Series Prediction based on Algebraic Approximants

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Abstract

It is described how the Hermite-Padé polynomials corresponding to an algebraic approximant for a power series may be used to predict coefficients of the power series that have not been used to compute the Hermite-Padé polynomials. A recursive algorithm is derived and some numerical examples are given.

Key words: Hermite-Padé polynomial, Algebraic approximant, Padé approximant, prediction of coefficients
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1 Introduction

Using sequence transformation and extrapolation algorithms for the prediction of further sequence elements from a finite number of known sequence elements is a topic of growing importance in applied mathematics. For a short introduction see the book of Brezinski and Redivo Zaglia [3, Sec. 6.8]. We mention theoretical work on prediction properties of Padé approximants and related algorithms like the epsilon algorithm, and the iterated Aitken and Theta algorithms [2, 5, 7, 11], Levin-type sequence transformations [8, 9], the E algorithm [2, 10], and applications on perturbation series of physical problems [6, 8].

Here, we will concentrate on a different class of approximants, namely, the algebraic approximants. For a general introduction to these approximants and

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the related Hermite-Padé polynomials see [1]. Programs for these approximants are available [4]. We summarize those properties that are important for the following.

Consider a function f of complex variable z with a known (formal) power series

$$f(z) = \sum_{j=0}^{\infty} f_j \, z^j \; . \tag{1}$$

The Hermite-Padé polynomials (HPPs) corresponding to a certain algebraic approximant are $N+1$ polynomials $P_n(z)$ with degree $p_n = deg(P_n)$, $n = 0..N$ such that the order condition

$$\sum_{n=0}^{N} P_n(z) f(z)^n = O(z^M) \tag{2}$$

holds for small z. Since one of the coefficients of the polynomials can be normalized to unity, the order condition (2) gives rise to a system of M linear equations for $N + \sum_{n=0}^{N} p_n$ unknown polynomial coefficients. Thus, the coefficient of z^m of the Taylor expansion at $z = 0$ of the left hand side of Eq. (2) must be zero for $m = 0, \ldots, M-1$. In order to have exactly as many equations as unknowns, we choose

$$M = N + \sum_{n=0}^{N} p_n \tag{3}$$

and assume that the linear system (2) has a solution. Then, the HPPs $P_n(z)$ are uniquely defined upon specifying the normalization. The algebraic approximant under consideration then is that pointwise solution $a(z)$ of the algebraic equation

$$P_0(z) + \sum_{n=1}^{N} P_n(z) a(z)^n = 0 \tag{4}$$

for which the Taylor series of $a(z)$ coincides with the given power series at least up to order z^{M-1}.

We note that for $N = 1$, the algebraic approximants are nothing but the well-known Padé approximants.

Although we assumed that the power series of f is known, quite often in practice, only a finite number of coefficients *is* really known. These coefficients then may be used to compute the Hermite-Padé polynomials and the algebraic approximant under consideration.

We note that the higher coefficients of the Taylor series of $a(z)$ may be considered as predictions for the higher coefficients of the power series. The latter are also of interest in applications.

The question then arises how to compute the Taylor series of $a(z)$. If it is possible to solve the equation (4) explicitly, i.e. for $N \leq 4$, a computer algebra system may be used to do the job. But even then, a recursive algorithm for the computation of the coefficients of the Taylor series would be preferable in order to reduce computational efforts.

In the following section, such a recursive algorithm is obtained. In a further section, we will present numerical examples.

2 The recursive algorithm

We consider the HPPs

$$P_n(z) = \sum_{j=0}^{p_n} p_{n,j}\, z^j \tag{5}$$

as known. Putting

$$a(z) = \sum_{k=0}^{\infty} a_k\, z^k \tag{6}$$

we obtain from Eq. (4)

$$\sum_{j=0}^{p_0} p_{0,j} z^j + \sum_{n=1}^{N} \sum_{j=0}^{p_n} p_{n,j} z^j \sum_{k_1=0}^{\infty} \ldots \sum_{k_n=0}^{\infty} z^{k_1+\ldots+k_n} \prod_{m=1}^{n} a_{k_m} = 0 \tag{7}$$

whence, by equating the coefficient of z^J to zero, we obtain an infinite set of equations. Due to Eq. (2), all the equations for $J < M$ are satisfied exactly for $a_j = f_j$, $j = 0, \ldots, M-1$.

