{40^{21}}[3.6889-3.5977]$$

which is certainly negligible to the precision tabulated.

We now turn to the case of $\gamma_2$. The analogue of Lemma 1 is

LEMMA 2. *If* $\mathrm{f}_2(\mathrm{x}) = (\log \mathrm{x})^2/\mathrm{x}$ *then for* $\mathrm{r} \geqslant 0$

$$\mathrm{f}_2^{(\mathrm{r})}(\mathrm{r}) = \frac{(-1)^{\mathrm{r}}\mathrm{r}!}{\mathrm{x}^{\mathrm{r}+1}}[\mathrm{a}_\mathrm{r}-\mathrm{b}_\mathrm{r}\log \mathrm{x}+(\log \mathrm{x})^2] \tag{7.8}$$

*where* $\quad \mathrm{a}_0 = \mathrm{b}_0 = 0$ *and for* $\mathrm{r} \geqslant 0$

$$\mathrm{b}_{\mathrm{r}+1} = \mathrm{b}_\mathrm{r} + 2/(\mathrm{r}+1) \text{ giving } \mathrm{b}_\mathrm{r} = 2\left[1+\frac{1}{2}+\ldots+\frac{1}{\mathrm{r}}\right],\ \mathrm{a}_{\mathrm{r}+1} = \mathrm{a}_\mathrm{r} + \mathrm{b}_\mathrm{r}/(\mathrm{r}+1). \tag{7.9}$$

PROOF. Induction.

In order to apply our estimates we have to find a value of $x_0(r)$ such that

$$E(r,x) \equiv [a_r - b_r \log x + (\log x)^2] \geqslant 0$$

if $x \geqslant x_0(r)$. From the recurrence relations defining the $\{a_r\}$, $\{b_r\}$ we conclude that $b_r \sim 2\log r$, $a_r \sim (\log r)^2$ which suggests that the critical value will be $O(r)$. Computations also suggest that we may take $x_0 = O(r)$. We examine this theoretically.

From the recurrence relations (7.9) we have

$$E(r+1,x)-E(r,x)=\frac{b_r}{r+1}-\frac{2\log x}{r+1}.$$

Summing this we find

$$E(r, x) = (\log x)^2 - 2(\log x)d_r + \sum_{s=1}^{r-1} (b_s/(s+1)).$$

We shall use our estimates (7.4), (7.5) to approximate $E(r, x)$. We have, with errors of O(1),

$$E(r, x) \doteqdot (\log x)^2 - 2(\log x)\{\log r + \gamma\} + 2\sum_{s=1}^{r-1}\left\{\frac{\log(s+1)}{s+1} + \frac{\gamma}{s+1} - \frac{1}{2(s+1)^2}\right\}$$

$$\doteqdot (\log x)^2 - 2(\log x)\{\log r + \gamma\} + (\log r)^2 + 2\gamma \log r.$$

Trying $x = 2r$, i.e., $\log x = \log r + \log 2$, in this we get, to the same accuracy,

$$\begin{aligned} E(r, 2r) &\doteqdot (\log r)^2 + 2(\log r)(\log 2) - 2(\log r)^2 - 2(\log r)(\log 2 + \gamma) \\ &\quad + (\log r)^2 + 2\gamma(\log r) \\ &= 0. \end{aligned}$$

More precise investigations can be made but this discussion seems adequate in the context of practical computation.

We shall now indicate an alternative approach. Let $t_r$ be the larger root of the quadratic $a_r - b_r t + t^2 = 0$, i.e., $t_r = \frac{1}{2}(b_r + \sqrt{b_r^2 - 4a_r})$. Then any number larger than $\exp t_r$ can be taken as $x_0$. From the recurrence relations (7.9) we have, if $\Delta_r = b_r^2 - 4a_r$,

$$\Delta_{r+1} - \Delta_r = 4(r+1)^{-2}.$$

Summing this we find

$$\Delta_r = 4\left(1 + \frac{1}{2^2} + \cdots + \frac{1}{r^2}\right)$$

$$= 4\left\{\frac{\pi^2}{6} - \left(\frac{1}{(r+1)^2} + \frac{1}{(r+2)^2} + \cdots\right)\right\}$$

$$< \frac{2\pi^2}{3} - 4\left\{\frac{1}{(r+1)(r+2)} + \frac{1}{(r+2)(r+3)} + \cdots\right\}$$

$$= \frac{2\pi^2}{3} - \frac{4}{r+1}.$$

From (7.4) we find

$$t_r < \log r + \gamma + \frac{1}{2r} + \left(\frac{\pi^2}{6} - \frac{1}{r+1}\right)^{1/2}$$

$$< \log r + \gamma + \frac{1}{2r} + \frac{\pi}{\sqrt{6}}\left(1 - \frac{3}{\pi^2(r+1)}\right)$$

$$< \log r + \left(\gamma + \frac{\pi}{\sqrt{6}}\right) + \frac{1}{2r} - \frac{\sqrt{3}}{\sqrt{2}\,\pi(r+1)}$$

$$\doteqdot \log r + 1.8599.$$

This estimate is in agreement with computations. We find

$$a_{25}=0.1296\times 10^2, \qquad b_{25}=0.7632\times 10^1, \qquad \log 25=0.3219\times 10^1, \qquad t_{25}=0.5083\times 10^1$$

