JOURNAL OF APPROXIMATION THEORY 25, 295–317 (1979)

Rational Approximation to Formal Power Series

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Communicated by Richard S. Varga

Received October 20, 1977

A general method for obtaining rational approximations to formal power series is defined and studied. This method is based on approximate quadrature formulas. Newton–Cotes and Gauss quadrature methods are used. It is shown that Padé approximants and the ϵ-algorithm are related to Gaussian formulas while linear summation processes are related to Newton–Cotes formulas. An example is exhibited which shows that Padé approximation is not always optimal. An application to e^{-t} is studied and a method for Laplace transform inversion is proposed.

1. STATEMENT OF THE PROBLEM

Let f be the formal power series

$$f(t) = \sum_{i=0}^{\infty} c_i t^i.$$

If the series in the right-hand side converges, then $f(t)$ is equal to its sum; if the series diverges, f represents its analytic continuation (assumed to exist). We consider a linear functional c associated with f satisfying

$$c(x^i) = c_i\,, \qquad i = 0, 1,\dots\,;$$

c can be regarded as a formal integration process. The basic idea is that

$$c\left(\frac{1}{1-xt}\right) = f(t),$$

where c acts on the variable x and where t is a parameter. Thus computing $f(t)$ for a fixed value of t is nothing else than computing $c((1-xt)^{-1})$ since $c((1-xt)^{-1}) = c(1 + xt + x^2t^2 + \cdots) = c_0 + c_1 t + c_2 t^2 + \cdots$.

It arises very often in practice that only a few coefficients c_i of the series are known or that it converges too slowly. Thus the function $(1-xt)^{-1}$

0021-9045/79/040295–23$02.00/0

has to be replaced by a polynomial P and $f(t)$ is approximated by $c(P)$: This is an approximate quadrature formula.

There are two main ways for replacing a function by a polynomial. The first one is to use interpolation polynomials which leads to the so-called interpolatory quadrature formulas. The second is to use certain other approximation polynomials; the corresponding quadrature formulas will be called approximatory quadrature formulas. They are not studied herein. The results presented in this paper have some connection with the ideas of Larkin [8, 9] on the approximation of a linear functional but this connection has not yet been studied in detail.

2. Interpolatory Quadrature Formulas

Let $x_1, x_2, \ldots, x_k$ be the (complex distinct) points of interpolation. These points can also depend on k, that is we can have a triangular set of interpolation points $x_i^{(k)}$ for $i = 1, \ldots, k$. Set

$$v(x) = (x - x_1) \cdots (x - x_k),$$

$$w(t) = c\left(\frac{v(x) - v(t)}{x - t}\right),$$

where c acts on the variable x and t is a parameter. Setting $v(x) = a_0 + a_1 x + \cdots + a_k x^k$, it is easily seen that w is a polynomial of degree $k - 1$: $w(t) = b_0 + b_1 t + \cdots + b_{k-1} t^{k-1}$ with

$$b_i = \sum_{j=0}^{k-i-1} c_j a_{i+j+1}, \qquad i = 0, \ldots, k - 1. \tag{1}$$

Finally, note that the Lagrange interpolation polynomial of a function g at $x_1, x_2, \ldots, x_k$ is

$$P(x) = v(x) \sum_{i=1}^{k} \frac{g(x_i)}{(x - x_i)\, v'(x_i)}.$$

Theorem 1. *If P is the Lagrange interpolation polynomial of $g(x) = (1 - xt)^{-1}$ constructed on the distinct abscissae $x_1, \ldots, x_k$, then*

$$c(P) = \tilde{w}(t)/\tilde{v}(t),$$

where

$$\tilde{w}(t) = t^{k-1} w(t^{-1}) \qquad \textit{and} \qquad \tilde{v}(t) = t^k v(t^{-1}).$$

Proof.

$$P(x) = \sum_{i=1}^{k} \frac{(v(x) - v(x_i))/(x - x_i)}{v'(x_i)} \frac{1}{1 - x_i t}.$$

By using the definition of w, we obtain

$$c(P) = \sum_{i=1}^{k} \frac{w(x_i)}{v'(x_i)} \frac{1}{1 - x_i t} = x \sum_{i=1}^{k} \frac{w(x_i)}{v'(x_i)} \frac{1}{x - x_i}$$

with $x = 1/t$. This is the partial fraction decomposition of $xw(x)/v(x)$. Thus

$$x \frac{w(x)}{v(x)} = \frac{1}{t} \frac{w(t^{-1})}{v(t^{-1})} = \frac{\tilde{w}(t)}{\tilde{v}(t)}.$$

Let $A_i^{(k)} = w(x_i)/v'(x_i)$. Then $c(P) = \sum_{i=1}^{k} A_i^{(k)}(1 - x_i t)^{-1}$ is the Newton–Cotes quadrature formula. Expressing the interpolation polynomial P as the ratio of two determinants we get

$$c(P) = \frac{\begin{vmatrix} 0 & c_0 & c_1 & --- & c_{k-1} \\ (x_1 t - 1)^{-1} & 1 & x_1 & --- & x_1^{k-1} \\ ----- & ----- & ----- & ----- & ----- \\ (x_k t - 1)^{-1} & 1 & x_k & --- & x_k^{k-1} \end{vmatrix}}{\begin{vmatrix} 1 & x_1 & --- & x_1^{k-1} \\ ----- & ----- & ----- & ----- \\ 1 & x_k & --- & x_k^{k-1} \end{vmatrix}}. \tag{2}$$

Letting

$$V_k = \begin{pmatrix} 1 & --- & 1 \\ x_1 & --- & x_k \\ ----- & ----- & ----- \\ x_1^{k-1} & --- & x_k^{k-1} \end{pmatrix} \qquad g_k = \begin{pmatrix} (1 - x_1 t)^{-1} \\ | \\ | \\ (1 - x_k t)^{-1} \end{pmatrix} \qquad \gamma_k = \begin{pmatrix} c_0 \\ | \\ | \\ c_{k-1} \end{pmatrix}$$

then, by a formula given by Magnus [13, p.i 17]

$$c(P) = (V_k^{-1} \gamma_k, g_k). \tag{3}$$

THEOREM 2. *Under the assumptions of Theorem* 1

$$c(P) - f(t) = O(t^k), \qquad (as\ t \to 0)$$

$$c(P) = \sum_{i=0}^{\infty} e_i t^i \qquad with \qquad e_i = \sum_{j=1}^{k} A_j^{(k)} x_j^{\ i}, \qquad i = 0, 1, \ldots,$$

and $e_i = c_i$ *for* $i = 0, \ldots, k - 1$.

