JOURNAL OF COMPUTATIONAL PHYSICS 47, 477–488 (1982)

Note

Application of Generalized Padé Approximants to the Special Function Evaluation Problem

A new approach to generalized Padé approximants is presented. Its main interest lies in the fact that it avoids instability and/or round-off errors which occur in traditional algorithms for evaluating Padé approximants. Moreover, the approximants are readily obtained. Applications concerned with the tabulation of some transcendental functions in their critical domain (Weber and Bessel functions) illustrate the power of the method.

I. Introduction

Theoretical physicists are often confronted with the problem of poor convergence. A possible key to that problem is furnished by the theory of the acceleration of convergence [1]; consider the slowly convergent sequence

$$S_n = S + O(n).$$

It is possible to find an algorithm which replaces the sequence (S_n) by another sequence (Σ_n) which converges faster than (S_n). There are many such algorithms available; however, their applicability is closely dependent on the form of the original sequence. The best known are the algorithms ε [2], ρ, and θ [1]. A more general algorithm has been found recently by Håvie [3] and Brezinski [4] (E-algorithm).

Physicists almost always have recourse to Padé approximants [5] which are intimately correlated with the ε-algorithm. Note that this algorithm is most efficient when the original sequence (S_n) is exponentially convergent (or divergent), i.e., if $O(n) \simeq \lambda\rho^n$ but performs poorly otherwise.

In this paper, we shall develop a new approach to Padé approximants which will exhibit several advantageous features: compactness, stability, and rapid convergence.

II. Variations on a Theme of Padé

1. *Theme*

Suppose that we need to tabulate the function $f(z)$ defined by its MacLaurin expansion

$$f(z) = c_0 + c_1 z + c_2 z^2 + \cdots . \tag{1}$$

0021-9991/82/090477-12$02.00/0

The classical theory of Padé defines approximants $[L/M]$ given by

$$[L/M] = (a_0 + a_1 z + \cdots + a_L z^L)/(b_0 + b_1 z + \cdots + b_M z^M)$$

with the following properties [5]:

(a) $b_0 = 1$,

(b) the MacLaurin expansion of $[L/M]$ coincides with that of $f(z)$ up to an including order z^{L+M}.

Even when (1) is divergent, it is known that suitable sequences $[L/M]$ may converge to the value of $f(z)$.

Various methods have been proposed to evaluate the successive approximants $[L/M]$. Recurrent algorithms have been found, but the drawback of possible round-off errors and/or instability exists. The problem has been discussed recently by Graves-Morris [6].

2. *First Variation*

It is possible to express the special Padé approximant $[s - 1/s]$ in a different way

$$f(z) \sim [s - 1/s] = \sum_{i=1}^{s} \lambda_i/(1 - \omega_i z).$$

The idea naturally arises to generalize this approximant by considering the expansion

$$f(z) \sim \sum_{i=1}^{s} \lambda_i F(\omega_i z), \tag{2}$$

where the function F is given. General properties of such generalized approximants have been studied by Baker and Gammel [17]. In practical applications, however, the most widely used examples are $F(z) = 1/(1 - z)$ (ordinary Padé approximants) and $F(z) = \exp(-z)$ (exponential interpolation [7]). Our aim is to try a more systematic use of the other cases.

We shall first study the general case where the function $F(z)$ is defined by its MacLaurin expansion

$$F(z) = \alpha_0 + \alpha_1 z + \alpha_2 z^2 + \cdots . \tag{3}$$

The starting equation is written as

$$\sum_{0}^{\infty} c_k z^k \simeq \sum_{i=1}^{s} \lambda_i F(\omega_i z) = \sum_{0}^{\infty} \alpha_k z^k \sum_{i=1}^{s} \lambda_i \omega_i^k .$$