Hence we can take $x_0(r) = 6.5 \times r$.

We give here a typical exploratory calculation which we made in the case of $\gamma_2$:

| | | | | |
|---|---|---|---|---|
| $n=400$: 3 Bernoulli terms give | $-0.12455$ | 57727 | 57476 | $(-4)$ |
| which with the head of series gives $\gamma_2=$ | $-0.96903$ | 63192 | 87234 | $(-2)$ |

We use the Ostrowski error estimate (7.7) which in the present case is:

$$\frac{1}{2}\left(1-\frac{1}{2^6}\right)\frac{B_6}{6!}\left[\frac{6!}{n^7}\{a_6-b_6\log n+(\log n)^2\}\right];$$

This is valid if $\log n$ exceeds the larger root of $a_6-b_6\,t+t^2=0$, where $a_6=203/45$ and $b_6=49/10$, which is $t_6=3.6712$. With $n=400$, $\log n \doteqdot 6$. The term in braces $\{\ldots\}$ is about 11 and so the truncation error estimate is about $10^{-19}$—so that the round off errors will dominate. Note that in dealing with the head of the series we are summing 400 terms, each involving the square (or cube) of a logarithm.

We have not made any detailed error analyses for the cases of $\gamma_m$, for $m>2$. In our final computations we have taken $n=400$. For instance, in the case of $\gamma_{15}$,

| | | | | |
|---|---|---|---|---|
| 3 Bernoulli terms give | 0.36042 | 49967 | 32360 | $(+6)$ |
| which with the head of the series gives $\gamma_{15}=$ | $-0.28369$ | 16022 | 44191 | $(-3)$ |

so that there is a massive cancellation. Similarly, in the case of $\gamma_{19}$,

| | | | | |
|---|---|---|---|---|
| 3 Bernoulli terms give | 0.67068 | 88575 | 83315 | $(+9)$ |
| which with the head of the series gives $\gamma_{19}=$ | 0.21630 | 66613 | 69313 | $(-3)$ |

It is because of this that we used the Tooper multiple precision package, with quadruple precision.

We conclude this paragraph by recording the recurrence relations which we used to calculate the derivatives needed in the Bernoulli terms and in the error estimates.

LEMMA 3. *If* $f_m(x)=(\log x)^m/x$ *then*

$$f^{(r)}(x)=(-1)^r(r!)\,x^{-r-1}\,[(-1)^m\alpha_{0,r}-(-1)^{m-1}\alpha_{1,r}\log x+\ldots+\alpha_{m,r}(\log x)^m]. \tag{7.10}$$

where

$$\begin{cases} \alpha_{0,\,r+1}=\alpha_{0,\,r}+\dfrac{1}{r+1}\alpha_{1,\,r} \\ \alpha_{1,\,r+1}=\alpha_{1,\,r}+\dfrac{2}{r+1}\alpha_{2,\,r} \\ \quad\cdots \\ \alpha_{m-1,\,r+1}=\alpha_{m-1,\,r}+\dfrac{m}{r+1}\alpha_{m,\,r} \\ \alpha_{m,\,r}\equiv 1 \end{cases} \tag{7.11}$$

with appropriate initial conditions:

$$\alpha_{0,0}=\alpha_{1,0}=\ldots=\alpha_{m-1,0}=0,\ \alpha_{m,0}=1.$$

PROOF. Induction.

Using the same ideas as in our discussion of $f_2^{(r)}$ we can estimate

$$\alpha_{s,r} \doteqdot \binom{m}{s}(\log r)^{m-s}$$

which gives

$$f_m^{(r)}(x) \doteqdot (-1)^r r!\, x^{-r-1}[\log x-\log r]^m$$

and indicates that $f_m^{(r)}(x)$ will be of one sign for $x \geqslant x_0(r)$ where $x_0(r)=O(r)$.