Proof. $c(P) = \sum_{i=1}^{k} A_i^{(k)}(1 + x_i t + x_i^2 t^2 + \cdots) = \sum_{i=0}^{\infty} e_i t^i$ with

$$e_i = \sum_{j=1}^{k} A_j^{(k)} x_j^{\,i} \qquad \text{for} \quad i = 0, 1, \ldots .$$

From the fact that the Newton–Cotes quadrature formula is exact for polynomials of degree less than k, it follows that $c(P) - f(t) = O(t^k)$ and thus $e_i = c_i$ for $i = 0, \ldots, k - 1$.

Let us now study the error.

THEOREM 3. *Under the assumptions of Theorem* 1

$$c(P) - f(t) = \frac{t^k}{\tilde{v}(t)}\, c\left(\frac{v(x)}{xt - 1}\right).$$

Proof.

$$\tilde{w}(t) = t^{k-1} w(t^{-1}) = t^{k-1} c\left(\frac{v(x) - v(t^{-1})}{x - t^{-1}}\right) = c\left(\frac{t^k v(x) - t^k v(t^{-1})}{xt - 1}\right)$$

$$= t^k c\left(\frac{v(x)}{xt - 1}\right) - \tilde{v}(t)\, c\left(\frac{1}{xt - 1}\right)$$

and the result of the theorem immediately follows.

Remark 1. From the proof of the preceeding theorem we get

$$\frac{\tilde{w}(t)}{\tilde{v}(t)} = \frac{1}{v(t^{-1})}\, c\left(\frac{v(t^{-1}) - v(x)}{1 - xt}\right).$$

This relationship shows that any interpolatory quadrature method for $(1 - xt)^{-1}$ can be looked as replacing $(1 - xt)^{-1}$ by $(1 - v(x)/v(t^{-1})/(1 - xt)$ with $v(x) = (x - x_1) \cdots (x - x_k)$. From this theorem we also obtain

$$c(P) - f(t) = \frac{t^k}{\tilde{v}(t)} \sum_{i=0}^{\infty} d_i t^i$$

with $d_i = -c(x^i v) = -(a_0 c_i + a_1 c_{i+1} + \cdots + a_k c_{i+k})$.

Although the abscissae are not always equidistant such interpolatory quadrature methods will be called Newton–Cotes methods. The approximants obtained will be called Padé-type approximants and will be denoted by $(k - 1/k)_f(t)$, where f is the function to be approximated and t is the variable.

Let us now turn to Gaussian quadrature formulas. It is well known that, in Gaussian methods, the interpolation points x_i are chosen so that the quadrature formula is exact for polynomials of degree less than $2k$. It is also well known that the x_i are the roots of orthogonal polynomials. Thus let us now consider the family of orthogonal polynomials $\{P_k\}$ with respect to the functional c, that is,

$$c(x^i P_k) = 0 \qquad \text{for} \quad i = 0,..., k-1,$$

where k is the degree of P_k. Such polynomials are given by

$$P_k(x) = \begin{vmatrix} c_0 & c_1 & --- & c_k \\ c_1 & c_2 & --- & c_{k+1} \\ -- & -- & -- & -- \\ c_{k-1} & c_k & --- & c_{2k-1} \\ 1 & x & --- & x^k \end{vmatrix}.$$

Let us now chose the x_i's, for fixed k, as the roots of P_k. We assume that these roots are distinct and that the Hankel determinants

$$H_k(c_0) = \begin{vmatrix} c_0 & c_1 & --- & c_{k-1} \\ c_1 & c_2 & --- & c_k \\ -- & -- & -- & -- \\ c_{k-1} & c_k & --- & c_{2k-2} \end{vmatrix}$$

are all different from zero such that P_k has the exact degree k. Let Q_k be the associated polynomials defined by

$$Q_k(t) = c\left(\frac{P_k(x) - P_k(t)}{x - t}\right)$$

and let $\tilde{P}_k(t) = t^k P_k(t^{-1})$, $\tilde{Q}_k(t) = t^{k-1} Q_k(t^{-1})$. Then P_k is identical to v apart from a multiplying factor and Q_k is identical to w apart from the same factor. Thus

$$\tilde{w}(t)/\tilde{v}(t) = \tilde{Q}_k(t)/\tilde{P}_k(t) \tag{4}$$

and Theorems 1, 2, and 3 remain true for Gaussian quadrature formulas. Moreover we get:

THEOREM 4. *If the x_i are the roots of P_k which are assumed to be distinct, then*

$$e_i = c_i \qquad \textit{for} \quad i = 0,..., 2k-1,$$

$$c(P) - f(t) = O(t^{2k}),$$

$$c(P) - f(t) = \frac{t^{2k}}{\tilde{P}_k(t)}\, c\left(\frac{x^k P_k(x)}{xt - 1}\right) = \frac{t^{2k}}{\tilde{P}_k^2(t)}\, c\left(\frac{P_k^2(x)}{xt - 1}\right),$$

$$c(P) = [k - 1/k]_f(t),$$

where $[p/q]_f(t)$ is the Padé approximant to f whose numerator has degree p and whose denominator has degree q.

Proof. Gaussian quadrature formulas are exact for polynomials of degree less than $2k$; then the first two statements of the theorem immediately follow. The identity with Padé approximants comes out from the unicity of Padé approximants or from their definition as the ratio of two determinants. From the orthogonality property of P_k we get

$$c\left(\frac{v(x)}{1-xt}\right) = c(v(x)(1+xt+\cdots)) = c(v(x)(x^k t^k + x^{k+1}t^{k+1}+\cdots))$$
$$= t^k c\left(\frac{x^k v(x)}{1-xt}\right)$$

and the first part of the third statement follows. $(P_k(x) - P_k(t^{-1}))/(1-xt)$ is a polynomial of degree $k-1$ in x; then

$$c\left(P_k(x)\,\frac{P_k(x)-P_k(t^{-1})}{1-xt}\right) = 0 = c\left(\frac{P_k^2(x)}{1-xt}\right) - P_k(t^{-1})\,c\left(\frac{P_k(x)}{1-xt}\right)$$

which ends the proof of this theorem.

