Referee Report on Manuscript NUMA948

An Efficient Algorithm for Accelerating the Convergence of Oscillatory Series, Useful for Computing the Polylogarithm and Hurwitz Zeta Functions

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(submitted to Numerical Algorithms)

Polylogarithms and zeta functions are very important special functions, and there is a very detailed literature on these functions. However, it is also well known that the efficient and reliable numerical evaluation of these functions is much more difficult than it may look at first sight. Accordingly, articles dealing with the evaluation of these functions are certainly welcome and useful.

Nevertheless, I cannot recommend the publication of this manuscript in its present form in Numerical Algorithms. As explained in the following text, this manuscript has to be improved considerably before it could be published.

First, a purely technical remark. In Numerical Algorithms, it is customary to enclose equation numbers in the text in parentheses `()`. The author should follow this convention since it improves readability.

Secondly, the author should give more references. Too often, the author uses mathematical results, that are too special to be known by the hypothetical typical reader of Numerical Algorithms, without giving appropriate references.

The phrase "oscillatory sequence" or "oscillatory series" plays a major role in this manuscript. I have the impression that it would be desirable to provide more background information on these concepts and also define these things properly. In the literature on convergence acceleration, which predominantly considers real sequences, a different terminology is used. For example, in the book by Brezinski and Redivo Zaglia [1, pp. 97 and 90], *totally montonic* and *totally oscillatory* sequences are defined.

A better motaivation of the terms mentioned above would be desirable also because the zeta Hurwitz function $\zeta(s, q))$ and the polylogarithm $\mathrm{Li}_s(z)$ are defined by the series expansions (1.1) and (1.4) on pp. 1 and 2, respectively, which for positive s, q, and z can be viewed to be prototypes of monotonic series.

In the 1st line of the 1st paragraph of Section 1 on p. 1, the author calls his manuscript a "note". In my opinion, this manuscript is far too long for that. Therefore, I suggest to replace "note" by "article".

In Eq. (1.1) on p. 1, the Hurwitz zeta function is defined by the following Dirichlet series:

$$\zeta(s, q) \;=\; \sum_{n=0}^{\infty} (n+q)^{-s} \,. \tag{1}$$

As is well known, this Dirichlet series converges if $\Re(s) > 1$. Accordingly, it cannot be used in the so-called *critical strip* $s = \sigma + \mathrm{i}\tau$ with $0 \le \sigma \le 1$.

The author ignores the fact that in the Dirichlet series (1) there is a restriction on the 2nd parameter q. As for instance emphasized in [2, p. 22], we must have $q \neq 0, -1, -2, \ldots$ in (1). This negligence is hard to understand since in Figure .2 on p. 30 the author shows that $\zeta(s, q)$ has a pole for $q = 0$.

The fact, that the Dirichlet series (1) for $\zeta(s, q)$ is undefined for $q = 0, -1, -2, \ldots,$ is quite important for the series expansion (1.3) on p. 2, which was derived by doing a power series expansion of (1) about $q = 0$. Since we also have (see for example [2, p. 22])

$$\zeta(s, 1) \;=\; \zeta(s) \,, \tag{2}$$

where $\zeta(s)$ is Riemann's zeta function defined by the Dirichlet series

$$\zeta(s) \;=\; \sum_{n=0}^{\infty} (n+1)^{-s} \,, \qquad \Re(s) > 1 \,, \tag{3}$$

we must expand $\zeta(s, q)$ about $q = 1$. If we also use (see for example [2, p. 23])

$$\frac{\mathrm{d}^m}{\mathrm{d}q^m} \zeta(s, q) \;=\; (-1)^m \, (s)_m \, \zeta(s+m, q) \,, \qquad m \in \mathbb{N}_0 \,, \tag{4}$$

we obtain the following expansion:

$$\zeta(s, q) \;=\; \sum_{m=0}^{\infty} (1-q)^m \, \frac{(s)_m}{m!} \, \zeta(s+m) \,. \tag{5}$$

