A NEW SUMMATION METHOD FOR POWER SERIES WITH RATIONAL COEFFICIENTS

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ABSTRACT. We show that an asymptotic summation method, recently proposed by the authors, can be conveniently applied to slowly convergent power series whose coefficients are rational functions of the summation index. Several numerical examples are presented.

1. Asymptotic summation

Consider a power series

$$(1) \sum_{j=1}^{\infty} f_j z^j ,$$

where $z \in \mathbb{C}$ and $f_j \in \mathbb{C}$. In [3] we proved that, when the coefficients f_j possess an asymptotic expansion

(2)
$$f_j \sim a_1 j^{-p_1} + a_2 j^{-p_2} + \dots, \quad j \to \infty, \quad 0 < p_1 < p_2 < \dots,$$

and $p_{k+1} - p_k \in \mathbb{N}$, then also the remainder of (1) has an asymptotic expansion

(3)
$$\sum_{j=n}^{\infty} f_j z^j \sim z^n n^{-q} \{ b_1(z) n^{-1} + b_2(z) n^{-2} + \cdots \} , \quad n \to \infty ,$$

where $q = p_1 - 1$ if $|z| \le 1$ and $z \ne 1$, and $q = p_1 - 2$ if z = 1. In particular, we provided *explicit formulas* for the computation of the coefficients $b_k(z)$, which allow for a direct use of expansion (3) for the numerical summation of (2). It is worth recalling that in [11] Sidi already showed the mere *existence* of an asymptotic expansion for the remainder, as a basis for acceleration of convergence by means of Levin's T-transformation. Convergence of the series (2), in fact, can be very slow (when p_1 is "small") for z on (or close to) the boundary of the unit circle.

When $p_{k+1} - p_k \equiv 1$, which is the most common case in applications, the quoted formulas are simple and easy to implement. In fact, for $z \neq 1$ we have

(4)
$$b_k(z) = -\sum_{i=0}^{k-1} a_{k-i} \varphi_i(k, z) ,$$

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where the φ_i are recursively defined by

(5)
$$\varphi_0(k,z) = \frac{1}{z-1},$$

$$\varphi_i(k,z) = \frac{z}{1-z} \sum_{r=0}^{i-1} {i+1-k-p_1 \choose i-r} \varphi_r(k,z), \quad i = 1, 2, \dots,$$

while for z = 1 we have

(6)
$$b_k(1) = \sum_{i=1}^k \frac{a_i}{p_1 + i - 2} \begin{pmatrix} 2 - p_1 - i \\ k - i \end{pmatrix} B_{k-i} ,$$

where B_k are the Bernoulli numbers; cf. [2], [3, Formula (24)]. Observe that the more general formula (5) of [3] contains a misprint: the number $k + p_{\ell} - p_1 - 1$ in the binomial coefficient, should be $k + p_1 - p_{\ell} - 1$ instead.

As a numerical application, we considered in [3] the evaluation of the special function

(7)
$$S(z; j_0, \nu, a, b, p) = \sum_{j=j_0}^{\infty} z^j (j+b)^{\nu-1} (j+a)^{-p} , \quad |z| \le 1 ,$$
$$0 < \nu \le 1 , \quad a, b \in \mathbb{C} \setminus \{-j_0, -j_0 - 1, \ldots\} ,$$

generalizing various summation problems that appeared in the recent literature on convergence acceleration of numerical and power series; cf., e.g., [1, 4, 5, 6, 8, 9, 10]. When z is on or close to the boundary of the unit circle, summation of (7) was accomplished by a numerical algorithm based directly on the expansion (3) and the formulas (4)-(6).

2. The case of rational coefficients

In the present work, we show that the approach briefly described in the previous section can be also applied to the numerical summation of series whose coefficients are *rational functions* of the *index*, i.e.,

(8)
$$S = S(z) = \sum_{j=j_0}^{\infty} z^j (j+b)^{\nu-1} r(j) , \quad |z| \le 1 ,$$

$$0 < \nu \le 1 , \quad b \in \mathbb{C} \setminus \{-j_0, -j_0 - 1, \ldots\} , \quad r(j) = \frac{\alpha(j)}{\beta(j)} = \frac{\alpha_s j^s + \cdots + \alpha_0}{\beta_t j^t + \cdots + \beta_0}$$

where $t-s>\nu$ if $z=1,\,t-s>\nu-1$ if $|z|\leq 1$ and $z\neq 1$, and $\beta(j)\neq 0$ for all integers $j\geq j_0$.