Remark 2. Formulas (2) and (3) provide new expressions for Padé approximants.

Remark 3. From the third result of Theorem 4 it is easy to prove that

$$f(t) - [k-1/k]_f(t) = \frac{H_{k+1}(c_0)}{H_k(c_0)}\,t^{2k} + O(t^{2k+1}).$$

Remark 4. For arbitrary distinct x_i we get $f(t) - c(P) = O(t^k)$ but the computation of $(k-1/k)$ only requires the knowledge of $c_0,\ldots,c_{k-1}$. If the x_i are the roots of P_k, then $f(t) - c(P) = O(t^{2k})$ but, as it can be seen from (4), the computation of $[k-1/k]$ requires the knowledge of $c_0,\ldots,c_{2k-1}$. Thus, from the algebraic point of view, nothing is gained by using Padé approximants and Gaussian quadrature formulas with k points have to be compared with Padé-type approximants using $2k$ points. Moreover, in Padé-type approximants, the poles of the rational approximation $\tilde{w}(t)/\tilde{v}(t)$ can be arbitrarily chosen since the roots of $\tilde{v}$ are equal to x_i^{-1}. The relationships (1) between the coefficients of the numerator and those of the denominator come out from equating the coefficients of t^i to zero for $i = 0,\ldots,k-1$ in $f(t) - c(P)$. If the coefficients of t^i must also be zero for $i = k,\ldots,2k-1$ then we must have $c(x^i v(x)) = 0$ for $i = 0,\ldots,k-1$ which shows that v is identical to P_k. However if f is a rational function of degree $k-1$ over degree k then, for arbitrary distinct x_i, $(k-1/k)_f(t)$ is not identical to f while the Padé approximant $[k-1/k]_f(t)$ is.

Remark 5. The difference between the approximants obtained by Newton–Cotes formulas or by Gauss formulas is that the first are linear with respect to the c_i's while the second are not.

These quadrature methods can be applied to the computation of the limit S of a sequence $\{S_n\}$. Let us consider the series f defined by $c_i = S_{i+1} - S_i$. Then $S = S_0 + f(1)$ will be approximated by $S_0 + w(1)/v(1)$. It is easy to see that $S_0 + w(1)/v(1) = (a_0 S_0 + \cdots + a_k S_k)/(a_0 + \cdots + a_k)$. In the case where the x_i's are arbitrarily chosen this is a summation method. If the x_i's are the roots of P_k then we obtain $\epsilon_{2k}^{(0)}$ given by the ϵ-algorithm of Wynn [19]. This fact had been proved some years ago by Brezinski [2] in a very different way.

A consequence of Theorem 4 is the

COROLLARY 1. *Under the assumptions of Theorem* 1 *and if* $v(x) = (x - x_1) \cdots (x - x_k) = u(x) P_m(x)$ *with* $m \leqslant k \leqslant 2m$ *then*

$$\tilde{w}(t)/\tilde{v}(t) = [m - 1/m]_f(t).$$

Proof.

$$\begin{aligned} w(t) &= c\left(\frac{u(x) P_m(x) - u(t) P_m(t)}{x - t}\right) \\ &= c\left(u(t) \frac{P_m(x) - P_m(t)}{x - t} + P_m(x) \frac{u(x) - u(t)}{x - t}\right) \\ &= u(t)\, c\left(\frac{P_m(x) - P_m(t)}{x - t}\right) \end{aligned}$$

since P_m is orthogonal to every polynomial of degree less than m and since the degree of u is $k - m \leqslant m$. Thus $\tilde{w}(t)/\tilde{v}(t) = [m - 1/m]_f(t)$ by Theorem 4.

Remark 6. Replacing v by uP_m in the error term of Theorem 3 we get the error term of Theorem 4 since

$$c\left(\frac{v(x)}{xt - 1}\right) = u(t^{-1})\, c\left(\frac{P_m(x)}{xt - 1}\right).$$

The two preceeding results show that the theory of general orthogonal polynomials plays a fundamental role in the algebraic theory of Padé approximants. In fact almost all the known algebraic results about Padé approximants follow in a very easy and natural way from the theory of orthogonal polynomials and new results can also be obtained [3, 4].

Let us now mix up the two preceding methods in the following way: Let some of the x_i, say $x_1, \ldots, x_m$, be arbitrarily chosen and let the remainding points, $x_{m+1}, \ldots, x_k$, be taken such that the quadrature method be exact for polynomials of degree less than $2k - m$. Such quadrature formulas exist and are well known. Let $u(x) = (x - x_1) \cdots (x - x_m)$ and let the functional $\bar{c}$ be defined by

$$\bar{c}(x^i) = c(x^i u(x)), \qquad i = 0, 1, \ldots .$$

Let $\bar{P}_{k-m}$ be the orthogonal polynomial of degree $k - m$ with respect to $\bar{c}$. We assume that it has the exact degree $k - m$; then $x_{m+1}, \ldots, x_k$ must be chosen as the roots of $\bar{P}_{k-m}$. Thus we have

$$v(x) = \bar{P}_{k-m}(x)\, u(x).$$

w is defined in the usual way from c and $c(P) = \tilde{w}(t)/\tilde{v}(t)$. For such quadrature formulas we get:

THEOREM 5. *If $x_1, \ldots, x_m$ are arbitrary distinct points and if $x_{m+1}, \ldots, x_k$ are the roots of $\bar{P}_{k-m}$ that are assumed to be distinct and distinct from $x_1, \ldots, x_m$, then*

$$e_i = c_i \qquad \textit{for} \quad i = 0, \ldots, 2k - m - 1,$$

$$c(P) - f(t) = O(t^{2k-m}),$$

$$\begin{aligned} c(P) - f(t) &= \frac{t^{2k-m}}{\tilde{v}(t)}\, c\left(\frac{x^{k-m} v(x)}{xt - 1}\right) \\ &= \frac{1}{v(t^{-1})\, \bar{P}_{k-m}(t^{-1})}\, c\left(\frac{v(x)\, \bar{P}_{k-m}(x)}{xt - 1}\right). \end{aligned}$$

Proof. Essentially the same as for Theorem 4. The first two statements are properties of such quadrature methods. The last two statements follow from Theorem 3 and from the orthogonality properties of $\bar{P}_{k-m}$.