Obviously, this power series in $1 - q$ converges if $|1 - q| < 1$. Of course, the ratio $(s)_m / m!$ can also be expressed as a binomial coefficient according to

$$\binom{s+m-1}{m} \;=\; \frac{(s)_m}{m!} \,. \tag{6}$$

If we replace in (5) q by $q + 1/2$, we immediately obtain the following power series expansion:

$$\zeta(s, q+1/2) \;=\; \sum_{m=0}^{\infty} (1/2-q)^m \, \frac{(s)_m}{m!} \, \zeta(s+m) \,, \qquad |1/2 - q| < 1 \,. \tag{7}$$

I also have some problems with the unnumbered series expansion for $\zeta(s, q+1/2)$ on p. 2. In my opinion, the author should explain more clearly that this expansion is the Taylor expansion of $\zeta(s, q+1/2)$ about $q = 0$. If we use (4), we obtain:

$$\zeta(s, q+1/2) \; = \; \sum_{m=0}^{\infty} (-q)^m \, \frac{(s)_m}{m!} \, \zeta(s+m, 1/2) \, . \tag{8}$$

If we now use [3, Example 2 on p. 267]

$$(2^s - 1) \, \zeta(s) \; = \; \zeta(s, 1/2) \, , \tag{9}$$

we obtain

$$\zeta(s, q+1/2) \; = \; \sum_{m=0}^{\infty} (-q)^m \, \frac{(s)_m}{m!} \, (2^{s+m} - 1) \, \zeta(s+m) \, . \tag{10}$$

In intermediate formula (8) is nevertheless helpful because from it we can understand more easily that both (8) and (10) converge for $|q| < 1/2$.

In this manuscript, Taylor expansions are used for the evaluation of Hurwitz zeta functions. In this context, it may well be a useful idea to combine these expansions with suitable convergence acceleration techniques. As is well known, convergence acceleration techniques such as Wynn's epsilon algorithm [4], Brezinski's theta algorithm [5], or the various Levin-type transformations described in [6, 7, 8] are particularly powerful in the case of strictly alternating series. I am convinced that the use of suitable convergence acceleration techniques can greatly enhance the efficiency of the Taylor expansions mentioned above. The author should definitely investigate this, but not necessarily in this manuscript.

In the 4th line of the 1st paragraph of Section 1 on p. 1, "principle" should be replaced by "principal".

In the text following the unnumbered equation after Eq. (1.3) on p. 2. "of the Riemann zeta;" and "compute time" should be replaced by "of the Riemann zeta function;" and "computing time", respectively.

In the text following Eq. (1.5) on p. 2, effective algorithms for polylogarithms are mentioned. In this respect, it may be of interest for the author that in recent years some alternative techniques had been developed that can be quite useful for monotone power series with arguments close to the boundary of its circle of convergence. A discussion of these topics and several numerical examples can be found in the article [9]. This article uses a condensation transformation introduced by Van Wijngaarden, which transforms a monotone series to an alternating series. Van Wijngaarden's condensation transformation was first mentioned in the book by Clenshaw, Goodwin, Martin, Miller, Olver, and Wilkinson [10, p. 126] and only later described by Van Wijngaarden [11]. Being unaware of the previous work on the Van Wijngaarden transformation, Pelzl and King [12] rediscovered this condensation transformation.

Later, Van Wijngaarden's condensation transformation was used by Daniel [13] who accelerated the convergence of the transformed alternating series with the help of Euler's series transformation. The same approach was also pursued by Wallén and Sihvola [14]. In my opinion, the combination of Van Wijngaarden's condensation transformation with the Euler transformation does not seem to be such a good idea: The Euler transformation is in general an at most moderately powerful accelerator. Later, the more effective approach described in [9] based on the so-called delta transformation introduced in [6, Eq. (8.4-4)] or on other powerful nonlinear sequence transformations was also used in [15, 16, 17, 18]. This approach is also discussed on p. 217 of the most recent (3rd) edition of the book *Numerical Recipes* [19] which came out just a few days ago.