The coefficients of the lowest powers of z can be identified up to and including order $2s - 1$. This leads to the following nonlinear system for the $2s$ unknowns λ_i and ω_i:

$$\begin{aligned}
\lambda_1 &+ \cdots + \lambda_s &&= \gamma_0,\\
&&&\vdots\\
\lambda_1\omega_1^{s-1} &+ \cdots + \lambda_s\omega_s^{s-1} &&= \gamma_{s-1},\\
\lambda_1\omega_1^{s} &+ \cdots + \lambda_s\omega_s^{s} &&= \gamma_{s},\\
&&&\vdots\\
\lambda_1\omega_1^{2s-1} &+ \cdots + \lambda_s\omega_s^{2s-1} &&= \gamma_{2s-1},
\end{aligned} \tag{4}$$

where $\gamma_k = c_k/\alpha_k$. A quite similar system appears in the theory of Gaussian quadratures [8]. Its solution is obtained by first eliminating the λ_i. One finds

$$\begin{aligned}
\gamma_s &= \gamma_{s-1}A_1 - \gamma_{s-2}A_2 + \cdots + (-1)^{s+1}\gamma_0 A_s,\\
\gamma_{s+1} &= \gamma_s A_1 - \gamma_{s-1}A_2 + \cdots + (-1)^{s+1}\gamma_1 A_s,\\
&\vdots\\
\gamma_{2s-1} &= \gamma_{2s-2}A_1 - \gamma_{2s-3}A_2 + \cdots + (-1)^{s+1}\gamma_{s-1}A_s,
\end{aligned} \tag{5}$$

where the A_i are the fundamental symmetrical polynomials acting on the ω_i

$$A_1 = \sum_i \omega_i, \qquad A_2 = \sum_{i<j}\sum \omega_i\omega_j\ , \qquad \ldots, \qquad A_s = \prod_i \omega_i.$$

Solving system (5) leads to the values of $A_1,\ldots,A_s$. The ω_i are then found as the roots of the polynomial equation

$$z^s - A_1 s^{s-1} + A_2 z^{s-2} + \cdots + (-1)^s A_s = 0.$$

Finally, the λ_i are deduced from the first s equations of system (4). That approach is not very efficient in practice because it needs the resolution of two linear systems of order s.

Fortunately, an alternative exists, the recurent computation of the ω_i and of the λ_i. Hence, system (4) exactly describes the $[s-1/s]$ Padé approximant of the function $\sum_0^\infty \gamma_k/z^{k+1}$. In greater detail [9]

$$\sum_0^\infty \gamma_k z^{k+1} \sim \sum_{i=1}^{s} \lambda_i/(z-\omega_i) = P_s(z)/Q_s(z)$$

$$= \cfrac{\gamma_0}{z - a_0 - \cfrac{b_1}{z - a_1 - \cfrac{b_2}{z - a_2 - \cfrac{\ddots}{\ddots - \cfrac{b_{s-1}}{z - a_{s-1}}}}}}$$

The coefficients a_k and b_k in the continued fraction are calculated with the aid of the $q-d$ algorithm of Rutishauser (see Appendix A). Polynomials $Q_s(z)$ and $P_s(z)$ are of degree s and $s-1$, respectively. They are calculated recursively through the scheme

$$X_{k+1} = (z - a_k) X_k - b_k X_{k-1}, \qquad (k = 0, 1, 2,...), \tag{6}$$

together with the initial conditions

$$Q_{-1} = 0, \qquad Q_0 = 1, \qquad P_{-1} = \gamma_0, \qquad P_0 = 0 \qquad (\text{and } b_0 = -1).$$

The ω_i are the roots of $Q_s(z)$, while the λ_i are known as the Christoffel constants [10]

$$\lambda_i = P_s(\omega_i)/Q_s'(\omega_i). \tag{7}$$

In summary, the strategy is as follows:

(1) In Eqs. (1), (3), the c_k and the α_k are given. We fix s, a positive integer. We define $\gamma_k = c_k/\alpha_k$ $(k = 0, 1,..., 2s-1)$.

(2) The $q-d$ algorithm is applied to the sequence (γ_k) in order to find the a_k and the b_k $(k = 0, 1,..., s-1)$ (see Appendix A).

(3) The polynomials $Q_k(z)$ and $P_k(z)$ are calculated recursively $(k = 1,..., s)$ with the aid of Eq. (6).

(4) The roots of $Q_s(z)$ are the desired ω_i and Eq. (7) leads to the corresponding λ_i.

(5) Those λ_i and ω_i are introduced in Eq. (2) to obtain the approximation of order s. Increasing s theoretically improves the precision.