Remark 7. The computation of such a quadrature formula requires the knowledge of $c_0, \ldots, c_{2k-m-1}$.

Let now P be the general Hermite interpolation polynomial such that

$$P^{(j)}(x_i) = \frac{d^j}{dx^j}\left(\frac{1}{1 - xt}\right)_{x = x_i}, \qquad i = 1, \ldots, n \text{ and } j = 0, \ldots, k_i - 1 \geqslant 0. \quad (5)$$

We assume that the interpolation points x_i are distinct. Let $k = \sum_{i=1}^{n} k_i$ and

$$v(x) = (x - x_1)^{k_1} \cdots (x - x_n)^{k_n}.$$

Let w, $\tilde{v}$ and $\tilde{w}$ be defined as above. We get:

THEOREM 6. *Let P be the general Hermite interpolation polynomial which is assumed to satisfy the preceding conditions; then*

$$c(P) = \tilde{w}(t)/\tilde{v}(t),$$

$$c(P) - f(t) = O(t^k) = \frac{t^k}{\tilde{v}(t)} c\left(\frac{v(x)}{xt-1}\right).$$

Proof. It is well known that the general Hermite interpolation polynomial can be deduced from the Lagrange interpolation polynomial by continuity arguments when some points coincide. Thus the first part of the theorem immediately follows. The proof of the second part of the theorem is as in Theorem 3.

Remark 8. This theorem can also be proved by writing down P and showing that $c(P)$ is the partial fraction decomposition of $\tilde{w}(t)/\tilde{v}(t)$.

Remark 9. $\tilde{v}$ has the exact degree k and the computation of $\tilde{v}(t)/\tilde{w}(t)$ requires the knowledge of $c_0, \ldots, c_{k-1}$.

Remark 10. If $v(x) = (x - x_1)^{k_1} \cdots (x - x_n)^{k_n} = u(x) P_m(x)$ with $m \leqslant k \leqslant 2m$ then Corollary 1 applies and $\tilde{w}(t)/\tilde{v}(t) = [m - 1/m]_f(t)$. In particular if $k_i = 2 \forall i$ and if $x_1, \ldots, x_n$ are the roots of P_n then $\tilde{w}(t)/\tilde{v}(t) = [n - 1/n]_f(t)$. Replacing v by $P_n{}^2$ in the error term of Theorem 6 we get the result of Theorem 4. If $v(x) = P_k(x)$ then $c(P) = [k - 1/k]_f(t)$ which shows that the roots of P_k have not to be distinct as in Theorem 4 but that, in case of multiple roots, P must be taken as the general Hermite interpolation polynomial.

Remark 11. If $n = 1$ then $v(x) = (x - x_1)$ and $\tilde{w}(t)/\tilde{v}(t) = \tilde{w}(t)/(1 - x_1 t)^k$. In particular if $x_1 = 0$ then

$$w(t) = c\left(\frac{x^k - t^k}{x - t}\right) = c_{k-1} + c_{k-2} t + \cdots + c_0 t^{k-1},$$

$\tilde{w}(t)/\tilde{v}(t) = c_0 + c_1 t + \cdots + c_{k-1} t^{k-1}$ and P is the Taylor interpolation polynomial at $x_1 = 0$ that is $P(x) = 1 + xt + \cdots + x^{k-1} t^{k-1}$.

Remark 12. Conversely let

$$v(x) = (x - x_1)^{k_1} \cdots (x - x_n)^{k_n}$$

with $k = \sum_{i=1}^{n} k_i$, let $x_1, \ldots, x_n$ be distinct and let $w(x)$, $\tilde{v}(t)$ and $\tilde{w}(t)$ be defined in the usual way. Then $\tilde{w}(t)/\tilde{v}(t)$ is a rational approximation to $f(t)$ obtained by replacing $(1 - xt)^{-1}$ by its general Hermite interpolation polynomial such that (5) holds and then computing $c(P)$.

All the preceding rational approximations have the same form $\tilde{w}(t)/\tilde{v}(t)$ and a general compact formula which generalizes Nuttall's compact formula [16] can be derived for them. The basic idea for such a compact formula in the case of Padé approximants for some special series is due to Magnus [14] and we only extend here this idea. It is easy to see that

$$\frac{1}{v(t^{-1})}\frac{v(t^{-1}) - v(x)}{1 - xt}$$

is a polynomial of degree $k - 1$ in x whose coefficients depend on t. Let $\{q_n\}$ be any sequence of polynomials such that q_n has the exact degree n for all n. Thus

$$\frac{1}{v(t^{-1})}\frac{v(t^{-1}) - v(x)}{1 - xt} = \beta_0 q_0(x) + \cdots + \beta_{k-1} q_{k-1}(x)$$

and, by Remark 1

$$\tilde{w}(t)/\tilde{v}(t) = \beta_0 c(q_0) + \cdots + \beta_{k-1} c(q_{k-1}).$$

For $i = 0,..., k - 1$ we get

$$c(q_i(x)(1 - v(x)/v(t^{-1})) = c(q_i(x)(1 - xt)(\beta_0 q_0(x) + \cdots + \beta_{k-1} q_{k-1}(x))).$$

