On Transforming Logarithmic to Linear Convergence by Interpolation*

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Abstract

We propose to map logarithmically converging sequences to linearly converging sequences using interpolation. After this, convergence accelerators for linear convergence become effective. The interpolation approach works also if only relatively few members of the problem sequence are known, contrary to several other approaches. The effectiveness of the approach is demonstrated for a particular example.
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1 Description of the Method

Many slowly convergent sequences $\{s_n\}_{n\in\mathbb{N}}$ satisfy the equation

$$\lim_{n\to\infty} (s_{n+1} - s)/(s_n - s) = \rho \tag{1}$$

and are called *linearly convergent* if $0 < |\rho| < 1$, and *logarithmically convergent* for $\rho = 1$. In particular, logarithmically convergent sequences are slowly convergent and notoriously difficult to extrapolate and so, there is quite a large literature on special methods to deal with this problem. A necessarily incomplete list of references is [1–22]. More general references for extrapolation, convergence acceleration, and summation of divergence are [4, 9, 20, 21].

The reason for the problems with logarithmically convergent sequences is that there is no single method that is able to provide convergence acceleration for

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all such sequences as shown by Delahaye and Germain-Bonne [5]. This implies that a large variety of methods are required, although there are some methods that seem to work for larger subsets of the set of logarithmically convergent sequences [7, 19].

For linearly convergent sequences, many methods are known to work [4, 8, 10, 20, 23]. Thus, there have been attempts to use only linearly convergent subsequences of the logarithmically convergent sequence [3, 18]. In this way, the usual convergence accelerators for linearly convergent sequences, like the ϵ algorithm [23], the Levin transformation [10], and the iterated version [4, 20, 21] of the famous Δ^2 process [24] become applicable. The main problem of these approaches is that usually a very large number of sequence elements is needed in order to extract the linear subsequences. Here, we describe an alternative method. For a further approach see [25].

For simplicity, we consider here only logarithmically convergent sequences with $s_n - s = O((n+1)^{-\alpha})$ with $\alpha > 0$ for $n \to \infty$. Also, we assume that only a finite set of sequence elements s_n with $0 \le n \le N$ is available. Then, regarding n as a continuous parameter, we define a mapping

$$s_n \to \tilde{s}_m = s_{f(m)} \,, \qquad n = f(m) = \sigma^m - 1 \,, \quad \sigma > 1 \tag{2}$$

and obtain

$$\lim_{m\to\infty} (\tilde{s}_{m+1} - s)/(\tilde{s}_m - s) = \sigma^{-\alpha} =: \tilde{\rho} \,. \tag{3}$$

This equation holds also under the weaker condition

$$(s_{n+1} - s)/(s_n - s) \sim 1 - \alpha/n \quad \text{as} \quad n \to \infty \tag{4}$$

since this implies

$$\ln[(s_{\sigma(n+1)-1} - s)/(s_n - s)] \sim (-\alpha) \sum_{j=n}^{\sigma n} 1/j \sim -\alpha \ln \sigma \quad \text{as} \quad n \to \infty \tag{5}$$

where now one may put $n = f(m)$ and use the identity $f(m+1) = \sigma(f(m) + 1) - 1$. Since $0 < |\tilde{\rho}| < 1$, the "sequence" $\{\tilde{s}_m\}$ would be linearly convergent. There is, however, the problem that for integer n the values of m are in general noninteger (with the possible exception of some special values of σ and n). The way out is to use noninteger values of n by computing an continous interpolating function $\phi : [0, N] \to \mathbb{C}$. The interpolation conditions are $\phi(n) = s_n$ for $n = 1, \ldots, N$. We choose the desired range of m values as $[0, M]$ and put $\sigma = (N + 1)^{1/M}$ accordingly. Then, we may put $\tilde{s}_m = \phi(f(m))$ for integer m. Obviously, this new sequence may be regarded as linearly convergent. Formally, the limit s is unchanged if f is an bijective mapping of $[0, \infty)$ onto itself. The $M+1$ sequence elements $\tilde{s}_0, \ldots, \tilde{s}_M$ depend only on the $s_0, \ldots, s_N$ and the choice of the interpolation scheme, and the former can now be input to a standard convergence accelerator for linear convergence like the ϵ algorithm to compute an approximation of the limit s.

