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A METHOD FOR THE RAPID NUMERICAL CALCULATION OF PARTIAL SUMS OF GENERALIZED HARMONICAL SERIES WITH PRESCRIBED ACCURACY

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Se propune o metodă nouă pentru calculul rapid al sumelor parțiale ale seriilor armonice generalizate, cu o precizie prestabilită. Folosind integrări pe intervale alese avantajos se obțin expresii simple de calcul care reduc sumarea cu mai multe ordine de mărime.

De asemenea, metoda permite găsirea unor expresii simple pentru margini ale erorilor suficient de strânse. Reducerea timpului de calcul față de rutinele extinse pe calculatoarele actuale este semificativă.

One proposes a new method for the rapid calculation of partial sums of generalized harmonical series with prescribed accuracy. By using integration on advantageously selected intervals one obtains simple expressions of calculus reducing the summation to serval orders of magnitude.

As well, the given method allows finding simple expressions for error bounds in restricted intervals.

The reduction of computation time as compared to the existing rutines is significant.

1. Problem formation

Let $S_m^{(\alpha)}$ be the sum:

$$S_m^{(\alpha)} = \sum_{i=1}^{m} \frac{1}{i^{\alpha}} \quad , \quad \alpha \in R^{+}. \tag{1.1}$$

For m → α from (1.1) one obtaines the harmonical generalized series that for α > 1 is convergent. We call $S_N^{(\alpha)}$ a partial sum. The problem is to accurate and rapid compute this sum for very large *m,* in particular $m \to \infty$ for convergent series.

To this aim, one considers the function:

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$$f(x) = \frac{1}{x^{\alpha}}, \quad x > 0, \quad \alpha \in R^{+}, \tag{1.2}$$

which is infinite differentiable. Then we write a Taylor formula of the form:

$$f(x) = \frac{1}{i^2} - (x-i)\frac{\alpha}{i^{\alpha+1}} + \frac{(x-i)^2}{2}\frac{\alpha(\alpha+1)}{i^{\alpha+2}} + \\ + (x-i)^3 \frac{C_{-\alpha}^3}{i^{\alpha+3}} + R_4(x,i,\alpha), \ i \in N^*, \tag{1.3}$$

where the rest R_4 has the expression:

$$R_4(x,i,\alpha) = \frac{(x-i)^4 C_{-\alpha}^4}{\xi_{i(x)}^{\alpha+4}} \ ; \ \xi_i(x) = (1-\theta)i + \theta x, \ \theta \in (0,1); \tag{1.4}$$

Further, one integrates the function f (x) within the limits [i - a, i + a], $a \in (0;1)$ conveniently chosen. By denoting I_{ia} this integral, and taking (1.3) into account, one yealds:

$$I_{ia} = \int_{i-a}^{i+a} \frac{dx}{x^{\alpha}} = \frac{2a}{i^{\alpha}} + \frac{2a^3}{3\,i^{\alpha+2}} + \frac{2a^5}{5}\frac{C_{-\alpha}^4}{\overline{\xi}_{ia}^{\alpha+4}}, \quad \overline{\xi}_{ia} \in (i-a, i+a). \tag{1.5}$$

For the rest R_4, we have applied the mean value theorem.
On the other hand, by direct integration of f(x), one obtains:

$$I_{ia} = \begin{cases} \ln\dfrac{i+a}{i-a}, & \text{for } \alpha = 1; \\ \dfrac{1}{1-\alpha}\left[(i+a)^{1-\alpha} - (i-a)^{1-\alpha}\right], & \text{for } \alpha \neq 1 \end{cases}. \tag{1.6}$$