That is,

$$\begin{pmatrix} c((1-xt)\,q_0^2) & c((1-xt)\,q_0q_1) & \cdots & c((1-xt)\,q_0q_{k-1}) \\ c((1-xt)\,q_1q_0) & c((1-xt)\,q_1^2) & \cdots & c((1-xt)\,q_1q_{k-1}) \\ \hdashline c((1-xt)\,q_{k-1}q_0) & c((1-xt)\,q_{k-1}q_1) & \cdots & c((1-xt)\,q_{k-1}^2) \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \\ \beta_{k-1} \end{pmatrix}$$

$$= \begin{pmatrix} c_0' \\ c_1' \\ \\ c_{k-1}' \end{pmatrix}$$

with $c_i' = c(q_i(x)(1 - v(x)/v(t^{-1}))$. Let V be the matrix and v' the second member of the preceding system; let v be the vector whose components are $c(q_i)$. Then we get

$$\tilde{w}(t)/\tilde{v}(t) = (v, V^{-1}v'). \tag{6}$$

If $q_n(x) = x^n$ the elements V_{ij} of V are $V_{ij} = c_{i+j-2} - tc_{i+j-1}$ for i, $j = 1,..., k$ while the components v_i of v are c_{i-1} for $i = 1,..., k$. This is a generalization of Nuttall's compact formula. If the x_i are the roots of P_k then $v(x) = P_k(x)$, $v = v'$ and we obtain Nuttall's formula for Padé approximants.

If we choose $q_n(x) = P_n(x)$, then we obtain a result which is closely related to the matrix interpretation of Padé approximants [7]

$$[k-1/k]_f(t) = c_0(e, (I_k - J_k t)^{-1} e),$$

where e is the vector all of whose components are equal to zero except the first one which is one. J_k is the tridiagonal matrix

$$J_k = \begin{bmatrix} -B_1 & C_2 & & & \\ 1 & -B_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & C_k \\ & & & 1 & -B_k \end{bmatrix},$$

where B_i and C_i are the coefficients of the recurrence relationship of the orthogonal polynomials

$$P_{k+1}(x) = (x + B_{k+1})\, P_k(x) - C_{k+1} P_{k-1}(x).$$

From this formula, formula (3) can also be easily obtained. A similar formula holds for $\tilde{w}(t)/\tilde{v}(t)$.

Remark 13. If the x_i are not the roots of P_k then $\tilde{w}(t)/\tilde{v}(t)$ only depends on $c_0, \ldots, c_{k-1}$. Thus in formula (6) arbitrary values can be given to $c_k, \ldots, c_{2k-1}$ and, in particular, $c_i = 0$ for $i = k, \ldots, 2k-1$.

Remark 14. Let A and B be the matrices whose coefficients are, respectively, $c(q_i\, q_j)$ and $c(x\, q_i\, q_j)$ for $i, j = 0, \ldots, k-1$. Then $V = A - tB$ and

$$\tilde{w}(t)/\tilde{v}(t) = \sum_{i=0}^{\infty} (v, (A^{-1}B)^i A^{-1} v')\, t^i.$$

Thus $c_i = (v, (A^{-1}B)^i A^{-1} v')$ for $i = 0, \ldots, k-1$. For Padé approximants this relation is valid until $i = 2k-1$ and from (7) we also get

$$c_i = c_0(e, J_k{}^i e), \qquad i = 0, \ldots, 2k-1.$$

Let us now show how to construct rational approximations of series with arbitrary degrees in the numerator and denominator. We have

$$\frac{1}{1-xt} = 1 + xt + \cdots + x^n t^n + \frac{x^{n+1} t^{n+1}}{1-xt}.$$

Then

$$f(t) = c\left(\frac{1}{1-xt}\right) = c_0 + c_1 t + \cdots + c_n t^n + t^{n+1} c\left(\frac{x^{n+1}}{1-xt}\right).$$

Let P be the interpolation polynomial of the function $(1 - xt)^{-1}$ on some points $x_1, \ldots, x_k$. Then $f(t)$ can be approximated by

$$c_0 + c_1 t + \cdots + c_n t^n + t^{n+1} c(x^{n+1} P).$$

If we define the functional $c^{(m)}$ by $c^{(m)}(x^i) = c(x^{m+i}) = c_{m+i}$ for $i = 0, 1, \ldots,$ and if

$$w(t) = c^{(n+1)}\left(\frac{v(x) - v(t)}{x - t}\right),$$

then the preceding approximation of $f(t)$ can be written as

$$c_0 + c_1 t + \cdots + c_n t^n + t^{n+1} c^{(n+1)}(P)$$
$$= c_0 + c_1 t + \cdots + c_n t^n + t^{n+1} \frac{\tilde{w}(t)}{\tilde{v}(t)} \tag{8}$$

which is the ratio of a polynomial of degree $n + k$ in t over a polynomial of degree k.

We also have

$$\frac{1}{1-xt} = \frac{x^{-n+1} t^{-n+1}}{1-xt} - \frac{1}{xt} - \cdots - \frac{1}{x^{n-1} t^{n-1}}.$$

Let us apply the functional c to this identity. Then, since $c(x^i) = c_i = 0$ for $i < 0$, we get

$$f(t) = c\left(\frac{1}{1-xt}\right) = t^{-n+1} c\left(\frac{x^{-n+1}}{1-xt}\right).$$

Let P be the interpolation polynomial of the function $(1 - xt)^{-1}$ on some points $x_1, \ldots, x_{n+k}$. $f(t)$ can be approximated by

$$t^{-n+1} c(x^{-n+1} P).$$

Let $v(x) = (x - x_1) \cdots (x - x_{n+k})$, let $c^{(-n+1)}$ be defined by $c^{(-n+1)}(x^i) = c(x^{-n+1+i}) = c_{-n+1+i}$ for $i = 0, 1, \ldots,$ with $c_{-n+1+i} = 0$ if $i < n - 1$, and let w be defined in the usual manner. It can easily be seen from its definition that w has the degree k for $n = 1, 2, \ldots$.

Let $\tilde{w}$ be defined by

$$\tilde{w}(t) = t^{n+k-1} w(t^{-1}).$$

Then

$$t^{-n+1}c(x^{-n+1}P) = t^{-n+1}c^{(-n+1)}(P) = t^{-n+1}\frac{\tilde{w}(t)}{\tilde{v}(t)} \tag{9}$$

which is the ratio of a polynomial of degree k in t over a polynomial of degree $n+k$.

