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SHARP BOUNDS FOR THE PSI FUNCTION AND HARMONIC NUMBERS

NECDET BATIR

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Abstract. We establish several new bounds for the psi function ψ and harmonic numbers H_n. For example, we prove that

$$\gamma+\frac{1}{2}\log(n^2+n+c)<H_n<\gamma+\frac{1}{2}\log(n^2+n+d),$$

where the constants $c=e^{2(1-\gamma)}-2=0.329302...$ and $d=1/3=0.3333...$ are the best possible, and

$$\gamma+\frac{1}{2}\log\left(\frac{2n+a}{e^{2/(n+1)}-1}\right)<H_n\leqslant\gamma+\frac{1}{2}\log\left(\frac{2n+b}{e^{2/(n+1)}-1}\right),$$

where $a=2$ and $b=e^{2-2\gamma}(e-1)-2=2.0024...$ are the best possible constants. Our estimations give extremely accurate values for γ, and they improve some estimations for γ deduced very recently by C. Mortici.

1. Introduction

The n'th harmonic number H_n is defined by the finite sum $H_n=\sum_{k=1}^{n}\frac{1}{k}$. There is a close connection between the harmonic numbers and the psi (or digamma) function $\psi=\Gamma'/\Gamma$, the logarithmic derivative of the gamma function $\Gamma(z)=\int_0^\infty u^{z-1}e^{-u}du$ $(z>0)$, $\psi(n+1)=H_n-\gamma$ for $n\in\mathbb{N}$. Here $\gamma=0.5772156...$ is the Euler's constant. The harmonic numbers have important applications in mathematics. For example, they have applications in number theory, analysis, combinatorics and differential equations. The most important properties of these numbers can be found in sections 6.3 and 6.4 of [10]. Recently, interesting inequalities for the psi function and these numbers have been published; see [2, 3, 4, 5, 15, 16] and references therein. In particular, we want to recall some of them (H. Alzer [2]):

$$\alpha\cdot\frac{\log(\log n+\gamma)}{n^2}\leqslant H_n^{1/n}-H_{n+1}^{1/(n+1)}<\beta\cdot\frac{\log(\log n+\gamma)}{n^2}$$

with best possible constants $\alpha=0.0140....$ and $\beta=1$, and

$$a\leqslant\exp(H_{n+1})-\exp(H_n)<b \tag{1.1}$$

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where the constants $a = 1+\log(\sqrt{e}-1) = 0.5672...$ and $b = \gamma = 0.57721...$ are the best possible, and for $x > 0$ and $n \in \mathbb{N}$. Elezović et al [9, Corollary 3] proved in 2000 that

$$\log(x+n-1/2) < \psi(x+n) < \log(x+e^{-\gamma+H_{n-1}}).$$

Finally for $x > 0$ (N. Batir [4]),

$$-\gamma-\log(e^{2/x}-1) < \psi(x) < -\log(e^{2/x}-1).$$

In this work we continue our investigations of the psi functions and harmonic numbers and establish various new upper and lower bounds for them. One of our theorems provides the best possible constants α and β in

$$\gamma+\frac{1}{2}\log(n^2+n+\alpha) \leqslant H_n < \gamma+\frac{1}{2}\log(n^2+n+\beta).$$

Another theorem presents the following sharp bounds for H_n

$$\gamma+\frac{1}{2}\log\left(\frac{2n+a}{e^{2/(n+1)}-1}\right) < H_n \leqslant \gamma+\frac{1}{2}\log\left(\frac{2n+b}{e^{2/(n+1)}-1}\right),$$

where $a = 2$ and $b = e^{2-2\gamma}(e-1)-2 = 2.0024...$ are the best possible constants. As it is shown in the last section our estimations give extremely good approximations for Euler's constant and improve some formulas due to C. Mortici [11, 13]. The numerical and algebraic computations have been carried out with the computer program *Mathematica 5*. We need the following elementary but very useful lemmas in order to prove our main results. The first lemma, despite of its simple appearance, is a strong tool to accelerate and measure the speed of convergence of some sequences having limit 0, and has proved by C. Mortici in [12]. It is evident from this lemma that the speed of convergence of the sequence (ω_n) is as higher as the value of k is greater.

