

A RECURSIVE ALGORITHM FOR PADÉ-HERMITE APPROXIMATIONS*

A.V. SERGEYEV

An algorithm for the successive calculation of multiple-valued approximations, or Padé-Hermite approximations, is proposed. Simple formulas which generalize the recurrence formulas between the numerators and denominators of appropriate continued fractions are obtained for the polynomials which take part in the determination of Padé-Hermite approximations. General expressions for the coefficients of the recurrence formulas are obtained in cases of quadratic and cubic approximations to the functions $(1+x)^a$ and e^x .

1. Introduction.

If the function φ is specified in the form of the expansion

$$\varphi(x) = \sum_{i=0}^{\infty} \varphi_i x^i, \quad (1.1)$$

then Padé approximations are often used to calculate approximately the sum of series (1.1). By definition, the proportion of the polynomials $A^{(2)}$ and $A^{(1)}$ of powers no higher than n_2 and n_1 respectively, which has the same n_1+n_2+1 first coefficients of Maclaurin's expansion as the function φ , is called a Padé approximation $[n_1, n_2]$. The polynomials $A^{(1)}$ and $A^{(2)}$ in this case satisfy the equation

$$A^{(1)}(x)\varphi(x) - A^{(2)}(x) = o(x^{n_1+n_2}).$$

The papers of Hermite /1/ and Padé /2/ also consider the more general case when several polynomials occur - as coefficients - in the linear equations between certain functions.

Suppose $f^{(1)}, \dots, f^{(k)}$ are functions which can be expanded in a Maclaurin series.

Then, according to /3, 4/, the set of polynomials $(A^{(1)}, \dots, A^{(k)})$ of a power no higher than n_1, \dots, n_k respectively, is called a Padé-Hermite form of the type $[n_1, \dots, n_k]$ associated with the system $(f^{(1)}, \dots, f^{(k)})$, if

$$\sum_{p=1}^k A^{(p)}(x) f^{(p)}(x) = o(x^{N-2}), \quad N = \sum_{i=1}^k n_i + k. \quad (1.2)$$

We shall call the residual function

$$S(x) = \frac{1}{x^{N-1}} \sum_{p=1}^k A^{(p)}(x) f^{(p)}(x). \quad (1.3)$$

The Padé-Hermite approximation $(f^{(1)}, \dots, f^{(k)})$ is obtained from the equation

$$\sum_{p=1}^k A^{(p)}(x) f^{(p)}(x) = 0.$$

In order for the functions $f^{(1)}, \dots, f^{(k)}$ to be uniquely defined, some kind of limitations or connections are usually imposed on both $f^{(1)}, \dots, f^{(k)}$ and $f^{(1)}, \dots, f^{(k)}$. When $k=3$, for example (see /5/), for the quadratic approximations $f^{(1)}(x)=1, f^{(2)}(x)=[f^{(2)}(x)]^2$ and for the integral approximations $f^{(1)}(x)=1, f^{(3)}(x)=(d/dx)f^{(2)}(x)$.

The Padé-Hermite approximations are used to calculate approximately the sum of series (1.1) in the vicinity of the features of the function φ , which can differ from the poles /5/. For example, if the function φ has branching points of the square-root type, the quadratic approximations $(f^{(1)}=1, f^{(2)}=\varphi, f^{(3)}=\varphi^2)$ are usually used. The approximate value of the function φ is obtained in this case by solving the quadratic equation

$$\bar{\varphi} = \frac{-A^{(2)} \pm [(A^{(2)})^2 - 4A^{(1)}A^{(3)}]^{1/2}}{2A^{(3)}}. \quad (1.4)$$

We can also write Eq. (1.2) in the form of a set of $N-1$ homogeneous linear equations for N coefficients of the polynomials $A^{(1)}, \dots, A^{(k)}$. When calculating the Padé-Hermite form by solving the set of linear equations using the general method, the number of operations increases in proportion to N^3 as N increases, and the memory capacity increases in proportion to N^2 .

In this paper we use equations which generalize the well-known recurrence formulas between the numerators and denominators of convergent valuable fractions to calculate the Padé-Hermite forms with values N which successively increase to unity. The required number of operations increases in proportion to N^2 , and the memory capacity increases in proportion to N .

