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SUMMATION OF SERIES BY SOME SUBSTITUTIONS

The method of integration by variable transformation is adapted to numerical summation of some functions. Some substitutions provide valuable methods at least for analytic functions with singularities of algebraic-logarithmic type at infinity. Any details about the kind of singularity are unnecessary while making use of these methods.

1. Introduction. The Euler–Maclaurin summation formula is commonly known. Sometimes it yields the very useful method of calculating sums of some series. It is then employed in the form

$$(1)\qquad \sum_{n=0}^{\infty} s(n) = \int_{0}^{\infty} s(x)dx+\frac{1}{2}s(0)-\sum_{j=1}^{m}\frac{B_{2j}}{(2j)!}s^{(2j-1)}(0) -\frac{1}{(2m)!}\int_{0}^{\infty} B_{2m}^{*}(x)s^{(2m)}(x)dx,$$

where m is natural, B_{2j} denotes the $2j$-th Bernoulli number, and B_{2m}^{*} is a periodic function, with period 1, which in the interval $[0, 1)$ is identical with the $2m$-th Bernoulli polynomial (see [2]).

We assume that the function s and its first $2m$ derivatives are integrable in the interval $[0, \infty)$, and $s^{(2m)}$ is absolutely integrable.

There are different applications of summation formula (1). Perhaps its most important advantage is the fact that it shows how the error with which an integral approximates a sum (or vice versa) depends on the behaviour of the function s near the zero-point.

While computing an integral one can, as is well known, change the integration variable. Certain substitutions are specially useful and lead to quite good methods of numerical integration (see, e.g., [1], [3], [4]). The problem arises whether similar ideas can be taken advantage of in calculating sums of series.

2. Summation by substitution. Let φ be a function which in the interval

$[0, \infty)$ has a continuous $(2m+1)$-st derivative and which maps this interval onto itself in such a way that $\varphi(0) = 0$, $\varphi(\infty) = \infty$. Let us put

$$r(x) = \varphi'(x)s(\varphi(x)).$$

Using the Euler–Maclaurin formula to the function $s-r$, we obtain

THEOREM 1. *If formula* (1) *is true for the functions* s *and* r, *then*

$$(2)\quad \sum_{n=0}^{\infty} s(n) = \sum_{n=0}^{\infty} r(n) + \frac{s(0)-r(0)}{2} - \sum_{j=1}^{m} \frac{B_{2j}}{(2j)!}\big(s^{(2j-1)}(0) - r^{(2j-1)}(0)\big) - \frac{1}{(2m)!}\int_0^{\infty} B_{2m}^*(x)\big(s^{(2m)}(x) - r^{(2m)}(x)\big)dx.$$

Let us notice that it is possible for (1) to be true for s but not for r. For example, if

$$s(x) = \frac{\sin(x+1)}{(x+1)^{1.5}}, \qquad \varphi(x) = e^x - 1,$$

then

$$r(x) = e^{-x/2}\sin e^x, \qquad r'(x) = e^{x/2}\cos e^x - \tfrac{1}{2}e^{-x/2}\sin e^x,$$

and there is no limit of $r'(x)$ as $x \to \infty$, which means that r'' is not integrable in the interval $[0, \infty)$.

In spite of that we may take the expression

$$\sum_{n=0}^{\infty} r(n) = \sum_{n=0}^{\infty} \alpha_n s(\xi_n), \qquad \text{where } \alpha_n = \varphi'(n),\ \xi_n = \varphi(n),$$

for the approximation of the sum of the function s. The method arising from that will be called a *summation by substitution.*

Formula (2) shows that in the method the main part of the error is usually $(s(0)-r(0))/2$. The value can be decreased to zero if we assume $\varphi'(0) = 1$.