One may say about the above strategy that the algorithm works effectively. It solves the classical problem of expanding $f(z)$ in the form of an $[s-1/s]$ Padé approximant (i.e., $\gamma_k = c_k$) or as a sum of exponentials (i.e., $\gamma_k = (-1)^k k! c_k$). The advantage is that $f(z)$ is expanded in terms of known functions $F(z)$. The sole drawback is the recourse to the $q-d$ algorithm which might be unstable or develop large round-off errors.

3. *Second Variation*

In place of giving simple algebraic values to the α_k (corresponding to an expansion in terms of simple known functions $F(z)$, it is preferable to do that with the γ_k. Only those values of γ_k which allow the exact resolution of the $q-d$ scheme will be considered, since the $q-d$ scheme is the sole critical point in the above strategy. In Appendix A, the details of the exact resolution of the $q-d$ algorithm are presented. The improved strategy runs, therefore, as follows:

The function $f(z) = c_0 + c_1 z + c_2 z^2 + \cdots$ is given; s is fixed.

The γ_k are chosen so that the $q-d$ scheme is exactly calculable. Examples are $\gamma_k = \Gamma(k+a)$, $\gamma_k = a^{k(k-1)/2}$, $\gamma_k = 1/(k+\alpha)$,.... The a_k and b_k are therefore also known exactly.

The polynomials Q_s and P_s are computed recursively through (6). The λ_i and the ω_i are deduced as indicated previously.

One has the approximation of order s

$$f(z) \simeq \sum_{i=1}^{s} \lambda_i F(\omega_i z) \qquad \text{with} \quad F(z) = c_0/\gamma_0 + c_1 z/\gamma_1 + c_2 z^2/\gamma_2 + \cdots .$$

Our method computes stable approximations to $f(z)$ very rapidly. Even when the starting expansion (1) is divergent, the algorithm remains efficient provided that the expansion defining $F(z)$ is convergent.

III. Numerical Examples

Details of the numerical algorithms used to obtain the λ_i and the ω_i are reported in Appendix B.

Example One: $f(z) = \ln(1+z)/z$. In this case we have $c_k = (-1)^k/(k+1)$. We choose $\gamma_k = k!$ so that

$$F(z) = (1 - \exp(-z))/z.$$

The final result is written as:

$$f(z) = \ln(1+z)/z \simeq \sum_{i=1}^{s} \lambda_i \frac{1 - \exp(-\omega_i z)}{\omega_i z},$$

where the ω_i are the roots of the Laguerre polynomials and λ_i the corresponding Christoffel constants [11]. Table I presents the numerical results in two cases, $z = 1$ and $z = 2$ (i.e., outside the circle of convergence of $f(z)$).

TABLE I

Successive Approximations of the Function $\ln(1+z)/z$; the Precision Increases with s.

s	$z = 1$	$z = 2$
1	0.632120558828	0.432332358381
2	0.687464136346	0.524213272629
3	0.692593688196	0.543742419715
4	0.693091785341	0.548044127255
10	0.693147180488	0.549305929851
14	0.693147180559	0.549306143611
$\ln(z+1)/z$	0.693147180559	0.549306144334

EXAMPLE TWO: $f(z) = U(a, z)$ (Weber–Hermite function) $(a \geqslant 0)$. It is well known that the tabulation of certain transcendental functions is difficult in some critical domains. Two examples are the Weber function $U(a, z)$ and the Bessel functions $K_\nu(z)$. In both cases, there exists a MacLaurin expansion valid near the origin and an asymptotic expansion valid when $|z|$ is sufficiently large. In the intermediate domain, say, $3 < z < 9$, accurate computation is difficult. The case of the Weber function is particularly difficult [12]. Consider the asymptotic expansion of the Weber function [13]

$$U(a, z) \sim \frac{\exp(-z^2/4)\, z^{-a-1/2}}{\Gamma(a+1/2)} [\Gamma(a+\tfrac{1}{2}) - \Gamma(a+\tfrac{5}{2})\, u^2/1! + \Gamma(a+\tfrac{9}{2})\, u^4/2! + \cdots],$$