LEMMA 1.1. *If* $(\omega_n)_{n\geqslant 1}$ *is convergent to zero and there exists the limit*

$$\lim_{n\to\infty} n^k(\omega_n-\omega_{n+1}) = c \in \mathbb{R},$$

with $k > 1$, *then there exists the limit*

$$\lim_{n\to\infty} n^{k-1}\omega_n = \frac{c}{k-1}.$$

The next lemma, as far as we know, was first used in [8] (without proof) to establish some monotonicity results for the gamma function.

LEMMA 1.2. *Let* f *be a function defined on an interval* I *and* $\lim_{x\to\infty} f(x) = 0$. *If* $f(x+1)-f(x) > 0$ *for all* $x \in I$, *then* $f(x) < 0$. *If* $f(x+1)-f(x) < 0$, *then* $f(x) > 0$.

Proof. Let $f(x+1)-f(x) > 0$ for all $x \in I$. By mathematical induction we have $f(x) < f(x+n)$ for all $n \in \mathbb{N}$. Letting $n \to \infty$, we find $f(x) < 0$. The proof of second part of the lemma follows from the same argument. □

LEMMA 1.3. *Let x be a positive real number. Then*

$$\psi^{(n)}(x+1)-\psi^{(n)}(x)=\frac{(-1)^n n!}{x^{n+1}}\ \ n=0,1,2,3,\dots; \tag{1.2}$$

$$\psi(x)\sim\log x-\frac{1}{2x}-\frac{1}{12x^2}+\frac{1}{120x^4}+\dots\quad (as\ x\to\infty); \tag{1.3}$$

$$\psi'(x)\sim\frac{1}{x}+\frac{1}{2x^2}+\cdot\frac{1}{6x^3}-\frac{1}{30x^5}+\dots\quad (as\ x\to\infty) \tag{1.4}$$

and

$$\psi''(x)\sim-\frac{1}{x^2}-\frac{1}{x^3}-\frac{1}{2x^4}+\frac{1}{120x^4}+\dots\quad (as\ x\to\infty); \tag{1.5}$$

see [1, pp. 258–260].

2. Main results

Our first theorem is the key for the next theorems.

THEOREM 2.1. *For real number $x>-1$, we define*

$$\phi(x)=e^{2\psi(x+1)}-x^2-x. \tag{2.1}$$

Then ϕ is strictly increasing and concave in $(-1,\infty)$.

Proof. By differentiating we get

$$\phi'(x)=2\psi'(x+1)e^{2\psi(x+1)}-2x-1, \tag{2.2}$$

$$\phi''(x)=[2\psi''(x+1)+4(\psi'(x+1))^2]e^{2\psi(x+1)}-2, \tag{2.3}$$

and

$$\begin{aligned}\frac{1}{2}e^{-2\psi(x+1)}\phi^{(3)}(x)&=\psi^{(3)}(x+1)+6\psi'(x+1)\psi''(x+1)+4(\psi'(x+1))^3\\&=\phi_1(x),\ \text{say}.\end{aligned} \tag{2.4}$$

Applying (1.2), we find

$$\begin{aligned}\frac{x^2}{2}(\phi_1(x+1)-\phi_1(x))=&-\frac{3x^2+6x+2}{x^4}-6(\psi'(x+1))^2+\frac{6}{x^2}\psi'(x+1)\\&+\frac{6}{x}\psi'(x+1)-3\psi''(x+1)=\phi_2(x),\ \text{say}.\end{aligned} \tag{2.5}$$

Similarly, we have

$$\begin{aligned}&\frac{(x+1)^2(x+2)^2}{6(x^2+3x+3)}(\phi_2(x+1)-\phi_2(x))\\&=\psi'(x+1)-\frac{114+298x+321x^2+178x^3+51x^4+6x^5}{6(x+1)^2(x+2)^2(x^2+3x+3)}=\phi_3(x),\ \text{say}.\end{aligned} \tag{2.6}$$