Formulas (8) and (9) can both be written as

$$\sum_{i=0}^{n} c_i t^i + t^{n+1}\frac{\tilde{w}(t)}{\tilde{v}(t)}$$

for $n = 0, \pm 1, \pm 2,\ldots$ with the convention that the sum is equal to zero if n is negative.

If this approximant is written as $[\tilde{v}(t)\sum_{i=0}^{n} c_i t^i + t^{n+1}\tilde{w}(t)]/\tilde{v}(t)$ it can easily be seen that the relations between the coefficients of the numerator and the coefficients of the denominator are exactly the same as those occuring for Padé approximants. We shall designate by $(p/q)_f(t)$ these approximants in the general case and by $[p/q]_f(t)$ the Padé approximants. p is the degree of the numerator, q that of the denominator, f is the function which is approximated, and t is the variable. There is, in general, no connection between the upper and the lower part of the table of the (p/q) approximants as it occurs for the Padé table. Let $(k-1/k)_f(t)$ be the Padé-type approximant and let $\tilde{v}$ be its denominator. Let us now consider the reciprocal series g defined by $f(t)\,g(t) = 1$ and let $(k/k-1)_g(t)$ be the Padé-type approximant to g with $\tilde{w}$ as denominator. It is easy to see that we can have $(k-1/k)_f(t) = 1/(k/k-1)_g(t)$ only if v is such that $c(v) = 0$. In the Padé table this property is true since v is P_k.

If we look at the degrees of approximation of both parts of the table, as we now will proceed, it is also obvious that, in the general case, no connection can occur between the two parts of the table. However if $(k/k)_f(t)$ is the Padé-type approximant to f with $\tilde{v}$ as denominator and if $(k/k)_g(t)$ is the approximant to g with $c_0\tilde{v}(t) + t\tilde{w}^{(1)}(t)$ as denominator where

$$w^{(1)}(t) = c^{(1)}\left(\frac{v(x)-v(t)}{x-t}\right)$$

then we always have

$$(k/k)_f(t) = 1/(k/k)_g(t).$$

Let us now proceed to the degree of approximation.

From the definition of $c^{(n+1)}$ it is easy to see that $c^{(n+1)}(P)$ is an approximation to $c^{(n+1)}((1-xt)^{-1})$; thus

$$c^{(n+1)}(P) = c_{n+1} + c_{n+2}t + \cdots + c_{n+k}t^{k-1} + O(t^k)$$

and it follows from (8) that

$$c_0 + c_1 t + \cdots + c_n t^n + t^{n+1} \frac{\tilde{w}(t)}{\tilde{v}(t)} - f(t) = O(t^{n+k+1}).$$

From (9) we only obtain that

$$t^{-n+1} \frac{\tilde{w}(t)}{\tilde{v}(t)} - f(t) = O(t^{k+1}).$$

If P is the Hermite interpolation polynomial then v must be defined as $v(x) = (x - x_1)^{k_1} \cdots (x - x_n)^{k_n}$. If the points of interpolation are the roots of the polynomial $P_k^{(n+1)}$ which is orthogonal with respect to the functional $c^{(n+1)}$, if these roots are distinct and if $P_k^{(n+1)}$ has the exact degree k then

$$\sum_{i=0}^{n} c_i t^i + t^{n+1} \frac{\tilde{w}(t)}{\tilde{v}(t)} = [n + k/k]_f(t) = f(t) + O(t^{n+2k+1}).$$

If the points of interpolation are the roots of $P_{n+k}^{(-n+1)}$ which is orthogonal with respect to the functional $c^{(-n+1)}$, if these roots are distinct and if $P_{n+k}^{(-n+1)}$ has the exact degree $n + k$ then

$$t^{-n+1} \frac{\tilde{w}(t)}{\tilde{v}(t)} = [k/n + k]_f(t) = f(t) + O(t^{n+2k+1}).$$

Remark 15. The condition for $P_k^{(n)}$ to be of the exact degree k is that the Hankel determinant

$$H_k(c_n) = \begin{vmatrix} c_n & --- & c_{n+k-1} \\ c_{n+1} & --- & c_{n+k} \\ ---- & ---- & ---- \\ c_{n+k-1} & --- & c_{n+2k-2} \end{vmatrix} = H_k^{(n)}$$

is different from zero. If the roots of the orthogonal polynomials are not distinct similar results hold with P as the Hermite interpolation polynomial. Finally if the points $x_1, \ldots, x_m$ are arbitrarily chosen and if the remainding points $x_{m+1}, \ldots, x_k$ are the roots of the polynomial $\bar{P}_{k-m}^{(n+1)}$ which is orthogonal to the functional $\bar{c}^{(n+1)}$ defined by $\bar{c}^{(n+1)}(x^i) = c^{(n+1)}(x^i u(x))$ then results similar to those of Theorem 5 can be obtained.

Let us now study the convergence of such methods for obtaining rational approximation of series when n or k goes to infinity.

Let $S_n = \sum_{i=0}^{n} c_i t^i$ and $v(x) = a_0 + a_1 x + \cdots + a_k x^k$; then, by using (1), it is easy to see that

$$\frac{\tilde{w}(t)}{\tilde{v}(t)} = B_1 S_0 + \cdots + B_k S_{k-1}$$

and

$$\sum_{i=0}^{n} c_i t^i + t^{n+1} \frac{\tilde{w}(t)}{\tilde{v}(t)} = B_0 S_n + \cdots + B_k S_{n+k} \qquad \text{for} \quad n = 0, 1,...$$

with

$$B_i = a_i t^{k-i}/\tilde{v}(t) \qquad \text{and} \qquad \sum_{i=0}^{k} B_i = 1.$$

In fact, since the roots x_i of v can depend on k and n, the B_i's also depend on k and n. The convergence of these sequences of approximations when n or k goes to infinity can be studied by using the Toeplitz theorem for the convergence of summation processes [18] and we immediately obtain