THEOREM 2. *If for* x *near zero the functions* s, r *and* φ *have the expansions*

$$s(x) = s_0 + s_1x + s_2x^2 + \ldots, \qquad r(x) = r_0 + r_1x + r_2x^2 + \ldots,$$
$$\varphi(x) = x + \varphi_k x^k + \varphi_{k+1}x^{k+1} + \ldots,$$

where $k \geqslant 4$, *then*

$$r_0 = s_0, \qquad r_1 = s_1, \qquad \ldots, \qquad r_{k-2} = s_{k-2},$$
$$r_{k-1} = s_{k-1} + k\varphi_k s_0, \qquad r_k = s_k + (k+1)(\varphi_k s_1 + \varphi_{k+1}s_0),$$
$$r_{k+1} = s_{k+1} + (k+2)(\varphi_k s_2 + \varphi_{k+1}s_1 + \varphi_{k+2}s_0),$$
$$r_{k+2} = s_{k+2} + (k+3)(\varphi_k s_3 + \varphi_{k+1}s_2 + \varphi_{k+2}s_1 + \varphi_{k+3}s_0).$$

Furthermore, if k *is odd and* $k \leqslant 2m-3$, *then* (2) *takes the form*

(3) $$\sum_{n=0}^{\infty} s(n) = \sum_{n=0}^{\infty} r(n) + B_{k+1}(\varphi_k s_1 + \varphi_{k+1} s_0) + B_{k+3}(\varphi_k s_3 + \varphi_{k+1} s_2 + \varphi_{k+2} s_1 + \varphi_{k+3} s_0) + \ldots$$

Proof. Since

$$\varphi(x) = x + \varphi_k x^k + \varphi_{k+1} x^{k+1} + \varphi_{k+2} x^{k+2} + \ldots,$$
$$\varphi^2(x) = x^2 + 2\varphi_k x^{k+1} + 2\varphi_{k+1} x^{k+2} + \ldots,$$
$$\varphi^3(x) = x^3 + 3\varphi_k x^{k+2} + \ldots,$$

etc., we have

(4) $$r(x) = (1 + k\varphi_k x^{k-1} + (k+1)\varphi_{k+1} x^k + \ldots)(s_0 + s_1 x + \ldots + s_{k-1} x^{k-1} + (s_k + \varphi_k s_1) x^k + (s_{k+1} + 2\varphi_k s_2 + \varphi_{k+1} s_1) x^{k+1} + (s_{k+2} + 3\varphi_k s_3 + 2\varphi_{k+1} s_2 + \varphi_{k+2} s_1) x^{k+2} + \ldots).$$

Ordering the terms on the right-hand side of (4), we obtain the required identities of the first part of the theorem. Now we substitute the obtained values in place of

$$s(0) - r(0) = s_0 - r_0, \qquad \frac{s^{(2j-1)}(0) - r^{(2j-1)}(0)}{(2j-1)!} = s_{2j-1} - r_{2j-1}$$

appearing in (2), and we have got formula (3).

3. Two propositions of substitutions. Of many possible substitutions we propose here two. In both cases the function φ depends additionally on a parameter w.

The first proposition:

(5) $$\varphi(x) = \frac{\mathrm{sh}(wx)^3}{w(wx)^2}.$$

It is easy to check that

$$\varphi'(x) = 3\,\mathrm{ch}(wx)^3 - \frac{2\varphi(x)}{x}, \qquad \varphi(x) = x + \frac{w^6}{6} x^7 + \frac{w^{12}}{120} x^{13} + \ldots$$

Formula (3) is now of the form

$$\sum_{n=0}^{\infty} s(n) = \sum_{n=0}^{\infty} r(n) - \frac{w^6}{6}\left(\frac{1}{30} s'(0) - \frac{5}{66}\frac{s'''(0)}{3!} + \ldots\right),$$

since $B_8 = -\frac{1}{30}$ and $B_{10} = \frac{5}{66}$.