Table 1: Coefficients of the rational interpolant

j	p_j	q_j
0	$2.4156362287713252e+23$	$1.2650340186680030e+23$
1	$-6.9466187687642456e+22$	$4.6197728641881184e+22$
2	$1.7472782389930610e+22$	$8.2730873509423696e+21$
3	$-9.9302425597562704e+20$	$9.5926044596699824e+20$
4	$1.3495942609493410e+20$	$8.0424150701645184e+19$
5	$-3.7019467489948920e+18$	$5.1624254245533744e+18$
6	$2.5551801989536920e+17$	$2.6199945009733000e+17$
7	$-3.9506222548065600e+15$	$1.0725800946057290e+16$
8	$7.3970350942840384e+13$	$3.5531621772820436e+14$
9	$7.7882811808294000e+11$	$9.6750555948722976e+12$
10	$-8.6214475699912304e+10$	$2.0510651146889728e+11$
11	$1.8887209977950680e+09$	$3.7648101375003456e+09$
12	$-2.0741676247961408e+07$	$4.1591020534348688e+07$
13	$1.2896941144609298e+05$	$6.1092646461362344e+05$
14	$-4.3922131631892304e+02$	$2.2797801442194008e+03$
15	$6.4544236191649008e-01$	$3.7786526415900824e+01$

2 A Numerical Example

All calculations in this section were done using `MAPLE V`$^{\mathrm{TM}}$ Release 3. As interpolation scheme defining ϕ, we used rational interpolation based on Thiele's interpolation formula involving reciprocal differences [26, Chap. 25, p. 881, Eq. 25.2.50]. The interpolating function was calculated in `MAPLE V`$^{\mathrm{TM}}$ by procedure `thiele` using an accuracy of 64 decimal digits in order to exclude numerical instabilities in this step. All other `MAPLE V`$^{\mathrm{TM}}$ calculations were done with an accuracy of 32 decimal digits.

As example, we apply the interpolation approach to the sequence (=problem sequence)

$$s_n = \ln(a\,(n+1))(n+1)^{-a} + \ln(n+1)/(n+1)\,, \quad a = 27/4\,, \tag{6}$$

that has the limit $s = 0$. The maximal values of n and m are chosen as $N = M = 30$, whence $\sigma \approx 1.121$. We have for $n \to \infty$

$$(s_{n+1} - s)/(s_n - s) = s_{n+1}/s_n \sim 1 - 1/n + (\ln(n)n)^{-1}\,. \tag{7}$$

Hence, $\alpha = 1$ and $\tilde{\rho} = 1/\sigma \approx 0.8918$. As interpolant $\phi(n)$, the rational interpolant

$$\rho(n) = \sum_{j=0}^{15} p_j\, n^j \Bigg/ \sum_{j=0}^{15} q_j\, n^j \tag{8}$$

with (rounded) coefficients p_j and q_j displayed in Table 1 is obtained. The noninteger n values corresponding to integer m are plotted in Table 2.

Table 2: Noninteger n values

m	$n = f(m)$	m	$n = f(m)$
1	0.1212747863558303	16	5.2429937964118392
2	0.2572571465173129	17	6.0001115352924576
3	0.4097307383555408	18	6.8490485662020336
4	0.5806955324688557	19	7.8009402541647200
5	0.7723940454626317	20	8.8682724032189696
6	0.9873407546644578	21	10.0650450306204896
7	1.2283550801026244	22	11.4069560027266320
8	1.4985983663669992	23	12.9116069412834896
9	1.8016153494371840	24	14.5987341009539296
10	2.1413806523913928	25	16.4904672464685248
11	2.5223509198724976	26	18.6116199250476384
12	2.9495232751502968	27	20.9900149415495360
13	3.4285008665515280	28	23.6568493055474688
14	3.9655663630191744	29	26.6471034372856352
15	4.5677643628300224	30	30.0000000000000000