A possible approach to the summation of (8) in instances of slow convergence is given by partial fraction decomposition of the rational function, together with suitable algorithms for the computation of (7). The series involved in the partial fractions are indeed of that form, with $p \in \mathbb{N}$. This represents a motivation for the development of special summation methods for the series in (7), as pointed out in several recent papers (cf. [4, 6, 8]). On the other hand, though the basic step of partial fraction decomposition can be accomplished in an efficient manner (cf. [7, §7.1]), it is still quite costly.

For this reason, it is worth pursuing a direct use of asymptotic summation via (3)-(5), provided an asymptotic expansion like (2) exists for the coefficient $(j+b)^{\nu-1}r(j)$ and can be easily constructed. This is indeed the case for a rational function

 $r(z) = \alpha(z)/\beta(z)$, which admits an asymptotic expansion in powers of z^{-1} , the convergent Laurent expansion, in a suitable neighborhood of ∞ which omits the poles of r(z). Thus the following asymptotic relation holds:

(9)
$$\alpha(j) = j^{s-t}\beta(j) \left(\sum_{k=0}^{m} c_k j^{-k} + O(j^{-m-1}) \right), \quad m = 0, 1, 2, \dots, \quad j \ge \tilde{n},$$

where \tilde{n} is the least positive integer such that r(z) has no poles for $|z| \geq \tilde{n}$, and the c_k 's are the coefficients of the Laurent expansion of r(z).

From (9) we can compute recursively the coefficients c_k by means of the α_i 's and β_i 's (cf. (8)). In fact, substituting from (8) the explicit expressions for $\alpha(j)$ and $\beta(j)$ and comparing the coefficients of like powers of j on the left and right of (9), we obtain the infinite triangular system

(10)
$$\sum_{k=0}^{\ell} c_k \beta_{t-\ell+k} = \begin{cases} \alpha_{s-\ell} & \text{if } 0 \le \ell \le s, \\ 0 & \text{if } \ell > s, \end{cases}$$

and, by forward substitution, we find that

(11)
$$c_k = \begin{cases} \left(\alpha_{s-k} - \sum_{i=0}^{k-1} c_i \beta_{t-k+i} \right) / \beta_t & \text{if } 0 \le k \le s, \\ -\sum_{i=0}^{k-1} c_i \beta_{t-k+i} / \beta_t & \text{if } k > s. \end{cases}$$

In this way we get the asymptotic expansion

(12)
$$f_j := (j+b)^{\nu-1} r(j) = \sum_{k=1}^m a_k j^{-p_k} + O(j^{-p_{m+1}}), \ m = 1, 2, \dots, \ j \ge n^*,$$

with

(13)
$$a_k = \sum_{i=1}^k \binom{\nu-1}{k-i} c_{i-1} b^{k-i}, \ p_k = k+t-s-\nu, \ k=1,2,\dots,$$

and

(14)
$$n^* = \begin{cases} \tilde{n} & \text{if } b \in \mathbb{C} \setminus (-\infty, -j_0], \\ \max\{\tilde{n}, [|b|] + 1\} & \text{if } b \in (-\infty, j_0] \setminus \{-j_0, -j_0 - 1, ...\}. \end{cases}$$

In (13), indeed, a_k is the kth coefficient of the product of the asymptotic expansions for r(j) and $(j+b)^{\nu-1}$. The fact that $(j+b)^{\nu-1}=j^{\nu-1}(1+b/j)^{\nu-1}$ possesses an asymptotic expansion in powers of j^{-1} is a trivial consequence of the Maclaurin formula for the binomial function $(1+w)^{\nu-1}$ when $w=b/j\in\mathbb{C}\setminus(-\infty,-1]$ (where j>|b| when b<0).