The approach described above is also of interest in connection with zeta functions. In [9, Eqs. (4.1) - (4.3))] it was shown that the application of Van Wijngaarden's condensation transformation to the Dirichlet series (3) of the Riemann zeta function can be expressed in closed form, yielding the following well known alternating series representation [20, Eq. (23.2.19)]:

$$\zeta(s) \; = \; \frac{1}{1-2^{1-s}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)^s} \, . \tag{11}$$

From a computational point of view, this alternating series expansion, which converges for $\Re s > 0$, is much more attractive than the Dirichlet series (3), in particular if it is combined with suitable convergence acceleration techniques. Experience has shown that the acceleration of the convergence of strictly alternating series is a remarkably stable process. Accordingly, it is normally possible to compute $\zeta(s)$ via (11) with an accuracy that is close to machine accuracy.

Unfortunately, Van Wijngaarden's condensation transformation does not lead to a simple closed form expression of the type of (11) in the case of the Hurwitz zeta function $\zeta(s,q)$. Nevertheless, the resulting alternating series expansion for $\zeta(s,q)$ should have much better numerical properties than the Dirichlet series (1). I suspect that it would be of considerable interest to investigate this approach.

In the 4th line from below on p. 2, the author cites two articles by Borwein as his Refs. [4, 5]. In this context, an article by Borwein, Bradley, and Crandall [21] may also be of interest.

In the 3rd line from below on p. 2, the author speaks of "Padé-approximant type algorithm". Here, the author should be more specific and explain more carefully what he means. In particular, the author should take into account that in addition to Padé approximants, which are named after Padé's thesis [22], there are also the so-called *Padé-type approximants* which were introduced in [23] and fully developed in [24].

In the 3rd paragraph of p. 3, the evaluation of the Hurwitz zeta function via the Euler-Maclaurin summation formula is discussed. In this respect, it may be of interest for the author that the evaluation of the Riemann zeta function via the Euler-Maclaurin summation formula was discussed in a relatively detailed way in [25, Section 2]. By considering the example $\zeta(1.01)$, it was shown there that the convergence of an infinite series and its usefulness as a computational tool are at best loosely connected.

An alternative approach for the Euler-Maclaurin summation formula was discussed in [26, Section 2]. I am confident that the approach described in [26, Section 5] for the Riemann zeta function will also work for the Hurwitz zeta function.

In the 3rd paragraph of p. 3, there occurs the sentence "It is faster then evaluating 1.5 (which can be computed for real values of q)." which I do not really understand.

In the 7th line of 3rd paragraph of p. 3, "application of the Euler Maclaurin summation" should be replaced by "application of Euler Maclaurin summation".

In the Proof of Lemma 2.1 on p. 4, I suggest to replace "This identity is easily obtained by inserting the integral representation of the Gamma function:" by "This identity is easily obtained by inserting the integral representation of the Gamma function into (1.4):".

In the last line of Section 2, "Costin[6, Thm. 1]" should be replaced by "Costin and Garoufalidis [6, Thm. 1]". This applies also to "Costin[6, eqn 14]" in the 2nd paragraph on p. 18.

Section 3 on p. 4 is called "THE BORWEIN TRICK". In my opinion, one should also indicate via suitable references where this Borwein trick can be found.

In the Proof of Lemma 2.1 on p. 4, the author states "This identity is easily obtained by inserting the integral representation of the Gamma function:". In my opinion, one should always state clearly into which expression something should be inserted.