where $u^2 = 1/(2z^2)$. Choose $\gamma_k = \Gamma(k + a + \frac{1}{2})$. We immediately deduce the remarkable result

$$U(a, z) \simeq \frac{\exp(-z^2/4)\, z^{-a-1/2}}{\Gamma(a+1/2)} \sum_{i=1}^{s} \lambda_i \exp(-\omega_i^2/2z^2),$$

where the ω_i are the roots of the associated Laguerre polynomials $L_s^{(a-1/2)}(z)$, and the λ_i are the corresponding Christoffel constants. In Table II, we see an increase in precision as s increases. The figures which remain stable may be considered as exact. A check performed with the aid of the existing tables [13] confirms the assertion. The tabulation of $U(a, z)$ outside the range $0 \leqslant a \leqslant 2$ is performed by using the well-known recurrence relation which connects $U(a+1)$, $U(a)$, and $U(a-1)$ backwards (Miller's algorithm [23]).

EXAMPLE THREE: $f(z) = K_\nu(z)$ (Bessel function of the third kind) $(\nu > 0)$. Working as in the second example, we start with the asymptotic expansion of $K_\nu(z)$ [13].

$$K_\nu(z) \sim \sqrt{\pi/2z} \exp(-z) \left[1 + \frac{\mu-1}{8z} + \frac{(\mu-1)(\mu-9)}{2!(8z)^2} + \frac{(\mu-1)(\mu-9)(\mu-25)}{3!(8z)^3} + \cdots\right]$$

(with $\mu = 4\nu^2$ and z large). We choose $\gamma_k = \Gamma(k + \nu + \frac{1}{2})$ and after the calculation of $F(z)$ we find another remarkable result:

$$K_\nu(z) \simeq \frac{\sqrt{\pi/2z}\, \exp(-z)}{\Gamma(\nu+1/2)} \sum_{i=1}^{s} \lambda_i (1 + \omega_i/2z)^{\nu-1/2},$$

where the ω_i are the roots of the associated Laguerre polynomials $L_s^{(\nu-1/2)}(z)$ and the λ_i are the corresponding Christoffel constants. Exhibited in Table III is the increase in precision as s increases. Outside the range $0 \leqslant \nu \leqslant 2$, the reader may have recourse to the recurrence satisfied by $K_\nu(z)$ and to Miller's algorithm. It should be mentioned that the same formula seems to be valid in the whole complex plane. That point will be investigated more closely in future studies.