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A recursive algorithm, based on the generalized Frobenius identity /3/, was previously suggested to construct a table of Padé-Hermite approximations of all kinds of types $[n_1, \dots, n_k]$. The new algorithm calculates only the sequence of approximations on the main diagonal of the table ($n_1 = \dots = n_k$), or of the extra-diagonal approximations nearest to them. These approximations are usually used for the generalized summation of series. The algorithm from /3/ is inconvenient for constructing a diagonal sequence of approximations, since, to determine the Padé-Hermite forms of the type $[n_1, \dots, n_k]$, we are obliged to calculate a large number of forms of the types $[n'_1, \dots, n'_k]$, for which

$$\sum_{i=1}^k n'_i < \sum_{i=1}^k n_i.$$

Equations similar to those we will derive in Sect. 2 are obtained in /1, 2/.

Note that the construction of Padé-Hermite approximations enables a number of changes to be made. Consider, for example, two sets of non-negative integrals: (r_0, \dots, r_k) and (s_1, \dots, s_k) , such that

$$\sum_{i=0}^k r_i = \sum_{p=1}^k s_p.$$

We shall specify a set of polynomials $B^{(i)}$, $i=0, 1, \dots, k$ of a power no higher than r_i using the relations $B^{(0)}(x)f^{(p)} - B^{(p)}(x) = o(x^{r_p})$, $p=1, 2, \dots, k$ which are equivalent to the system

$$N-1 = \sum_{p=1}^k s_p + k$$

of homogeneous linear equations for

$$N = \sum_{i=0}^k r_i + k + 1$$

unknown coefficients of the polynomials. It is natural to assume that the fractions $B^{(p)}(x)/B^{(0)}(x)$ for $p=1, 2, \dots, k$ are approximations of the functions $f^{(p)}(x)$ (see /6/). The algorithm for constructing continued fractions was generalized to similar joint approximations in /7, 8/ when using the Jacobi-Perron algorithm.

2. Description of the algorithm.

As is well known /9/, to calculate a diagonal ladder sequence of Padé approximations ($n_1 = n_2$ or $n_1 = n_2 + 1$) it is convenient to transform the function into a continued fraction.

Suppose S_0, S_1, \dots is a sequence of functions, defined by the equations

$$S_0(x) = -1, \quad S_1(x) = \varphi(x), \quad (2.1a)$$

$$xS_N(x) = S_{N-2}(x)S_{N-1}(0) - S_{N-2}(0)S_{N-1}(x). \quad (2.1b)$$

Then for any $N \geq 2$ we can represent the function φ in the form of the continued fraction:

$$\varphi(x) = \frac{c_0^{(0)}}{c_0^{(1)} + \sum_{i=1}^{N-2} \frac{xc_i^{(0)}}{c_i^{(1)} - \frac{xS_N(x)}{S_{N-1}(x)}}$$

where $c_i^{(0)} = S_{i+1}(0)$, $c_i^{(1)} = -S_i(0)$.

The convergent fraction

$$\frac{A_N^{(2)}(x)}{A_N^{(1)}(x)} = \frac{c_0^{(0)}}{c_0^{(1)} + \sum_{i=1}^{N-2} \frac{xc_i^{(0)}}{c_i^{(1)}}$$

is the Padé approximation $[(N-2)/2, (N-2)/2]$, if N is even, or $[(N-1)/2, (N-3)/2]$, if N is odd.

To calculate the numerators and denominators of the convergent fractions it is convenient to use the simple equations

$$A_1^{(1)} = 1, \quad A_1^{(2)} = 0, \quad A_2^{(1)} = 1, \quad A_2^{(2)} = \varphi(0),$$

$$A_N^{(p)}(x) = xc_{N-2}^{(0)}A_{N-2}^{(p)}(x) + c_{N-2}^{(1)}A_{N-1}^{(p)}(x), \quad (2.2)$$

where $p=1, 2$.

Note, also, that for any $N \geq 1$

$$A_N^{(1)}(x)\varphi(x) - A_N^{(2)}(x) = x^{N-1}S_N(x). \quad (2.3)$$

The (2.1) procedure is known as the Viskovatov algorithm /10/ and is a successive division of the residue of the power series.