From (3)-(6) we can finally write the representation

(15)
$$S = S_n + R_n = \sum_{j=j_0}^{n-1} z^j (j+b)^{\nu-1} r(j) + \sigma_{n,m} + \varepsilon_{n,m} , \quad m = 1, 2, \dots ,$$
$$\sigma_{n,m} = z^n n^{-q} \sum_{k=1}^m b_k(z) n^{-k} , \quad \varepsilon_{n,m} = z^n O\left(n^{-(m+q+1)}\right) , \quad n \ge n^* ,$$

where $q = t - s - \nu$ if $z \neq 1$, and $q = t - s - \nu - 1$ if z = 1.

3. The summation algorithm

The representation (15) gives rise to the problem of constructing an algorithm that finds a pair (n,m) such that the relative error $|\varepsilon_{n,m}/S|$ is below a given tolerance and at the same time the computational cost is low. Recall that, because of the asymptotic nature of the approximation in (15), the error term $\varepsilon_{n,m}$ tends to 0 as $n \to \infty$, but is not infinitesimal as $m \to \infty$; indeed, $|\varepsilon_{n,m}|$ exhibits for each fixed value of n a minimum in m which is infinitesimal as $n \to \infty$. As in [3], however, we forgo a procedure based on finding (empirically) such a minimum for a given subsequence of indices $\{n_s\}$: in fact, the complexity in the computation of $\sigma_{n,m}$ increases quadratically (z=1) or cubically $(z\neq 1)$ with m, so that this approach turns out to be quite costly.

An alternative strategy, which is that adopted in [3], consists in trying to balance the computational cost of the partial sum S_n with that of $\sigma_{n,m}$ in terms of the order of magnitude of the respective flops number. While the computation of $\sigma_{n,m}$ requires basically only elementary arithmetic operations, that of S_n may involve the evaluation of logarithms (when $\nu < 1$). In this regard we have assumed that the computation of a logarithm corresponds to 10 flops: this value was obtained by averaging the results obtained with various programming languages and compilers, on various processors.

The summation algorithm can then be summarized as follows:

- (i) k := 1, $n_0 := j_0 1$, $S_{n_0} := 0$, $c_0 := \alpha_s / \beta_t$;
- (ii) compute the coefficient a_k by (11), (13), and $b_k(z)$ by (4)-(6);
- (iii) compute the partial sum S_{n_k} as

(16)
$$S_{n_k} := S_{n_{k-1}} + \sum_{j=n_{k-1}+1}^{n_k} z^j (j+b)^{\nu-1} r(j) ,$$

where n_k is choosen in such a way as to balance the cost of (ii) with the cost of (16), as described above;

- (iv) for i = 1, ..., k
 - compute $\sigma_{n_k,i}$ as in (15);
 - if i < k, then if

(17)
$$\mu_{k,i} \left| \frac{\varepsilon_{n_k,i}}{S} \right| \cong \left| \frac{S_{n_k} - S_{n_{k-1}} + \sigma_{n_k,i} - \sigma_{n_{k-1},i}}{S_{n_k} + \sigma_{n_k,i}} \right| \leq \mu_{k,i} \cdot reltol ,$$
where
$$\mu_{k,i} = \left| 1 - z^{n_{k-1} - n_k} \left(\frac{n_k}{n_{k-1}} \right)^{q+i+1} \right| ,$$

then EXIT;

(v) go to step (ii) with k := k + 1.

A key observation is now in order. In principle, representation (15) can be used only for $n \geq n^*$ (cf. (14)), so that in step (i) one should choose $n_0 \geq n^*$ and compute the initial sum S_{n_0} to start the iterative process, making an appropriate use of the *a posteriori estimate* (17). Such an estimate is strongly based on the asymptotic nature of (15): in fact by (15) we obtain $\varepsilon_{n,i} \cong z^n b_{i+1}(z) n^{-(q+i+1)}$ for

 $n > n^*$ sufficiently large, and moreover, we have

(18)
$$\left| S_{n_k} - S_{n_{k-1}} + \sigma_{n_k,i} - \sigma_{n_{k-1},i} \right| = \left| \varepsilon_{n_k,i} - \varepsilon_{n_{k-1},i} \right|$$

$$\cong \left| \left(1 - z^{n_{k-1} - n_k} \left(\frac{n_k}{n_{k-1}} \right)^{q+i+1} \right) \varepsilon_{n_k,i} \right|$$

for k sufficiently large.