## 8. Gram's Calculations

Gram [7] gives few details of his computations but we can indicate the lines along which they went. He realized that it was not attractive to extend the calculations of Jensen [9] which were based on the definition

$$\zeta(s)=\lim\left\{\sum_{r=1}^{n} r^{-s}-\frac{n^{1-s}}{1-s}\right\}$$

and sought another approach.

The function

$$\xi(s)=\frac{1}{2}s(s-1)\pi^{-s/2}\Gamma\left(\frac{1}{2}s\right)\zeta(s) \tag{8.1}$$

is entire and satisfies the functional equation

$$\xi(s)=\xi(1-s).$$

If we write

$$\Xi(t)=\xi(s),\qquad s=\frac{1}{2}+it \tag{8.2}$$

then $\Xi(t)$ is an even entire function which does not vanish at $t=0$ since $\Xi(0)=\xi\left(\frac{1}{2}\right)=-\frac{1}{8}\pi^{-1/4}\Gamma\left(\frac{1}{4}\right)\zeta\left(\frac{1}{2}\right)$. We can write

$$\log\Xi(it)=a_0+a_1t^2+a_2t^4+\ldots$$

where $a_0=\log\xi\left(\frac{1}{2}\right)$. If we can compute the $a$'s, we can, by exponentiating, get the coefficients in the Maclaurin expansion of $\Xi(t)$ and from this, using (8.1) and (8.2) obtain the coefficients in the Laurent expansion of $\zeta(s)$ about $s=1$.

Gram had available Stieltjes' $32D$ values of $\zeta(s)$, $s=2(1)70$, i.e., in principle, the values of $\log\Xi(it)$ for $\pm it=\frac{3}{2}(1)\frac{139}{2}$. The $a$'s are essentially the values of the (even) derivatives of



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$\log \Xi(it)$ at 0 and can be calculated by using appropriate Lagrangian expressions. For instance, we have (see, e.g., [23])

$$f_{1/2}=\frac{1}{256}(3f_{-2}-25f_{-1}+150f_0+150f_1-25f_2+3f_3)-\frac{5}{1024}\mu\delta^6 f_{1/2}+\ldots$$

$$h^2 f''_{1/2}=\frac{1}{48}(-5f_{-2}+39f_{-1}-34f_0-34f_1+39f_2-5f_3)+\frac{259}{5760}\mu\delta^6 f_{1/2}-\ldots.$$

From these expressions we find, when $f_{-n}=f_{n+1}=\log \Xi\,(i(1/2+n))=\log \xi(n+1)$,

$$a_0 \doteqdot -0.69892\,210,$$

$$a_1 \doteqdot +0.02310\,424.$$

These are to be compared with the values given by Gram

$$a_0=-0.69892\,22679\,45331\,4,$$

$$a_1=+0.02310\,49931\,15419\,0.$$

Gram, actually, made use of independent calculations by himself and Stieltjes of $\zeta(\frac{1}{2})$ which gave $a_0$ directly and his calculations were more complicated and elaborate than ours, e.g., he used the values of $\log \Xi\,(t)$ for $it=\frac{1}{2}\,(1)\,\frac{29}{2}$.

## 9. Tooper's Multiple Precision Package

When we realized that we needed multiple precision calculations we were fortunate to have available a package produced by Professor R. F. Tooper. In this we used one storage place for the exponent of our numbers and four for the mantissa (actually it is possible to use up to 19). Besides the usual arithmetic operations included in this package we used the logarithm subroutine. The logarithms were calculated from the usual series

$$\log\frac{1-x}{1+x}=-2\,[x+\tfrac{1}{3}x^3+\tfrac{1}{3}x^5\ \ldots]$$

after a reduction in the range to $(\frac{1}{2},1)$; a "long division" process was used.

Our preliminary calculations were made on the IBM 360/75 at the California Institute of Technology and the final ones on the IBM 370/155 at the University of South Florida.

We used (7.3), with $n=400$, to compute the $\gamma$'s and $A$'s, and (3.6) to derive the $\tau$'s.

## 10. Tables

*The Stieltjes constants $A_r$*

| | (1) Jensen | | (2) Gram | | | |
|---|---|---|---|---|---|---|
| 0 | 0.57721 | 5665 | 0.57721 | 56649 | 01532 | 9 |
| 1 | .07281 | 5845 | .07281 | 58454 | 83676 | 7 |
| 2 | −.00484 | 5182 | −.00484 | 51815 | 96436 | 1 |
| 3 | −.00034 | 2306 | −.00034 | 23057 | 36717 | 2 |
| 4 | .00009 | 6889 | .00009 | 68904 | 19394 | 4 |