In my opinion, the derivation of Eq. (3.1) on p. 4 is messy and basically incomprehensible for the uninitiated reader. In particular, the author should explain the role of $\xi(s,z)$ which is introduced via Eq. (3.1) without any additional comments or remarks. Please clarify and improve. In my opinion, the author should start from the integral representation for $\mathrm{Li}_s(z)$. I am also not completely happy with the notation $\xi(s,z)$. The problem is that in the theory of the Riemann zeta function there occurs also the function [27, Eq. (2.1.12) on p. 16]

$$\xi(s) \; = \; \frac{s(s-1)\,\Gamma(s/2)\,\zeta(s)}{2\pi^{s/2}} \, , \tag{12}$$

which satisfies the exceptionally simple functional equation [27, Eq. (2.1.13) on p. 16]

$$\xi(s) \; = \; \xi(1-s) \, . \tag{13}$$

Therefore, an alternative notation for $\xi(s,q)$ would be desirable.

In the 1st paragraph of Section 4 on p. 5, the author states " ...a particularly efficient algorithm for Euler's method is given by van Wijngaarden[19]." Here, the author's Ref. [19] corresponds to an older edition of the well known book *Numerical Recipes*. However, it would be better to cite the original reference, which is the book by Clenshaw *et al.* [10, pp. 125 - 16].

In the 1st paragraph of Section 4 on p. 5, "Cohen etal[18]" should be replaced by "Cohen et al. [18]".

I have the impression that in the 1st unnumbered equation on p. 7, "$\xi(z)$" should be replaced by "$\xi_n(z)$".

In the 2nd paragraph on p. 7, the power series (4.1) on p. 6 is called "geometric series". However, the geometric series is the special power series $1/(1-z) = \sum_{n=0}^{\infty} z^n$.

In the 3rd paragraph from below on p. 7, there occurs "(mostly) positive". Please explain.

In the 1st paragraph on p. 8, the polynomials $p_n(y) = y^a(1-y)^{n-a}$ are introduced. However, this is a bad notation this it does not provide any information on the parameter a. It is also inconsistent with the notation for the polynomials $p_{2n}(y) = y^n(1-y)^n$ occurring in 2nd paragraph on p. 8.

I do not really understand the 1st unnumbered equation on p. 8. The Landau symbol `big-O` is normally used to describe the behavior of a function $f(y)$ in the vicinity of a point, say y_0. It may well be that here we have $y_0 = 1/2$, but the author should be more specific. Moreover, I am wondering whether the 1st unnumbered equation on p. 8 is new or whether it had already been treated elsewhere in the literature.

Assuming $|\sigma| \ll n$, the author derived on p. 10 the following estimate:

$$\frac{\Gamma(n+1)\Gamma(n+\sigma)}{\Gamma(2n+\sigma+1)} \le \frac{2^{1-\sigma}}{4^n} \,. \tag{14}$$

Please explain the derivation of this estimate.

Please give suitable references for the 1st three unnumbered equations on p. 11. This applies also to Eq. (7.1) on p. 11 and to the unnumbered equations on p. 12.

In the 3rd unnumbered equation on p. 11, the author uses a notation for the Stirling numbers of the second kind that was introduced by Knuth [28]. Unfortunately, a bewildering multitude of different conventions and notations for Stirling numbers occurs in the literature. In particular, there are *signed* and *unsigned* Stirling numbers. Therefore, a precise definition of the Stirling numbers of the second kind would be desirable, for example via its generating function which expresses an integral power in terms of Pochhammer symbols:

$$z^n = \sum_{\nu=0}^{n} \left\{ {n \atop \nu} \right\} (z-\nu+1)_\nu \,. \tag{15}$$

Personally, I would replace $s(s+1)(s+2)\ldots(s+2k)$ in the 1st unnumbered equation on p. 12 by the Pochhammer symbol $(s)_{2k+1}$.

In the 2nd unnumbered equation on p. 12, the *integral part* $\lfloor x \rfloor$ should be explained properly.

The last line of Section 7 on p. 12,

> "XXX to do: characterize the region of convergence for this algo."

creates the impression that the author had submitted an only partly finished manuscript. This applies also to the sentences "XXX Expand on this remark." and "XXX Expand on this." occurring on p. 24.

In the caption of Fig. 8.1 on p. 13, I suggest to replace "closer to the troublesome branch point at $z = +1$ than algorithmically optimum $z = -1$." by "closer to the troublesome branch point at $z = +1$ than the algorithmically optimal argument $z = -1$.".