As a first step, we compute a_M. We note that $M > p_0$. Hence, the coefficient of z^M does not involve any terms with $p_{0,j}$. For this coefficient R_M, we only need to consider terms in Eq. (7) such that $M = j + k_1 + \ldots + k_n$ and we obtain $R_M = 0$ for

$$R_M = \sum_{n=1}^{N} \sum_{j+k_1+\ldots+k_n=M} p_{n,j} \prod_{m=1}^{n} a_{k_m} \tag{8}$$

The only terms on the RHS involving a_M are obtained if exactly one of the k_m is equal to M, i.e., we have $k_m = M$, $j = 0$ and $k_j = 0$ for $j \neq m$. Thus, we may rewrite all these terms as $a_M C$ where

$$C = \sum_{n=1}^{N} n\, p_{n,0} f_0^{n-1} \tag{9}$$

and note that the rest $D_M = R_M - a_M C$ is independent of a_M. Recalling $R_M = 0$, we obtain

$$a_M = -D_M/C \tag{10}$$

Proceeding analogously for $J > M$, only terms with $J = j + k_1 + \ldots + k_n$ need to be considered. Hence, $R_J = 0$ for

$$R_J = \sum_{n=1}^{N} \sum_{j+k_1+\ldots+k_n=J} p_{n,j} \prod_{m=1}^{n} a_{k_m} \tag{11}$$

Now, the only terms on the RHS involving a_J are obtained if exactly one of the k_m is equal to J, i.e., we have $k_m = J$, $j = 0$ and $k_j = 0$ for $j \neq m$. Thus, we may rewrite all these terms as $a_J C$ where C is defined above. Proceeding as before, we put $D_J = R_J - a_J C$ and obtain

$$a_J = -D_J/C \tag{12}$$

An equivalent form of the recursive algorithm is obtained in the following way:

Consider for known P_n and $a_0, \ldots, a_{J-1}$ the expression

$$U_J = \left.\frac{d^J}{J!dz^J}\right|_{z=0} \sum_{n=1}^{N} P_n(z) \left(\sum_{j=0}^{J} a_j\, z^j\right)^n \tag{13}$$

It is easy to see, that this expression is exactly equal to R_J, and hence, is linear in the unknown a_J. Thus, we may compute the quantities D_J by substituting

$a_J = 0$ into U_J, which entails

$$D_J = \left.\frac{d^J}{J!dz^J}\right|_{z=0} \sum_{n=1}^{N} P_n(z) \left(\sum_{j=0}^{J-1} a_j\, z^j\right)^n \tag{14}$$

Thus, starting from $J = M$, one may compute all the a_J consecutively by repeated use of Eqs. (9), (14), and (12).

This concludes the derivation of the recursive algorithm.

3 Modes of application

Basically, there are two modes of application.

a) one computes a sequence of HPPs and for the resulting algebraic approximants, one predicts a fixed number of sofar unused coefficients, e.g., only one new coefficient. This mode is mainly for tests.

b) one computes from all available coefficients certain HPPs. For the best HPPs one computes a larger number of predictions for sofar unused coefficients.

In the following examples, we concentrate on mode b). Here, it is to be expected that the computed values have the larger errors the higher coefficients are predicted.

4 Examples

The examples serve to introduce to the approach. All numerical calculations in this section were done using Maple (Digits=16).

Example 1

As a first example, we consider $N = 2$, $p_0 = p_1 = p_2 = 1$ and, hence, $M = 5$. Since $N = 2$, we are dealing with a quadratic algebraic approximant. Then, the recursive algorithm is started by $a_j = f_j$, $j = 0, \ldots, 4$. For a_5, we obtain

$$a_5 = -\frac{p_{1,1} f_4 + p_{2,1}(2 f_0 f_4 + 2 f_1 f_3 + f_2^2) + p_{2,0}(2 f_1 f_4 + 2 f_2 f_3)}{p_{1,0} + 2 p_{2,0} f_0} \tag{15}$$

and for $J > 5$, we obtain

$$a_J = -\frac{p_{1,1}a_{J-1} + p_{2,1}\sum_{k=0}^{J-1} a_{J-k-1}a_k + p_{2,0}\sum_{k=1}^{J-1} a_k a_{J-k}}{p_{1,0} + 2p_{2,0}f_0} \tag{16}$$

For

$$f(z) = (2-3z)^{1/2} + 1/(5-z) \tag{17}$$

the HPPs are determined to be

$$P_0(z) = 1. - 1.544503593423590\, z \tag{18}$$
$$P_1(z) = .1947992842134984 + .06783822675080703\, z \tag{19}$$
$$P_2(z) = -.5044536972622500 - .01090573365920830\, z \tag{20}$$

The results for the predicted coefficients given in Table 1.