This implies that a (possibly sharp) overestimate of \tilde{n} should be produced (cf. (9)), for example by using for the denominator $\beta(z)$ one of the well-known a priori bounds of the complex zeros of a polynomial, or by applying a suitable localization algorithm for the zeros; cf. [7, Ch.6] for an extensive treatment of these topics. In fact, in excluding the zeros of $\beta(z)$ we exclude a fortiori the poles of r(z).

In practice, however, the summation algorithm sketched above turns out to be "robust" in the sense that it gives a correct answer also starting from $n_0 = j_0 - 1$, $S_{n_0} = 0$: our numerical experiments confirmed that in every case the exit index n_k is greater than n^* . On the other hand, it should also be noticed that this dependence on the value of n^* can represent a possible drawback of the method, when $b \ll -1$ or when r(z) exhibits poles with very large modulus.

4. Numerical examples

In this section we present the results of the application of the asymptotic summation method to several series of the form (8). In all the examples we set a relative tolerance $reltol = 10^{-14}$ in the termination test (17): in Tables I-X below $(n,i) = (n_k,i)$ is the first pair which satisfies (17).

All computations have been carried out in double-precision arithmetic within the Turbo Pascal programming framework, on a Pentium-based personal computer. The accuracy and (empirical) stability of the method are witnessed by the fact that the actual errors are always below the prescribed tolerance; the errors have been computed by comparison with the values obtained by the numerical summation tool *NSum* of *Mathematica* [12, §3.9.4].

Tables I-VIII refer to the summation of

(19)
$$\sum_{j=1}^{\infty} z^j j^{\nu-1} \frac{j^s + \dots + 1}{j^t + \dots + 1} , \quad z = e^{i\omega\pi/2} , \quad \omega \in [0, 2] ,$$

for various admissible quadruples ν, s, t, ω corresponding to very slow convergence. Observe that the algorithm behavior gets worse in the neighborhood of z=1 (i.e., for ω "small"), while it works satisfactorily at z=1 ($\omega=0$); as already pointed out in [3], this could be ascribed to the discontinuity of the coefficients $b_k(z)$ at z=1, since $b_k(z) \sim \text{const}/(z-1)^{k+2}$ as $z\to 1$, cf. (4)-(6) and [3, Remark 1.4].

In Tables IX-X we report the results corresponding to the summation of

(20)
$$\sum_{j=1}^{\infty} j^{\nu-1} \frac{\alpha_1 j + \alpha_0}{\beta_2 j^2 + \beta_0} ,$$

for $\nu = 1/2$ and $\nu = 9/10$, varying the relative weights of the coefficients of the rational function within a range of two orders of magnitude. Only the values of these coefficients which are not related by a scaling of the series have been considered.

Table I. Summation of (19) for $\nu = 1$, s = 1, t = 2

ω	2	1	0.8	0.6	0.4	0.2	0.1	0.05	0.01
n	67	90	90	117	149	230	336	547	2246
m	9	9	10	10	10	11	14	17	2246 21

Table II. Summation of (19) for $\nu = 1, s = 1, t = 3$

ω	2	1	0.8	0.6	0.4	0.2	0.1	0.05	0.01	0
n	60	81	81	105	134	167	300	490	2010	54
m	8	9	9	9	10	13	13	16	17	8

Table III. Summation of (19) for $\nu = 1$, s = 9, t = 10

	ω	2	1	0.8	0.6	0.4	0.2	0.1	0.05	0.01
ſ	n	31	52	65	65	97	138	253	468	2027
	m	10	11	11	13	13	17	18	20	2027 27

Table IV. Summation of (19) for $\nu = 1, s = 9, t = 11$

	ω	2	1	0.8	0.6	0.4	0.2	0.1	0.05	0.01	0
П	n	29	48	48	60	73	127	203	386	1516	16
I	m	10	10	12	11	13	13	17	15	1516 16	9