THEOREM 7. *Let the sequence $\{S_n\}$ converge to $f(t)$. The sequence $\sum_{i=0}^{n} c_i t^i + t^{n+1}\tilde{w}(t)/\tilde{v}(t)$ converges to $f(t)$ when n goes to infinity if*

$$\sum_{i=0}^{k} | B_i | \leqslant M \qquad \forall n.$$

The sequence converges to $f(t)$ when k goes to infinity if

$$\lim_{k\to\infty} B_i = 0 \qquad \text{for} \quad i = 0, 1,...$$

and

$$\sum_{i=0}^{k} | B_i | \leqslant M \qquad \forall k.$$

In practice it is a difficult matter to know if these conditions are satisfied or not. However it is possible to get the following partial results:

THEOREM 8. *If $x_i \leqslant 0$ $\forall i$ and $\forall n, k$, if $t \geqslant 0$ and if $\{S_n\}$ tends to $f(t)$ then the sequences $\sum_{i=0}^{n} c_i t^i + t^{n+1}\tilde{w}(t)/\tilde{v}(t)$ converge to $f(t)$, for every fixed $k \geqslant 0$, when n goes to infinity.*

The proof is elementary since all the B_i are positive.

THEOREM 9. *Let $\{x_i\}$ be an infinite sequence of negative numbers converging to zero and let $v(x) = (x - x_1) \cdots (x - x_k)$. If $t \geqslant 0$ and if $\{S_n\}$ tends to $f(t)$ then the sequences $\sum_{i=0}^{n} c_i t^i + t^{n+1}\tilde{w}(t)/\tilde{v}(t)$ converge to $f(t)$, for every fixed $n \geqslant -1$, when k goes to infinity.*

Proof. Let $v_k(x) = (x - x_1) \cdots (x - x_k)$ and let $B_i^{(k)}$ be the corresponding coefficients for fixed $n \geqslant -1$. Since $v_{k+1}(x) = v_k(x)(x - x_{k+1})$ it is easy to see that

$$B_0^{(k+1)} = x_{k+1} t B_0^{(k)}/(1 - x_{k+1} t),$$
$$B_i^{(k+1)} = (B_{i-1}^{(k)} - x_{k+1} t B_i^{(k)})/(1 - x_{k+1} t) \qquad \text{for} \quad i = 1,\dots, k,$$

and

$$B_{k+1}^{(k+1)} = B_k^{(k)}/(1 - x_{k+1} t)$$

with $B_0^{(0)} = 1$.

If $t \geqslant 0$, $x_i \leqslant 0$ and $\lim_{n\to\infty} x_n = 0$ then $B_i^{(k)} \geqslant 0$ and $\lim_{k\to\infty} B_0^{(k)} = 0$. Let us assume that $\lim_{k\to\infty} B_{i-1}^{(k)} = 0$. Then

$$\lim_{k\to\infty} x_{k+1} t (B_i^{(k)} - B_i^{(k+1)}) + B_i^{(k+1)} = 0.$$

If $B_i^{(k)} \leqslant M\ \forall k$ then $\lim_{k\to\infty} B_i^{(k)} = 0$. If such an M does not exist thus it is impossible that $\sum_{i=0}^{k} B_i^{(k)} = 1$ since $B_i^{(k)} \geqslant 0$. In conclusion $\lim_{k\to\infty} B_i^{(k)} = 0$ for $i = 0, 1,\dots$, and, by Theorem 7, the approximants converge to $f(t)$ when k goes to infinity and when $n \geqslant -1$ is fixed.

Let us now study the case where the coefficients c_i are given by

$$c_i = \int_a^b x^i \, d\alpha(x), \tag{10}$$

where α is bounded and nondecreasing in the finite or semi-infinite interval $[a, b]$. In that case the functional c is positive, that is, $c(p) \geqslant 0$ for every polynomial p such that $p(x) \geqslant 0$, $\forall x \in [a, b]$. If the x_i belong to $[a, b]$ and if t is real and does not belong to $[b^{-1}, a^{-1}]$ then $(1 - xt)^{-1}$ is continuous on $[a, b]$ and the convergence can be studied by convergence results on classical quadrature methods. Thus, for Padé approximants, the x_i belong to $[a, b]$, the coefficients $A_i^{(k)}$ of the quadrature formula are positive and the sequence $[k - 1/k]_f(t)$ converges to $f(t)$ for every $t \notin [b^{-1}, a^{-1}]$ when k goes to infinity. The general convergence result is the following:

THEOREM 10. *If the coefficients c_i are given by* (10) *and if the x_i are distinct and belong to $[a, b]$ then*

$$\lim_{k\to\infty} \tilde{w}(t)/\tilde{v}(t) = f(t) \qquad \forall t \in [b^{-1}, a^{-1}]$$

if there exists an M independent of k such that

$$\sum_{i=1}^{k} \left| \frac{w(x_i)}{v'(x_i)} \right| \leqslant M \qquad \forall k,$$

then moreover,

$$f(t) - [k-1/k]_f(t) = \frac{H_{k+1}^{(0)}}{H_k^{(0)}} \frac{t^{2k}}{(1-\xi t)^{2k+1}}, \qquad \xi \in [a, b].$$

Proof. The first part is the classical theorem on the convergence of quadrature processes: $\sum_{i=1}^{k} | A_i^{(k)} | < M$ while the second is the error term of Gaussian methods.

Remark 16. From this theorem one can obtain bounds for the error. For example if $a = 0$ and $b = 1/R$, where R is the radius of convergence of f then

$$| f(t) - [k-1/k]_f(t)| \leqslant \frac{H_{k+1}^{(0)}}{H_k^{(0)}} | t^{2k} | \qquad \forall t \in (-\infty, 0],$$

$$| f(t) - [k-1/k]_f(t)| \leqslant \frac{H_{k+1}^{(0)}}{H_k^{(0)}} \frac{t^{2k}}{(1-td)^{2k+1}} \qquad \forall t \in [0, d], \quad d < R.$$

Remark 17. For such series composite quadrature formulas, such as the trapezoidal rule, can also be used to generate rational approximations.