*The Stieltjes constants* $(-1)^r A_r$—Continued

| | (1) Jensen | | (2) Gram | | | |
|---|---|---|---|---|---|---|
| 5 | −. | 6611 | −.00006 | 66110 | 31810 | 8 |
| 6 | −. | 0332 | −. | 03316 | 24090 | 9 |
| 7 | . | 0105 | . | 01046 | 20945 | 9 |
| 8 | −. | 0009 | −. | 00087 | 33218 | 1 |
| 9 | | | . | | 94782 | 7 |
| 10 | | | . | | 56584 | 2 |
| 11 | | | −. | | 06768 | 7 |
| 12 | | | . | | 00349 | 2 |
| 13 | | | . | | 00004 | 4 |
| 14 | | | −. | | 00002 | 4 |
| 15 | | | . | | 00000 | 2 |

Jensen asserted that only the ninth decimal in his values was doubtful. Gram stated that he believed that his results were correct to 15$D$ but could not guarantee this. Our results confirm these statements—the only discrepancies are Jensen's value for $A_4$ and Gram's value for $A_2$, $A_9$.

NEW COMPUTATIONS

| r | The gammas $\gamma_r$ | The Stieltjes constants $A_r$ | The taus $\tau_{r+1}$ |
|---|---|---|---|
| 0 | 0.57721 56649 01533 | 0.57721 56649 01533 | 0.15986 89037 42431 |
| 1 | -0.72815 84548 36767 (-1) | 0.72815 84548 36767 (-1) | 0.65372 59255 88987 (-1) |
| 2 | -0.96903 63192 87232 (-2) | -0.48451 81596 43616 (-2) | 0.94139 50232 49318 (-2) |
| 3 | 0.20538 34420 30335 (-2) | -0.34230 57367 17224 (-3) | -0.17996 93810 68913 (-1) |
| 4 | 0.23253 70065 46730 (-2) | 0.96890 41939 44708 (-4) | -0.24514 90765 64097 (-1) |
| 5 | 0.79332 38173 01063 (-3) | -0.66110 31810 84219 (-5) | -0.16685 79600 04258 (-1) |
| 6 | -0.23876 93454 30200 (-3) | -0.33162 40908 75277 (-6) | -0.83440 13692 15834 (-3) |
| 7 | -0.52728 95670 57751 (-3) | 0.10462 09458 44792. (-6) | 0.16416 07577 68938 (-1) |
| 8 | -0.35212 33538 03039 (-3) | -0.87332 18100 27380 (-8) | 0.28113 16491 35773 (-1) |
| 9 | -0.34394 77441 80881 (-4) | 0.94782 77782 76236 (-10) | 0.27628 25192 88580 (-1) |
| 10 | 0.20533 28149 09065 (-3) | 0.56584 21927 60871 (-10) | 0.10215 12232 23534 (-1) |
| 11 | 0.27018 44395 43904 (-3) | -0.67686 89863 51370 (-11) | -0.24395 66978 16397 (-1) |
| 12 | 0.16727 29121 05140 (-3) | 0.34921 15936 67203 (-12) | -0.68551 96259 04596 (-1) |
| 13 | -0.27463 80660 37602 (-4) | 0.44104 24741 75775 (-14) | -0.10325 15678 59017 |
| 14 | -0.20920 92620 59300 (-3) | -0.23997 86221 77100 (-14) | -0.96775 02330 08802 (-1) |
| 15 | -0.28346 86553 20241 (-3) | 0.21677 31220 07268 (-15) | -0.90996 45657 46961 (-2) |
| 16 | -0.19969 68583 08970 (-3) | -0.95444 66076 36696 (-17) | 0.19238 77261 64982 |
| 17 | 0.26277 03710 99183 (-4) | -0.73876 76660 53864 (-19) | 0.49962 39621 32792 |
| 18 | 0.30736 84081 49253 (-3) | 0.48008 50782 48807 (-19) | 0.80971 09289 54417 |
| 19 | 0.50360 54530 47356 (-3) | -0.41399 56737 71331 (-20) | 0.85772 10307 17131 |

We are indebted to Peter Weinberger and Herman P. Robinson for detailed comments on our tables and especially to Henry C. Thacher, Jr. for showing us his manuscript [26] which includes a table of $\gamma_r$, $r=0(1)35, 44$ to 28 $S$ as well as the coefficients of $z\zeta(1+z)$ together with Chebyshev series for this function in the ranges $[-1/2, 1/2]$ and $[0, 1]$. His values were also obtained by the Euler-Maclaurin method and our values agree with his up to the last digit except as indicated: specifically Thacher has for $\gamma_8$ . . . 9|509 . . . and for $\gamma_9$ . . . 0|481 . . . where we have . . . 9| and . . . 1|.

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(Paper 76B3&4–369)