Table V. Summation of (19) for $\nu = 1/2$, s = 1, t = 2

ĺ	ω	2	1	0.8	0.6	0.4	0.2	0.1	0.05	0.01	0
ſ	n	40	52	65	65	97	138	253	468	2027	20
	m	10	11	11	13	12	16	17	18	2027 20	11

Table VI. Summation of (19) for $\nu = 1/2$, s = 1, t = 3

	ω	2	1	0.8	0.6	0.4	0.2	0.1	0.05	0.01	0
ĺ	n	30	49	49	62	76	133	211	401	1693	19
	m	10	10	12	12	14	14	20	18	1693 19	11

As a confirmation of the robustness of the summation algorithm, it is also interesting to quote the following result. For $\alpha_1=1$, $\alpha_0=1$, $\beta_2=1$, and $\beta_0=10^4$ we obtained (n,m)=(198,37) with $reltol=10^{-14}$, and (n,m)=(119,23) with $reltol=10^{-4}$, both starting from $n_0=0$, $S_{n_0}=0$: observe that $n>n^*=\tilde{n}=100$ for two very different values of the relative tolerance.

Table VII. Summation of (19) for $\nu=1/2,\,s=9,\,t=10$

										0.01	
Π	n	31	39	48	58	83	133	224	428	1909	13
	m	10	13	13	14	14	17	21	21	1909 25	12

Table VIII. Summation of (19) for $\nu=1/2,\,s=9,\,t=11$

	ω	2	1	0.8	0.6	0.4	0.2	0.1	0.05	0.01	0
I	n	30	38	47	57	68	112	119	379	1653	12
	m	10	12	12	12	15	19	17	21	1653 19	9

Table IX. Summation of (20) for $\nu = 1/2$

α_1	1	1	1	1	1	1	1	1	1	1	10	10	10
α_0	1	1	1	1	1	10	10	10	10	10	1	1	1
β_2	1	1	1	10	10^{2}	1	1	1	10	10^{2}	1	1	1
β_0	1	10	10^{2}	1	1	1	10	10^{2}	1	1	1	10	10^{2}
n	21	32	50	18	10	21	28	50	18	18	21	32	50
m	11	13	18	10	10	11	13	18	10	10	11	12	18

α_1	10	10	1	1	1	1	1	10^{2}	10^{2}	10^{2}	10^{2}	10^{2}
α_0	1	1	10^{2}	10^{2}	10^{2}	10^{2}	10^{2}	1	1	1	1	1
β_2	10	10^{2}	1	1	1	10	10^{2}	1	1	1	10	10^{2}
β_0	1	1	1	10	10^{2}	1	1	1	10	10^{2}	1	1
n	18	18	21	32	50	18	18	21	32	50	18	18
m	9	9	11	13	18	10	10	11	12	18	9	9

Table X. Summation of (20) for $\nu=9/10$

α_1	1	1	1	1	1	1	1	1	1	1	10	10	10
α_0	1	1	1	1	1	10	10	10	10	10	1	1	1
β_2	1	1	1	10	10^{2}	1	1	1	10	10^{2}	1	1	1
β_0	1	10	10^{2}	1	1	1	10	10^{2}	1	1	1	10	10^{2}
n	21	32	50	18	18	21	28	50	18	18	21	32	50
m	10	13	18	10	10	11	13	18	10	10	11	12	18

ſ	α_1	10	10	1	1	1	1	1	10^{2}	10^{2}	10^{2}	10^{2}	10^{2}
l	α_0	1	1	10^{2}	10^{2}	10^{2}	10^{2}	10^{2}	1	1	1	1	1
l	β_2	10	10^{2}	1	1	1	10	10^{2}	1	1	1	10	10^{2}
l	β_0	1	1	1	10	10^{2}	1	1	1	10	10^{2}	1	1
İ	n	18	18	24	32	55	18	18	21	28	50	18	15
l	m	9	9	11	13	18	10	10	11	12	18	9	9

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