The second proposition:

(6) $$\varphi(x) = \frac{1}{w}\left(\mathrm{sh}(\mathrm{sh}(wx)) - \frac{1}{3}(wx)^3 - \frac{1}{10}(wx)^5\right).$$

In this case we have

$$\varphi'(x) = \mathrm{ch}(wx)\cdot\mathrm{ch}(\mathrm{sh}(wx)) - (wx)^2 - \tfrac{1}{2}(wx)^4,$$

$$\varphi(x) = x + \frac{8}{315}w^6x^7 + \frac{13}{2520}w^8x^9 + \ldots,$$

$$\sum_{n=0}^{\infty} s(n) = \sum_{n=0}^{\infty} r(n) - \frac{8}{315}w^6\left(\frac{1}{30}s'(0) - \frac{5}{66}\left(\frac{s'''(0)}{3!} + \frac{13}{64}w^2 s'(0)\right) + \ldots\right).$$

As can be seen, in both propositions the error of summation by substitution is of order $O(w^6)$ for $w \to 0$. We have also $\varphi'(x) > 0$. Hence it follows that if $s(x) \geqslant 0$, then $r(n) \geqslant 0$, i.e., while summing the components $r(n)$, the *influence of rounding errors is of little importance.*

The evaluation of $\varphi(x)$ and $\varphi'(x)$ is not so expensive as it seems. Using, e.g., substitution (6), we only need to perform 10 additions, 9 multiplications, 4 divisions and calculate 1(!) exponential function value (the φ and φ' can be tabulated, if necessary).

TABLE 1

Substitution	w	(a)		(b)		(c)		(d)	
(5)	0.8	4.696188	5	7.303722	5	0.860599	4	3.082478	3
	0.4	4.594984	10	7.493632	9	0.808481	7	3.913795	5
	0.2	4.595112	20	7.491400	17	0.808510	14	3.997695	8
	0.1	4.595109	38	7.491400	34	0.808509	26	4.000000	15
(6)	1.0	4.713135	5	7.732122	5	0.834331	4	3.349187	3
	0.5	4.593062	10	7.493370	9	0.807773	8	3.899829	5
	0.25	4.595111	19	7.491401	18	0.808510	15	3.997818	9
	0.125	4.595111	38	7.491400	35	0.808509	28	4.000000	15

In Table 1 we give the results of calculations for the series

$$\text{(a)} \sum_{n=0}^{\infty} \frac{1}{(n+1)^{1.25}}, \quad \text{(b)} \sum_{n=0}^{\infty} \left(\frac{\ln(n+2)}{n+2}\right)^{1.5},$$

$$\text{(c)} \sum_{n=0}^{\infty} (n+1+\sqrt{n+1})^{-1.75}, \quad \text{(d)} \sum_{n=0}^{\infty} 0.75^n.$$

The summing of components in the transformed series was abandoned after encountering the first component of modulus not greater than 10^{-5}. The number of that component is given beside the obtained sum of the series.

One of the best methods for sequence (and series) convergence acceleration is the Levin u-transform (see, e.g., [5]). Especially, series of type (a) and (d) are model examples indicating the power of that method. It can be verified that about 10 terms of series (a) are enough for getting the absolute error 10^{-6}, but then – as can also be verified – at least 12-digit floating-point arithmetic (decimal) must be used; whereas the results of Table 1 were obtained by using 10-digit arithmetic, and 9 digits would be enough, too. From Table 1 we see that the methods of summation by substitutions (5) and (6) *do not make the greater difference among the given examples.* The Levin u-transform, however, does not work well in cases (b) and (c). For instance, in case (b) it gives the following results (the n-th result is obtained by the first n terms):

$$0.20, \quad -0.06, \quad 1.06, \quad 3.82, \quad 9.05, \quad 11.09, \quad 10.69, \quad 10.09,$$
$$9.62, \quad 9.28, \quad 9.02, \quad 8.82, \quad \ldots$$