TABLE II

Approximation of $U(a, z)$

z	$U(0, z)$	$U(0.4, z)$	$U(0.8, z)$	$U(1.2, z)$	$U(1.6, z)$	$U(2, z)$
			Approximation of order $s = 6$ of $U(a, z)$			
3	5.8756516232E–02	3.6283544939E–02	2.2141548422E–02	1.3363292097E–02	7.9825277964E–03	4.7224150536E–03
4	8.9669263325L–03	5.0176454685E–03	2.7861220146E–03	1.5357080443E–03	8.4057044174E–04	4.5701588556E–04
5	8.5135652459E–04	4.3948478188E–04	2.2565648439E–04	1.1526733209E–04	5.8586283093E–05	2.9633871624E–05
6	4.9885775382E–05	2.4060782657E–05	1.1559664057E–05	5.5325899371E–06	2.6381677509E–06	1.2534514722E–06
7	1.7953344927E–06	8.1670600629E–07	3.7042406599E–07	1.6752218334E–07	7.5545847121E–08	3.3973350473E–08
8	3.9561562719E–08	1.7096542941E–08	7.3711737584E–09	3.1708449080E–09	1.3609410040E–09	5.8283408488E–10
9	5.3266254100E–10	2.1991897953E–10	9.0628735016E–11	3.7279709518E–11	1.5307101182E–11	6.2738966701E–12
			Approximation of order $s = 7$			
3	5.8756551788E–02	3.6283613659E–02	2.2141633810E–02	1.3363368640E–02	7.9825742143E–03	4.7224223549E–03
4	8.9669263711E–03	5.0176457304E–03	2.7861225761E–03	1.5357088523E–03	8.4057135957E–04	4.5701676293E–04
5	8.5135652209E–04	4.3948477900E–04	2.2565648265E–04	1.1526733224E–04	5.8586285073E–05	2.9633874814E–05
6	4.9885775350E–05	2.4060782613E–05	1.1559664011E–05	5.5325899008E–06	2.6381677277E–06	1.2534514616E–06
7	1.7953344924E–06	8.1670600597E–07	3.7042406564E–07	1.6752218304E–07	7.5545846881E–08	3.3973350311E–08
8	3.9561562717E–08	1.7096542940E–08	7.3711737568E–09	3.1708449066E–09	1.3609410029E–09	5.8283408407E–10
9	5.3266254097E–10	2.1991897952E–10	9.0628735011E–11	3.7279709514E–11	1.5307101178E–11	6.2738966680E–12
			Approximation of order $s = 8$			
3	5.8756548628E–02	3.6283612342E–02	2.2141639137E–02	1.3363382908E–02	7.9825960536E–03	4.7224476913E–03
4	8.9669263241E–03	5.0176456369E–03	2.7861224538E–03	1.5357087302E–03	8.4057126449E–04	4.5701670960E–04
5	8.5135652203E 04	4.3948477868E–04	2.2565648209E–04	1.1526733149E–04	5.8586284243E–05	2.9633874033E–05
6	4.9885775353E–05	2.4060782612E–05	1.1559664011E–05	5.5325899000E–06	2.6381677260E–06	1.2534514593E–06
7	1.7953344925E–06	8.1670600593E–07	3.7042406566E–07	1.6752218305E–07	7.5545846887E–08	3.3973350312E–08
8	3.9561562718E–08	1.7096542939E–08	7.3711737569E–09	3.1708449067E–09	1.3609410029E–09	5.8283408410E–10
9	5.3266254099E–10	2.1991897951E–10	9.0628735012E–11	3.7279709514E–11	1.5307101179E–11	6.2738966681E–12

TABLE III

z	K_0	$K_{0.4}$	$K_{0.8}$	$K_{1.2}$	$K_{1.6}$	K_2
			Approximation of order $s = 6$ of $K_\nu(z)$			
3	3.4739504157E-02	3.5557831990E-02	3.8121704264E-02	4.2780694614E-02	5.0200215783E-02	6.1510458403E-02
4	1.1159676078E-02	1.1362192062E-02	1.1990729794E-02	1.3111728160E-02	1.4848255154E-02	1.7401425523E-02
5	3.6910983336E-03	3.7456131230E-03	3.9137908091E-03	4.2101632759E-03	4.6611733045E-03	5.3089437109E-03
6	1.2439943280E-03	1.2594895481E-03	1.3070920457E-03	1.3902821077E-03	1.5153132662E-03	1.6919675669E-03
7	4.2479574187E-04	4.2937137830E-04	4.4338468172E-04	4.6772383780E-04	5.0396983385E-04	5.5456216658E-04
8	1.4647070522E-04	1.4786059957E-04	1.5210717756E-04	1.5944802709E-04	1.7030298408E-04	1.8531300814E-04
9	5.0881312956E-05	5.1312810178E-05	5.2628693906E-05	5.4894865298E-05	5.8227099804E-05	6.2800649918E-05
			Approximation of order $s = 7$ of $K_\nu(z)$			
3	3.4739504350E-02	3.5557832029E-02	3.8121704192E-02	4.2780694561E-02	5.0200215798E-02	6.1510458465E-02
4	1.1159676085E-02	1.1362192063E-02	1.1990729790E-02	1.3111728157E-02	1.4848255154E-02	1.7401425529E-02
5	3.6910983339E-03	3.7456131231E-03	3.9137908087E-03	4.2101632757E-03	4.6611733044E-03	5.3089437122E-03
6	1.2439943280E-03	1.2594895481E-03	1.3070920456E-03	1.3902821076E-03	1.5153132661E-03	1.6919675672E-03
7	4.2479574185E-04	4.2937137830E-04	4.4338468169E-04	4.6772383779E-04	5.0396983383E-04	5.5456216669E-04
8	1.4647070522R-04	1.4786059957E-04	1.5210717755E-04	1.5944802709E-04	1.7030298407E-04	1.8531300817E-04
9	5.0881312955E-05	5.1312810178E-05	5.2628693903E-05	5.4894865297E-05	5.8227099802E-05	6.2800649929E-05
			Approximation of order $s = 8$ of $K_\nu(z)$			
3	3.4739504380E-02	3.5557832031E-02	3.8121704184E-02	4.2780694555E-02	5.0200215801E-02	6.1510458471E-02
4	1.1159676086E-02	1.1362192062E-02	1.1990729791E-02	1.3111728157E-02	1.4848255155E-02	1.7401425529E-02
5	3.6910983340E-03	3.7456131228E-03	3.9137908089E-03	4.2101632758E-03	4.6611733046E-03	5.3089437122E-03
6	1.2439943280E-03	1.2594895480E-03	1.3070920457E-03	1.3902821077E-03	1.5153132662E-03	1.6919675673E-03
7	4.2479574187E-04	4.2937137826E-04	4.4338468171E-04	4.6772383780E-04	5.0396983385E-04	5.5456216669E-04
8	1.4647070522E-04	1.4786059955E-04	1.5210717756E-04	1.5944802709E-04	1.7030298408E-04	1.8531300817E-04
9	5.0881312956E-05	5.1312810173E-05	5.2628693905E-05	5.4894865298E-05	5.8227099804E-05	6.2800649930E-05