For the extrapolation, the ϵ algorithm that is defined by the recursive scheme [23]

$$\begin{aligned} \epsilon_{-1}^{(n)} = 0\,, \qquad \epsilon_{0}^{(n)} = s_n\,, \\ \epsilon_{k+1}^{(n)} = \epsilon_{k-1}^{(n+1)} + 1/[\epsilon_{k}^{(n+1)} - \epsilon_{k}^{(n)}] \end{aligned} \tag{9}$$

was chosen as implemented in the `MAPLE V`$^{\mathrm{TM}}$ procedure `eps` in the `share` library (`numerics/trans`). Note that the ϵ algorithm computes the Shanks transforms $e_k(s_n)$ as defined in [20, 27] according to

$$\epsilon_{2k}^{(n)} \;=\; e_k(s_n) \tag{10}$$

and the elements $\epsilon_{2k+1}^{(n)} \;=\; 1/e_k(s_{n+1} - s_n)$ are only auxiliary quantities.

The extrapolation results using the ϵ algorithm on $\tilde{s}_0, \ldots, \tilde{s}_M$ are displayed in Table 3. In the second and third column, the absolute errors of the interpolation transformed sequence elements $\tilde{s}_m$, and of the approximation obtained by extrapolation using sequence elements up to the very same $\tilde{s}_m$ are displayed side by side. In this way, the rather dramatic convergence acceleration obtained using the interpolation approach is demonstrated clearly.

For comparison purposes, we also display in Table 3 in the fifth column the results of applying the u transform of Levin [10, 20] to the original sequence given in the fourth column. The u transform may be defined as

$$u_k^{(n)}(\beta, s_n) = \frac{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} (\beta+n+j)^{k-2} \frac{s_{n+j}}{s_{n+j} - s_{n+j-1}}}{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} (\beta+n+j)^{k-2} \frac{1}{s_{n+j} - s_{n+j-1}}} \tag{11}$$

Table 3: Extrapolation results

ℓ	$\vert\tilde{s}_\ell - s\vert$	$\vert e_{\ell/2}(\tilde{s}_0) - s\vert$	$\vert s_\ell - s\vert$	$\vert u_\ell^{(0)}(1, s_0) - s\vert$
10	$3.657288e-01$	$6.659871e-07$	$2.179909e-01$	$3.654954e-01$
12	$3.480963e-01$	$1.022220e-09$	$1.973039e-01$	$3.280363e-01$
14	$3.227984e-01$	$1.508087e-11$	$1.805367e-01$	$1.216766e-01$
16	$2.933784e-01$	$2.111858e-14$	$1.666596e-01$	$6.842084e-03$
18	$2.625058e-01$	$2.148373e-15$	$1.549705e-01$	$7.160873e-04$
20	$2.319892e-01$	$8.466160e-18$	$1.449773e-01$	$7.831881e-04$
22	$2.029716e-01$	$6.738586e-19$	$1.363258e-01$	$6.414774e-04$
24	$1.761162e-01$	$3.716722e-21$	$1.287550e-01$	$5.301551e-04$
26	$1.517530e-01$	$3.246768e-23$	$1.220680e-01$	$4.446611e-04$
28	$1.299864e-01$	$1.035807e-25$	$1.161137e-01$	$3.777645e-04$
30	$1.107738e-01$	$4.124996e-26$	$1.107738e-01$	$3.245145e-04$

and is implemented as a variant in the `MAPLE V`$^{\rm TM}$ procedure `lev` in the `share` library (`numerics/trans`). The u transform is one of the rather successful nonlinear accelerators for logarithmic convergence [19]. In this example, it is seen to be far inferior to the interpolation approach in combination with the ϵ algorithm. Direct extrapolation ($s \approx \rho(\infty) = p_{15}/q_{15} \approx 0.017$) is inferior, too.

We conclude that there are logarithmically convergent sequences where the interpolation approach can produce good results and is superior to other approaches. It is not to be expected, however, that the details of the approach (use of the nonlinear mapping f as in Eq. (2), Thiele interpolation, ϵ algorithm) will be optimal for all logarithmically convergent sequences. But we remark, that the basic approach can easily be varied by using different nonlinear mappings, interpolation schemes, and other convergence accelerators. This is regarded as a promising future work.

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References

[1] P. Bjørstad, G. Dahlquist, and E. Grosse, Extrapolations of asymptotic expansions by a modified Aitken δ^2-formula, *BIT* **21**, 56–65 (1981).

[2] C. Brezinski, Accélération de suites convergence logarithmique, *C. R. Acad. Sc. Paris* **273 A**, 727 – 730 (1971).