Remark. If a given series is very slowly convergent and the computations are made on a computer, then the limited range of floating-point numbers can obstruct obtaining the required accuracy. For instance:

$$\sum_{n=2^{255}}^{\infty} \frac{1}{n^{1.05}} \sim \int_{2^{255}}^{\infty} \frac{dx}{x^{1.05}} = \frac{20}{2^{12.75}} = 0.0029\ldots$$

4. Error in summing analytic functions. Let us consider now the sum

$$S(f) = \sum_{n=0}^{\infty} s(n) f(n+1)$$

and its approximation

$$A(f) = \sum_{n=0}^{\infty} a_n f(x_n+1). \tag{7}$$

We assume that the series $\Sigma s(n)$ and Σa_n are absolutely convergent.

Let f be a complex variable function that is regular at infinity, continuous on a contour C and analytic outside C. As is known from the theory of analytic functions, if the contour C includes point 0 and a point x lies outside C, then

$$f(x) = \frac{1}{2\pi i} \int_C \frac{f(z)}{z} \frac{x}{x-z} dz \tag{8}$$

(to prove (8), one can use the substitution $z = 1/\zeta$ and take advantage of Cauchy's integral formula). Putting (8) into the error expression

$$\mathrm{E}(f) = S(f) - A(f) = \sum_{n=0}^{\infty} \big(s(n) f(n+1) - a_n f(x_n+1)\big)$$

and assuming that the arguments $1, 2, \ldots, x_0+1, x_1+1, \ldots$ of f lie outside the contour C, we obtain

$$\mathrm{E}(f) = \frac{1}{2\pi i} \int_C \frac{f(z)}{z} \mathrm{E}(g_z) dz, \qquad \text{where } g_z(x) = \frac{x}{x-z}.$$

That means that the estimate of the error $\mathrm{E}(f)$ is of the order of the estimate of $\mathrm{E}(g_z)$. It is evident then that to verify the methods based on approximation (7), among them the methods of Section 3, we should test them on the series

$$\sum_{n=0}^{\infty} s(n) g_z(n+1) = \sum_{n=0}^{\infty} s(n) \frac{n+1}{n+1-z} = \sum_{n=0}^{\infty} \frac{s(n)}{1-z/(n+1)},$$

where z ranges over a neighbourhood of the zero-point.

For the methods of Section 3 and for the functions s from examples (a)–(d) such calculations were performed. The parameter z was given values $z = a+ib$, where

$$a = 0,\ \pm 0.5,\ \pm 1,\ \pm 1.5,\ 2,\ 2.5; \qquad b = 0,\ \pm 0.5,\ \pm 1,\ \pm 1.5,$$

obviously excepting $z = 1$ and $z = 2$. As previously, the components were being added as long as their moduli were greater than 10^{-5}, and as previously the parameter w was halved. Every time the number of components was the same as in Table 1, and almost every time the rate of getting digits fixed in the results obtained was also as there. Merely for $z = 2.5$ and in a small vicinity the rate

TABLE 2

Substitution	w	$z = -1+i$		$z = 2.5$	
(5)	0.8	$6.735113+i0.392868$	5	6.364513	5
	0.4	$6.972847+i0.322928$	9	8.068223	9
	0.2	$6.969543+i0.323752$	17	8.125136	17
	0.1	$6.969542+i0.323752$	34	8.126083	34
(6)	1.0	$7.178462+i0.377780$	5	6.923675	5
	0.5	$6.973444+i0.321760$	9	8.087991	9
	0.25	$6.969544+i0.323752$	18	8.125523	18
	0.125	$6.969543+i0.323752$	35	8.126090	35

was diminished. It will probably be worse and worse as z departs from 0 remaining near the positive real semi-axis. Table 2 shows some results obtained for the series

$$\sum_{n=0}^{\infty} \left(\frac{\ln(n+2)}{n+2}\right)^{1.5} \frac{n+1}{n+1-z}.$$

Roughly speaking, the summation of terms $s(n)f(n+1)$ proceeds similarly to the summation of $s(n)$.

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