We shall now generalize Viskovatov's algorithm to the case of an arbitrary number of functions $f^{(1)}, \dots, f^{(k)}$.

Suppose $(A_N^{(1)}, \dots, A_N^{(k)})$ and S_N for $N=1, 2, \dots, k$ are Padé-Hermite forms of the type $[0, \dots, 0]$, associated with $(f^{(1)}, \dots, f^{(k)})$, and the corresponding residual functions; $A_N^{(N+1)} = \dots = A_N^{(k)} = 0$.

We shall describe a recursive algorithm for calculating the Padé-Hermite forms $(A_N^{(1)}, \dots, A_N^{(k)})$ of the type

$$[\underbrace{n_1, \dots, n_1}_m, \underbrace{n-1, \dots, n-1}_{k-m}] \quad (2.4)$$

and the corresponding residual functions S_N , where $n=1, 2, \dots, m=1, 2, \dots, k, N=kn+m$.

We shall first determine S_N together with some subsidiary functions $S_{Nq}, q=1, 2, \dots, k-2$ using recurrence formulas which are used for $N=k+1, k+2, \dots$:

$$\begin{aligned} xS_{N1}(x) &= S_{N-k}(x)S_{N-k+1}(0) - S_{N-k}(0)S_{N-k+1}(x), \\ xS_{N2}(x) &= S_{N1}(x)S_{N-k+2}(0) - S_{N1}(0)S_{N-k+2}(x), \\ &\dots \\ xS_{N,k-2}(x) &= S_{N,k-3}(x)S_{N-2}(0) - S_{N,k-3}(0)S_{N-2}(x), \\ xS_N(x) &= S_{N,k-2}(x)S_{N-1}(0) - S_{N,k-2}(0)S_{N-1}(x). \end{aligned} \quad (2.5)$$

Later $A_N^{(p)}$ are constructed together with the subsidiary polynomials $A_{Nq}^{(p)}, q=1, 2, \dots, k-2$ using the recurrence formulas

$$\begin{aligned} A_{N1}^{(p)}(x) &= xA_{N-k}^{(p)}(x)S_{N-k+1}(0) - S_{N-k}(0)A_{N-k+1}^{(p)}(x), \\ A_{N2}^{(p)}(x) &= A_{N1}^{(p)}(x)S_{N-k+2}(0) - S_{N1}(0)A_{N-k+2}^{(p)}(x), \\ &\dots \\ A_{N,k-2}^{(p)}(x) &= A_{N,k-3}^{(p)}(x)S_{N-2}(0) - S_{N,k-3}(0)A_{N-2}^{(p)}(x), \\ A_N^{(p)}(x) &= A_{N,k-2}^{(p)}(x)S_{N-1}(0) - S_{N,k-2}(0)A_{N-1}^{(p)}(x). \end{aligned} \quad (2.6)$$

Using (2.5) and (2.6), we can prove, using induction over N , that for all $N=k+1, k+2, \dots$

$$\begin{aligned} \sum_{p=1}^k A_{N1}^{(p)}(x)f^{(p)}(x) &= x^{N-k+1}S_{N1}(x), \\ &\dots \\ \sum_{p=1}^k A_{N,k-2}^{(p)}(x)f^{(p)}(x) &= x^{N-2}S_{N,k-2}(x), \\ \sum_{p=1}^k A_N^{(p)}(x)f^{(p)}(x) &= x^{N-1}S_N(x). \end{aligned} \quad (2.7)$$

The last equation in (2.7) signifies that $(A_N^{(1)}, \dots, A_N^{(k)})$ and S_N satisfy Eqs. (1.2) and (1.3), which determine the Padé-Hermite form and the residual function; it is easy to estimate the powers of the polynomials from (2.6):

$$\deg A_N^{(p)} \leq \begin{cases} n, & \text{if } p \leq m \\ n-1, & \text{if } p > m, \end{cases}$$

where n is the integer part of the number $(N-1)/k, m=N-kn$.