FOURTH EXAMPLE: hypergeometric functions. Working as before, it is easy to establish the following approximations ($\gamma_n = \Gamma(n+b)/\Gamma(n+c)$):

$$ {}_2F_1(a, b; c; z) \simeq [\Gamma(c)/\Gamma(b)] \sum_{i=1}^{s} \lambda_i (1 - \omega_i z)^{-a}, $$

$$ {}_1F_1(a; c; z) \simeq [\Gamma(c)/\Gamma(a)] \sum_{i=1}^{s} \lambda_i \exp(\omega_i z), $$

where the ω_i are the roots of the Jacobi polynomials $F(-s, s+b-1; c; z)$ and the λ_i the corresponding Christoffel constants. Similar formulas can be written for reducing arbitrary ${}_pF_q$ generalized hypergeometric functions.

IV. DISCUSSION AND CONCLUSION

This paper develops an approach to generalized Padé approximants; we exchange a poorly convergent series $f(z) = c_0 + c_1 z + \cdots$ for a more rapidly convergent one $F(z) = \alpha_0 + \alpha_1 z + \cdots$, where we have

$$ \alpha_i = c_i/\gamma_i $$

γ_i being simple given algebraic expressions. We have shown that an orthogonal polynomial family $Q_s(s)$ arises naturally in the scheme. The connection with the classical problem of moments (20–22) then becomes obvious since it is immediately seen that

$$ \gamma_k = \int_a^b t^k w(t)\, dt, $$

the density $w(t)$ being associated with the family Q_s;

$$ \int_a^b Q_m(t)\, Q_m(t)\, w(t)\, dt = h_m\, \delta_{m,n}, $$

i.e., the integral equals zero if $m \neq n$. The associated polynomials $P_s(z)$ are given by the formula [18]

$$ P_s(z) = -\gamma_0 \int_a^b \frac{Q_s(z) - Q_s(t)}{z - t}\, w(t)\, dt. $$

Both Q_s and P_s obey the recurrence (6)

$$ X_{k+1} = (z - a_k)\, X_k - b_k X_{k-1}, $$

where the a_k and the b_k evolve from the γ_k through the $q-d$ scheme. Its minimal solution is given by

$$g_s(z)/\gamma_0 = Q_s(z)\left(\sum_0^\infty \gamma_k/z^{k+1}\right) - P_s(z) \sim Q_s(z)\, O(1/z^{2s+1}),$$

since it is easily proved that $\lim_{s\to\infty} g_s/Q_s = 0$.

Another integral representation of g_s is

$$g_s(z) = \gamma_0 \int_a^b \frac{Q_s(t)\, w(t)}{z-t}\, dt.$$

We applied the new scheme to the evaluation of certain special functions. With this new method

(a) The calculations are simple. The second and third examples of Section III are particularly convincing since one easily obtains surprisingly good approximations of functions which are well known to be difficult to evaluate in their critical domain.

(b) The convergence is as good as with ordinary Padé approximants.