We want a simple expression for the sum: $\sum_{i=n+1}^{n+p} I_{ia}$, $p \geq 1$. Then, according to (1.6), one can get reduction of terms, if there is a number $k \in N$, such as:

$$i + a = k - a \, ; \, k = i + 2a \, , \, a \in (0;1) \tag{1.7}$$

From (1.7), one gets two possible values:

$$a = a_1 = 1\,;\; a = a_2 = 1/2. \tag{1.8}$$

Now we write the relation (1.5) for a_1 and a_2:

$$\frac{1}{2} I_{i\,a_1} = \frac{1}{i^\alpha} + \frac{C_{-\alpha}^2}{3}\frac{1}{i^{\alpha+2}} + \frac{C_{-\alpha}^4}{5}\frac{1}{\overline{\xi}_{i\,a_1}^{\,\alpha+4}} \;\; ; \overline{\xi}_{i\,a_1} \in (i-1, i+1); \tag{1.9}$$

$$I_{i\,a_2} = \frac{1}{i^\alpha} + \frac{C_{-\alpha}^2}{12}\frac{1}{i^{\alpha+2}} + \frac{C_{-\alpha}^4}{80}\frac{1}{\overline{\xi}_{i\,a_1}^{\,\alpha+4}}; \overline{\xi}_{i\,a_2} \in \left(i-\frac{1}{2}, i+\frac{1}{2}\right). \tag{1.10}$$

By eliminating the term in $1/i^{\alpha+2}$, one gets:

$$I_{i\,a_2} - \frac{1}{8} I_{i\,a_1} = \frac{3}{4}\frac{1}{i^\alpha} - \frac{C_{-\alpha}^4}{20}\left(\frac{1}{\overline{\xi}_{i\,a_1}^{\,\alpha+4}} - \frac{0.25}{\overline{\xi}_{i\,a_2}^{\,\alpha+4}}\right). \tag{1.11}$$

Now we take the sum of (1.11) from i = n + 1, to i = n + p, p ≥ 1, to obtain:

$$\sum_{i=n+1}^{n+p} \frac{1}{i^\alpha} = S_{n+p}^{(\alpha)} - S_n^{(\alpha)} = \sum_{n+1}^{n+p}\left(\frac{4}{3} I_{i\,a_2} - \frac{1}{6} I_{i\,a_1}\right) + \delta_{np}^{(\alpha)}, \tag{1.12}$$

were $\delta_{np}^{(\alpha)}$ stands for the error term:

$$\delta_{np}^{(\alpha)} = \frac{C_{-\infty}^4}{15}\sum_{n+1}^{n+p}\left(\frac{1}{\overline{\xi}_{i\,a_1}^{\,\alpha+4}} - \frac{0.25}{\overline{\xi}_{i\,a_2}^{\,\alpha+4}}\right); \alpha \geq 0. \tag{1.13}$$

By denoting $\sigma_{n+p}^{(\alpha)}$ the sum:

$$\sigma_{n+p}^{(\alpha)} = \sum_{i=n+1}^{n+p}\left(\frac{4}{3} I_{i\,a_2} - \frac{1}{6} I_{i\,a_1}\right), \tag{1.14}$$

one gets the formula for calculation of the partial sum $S_m^{(\alpha)}$, m = n + p:

$$S_m^{(\alpha)} = S_n^{(\alpha)} + \sigma_m^{(\alpha)} + \delta_{np}^{(\alpha)}, \; m = n + p \tag{1.15}$$

By using (1.6), one yields:

$$\sigma_{n+p}^{(\alpha)} = \frac{4}{3}\left(\left(m+\frac{1}{2}\right)^{\alpha_1} - (n+\frac{1}{2})^{\alpha_1}\right)/\alpha_1 - \tag{1.16}$$

$$\left((m+1)^{\alpha_1} + m^{\alpha_1} - (n+1)^{\alpha_1} - n^{\alpha_1}\right)/6\alpha_1 ,$$

$$m = n+p, \alpha_1 = (1-\alpha).$$

In the limit $\alpha \to 1, \alpha_1 \to 0$, one gets:

$$\sigma_{n+p}^{(1)} = \frac{4}{3}\ln\frac{2(n+p)+1}{2n+1} - \frac{1}{6}\ln\frac{(n+p)(n+p+1)}{n(n+1)}. \tag{1.16-a}$$