We can represent system (2.6) in the form of one formula which generalizes the recurrence formulas for the numerators and denominators of the continued fractions:

$$A_N^{(p)}(x) = x c_{N-k}^{(0)} A_{N-k}^{(p)}(x) + \sum_{i=1}^{k-1} c_{N-k}^{(i)} A_{N-k+i}^{(p)}(x), \quad (2.8)$$

where

$$\begin{aligned} c_{N-k}^{(0)} &= \prod_{j=N-k+1}^{N-1} S_j(0), & c_{N-k}^{(1)} &= -S_{N-k}(0) \prod_{j=N-k+2}^{N-1} S_j(0), \\ c_{N-k}^{(i)} &= -S_{N-k+i-1}(0) \prod_{j=N-k+i+1}^{N-1} S_j(0) \text{ for } i=2, 3, \dots, k-2, \\ c_{N-k}^{(k-1)} &= -S_{N,k-2}(0). \end{aligned}$$

We can rewrite (2.5) in a similar way:

$$x^k S_N(x) = c_{N-k}^{(0)} S_{N-k}(x) + \sum_{i=1}^{k-1} x^{i-1} c_{N-k}^{(i)} S_{N-k+i}(x). \quad (2.9)$$

In the special case when $k=2, f^{(1)}=\varphi, f^{(2)}=-1$ Eqs. (2.8), (2.9) and the last equation in (2.7) convert, respectively, to (2.2), (2.1) and (2.3).

We can also directly determine the coefficients $c_{N-k}^{(i)}, i=0, 1, \dots, k-1$, apart from an unimportant common multiplier, from the equations

$$c_{N-k}^{(0)} S_{N-k}(x) + \sum_{i=1}^{k-1} x^{i-1} c_{N-k}^{(i)} S_{N-k+i}(x) = o(x^{k-2}), \quad (2.10)$$

which is equivalent to a set of $k-1$ homogeneous linear equations that occur after expanding the left-hand side of (2.10) in powers x and equating the coefficients to zero when x^0, \dots, x^{k-2} .

Eqs. (2.8) and (2.9) are invariant under the substitution

$$A_N^{(p)} \rightarrow d_N A_N^{(p)}, \quad S_N \rightarrow d_N S_N, \quad c_N^{(i)} \rightarrow d_{N+k} d_{N+1}^{-1} c_N^{(i)}, \quad (2.11)$$

where d_1, d_2, \dots are arbitrary numbers which differ from zero.

Since $A_N^{(1)}, \dots, A_N^{(k)}$ and S_N are determined, apart from a constant common multiplier, the coefficients $c_N^{(i)}$ in Eqs. (2.8) and (2.9) permit an arbitrary transformation of the form (2.11) provided that $d_1 = \dots = d_k = 1$. It is convenient, for example, to select the normalization constants d_{k+1}, d_{k+2}, \dots , such that after the substitution (2.11) we have $c_N^{(0)} = 1$ or $c_N^{(k-1)} = 1$.

Note that the recurrence formulas, similar to (2.8), also hold for the more general sequence of Padé-Hermite forms of the type $[n_1+n, \dots, n_m+n, n_{m+1}+n-1, n_{m+2}+n-1, \dots, n_k+n-1]$ with fixed n_1, \dots, n_k .

3. Examples.

We shall call the set of solutions of the algebraic equation

$$\sum_{p=1}^k A^{(p)} \bar{\varphi}^{p-1} = 0$$

with respect to the unknown $\bar{\varphi}$, where $(A^{(1)}, \dots, A^{(k)})$ is the Padé-Hermite form associated with $(1, \varphi, \varphi^2, \dots, \varphi^{k-1})$, an algebraic approximation of the $k-1$ degree to the function φ .

Algebraic approximations have recently been frequently used in physical applications [5, 11, 12]. Henceforth, we shall confine ourselves to considering only these approximations.

Using the obvious equation $[\varphi(x) - \varphi(0)]^{N-1} = o(x^{N-1})$, we shall arrange to choose $A_N^{(i)}$ and S_N when $N=1, 2, \dots, k$ in the following way:

$$A_N^{(i)} = \binom{N-1}{i-1} [-\varphi(0)]^{N-i}, \quad S_N(x) = \left[\frac{\varphi(x) - \varphi(0)}{x} \right]^{N-1}.$$

To evaluate the polynomials $A_N^{(p)}$ and the residual functions S_N when $N=k+1, k+2, \dots$ we will use the recurrence formulas (2.8) and (2.9) with the substitution (2.11). We shall choose the constants d_{k+1}, d_{k+2}, \dots , such that the coefficients $c_N^{(i)}$ are written in a simpler form.