And, finally we get

$$\phi_3(x+1)-\phi_3(x)=-\frac{p(x)}{q(x)}, \tag{2.7}$$

where

$$p(x)=144+720(x+1)+1560(x+1)^2+1872(x+1)^3+1308(x+1)^4 \\ +504(x+1)^5+84(x+1)^6$$

and

$$q(x)=36(x+1)^2(x+2)^4(x+3)^2(x^2+3x+3)(x^2+5x+7).$$

Since both p and q are positive for all x in $(-1,\infty)$, it results from (2.7) that $\phi_3(x+1)-\phi_3(x)<0$ for $x>-1$. By Lemma 1.2 this means that $\phi_3(x)>0$ since $\lim\limits_{x\to\infty}\phi_3(x)=0$, that is, $\phi_2(x+1)-\phi_2(x)>0$ for $x>-1$. But this says that $\phi_2(x)<0$ for $x>-1$ by Lemma 1.2 since $\lim\limits_{x\to\infty}\phi_2(x)=0$. Taking into account (2.5) this implies that $\phi_1(x)>0$ for $x>-1$ by Lemma 1.2, since $\lim\limits_{x\to\infty}\phi_1(x)=0$, that is, $\phi^{(3)}(x)>0$ by (2.4). This shows that ϕ'' is strictly increasing in $(-1,\infty)$. Utilizing the asymptotic formulas(1.3), (1.4) and (1.5), we get

$$\lim_{x\to\infty}\phi'(x)=\lim_{x\to\infty}\phi''(x)=0, \text{ and } \lim_{x\to\infty}\phi(x)=\frac{1}{3}. \tag{2.8}$$

In view of (2.8) and monotonic increase of ϕ'' we get $\phi''(x)<0$ for all $x\ -1$, consequently, $\phi'(x)>\lim\limits_{x\to\infty}\phi'(x)=0$. This proves the assertions of Theorem 2.1. $\square$

Monotonic increase of ϕ and the facts that $\phi(0)=e^{-2\gamma}$ and $\lim\limits_{x\to\infty}\phi(x)=\frac{1}{3}$ by (2.8) lead to the following:

COROLLARY 2.2. *Let $x\in[0,\infty)$. Then*

$$\frac{1}{2}\log\left(x^2+x+e^{-2\gamma}\right)\leqslant\psi(x+1)<\frac{1}{2}\log\left(x^2+x+\frac{1}{3}\right), \tag{2.9}$$

where the scalers $e^{-2\gamma}=0.329302...$ and $1/3=0.333...$ are the best possible.

By virtue of $\phi(1)=e^{2-2\gamma}-2$ and the relation $\psi(n+1)=H_n-\gamma$, we obtain

COROLLARY 2.3. *Let $n\in\mathbb{N}$. Then*

$$\gamma+\frac{1}{2}\log\left(n^2+n+\alpha^*\right)\leqslant H_n<\gamma+\frac{1}{2}\log\left(n^2+n+\beta^*\right), \tag{2.10}$$

where $\alpha^*=e^{2-2\gamma}-2$ and $\beta=\frac{1}{3}$ are the best possible constants.

THEOREM 2.4. *Let x be a non-negative real number. Then we have*

$$\frac{1}{2}\log\left(\frac{2x+a}{e^{2/(x+1)}-1}\right) < \psi(x+1) \leqslant \frac{1}{2}\log\left(\frac{2x+b}{e^{2/(x+1)}-1}\right), \tag{2.11}$$

where $a=2$ and $b=e^{-2\gamma}(e^2-1)$ are the best possible constants.