For $\alpha = 0$, one recover the trivial case $\sigma_{n+p}^{(0)} = p$, and $\delta_{np}^{(0)} = 0$. For $\alpha \rangle 1,\ m \to \infty$, from (1.16) one obtains:

$$\sigma_{\infty}^{(\alpha)} = \frac{-1}{3\alpha_1}\left[4\left(n+\frac{1}{2}\right)^{\alpha_1} - \frac{1}{2}\left((n+1)^{\alpha_1} + n^{\alpha_1}\right)\right],\ \alpha_1 = 1-\alpha < 0\ ; \tag{1.16-b}$$

$$S_{\infty}^{(\alpha)} \approx S_n^{(\alpha)} + \sigma_{\infty}^{(\alpha)}\ . \tag{1.16-c}$$

2. The error evaluation

In order to find a bound for the error $\delta_{np}^{(\alpha)}$ (see 1.13), we consider, from (1.9) and (1.10), the most desadvantageous combination of $\bar{\xi}_{i\,a_1}$ and $\bar{\xi}_{i\,a_2}$ to get a maximum positive value:

$$\delta_{np\max}^{(\alpha)} = \frac{C_{-\alpha}^4}{15}\sum_{n+1}^{n+p}\left(\frac{1}{(i-1)^{\alpha+4}} - \frac{0.25}{\left(i+\frac{1}{2}\right)^{\alpha+4}}\right), \tag{2.1}$$

i.e. the maximum difference of terms in paranthesis.

Further, we observe that for any twice differentiable function g(x), one obtains, by using a Taylor formula and an integation in the interval [i, i + 1], the expresion:

$$\int_i^{i+1} g(x)dx = g_{mean} = g\left(i+\frac{1}{2}\right)+\frac{1}{24}g''\left(\overline{\xi}_i\right),\ \overline{\xi}_i \in (i, i+1), \tag{2.2}$$

g_{mean} being the mean value of g(x) in the interval (i, i + 1).
Then, for g”(x) > 0, one obtain the ineguality:

$$g_{mean} < g\left(i+\frac{1}{2}\right);\quad g'' > 0\ , \tag{2.3}$$

that is, for g” > 0, the mean value is smaller than the function value in the middle of the interval $\left(i+\frac{1}{2}\right)$.

Now, consider the function:

$$g(x) = \frac{1}{\left(x-\frac{3}{2}\right)^{\alpha+4}} - \frac{0.25}{x^{\alpha+4}}\ ,\quad x > \frac{3}{2}\quad , \tag{2.4}$$

which is positive together with its derivative g”(x) for x > 3/2. Taking the interval [i, i + 1], i > 3/2, we find in the middle the value in parenthesis from (2.1):

$$g\left(i+\frac{1}{2}\right) = \frac{1}{(i-1)^{\alpha+4}} \frac{0.25}{\left(i+\frac{1}{2}\right)^{\alpha+4}}. \tag{2.5}$$

In fact, the index i takes larger values ($i \geq 7$).

Thus, we get the error evaluation:

$$\begin{aligned}\delta_{np\max}^{(\alpha)} &\leq \frac{C_{-\alpha}^4}{15}\sum_{i=n+1}^{n+p}\left(\int_i^{i=1} g(x)dx\right) = \frac{C_{-\alpha}^4}{15}\int_{n+1}^{n+p+1} g(x)dx = \\ &= \frac{\alpha(\alpha+1)(\alpha+2)}{360}\left(G(n=1)-G(n+p+1)\right).\end{aligned} \tag{2.6}$$

where the function G(x) comes from integration having the expression:

$$G(x) = \frac{1}{\left(x-\frac{3}{2}\right)^{\alpha+3}} - \frac{0.25}{x^{\alpha+3}}. \tag{2.7}$$