We shall present several examples of the coefficients $c_N^{(i)}$ fitting into some general formula which can be used below, for example to investigate the convergence of Padé-Hermite approximations.

In the case of algebraic approximations of the $k-1$ degree to the function $\varphi(x) = (1+x)^k$ it is easy to prove, by induction, that

$$c_N^{(0)} = 1, \quad c_N^{(i)} = -\binom{k}{i}, \quad i=1, 2, \dots, k-1, \quad S_N(x) = \left[\frac{\varphi(x) - 1}{x} \right]^{N-1}. \quad (3.1)$$

We can often select general formulas for the coefficients $c_N^{(i)}$ using a numerical experiment but we cannot strictly prove these formulas due to the awkwardness of the calculations.

For example, for quadratic ($k=3$) algebraic approximations to the function $(1+x)^3$

$$c_{3n+1}^{(0)} = (2\alpha+n)(\alpha+n), \quad c_{3n+1}^{(1)} = -(3n+1)(2\alpha+n), \quad (3.2a)$$

$$c_{3n+2}^{(0)} = -(2\alpha+n)(2\alpha-n-1), \quad c_{3n+2}^{(1)} = (3n+2)(2\alpha-n-1), \quad (3.2b)$$

$$c_{3n+3}^{(0)} = (2\alpha-n-1)(\alpha-n-1), \quad c_{3n+3}^{(2)} = \alpha - 3n^2 - 3n - 1, \quad (3.2c)$$

$$c_{3n+3}^{(1)} = c_{3n+2}^{(2)} = c_{3n+3}^{(3)} = -3, \quad (3.2d)$$

and for cubic ($k=4$) approximations to $(1+x)^4$

$$c_{4n+1}^{(0)} = (\alpha+n)(2\alpha+n)(3\alpha+n), \quad (3.3a)$$

$$c_{4n+2}^{(0)} = -(3\alpha+n)(2\alpha+n)(3\alpha-n-1), \quad (3.3b)$$

$$c_{4n+3}^{(0)} = (3\alpha+n)(2\alpha-n-1)(3\alpha-n-1), \quad (3.3c)$$

$$c_{4n+4}^{(0)} = -(\alpha-n-1)(2\alpha-n-1)(3\alpha-n-1), \quad (3.3d)$$

$$c_{4n+1}^{(1)} = -(4n+1)(2\alpha+n)(3\alpha+n), \quad (3.3e)$$

$$c_{4n+2}^{(1)} = (4n+2)(3\alpha+n)(3\alpha-n-1), \quad (3.3f)$$

$$c_{4n+3}^{(1)} = -(4n+3)(2\alpha-n-1)(3\alpha-n-1), \quad (3.3g)$$

$$c_{4n+1}^{(2)} = -(3\alpha+n)[(2n-1)\alpha + 6n^2 + 4n + 1], \quad (3.3h)$$

$$c_{4n+2}^{(2)} = -(3\alpha-n-1)[(2n+3)\alpha - 6n^2 - 8n - 3], \quad (3.3i)$$

$$c_{4n+1}^{(3)} = -(2n+1)(2\alpha^2 - 3\alpha + 2n^2 + 2n + 1), \quad (3.3j)$$

$$c_{4n+4}^{(1)} = c_{4n+2}^{(3)} = c_{4n+3}^{(2)} = c_{4n+4}^{(3)} = -4, \quad c_{4n+3}^{(2)} = c_{4n+4}^{(2)} = -6, \quad (3.3k)$$

where $n=0, 1, 2, \dots$

In the special case when $\alpha=1/k$ for $k=3, 4$ the coefficients (3.2) and (3.3) convert to (3.1) after the transformation of (2.11) with the constants

$$d_{N+k} = \prod_{n=0}^{[(N-1)/k]} \prod_{i=1}^{k-1} \left(n + \frac{i}{k}\right)^{-1}.$$