(c) The method is stable because the $q-d$ algorithm has been solved in an exact way.

(d) The calculation may be performed at a preassigned order s without first performing all the calculations at the successive orders $1, 2, \ldots, s-1$.

Many other problems remain open, properties of convergence, limits of validity of the method, etc. They will be investigated in future papers.

APPENDIX A

1. *The $q-d$ Algorithm* [9]

Starting with a sequence $\gamma_0, \gamma_1, \ldots, \gamma_{2s-1}$, the $q-d$ algorithm runs as follows:

$$\begin{aligned}
&e_0^{(n)} = 0 && (n = 0, 1, 2, \ldots, 2s-1),\\
&q_1^{(n)} = \gamma_{n+1}/\gamma_n && (n = 0, 1, 2, \ldots, 2s-2),\\
&e_k^{(n)} = e_{k-1}^{(n+1)} + q_k^{(n+1)} - q_k^{(n)},\\
&q_{k+1}^{(n)} = e_k^{(n+1)} q_k^{(n+1)}/e_k^{(n)} && (k = 1, 2, \ldots, s-1,\ n = 0, 1, \ldots).
\end{aligned}$$

Then the coefficients of Eq. (6) are given by

$$\begin{aligned}
&a_k = e_k^{(0)} + q_{k+1}^{(0)} && (k = 0, 1, \ldots, s-1),\\
&b_k = q_k^{(0)} e_k^{(0)} && (k = 1, 2, \ldots, s-1) \quad \text{but} \quad b_0 = -1.
\end{aligned}$$

2. *Exact Resolution of the $q-d$ Scheme*

For a given sequence γ_n, it is generally necessary to work recursively and numerically, since no simple expression exists for the general $q_k^{(n)}$ and $e_k^{(n)}$. Wynn [19] has presented the most general case which can be solved exactly in closed form

$$\gamma_n = \prod_{j=0}^{n} [(A - q^{\alpha+j})/(B - q^{\gamma+j})].$$

He has found

$$q_k^{(n)} = q^{k-1}(B - q^{\gamma+n+k-1})(A - q^{\alpha+n+k})/(B - q^{\gamma+n+2k-2})(B - q^{\gamma+n+2k-1}),$$
$$e_k^{(n)} = q^{n+k}(1 - q^k)(Bq^{\alpha} - Aq^{\gamma+k-1})/(B - q^{\gamma+n+2k-1})(B - q^{\gamma+n+2k}).$$

He has also described the associated orthogonal polynomial families $Q_s(z)$ and $P_s(z)$. Y. L. Luke [16] has studied in great detail various important special cases: $\gamma_n = \Gamma(n+a)$, $1/\Gamma(n+a)$, ρ^{an^2+bn}, $\Gamma(n+a)/\Gamma(n+b)$. He has shown that the associated orthogonal polynomials coincide with the classical ones (respectively, Laguerre, Bessel, Stieltjes–Wiegert, and Jacobi).

In each case, it can be shown that the function $\sum_0^{\infty} \gamma_k/z^{k+1}$ can be approximated by Padé approximants written in closed forms. The expressions for $Q_s(z)$ and $P_s(z)$ have been detailed by Y. L. Luke [16] who has shown that frequently the exact values of the approximants themselves are known, rather than the continued fraction representations.

Other apparently less useful examples might be considered; in fact, each family of orthogonal polynomials $Q_k(z)$ satisfies a recurrence of the type (6). The factors γ_n appear to be the moments of the family [15]. In these cases, both a_k and b_k can be written in closed form, while the whole $q-d$ scheme is not in general exactly soluble (i.e., $q_k^{(n)}$ and $e_k^{(n)}$ are not expressible in finite form). An extended list of convenient polynomials is given in [15].