By denoting $\delta^{(\alpha)}_{n\infty\ \max}$ the limit for p → ∞:

$$\delta^{(\alpha)}_{n\infty\ \max} = \frac{\alpha(\alpha+1)(\alpha+2)}{360}\left[\frac{1}{\left(n-\frac{1}{2}\right)^{\alpha+3}} - \frac{0.25}{(n+1)^{\alpha+3}}\right], \tag{2.8}$$

one gets the absolute error evaluation:

$$\left|\delta^{(\alpha)}_{np}\right| \langle \delta^{(\alpha)}_{np\max} \langle \delta^{(\alpha)}_{n\infty,\max} \tag{2.8}$$

3. Results. Comparisons.

In Tables 1,2,3 are given the sums $S^{(\alpha)}_n$ for α = 0.5, α = 1 (harmonical series) and α = 2 (convergent series) a desired accuracy of at least 5;6 and 7 exact decimal figures respectively.

Table 1.

α = 0.5

n	$S^{(0.5)}_{n\,exact}$	$\delta^{(0.5)}_{n\infty,\max}$
7	4.0178834	0.654 E - 5
12	5.6111844	0.845 E - 6
22	8.0266736	0.907 E - 7

Exemple 1.

Calculate sum $S^{0,5}_{100.000}$ with at least seven exact decimal figures, by using Table 1.

Answer. One calculates $\sigma^{(0..5)}_{100\,000}$ by using the relation (1.16):

$$\sigma^{(0.5)}_{100.000} = 622.97008496;$$

then:

$$S_{100000}^{(0.5)} = \sigma_{1000000}^{(0.5)} + S_{22}^{(0.5)} = 630.9967586$$

Table 2.

α = 1

n	$S_{n\,exact}^{(1)}$	$\delta_{n\infty,\,\max}^{(1)}$
8	2.7178571	0.832 E - 5
12	3.1032107	0.807 E - 6
20	3.5977397	0.938 E - 7

Example 2.

By using Table 2., calculate the sum of terms of the harmonical series found between one million and a billion, with at least seven exact decimal figures. Answer. One has to calculate the difference (see 1.16.a):

$$S_{10^9}^{(1)} - S_{10^6}^{(1)} \cong \sigma_{10^9}^{(1)} + (\,S_{20,exact}{}^{(1)}\;\;S_{20,exact}{}^{(1)}\,) - \sigma_{10^6}^{(1)} = \frac{4}{3} ln \frac{2.10^9 + 1}{2.10^6 + 1} -$$

$$-\frac{1}{6} ln \frac{10^9\left(10^9 + 1\right)}{10^6\left(10^6 + 1\right)} = 6.90777548\ .$$

Remark. In this case, we have a difference error:

$\delta_{n,10^9}^{(1)} - \delta_{n,10^6}^{(1)} \langle\, \delta_{n\,10^9}$ and one can expect even smaller errors than that presented in Table 2. By using a Pentium 3 computer at 500 MHz, the computation time is about 18 minutes.

Table 3

α = 2

n	$S_{n\,exact}^{(2)}$	$\delta_{n\infty,\,\max}^{(2)}$
7	1.5117971	0.524 E - 5
12	1.5649766	0.286 E - 6
22	1.6004969	0.119 E - 7

Example 3. Because for α = 2, one gets a convergent series we can calculate the sum (see 1.16.b; c):

$$S_{\infty}^{(2)} \cong S_{22}^{(2)} + \sigma_{\infty}^{(2)} = 1.6004969 + 0.04443712 = 1.6449340\,.$$

In Table 4., the maximum error variation for n = 12, $\delta_{12,\infty\max}^{(\alpha)}$ is presented: after an increasing on the interval [0; 0.75], the maximum error is decreasing constantly.

Table 4.

Error variation with α

α	0	0.1	0.25	0.50	0.75	1.0	1.5	2
$\delta_{12,\infty\,max}^{(\alpha)} \times 10^{6}$	0	0.274	0.580	0.895	0.890	0.807	0.526	0.287

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