The coefficients $c_N^{(j)}$ for approximations to the function e^x are directly obtained from (3.2) and (3.3) using the relation

$$e^x = \lim_{\alpha \rightarrow \infty} \left(1 + \frac{x}{\alpha}\right)^\alpha.$$

For quadratic approximations to e^x

$$(c_N^{(0)}, c_N^{(1)}, c_N^{(2)}) = \begin{cases} (2, -2N, 1), & N \equiv 1 \pmod{3}, \\ (-4, 2N, -3), & N \equiv 2 \pmod{3}, \\ (2, -3, -3), & N \equiv 0 \pmod{3}, \end{cases} \quad (3.4)$$

and for cubic approximations to e^x

$$(c_N^{(0)}, c_N^{(1)}, c_N^{(2)}, c_N^{(3)}) = \begin{cases} (6, -6N, -3/2(N-3), -N-1), & N \equiv 1 \pmod{4}, \\ (-18), 9N, -3/2(N+4), -4), & N \equiv 2 \pmod{4}, \\ (18, -6N, -6, -4), & N \equiv 3 \pmod{4}, \\ (-6, -4, -6, -4), & N \equiv 0 \pmod{4}. \end{cases} \quad (3.5)$$

Eqs. (3.2)-(3.5) generalize the well-known formulas for the coefficients of the representation in the form of a continued fraction of the functions $(1+x)^\alpha$ and e^x .

Note that sets of polynomials which satisfy (1.2) for an arbitrary set of exponents were examined in /1/. Diagonal quadratic approximations to the functions $(1+x)^\alpha$ and e^x were obtained in general form in /13/.

In quantum mechanics and field theory we often encounter perturbation-theory series, the terms of which increase factorially /9/. Consider as an example the generalized summation of series

$$\sum_{j=0}^{\infty} j! z^j \quad (3.6)$$

by constructing a sequence of approximations of the form (2.4).

Series (3.6) is asymptotic for the function

$$\psi(z) = \int_0^{\infty} \frac{e^{-t}}{1-zt} dt \quad (3.7)$$

as $z \rightarrow 0$, $|\arg z| > 0$. The quantities $\psi(z)$ for all z , which do not lie in $(0, \infty)$, where the function ψ has a branch cut, can be calculated by transforming series (3.6) into a continued fraction /9/.

As $z \rightarrow x \pm i0$, $x \in (0, \infty)$ the sequence of valuable fractions becomes divergent. In this case to calculate $\psi(z)$ it is convenient to use quadratic approximations, since we can use them to approximate functions which have branch cuts.

The first few coefficients $c_N^{(j)}$ are shown in the table. The approximate values $\psi_N(z)$ to $\psi(z)$ were calculated using Eq. (1.4), where $A^{(j)} = A_{N+j}^{(j)}$. To illustrate the convergence of the approximations the table gives the real and imaginary parts of $\psi_N(1)$.

N	$c_N^{(0)}$	$c_N^{(1)}$	$c_N^{(2)}$	Re $\psi_N(1)$	Im $\psi_N(1)$	N	$c_N^{(0)}$	$c_N^{(1)}$	$c_N^{(2)}$	Re $\psi_N(1)$	Im $\psi_N(1)$
1	1	-1	2	1.2500	± 0.6614	7	2	-1	2	0.5625	± 0.9662
2	1	-1	1	1.0000	± 1.0000	8	3	-1	1	0.7667	± 1.0703
3	2	-1	0	2.0000	0.0000	9	8	-1	4	0.7005	± 1.1268
4	1	1	2	$5/6 \pm 1/6$	0.0000	10	3	-3	-1	0.7762	± 1.1495
5	12	3	-2	0.9167	± 1.2219	11	60	5	8	0.6931	± 0.9903
6	9	-2	3	0.5833	± 1.1517	12	150	18	-5	0.6830	± 1.1567

The value of the integral (3.7) when $z=1$ depends on the direction in which the pole is bypassed, situated at the point $t=1$, and is

$$\psi(1) = P \int_0^{\infty} \frac{e^{-t}}{1-t} dt \pm \frac{\pi}{e} i \approx 0.6971 \pm 1.1557i.$$

The approximation $\psi_N(1)$ when $N=12$ differs little from the accurate value $\psi(1)$.

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