Proof. For $x \geqslant 0$, we define

$$f(x) = \phi(x+1) - \phi(x),$$

where ϕ is as defined in (2.1). Differentiation gives $f'(x) = \phi'(x+1) - \phi'(x)$. Concavity of ϕ shows that f is strictly decreasing in $[0,\infty)$. Hence, we get

$$\lim_{x\to\infty} f(x) = \lim_{x\to\infty}[\phi(x+1)-\phi(x)] = 0 < f(x) \leqslant f(0) = e^{-2\gamma}(e^2-1)-2,$$

which is equivalent with (2.11) since

$$f(x) = e^{2\psi(x+1)}\left\{e^{\frac{2}{x+1}}-1\right\} - 2x - 2. \qquad \square$$

Monotonic decrease of f, and the relations $f(1) = \phi(2) - \phi(1) = e^{2-2\gamma}(e-1)-4$ and $\lim_{x\to\infty} f(x) = 0$ yield the following interesting bounds for the harmonic numbers:

COROLLARY 2.5. *Let $n \in \mathbb{N}$. Then we have*

$$\gamma + \frac{1}{2}\log\left(\frac{2n+a}{e^{2/(n+1)}-1}\right) < H_n \leqslant \gamma + \frac{1}{2}\log\left(\frac{2n+b}{e^{2/(n+1)}-1}\right), \tag{2.12}$$

where $a=2$ and $b=e^{2-2\gamma}(e-1)-2 = 2.0024...$ are the best possible constants.

We note that (2.12) can be written in the form

$$e^{2\gamma}(2n+2) < \exp\{2H_{n+1}\} - \exp\{2H_n\} \leqslant e^{2\gamma}(2n+2.0024...),$$

which provides a companion of (1.1). Our next theorem gives a monotonicity result for the sequence $\sigma_n = H_n - \frac{1}{2}\log(n^2+n+1/3)$.

THEOREM 2.6. *For $n \in \mathbb{N}$, we define*

$$\sigma_n = H_n - \frac{1}{2}\log(n^2+n+1/3).$$

Then the sequence (σ_n) is strictly increasing. Furthermore, we have

$$\lim_{n\to\infty} n^4(\sigma_n - \gamma) = -\frac{1}{180}. \tag{2.13}$$

Proof. For $x \geqslant 1$ let

$$F(x) = \psi(x+1) - \frac{1}{2}\log(x^2+x+1/3).$$

Differentiation yields

$$F'(x) = \psi'(x+1) - \frac{2x+1}{2x^2+2x+2/3}$$

and

$$F'(x+1) - F'(x) = -\frac{1}{9(x+1)^2(x^2+x+1/3)(x^2+3x+7/3)} < 0, \tag{2.14}$$

so that by Lemma 1.2 we have $F'(x) > 0$, which means that F is strictly increasing. Thus, $F(n)$ is increasing for $n \in \mathbb{N}$, so is (σ_n). In order to prove (2.13) we use (2.14) and l'Hospital rule. We have

$$\begin{aligned}\lim_{n\to\infty} n^5(\sigma_n - \gamma - (\sigma_{n+1} - \gamma)) &= \lim_{n\to\infty} \frac{F(n) - F(n+1)}{1/n^5} \\ &= \frac{1}{5}\lim_{n\to\infty} n^6[F'(n+1) - F'(n)] = -\frac{1}{45},\end{aligned}$$

which implies by Lemma 1.1 that (2.13) is valid. This means that the sequence (σ_n) converges to γ like n^{-4}. □

Our last two theorems offer new bounds for the ψ'-function in terms of the psi function. In [9, Corollary] Elezovic et al proved that

$$\psi'(x) < \exp\{-\psi(x)\}$$

holds for all $x > 0$. See [5] for an elementary and short proof of this inequality. The following theorem provides an improvement and a converse to this result.

THEOREM 2.7. *For $x > 0$ the follwing inequalities hold*

$$(x+a^*)e^{-2\psi(x+1)} < \psi'(x+1) < (x+b^*)e^{-2\psi(x+1)}, \tag{2.15}$$

where the constants $a^* = \frac{1}{2}$ and $b^* = \frac{\pi^2}{6}e^{-2\gamma}$ are the best possible.