A suitable reference for the so-called p-adic identity in the last line of p. 16 should be given.

In the text following Eq. (9.1) on p. 17, I suggest to replace "to the equation 9.1 immediately above," by "to Eq. (9.1) immediately above," or by the even shorter "to Eq. (9.1),".

I suspect that in the 1st unnumbered equation on p. 18, there should be the restriction that q must not be integral, $q \notin \mathbb{Z}$.

References for the two unnumbered equations in Section 10 on p. 18 should be given. Moreover, it would help the reader if Bernoulli polynomials would also be defined. The following generating function should suffice for that purpose:

$$\frac{t\mathrm{e}^{zt}}{\mathrm{e}^t - 1} = \sum_{n=0}^{\infty} \frac{B_n(z)}{n!} t^n , \qquad |t| < 2\pi . \tag{16}$$

Whenever complex numbers occur, branch points are of course extremely important. Nevertheless, I am not convinced that an extensive discussion of "BRANCH POINTS AND MONODROMY" as it is done in Section 11 is really suited for a predominantly numerical journal like Numerical Algorithms. In my opinion, it would be better to publish this discussion elsewhere and to focus in this manuscript on numerical and computational aspects.

But even if Section 11 should be condensed substantially, I would nevertheless like to see additional references that could provide necessary background information. I do not think that the hypothetical typical reader of Numerical Algorithms is sufficiently familiar with the topics discussed in Section 11.

The lone "The" at the end of the 1st paragraph on p. 18 is superfluous and should be deleted.

I must admit that I do not really understand the meaning of "straddling value" in the 2nd paragraph from below on p. 18.

Figure 11.1 on p. 19 refers to Eq. (11.4) on p. 23. Why appears Fig. 11.1 on p. 19 and not later?

In Eq. (12.1) on p. 25, the so-called *periodic zeta function* $F(q; s)$ was introduced. Firstly, why now $F(q; s)$ and not $F(s; q)$ as in $\zeta(s, q)$? Secondly, in the so-called p-adic identity in the last line of p. 16, there also occurs a function $F(q; s)$. Are these two functions identical? If yes, explain, and if no, use a better and less bewildering notation.

In the 2nd paragraph from below of Section 13 on 27, Lerch's transcendent is mentioned. It may be of interest for the author that a C program for Lerch's transcendent plus additional diocumentation files can be downloaded from the homepage

`http://www.mpi-hd.mpg.de/personalhomes/ulj/`

of Ulrich Jentschura.

In the title of both Ref. [4] and Ref. [5] on pp. 27 and 28, "riemann" should be replaced by "Riemann".

The WWW address given in Ref. [4] on p. 27,

`http://www.cecm.sfu.ca/personal/pborwein/`

may well be somewhat outdated. When I searched Google for *Peter Borwein*, I was directed to the following WWW address:

`http://www.cecm.sfu.ca/~pborwein/PAPERS/papers.html`

However, on neither of the two WWW addresses given above I was able to find a file `P117.ps`. On these WWW addresses, I only found a file `P155.pdf` with the title *An efficient algorithm for the Riemann zeta function* which seems to refer to Ref. [5] on p. 28. However, I was later able to find file `P117.ps` by searching Google for *Peter Borwein* and *Riemann* simultaneously. A superficial look at the two files `P117.ps` and `P155.pdf` indicates that they are identical. Accordingly, Refs. [4] and [5] should be condensed to a single reference.

The WWW address given in Ref. [7] on p. 28 is wrong. Correct is:

`http://people.reed.edu/~crandall/papers/Polylog.pdf`

I suspect that the author overlooked the fact that in LaTeX the tilde "~" is normally interpreted as a space " " with fixed length. To avoid this, a `verbatim` environment has to be used.

The title of Ref. [10] on p. 28 is incomplete. Correct is:

Ein Summierungsverfahren für die Riemannsche ζ-Reihe

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