APPENDIX B: NUMERICAL PROCEDURE

The numerical tables included in this paper have been prepared by following the strategy detailed at the end of Section II-3. The polynomials Q_k, Q_k', Q_k'', and P_k are calculated recursively ($k = 1,..., s$) with the aid of Eq. (6) and of its derivatives, i.e.,

$$Q_{k+1} = (z - a_k)\,Q_k - b_k Q_{k-1}, \qquad Q'_{k+1} = Q_k + (z - a_k)\,Q'_k - b_k Q'_{k-1},$$
$$Q''_{k+1} = 2Q'_k + (z - a_k)\,Q''_k - b_k Q''_{k-1}, \qquad P_{k+1} = (z - a_k)\,P_k - b_k P_{k-1},$$

with the following initial conditions:

$$Q_{-1} = P_0 = Q'_{-1} = Q'_0 = Q''_{-1} = Q''_0 = 0, \qquad Q_0 = P_{-1}/\gamma_0 = 1.$$

The roots of $Q_s(z)$ (which are all real and distinct in the examples considered) have been determined by using an iterative method due to Laguerre [14].

$$z_{i+1} = z_i - sQ_s(z_i)/[Q_s'(z_i) \pm \text{sign}[Q_s(z_i)] \sqrt{H}],$$

where $H = (s-1)^2[Q_s'(z_i)]^2 - s(s-1)\,Q_s(z_i)\,Q_s''(z_i)$. This method is specially interesting since it is nonlocal and of cubic convergence for the simple roots (i.e., a few iterative steps lead to a root correct to ten significant figures, whatever initial value one has chosen).

REFERENCES

1. C. BREZINSKI, Lecture Notes in Mathematics, No. 584, Springer-Verlag, Berlin, 1977.
2. P. WYNN, *MTAC*, **10** (1956), 91.
3. T. HÅVIE, *BIT*, **19** (1979), 204.
4. C. BREZINSKI, *Numer. Math.* **35** (1980), 175.
5. G. A. BAKER, JR., "Essentials of Padé Approximants," Academic Press, New York, 1975.
6. P. R. GRAVES-MORRIS, Lecture Notes in Mathematics, No. 765, Springer-Verlag, Berlin, 1979.
7. R. W. HAMMING, "Numerical Methods for Scientists and Engineers," McGraw–Hill, New York, 1962.
8. I. S. BEREZIN AND N. P. ZHIDKOV, "Computing Methods," Vol. 1, Pergamon, Oxford, 1965.
9. P. HENRICI, *in* "Mathematical Methods for Digital Computers" (A. Ralston and H. S. Wilf, Eds.) Vol. II Wiley, New York, 1967.
10. A. H. STROUD AND D. SECREST, "Gaussian Quadratures Formulas," Prentice–Hall, Englewood Cliffs, N.J., 1966.
11. H. E. SALZER AND R. ZUCKER, *Bull. Amer. Math. Soc.* **55** (1949), 1004.
12. W. P. LATHAM AND R. W. REDDING, *J. Comput. Phys.* **16** (1974), 66; **20** (1976), 256.
13. M. ABRAMOWITZ AND I. A. STEGUN, "Handbook of Mathematical Functions," Dover, New York, 1964.
14. E. DURAND, "Solutions numériques des équations algébriques," Masson, Paris, 1960.
15. T. S. CHIHARA, "An Introduction to Orthogonal Polynomials," Gordon and Breach, New York, 1978.
16. Y. L. LUKE, "The Special Functions and Their Approximations," Vols. I and II, Academic Press, New York, 1969.
17. G. A. BAKER, JR. AND J. L. GAMMEL, "The Padé Approximants in Theoretical Physics," Academic Press, New York, 1970.
18. W. GAUTCHI, *Math. Comput.* **36** (1981), 547.
19. P. WYNN, *Quart. J. Math. (Oxford)* **18** (1967), 81.
20. F. BERNSTEIN, *Jahresber. Deutsch. Math.-Verein.* **28** (1919), 50; **29** (1920), 94; *Math. Ann.* **81** (1920) 46.
21. M. RIESZ, *Acta Litt. Sci. (Szeged)* **1** (1922), 209.
22. H. HAMBURGER, *Math. Ann.* **81** (1920) 31.
23. Z. SCHULTEN, R. G. GORDON, AND D. G. M. ANDERSON, *J. Comput. Phys.* **42** (1981), 213.

RECEIVED: March 30, 1981; REVISED: April 21, 1982

ANDRÉ HAUTOT

Institute of Physics,
Université of Liège, Sart Tilman par 4000, Liège 1, Belgium