Proof. Since ϕ, defined in (2.1), is concave and $\phi'(0) = \frac{\pi^2}{3}e^{-2\gamma} - 1$ and $\lim_{x\to\infty} \phi'(x) = 0$, which can be easily seen by using the asymptotic formulas (1.3) and (1.4), we find that

$$0 = \lim_{x\to\infty} \phi'(x) < \phi'(x) = 2\psi'(x+1)e^{-2\psi(x+1)} - 2x - 1 < \phi'(0) = \frac{\pi^2}{3}e^{-2\gamma} - 1,$$

which is equivalent to (2.15). □

THEOREM 2.8. *For $x>0$ we have*

$$\frac{1}{2}\left\{\frac{2}{x^2}-1+e^{\frac{2}{x+1}}-e^{-2\psi(x+1)}\right\}<\psi'(x)<\frac{1}{2}\left\{\frac{2}{x^2}+1-e^{-\frac{2}{x}}+e^{-2\psi(x+1)}\right\}. \quad (2.16)$$

Proof. Let ϕ be as given in (2.1). Applying the mean value theorem to ϕ on the interval $[x,x+1]$, we obtain

$$\phi(x+1)-\phi(x)=\phi'(x+\delta_x),\ 0<\delta_x<1.$$

Since ϕ is concave by Theorem 2.1 we get

$$\phi'(x+1)<\phi(x+1)-\phi(x)<\phi'(x).$$

In view of (1.2), this is equivalent with (2.16). □

3. Approximations of Euler's constant

The Euler's constant γ defined by the limit relation

$$\gamma=\lim_{n\to\infty}(H_n-\log n)=0.57721566...,$$

where $H_n=\sum_{k=1}^{n}\frac{1}{k}$ is the n'th harmonic number, is one of the most important constants in mathematics, maybe the third next to π and e. For a brief historical description of γ we refer to [6] and references therein. An important concern for this constant is to define new sequences convergent to this constant with increasingly higher speed. For this purpose many mathematicians have derived remarkable sequences to approximate γ. It is known that the classical sequence $D_n=H_n-\log n$ converges to γ very slowly. Indeed, Young [16] proved that the sequence D_n converges to γ as n^{-1}. A faster sequence introduced by DeTemple in [7]. More precisely, he proved that the sequence (R_n) given by the formula $R_n=H_n-\log(n+1/2)$ converges to γ like n^{-2}. The author [5] shows numerically that the sequence given by

$$\mu_n=\sum_{k=1}^{n}\frac{1}{k}+\frac{1}{2}\log\left(\frac{e^{1/(n+1)}-1}{n+1/2}\right) \quad (3.1)$$

gives better results than DeTemple's sequence R_n. In a very new paper C. Mortici [14] proved that

$$\lim_{n\to\infty}n^3(\mu_n-\gamma)=\frac{1}{48}, \quad (3.2)$$

which means that the sequence (μ_n) converges to γ with the rate of convergence n^{-3}. In a very recent paper C. Mortici [13] proved that the sequences (u_n) and (v_n) defined by, respectively,

$$u_n=H_{n-1}+\frac{1}{(6-2\sqrt{6})n}-\log(n+1/\sqrt{6}), \quad (3.3)$$

and

$$v_n = H_{n-1} + \frac{1}{(6+2\sqrt{6})n} - \log(n - 1/\sqrt{6}) \tag{3.4}$$

converge to γ like n^{-3} since

$$\lim_{n\to\infty} |n^3(u_n - \gamma)| = \lim_{n\to\infty} |n^3(v_n - \gamma)| = \frac{\sqrt{6}}{108}. \tag{3.5}$$