Table 1
The case of $N = 2$, $p_0 = p_1 = p_2 = 1$ for Eq. (17). Displayed are the coefficients of the Taylor series, the predicted coefficients and absolute and relative errors of the predicted coefficients.

j	f_j	a_j	$\lvert f_j - a_j \rvert$	rel. error (%)
5	-.294	-.294	.001	.18
6	-.330	-.332	.001	.38
7	-.389	-.392	.002	.58
8	-.475	-.478	.004	.76
9	-.593	-.599	.006	.93
10	-.756	-.765	.008	1.10

Example 2

As a second example, we consider again $N = 2$, $p_0 = p_1 = p_2 = 1$, and $M = 5$, but now the function

$$f(z) = 17(1-2z)^{-1/3} + z/(2-z) \tag{21}$$

with the HPPs

$$
\begin{aligned}
P_0(z) &= -49.52369318166839 - 6.946105600281359\, z & (22)\\
P_1(z) &= 1. + 1.695055482965655\, z & (23)\\
P_2(z) &= .1125387307324166 - .2732915349762758\, z & (24)
\end{aligned}
$$

The results for the predicted coefficients given in Table 2.

Table 2
The case of $N = 2$, $p_0 = p_1 = p_2 = 1$ for Eq. (21). Displayed are the coefficients of the Taylor series, the predicted coeffizients and absolute and relative errors of the predicted coefficients.

j	f_j	a_j	$\lvert f_j - a_j\rvert$	rel. error (%)
5	67.938	68.212	.274	.40
6	120.739	122.291	1.552	1.29
7	218.459	224.194	5.735	2.62
8	400.498	418.053	17.555	4.38
9	741.657	790.063	48.406	6.53
10	1384.425	1509.437	125.012	9.03

Example 3

As a final example, we consider the case $N = p_0 = p_1 = p_2 = 2$, whence $M = 8$, and the function

$$
f(z) = \exp(z)\,(2 - 3\,z)^{-1/3} + 1/(5 - z) \tag{25}
$$

The corresponding HPPs are

$$
\begin{aligned}
P_0(z) &= 1. - 1.027576803009053\, z + .02070967420422950\, z^2 & (26)\\
P_1(z) &= 2.617867885747464 - .6563757889994458\, z \\
&\quad - 3.118191126500581\, z^2 & (27)\\
P_2(z) &= -3.647182626894738 + 7.471780741166546\, z \\
&\quad - 3.356878399103086\, z^2 & (28)
\end{aligned}
$$

The results for the predicted coefficients are displayed in Table 3.

Table 3
The case of $N = 2$, $p_0 = p_1 = p_2 = 2$ for Eq. (25). Displayed are the coefficients of the Taylor series, the predicted coeffizients and absolute and relative errors of the predicted coefficients.

j	f_j	a_j	$\|f_j - a_j\|$	rel. error (%)
8	3.888956	3.878509	.010447	.27
9	5.356681	5.301047	.055634	1.04
10	7.451679	7.275227	.176452	2.37
11	10.447061	10.006950	.440111	4.21
12	14.739132	13.781978	.957155	6.49
13	20.903268	18.995972	1.907297	9.12

5 Conclusions

It is seen that even rather low-order algebraic approximants, or HPPs, respectively, can lead to quite accurate predictions of the unknown coefficients of the power series, especially for f_M, and the next few coefficients.

References

[1] G. A. Baker, Jr. and P. Graves-Morris. *Padé approximants.* Cambridge U.P., Cambridge (GB), second edition, 1996.

[2] C. Brezinski. Prediction properties of some extrapolation methods. *Appl. Numer. Math.*, 1:457 – 462, 1985.

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

[4] T. M. Feil and H. H. H. Homeier. Programs for the approximation of real and imaginary single- and multi-valued functions by means of Hermite-Padé-approximants. *Comput. Phys. Commun.*, 158:124–135, 2004. Computer Physics Communications Program Library, Catalogue number: ADSO.

[5] J. Gilewicz. Numerical detection of the best Padé approximant and determination of the Fourier coefficients of insufficiently sampled functions. In P. R. Graves-Morris, editor, *Padé Approximants and their Applications*, pages 99–103. Academic Press, New York, 1973.

[6] U. D. Jentschura, J. Becher, E. J. Weniger, and G. Soff. Resummation of QED perturbation series by sequence transformations and the prediction of perturbative coefficients. *Phys. Rev. Lett.*, 85:2446–2449, 2000.

[7] M. Prévost and D. Vekemans. Partial Padé prediction. *Numer. Algo.*, 20:23–50, 1999.

[8] Dhiranjan Roy and Ranjan Bhattacharya. Prediction of unknown terms of a sequence and its application to some physical problems. *Annals of Physics*, 321:1483–1523, 2006.

[9] A. Sidi and D. Levin. Prediction properties of the t-transformation. *SIAM J. Numer. Anal.*, 20:589–598, 1983.

[10] D. Vekemans. Algorithm for the E-prediction. *J. Comput. Appl. Math.*, 85:181–202, 1997.

[11] E. J. Weniger. Prediction properties of Aitken's iterated Δ^2 process, of Wynn's epsilon algorithm, and of Brezinski's iterated theta algorithm. In C. Brezinski, editor, *Numerical Analysis 2000 Vol. 2: Interpolation and Extrapolation*, pages 329 – 356. Elsevier, Amsterdam, 2000.