[3] C. Brezinski, J. P. Delahaye, and B. Germain-Bonne, Convergence acceleration by extraction of linear subsequences, *SIAM J. Numer. Anal.* **20**, 1099–1105 (1983).

[4] C. Brezinski and M. Redivo Zaglia, *Extrapolation methods. Theory and practice*, North-Holland, Amsterdam, (1991).

[5] J. P. Delahaye and B. Germain-Bonne, The set of logarithmically convergent sequences cannot be accelerated, *SIAM J. Numer. Anal.* **19**, 840–844 (1982).

[6] J. E. Drummond, Summing a common type of slowly convergent series of positive terms, *J. Austral. Math. Soc.* **B 19**, 416–421 (1976).

[7] J. E. Drummond, Convergence speeding, convergence, and summability, *J. Comput. Appl. Math.* **11**, 145 – 159 (1984).

[8] H. H. H. Homeier, Analytical and numerical studies of the convergence behavior of the $\mathcal{J}$ transformation, *J. Comput. Appl. Math.* **69**, 81–112 (1996).

[9] H. H. H. Homeier, *Extrapolationsverfahren für Zahlen-, Vektor- und Matrizenfolgen und ihre Anwendung in der Theoretischen und Physikalischen Chemie*, Habilitation thesis, Universität Regensburg, (1996).

[10] D. Levin, Development of non-linear transformations for improving convergence of sequences, *Int. J. Comput. Math. B* **3**, 371–388 (1973).

[11] D. Levin and A. Sidi, Two new classes of nonlinear transformations for accelerating the convergence of infinite integrals and series, *Appl. Math. Comput.* **9**, 175–215 (1981).

[12] S. Lubkin, A method of summing infinite series, *J. Res. Natl. Bur. Stand.* **48**, 228–254 (1952).

[13] N. Osada, A convergence acceleration method for some logarithmically convergent sequences, *SIAM J. Numer. Anal.* **27**, 178–189 (1990).

[14] N. Osada, Accelerable subsets of logarithmic sequences, *J. Comput. Appl. Math.* **32**, 217–227 (1990).

[15] N. Osada, An acceleration theorem for the ρ-algorithm, *Numer. Math.* **73**, 521–531 (1996).

[16] N. Osada, Vector sequence transformations for the acceleration of logarithmic convergence, *J. Comput. Appl. Math.* **66**, 391–400 (1996).

[17] L. F. Richardson, The deferred approach to the limit. I. Single lattice, *Phil. Trans. Roy. Soc. London A* **226**, 229–349 (1927).

[18] A. Sidi, Convergence analysis for a generalized Richardson extrapolation process with an application to the $d^{(1)}$ transformation on convergent and divergent logarithmic sequences, *Math. Comput.* **64** (212) 1627–1657 (1995).

[19] D. A. Smith and W. F. Ford, Acceleration of linear and logarithmic convergence, *SIAM J. Numer. Anal.* **16**, 223–240 (1979).

[20] E. J. Weniger, Nonlinear sequence transformations for the acceleration of convergence and the summation of divergent series, *Comput. Phys. Rep.* **10**, 189–371 (1989).

[21] J. Wimp, *Sequence transformations and their applications*, Academic Press, New York, (1981).

[22] P. Wynn, On a procrustean technique for the numerical transformation of slowly convergent sequences and series, *Proc. Cambridge Phil. Soc.* **52**, 663–671 (1956).

[23] P. Wynn, On a device for computing the $e_m(S_n)$ transformation, *Math. Tables Aids Comput.* **10**, 91–96 (1956).

[24] A. C. Aitken, On Bernoulli's numerical solution of algebraic equations, *Proc. Roy. Soc. Edinburgh* **46**, 289–305 (1926).

[25] H. H. H. Homeier. Convergence acceleration of logarithmically convergent series avoiding summation. Technical Report TC-NA-97-8, Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, (1997). *Appl. Math. Lett.* In press.

[26] M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Dover Publications, Inc., New York, (1965).

[27] D. Shanks, Non-linear transformations of divergent and slowly convergent sequences, *J. Math. and Phys. (Cambridge, Mass.)* **34**, 1–42 (1955).