A comparison between (3.2) and (3.5) enables us to conclude that our formula (3.1) is slightly better than formulas (3.3) and (3.4). Better estimations than (3.1), (3.3) and (3.4) are also proposed by Mortici in [13]. His sequences defined by

$$\alpha_n = H_{n-2} + \frac{23}{24(n-1)} + \frac{1}{24n} - \log(n - 1/2) \tag{3.6}$$

and

$$\delta_n = \frac{u_n + v_n}{2} = H_{n-1} + \frac{1}{2n} - \frac{1}{2}\log(n^2 - 1/6) \tag{3.7}$$

converge to γ as n^{-4}. Indeed he proved that

$$\lim_{n\to\infty} n^4(\alpha_n - \gamma) = -\frac{17}{960}. \tag{3.8}$$

$$\lim_{n\to\infty} n^4(\delta_n - \gamma) = \frac{11}{720}. \tag{3.9}$$

From (2.13), (3.8), and (3.9) it is clear that our sequence (σ_n) given in Theorem 2.6 gives much accurate values for γ than the approximations $\alpha_n \approx \gamma$ from (3.6) and $\delta_n \approx \gamma$ from (3.7). In view of our underestimate in (2.12) we set

$$\theta_n = H_n + \frac{1}{2}\log\left(\frac{e^{2/(n+1)} - 1}{2n+2}\right), \tag{3.10}$$

which can be easily seen that it converges to γ. Using l'Hospital rule it is easy to see that $\lim\limits_{n\to\infty} n^5(\theta_n - \theta_{n+1}) = \frac{1}{45}$, so that by Lemma 1.1 we get

$$\lim_{n\to\infty} n^4\theta_n = \frac{1}{180}. \tag{3.11}$$

Since $\theta_n \to \gamma$ and $\sigma_n \to \gamma$, the arithmetic mean of θ_n and σ_n also converges to γ. Let us define

$$\tau_n = \frac{\theta_n + \sigma_n}{2} = H_n + \frac{1}{4}\log\left(\frac{e^{2/(n+1)} - 1}{2n^3 + 4n^2 + 8n/3 + 2/3}\right).$$

From (2.13) and (3.11) it results that $\lim\limits_{n\to\infty} n^4\tau_n = 0$, which means that the sequence (τ_n) converges to γ at rate faster than n^{-4}. These facts can be seen in the following table. We note that C. Mortici has established some other new approximation formulas for γ in [11] but his results obtained in [13] are better than those from [11].

n	$\|\theta_n - \gamma\|$	$\|\sigma_n - \gamma\|$	$\|\tau_n - \gamma\|$	$\|\alpha_n - \gamma\|$	$\|\delta_n - \gamma\|$
1	0.00029	0.00086	0.00028	——-	0.0139451
2	0.00006	0.00012	0.00003	0.00004	0.00091
10	$3.7733 \cdot 10^{-7}$	$4.5428 \cdot 10^{-7}$	$3.8478 \cdot 10^{-8}$	$2.1725 \cdot 10^{-6}$	$1.5246 \cdot 10^{-6}$
25	$1.2145 \cdot 10^{-8}$	$1.3125 \cdot 10^{-8}$	$4.9028 \cdot 10^{-10}$	$4.9143 \cdot 10^{-8}$	$3.9098 \cdot 10^{-8}$
50	$8.2098 \cdot 10^{-10}$	$8.5397 \cdot 10^{-10}$	$1.6499 \cdot 10^{-11}$	$2.9494 \cdot 10^{-9}$	$2.4442 \cdot 10^{-9}$
100	$5.3384 \cdot 10^{-11}$	$5.4454 \cdot 10^{-11}$	$5.3557 \cdot 10^{-13}$	$1.8066 \cdot 10^{-10}$	$1.5277 \cdot 10^{-10}$
500	$9.5035 \cdot 10^{-14}$	$8.8817 \cdot 10^{-14}$	$3.5527 \cdot 10^{-15}$	$2.851 \cdot 10^{-13}$	$2.4424 \cdot 10^{-13}$

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Necdet Batir
Department of Mathematics, Faculty of Sciences and Arts
Nevşehır University
65080, Nevşehır
Turkey
e-mail: nbatir@hotmail.com