3. Examples and Applications

Let us first give an example to show that Padé approximants are not always optimal. For this purpose we consider the series

$$f(t) = t^{-1} \operatorname{Log}(1+t) = 1 - \frac{t}{2} + \frac{t^2}{3} - \frac{t^3}{4} + \cdots.$$

For this series Theorem 10 applies and the sequence $[k-1/k]_f(t)$ converges to $f(t)$. Let us compare the relative errors of $[1/2]_f(t)$ and of the Padé-type approximant with $k = 4$ constructed from the interpolation points $x_i = -i^{-1}$ for $i = 1, 2, 3$, and 4. The construction of these two rational approximations requires the knowledge of $c_0, \ldots, c_3$.

t	[1/2]	(3/4)
−0.8	$-0.27\ 10^{-1}$	$0.29\ 10^{-1}$
−0.5	$-0.12\ 10^{-2}$	$0.73\ 10^{-3}$
0.1	$-0.46\ 10^{-6}$	$0.92\ 10^{-7}$
0.5	$-0.15\ 10^{-3}$	$0.56\ 10^{-5}$
1.0	$-0.12\ 10^{-2}$	$-0.13\ 10^{-3}$
1.5	$-0.35\ 10^{-2}$	$-0.77\ 10^{-3}$
2.0	$-0.70\ 10^{-2}$	$-0.21\ 10^{-2}$
4.0	$-0.27\ 10^{-1}$	$-0.14\ 10^{-1}$

$$\frac{\tilde{w}(t)}{\tilde{v}(t)} = \frac{24 + 38t + 18t^2 + 19t^3/6}{24 + 50t + 35t^2 + 10t^3 + t^4}$$

$$[1/2]_f(t) = \frac{6+3t}{6+6t+t^2}$$

Some other choices of the points x_i have been made for Padé-type approximants but they produce less good numerical results. A very important question for further research will be the study of optimal interpolation points.

Let us now turn to rational approximations to the exponential function. Because of the search for A-stable methods for integrating stiff differential equations such approximations have a great practical interest and many papers on this subject have appeared in the past few years. The fundamental notion is the A-acceptability [6] which states that a rational approximation r to e^{-t} is A-acceptable if $|r(t)| \leqslant 1 \; \forall t$, $\mathrm{Re}(t) \geqslant 0$. It can be shown, by using the maximum modulus theorem, that r is A-acceptable iff $|r(it)| \leqslant 1 \; \forall t \in \mathbb{R}$, $\lim_{|t|\to\infty} |r(t)| \leqslant 1$ and r is analytic in the right half part of the complex plane [1, 15].

If we construct rational approximations to e^{-t} by using Padé-type approximants as described in Section 2 with the degree of the denominator greater than the degree of the numerator and with the x_i in the left half part of the complex plane then the second and the third conditions for the A-acceptability are satisfied; it is, in general, difficult to know if the first condition is true or not. However the following result can be obtained:

THEOREM 11. *Let r be a Padé-type approximant to e^{-t} with real coefficients, whose numerator has degree k and whose denominator has degree $n + k$. Let*

$$|r(it)|^2 = \frac{1 + \beta_1 t^2 + \cdots + \beta_k r^{2k}}{1 + \alpha_1 t^2 + \cdots + \alpha_{n+k} t^{2(n+k)}}.$$

If the interpolating points x_i have negative real parts, if $\beta_i \leqslant \alpha_i$ for $i = p + 1,\ldots, k$ and $0 \leqslant \alpha_i$ for $i = k + 1,\ldots, n + k$, where p is the integer part of $k/2$, then r is A-acceptable.

Proof. It follows the ideas of [5]. Since the points x_i have negative real parts r is analytic in the right half part of the complex plane. If $n \geqslant 1$ then $\lim_{|t|\to\infty} |r(t)| = 0$.

We have, by definition

$$r(t) = e^{-t} + O(t^{k+1}).$$

Thus

$$|r(it)|^2 = 1 + O(t^{k+1}).$$

This last condition implies that $\alpha_i = \beta_i$ for $i = 1,\ldots, [k/2]$, where $[p]$ denotes the integer part of p. Moreover we get

$$|r(it)|^2 = 1 + \frac{(\beta_{p+1} - \alpha_{p+1})\, t^{2(p+1)} + \cdots + (\beta_{n+k} - \alpha_{n+k})\, t^{2(n+k)}}{1 + \alpha_1 t^2 + \cdots + \alpha_{n+k} t^{2(n+k)}}$$

with the convention that $\beta_i = 0$ for $i \geqslant k+1$. Thus if $\beta_i \leqslant \alpha_i$ for $i = p+1,..., n+k$ then $|r(it)|^2 \leqslant 1$.

Moreover if $n = 0$, $\beta_k = b_0^2$ and $\alpha_k = a_0^2$ which imply that $\lim_{|t|\to\infty} |r(t)| \leqslant 1$.

This theorem is related to Theorem 3.2 of Norsett [15]. It seems to be difficult in practice to know if this condition is satisfied or not for fixed n and for every k even by applying Norsett's results although the C-polynomial exists.

We are now going to study a very interesting class of Padé-type approximations to the exponential function. If, for fixed k, we choose $x_i = -k^{-1}$ for $i = 1,..., k$ then we obtain rational approximations of the form $\tilde{w}(t)/(1 + t/k)^k$ which are very useful for integrating a linear system of ordinary differential equations since the denominator can be factored. Such approximations have been recently studied by Saff, Schönhage, and Varga [17] but with a different numerator.

Let us first study the convergence of such approximations:

THEOREM 12. *When k goes to infinity $\tilde{w}(t)/(1 + t/k)^k$ converges to e^{-t} for every $t \geqslant 0$.*

Proof. We shall use the second part of Theorem 7 with $n = -1$. It is obvious that $B_i \geqslant 0$; thus we only have to prove that the B_i's tend to zero when k tends to infinity since the series converges for every $t \geqslant 0$. Since $B_i = a_i t^{k-i}/\tilde{v}(t)$ and since $\tilde{v}(t)$ tends to e^t we only have to study the convergence of $a_i t^{k-i}$ to zero. We get

$$\begin{aligned}\tilde{v}(t) &= 1 + t + \sum_{i=2}^{k} \left(1 - \frac{1}{k}\right) \cdots \left(1 - \frac{i-1}{k}\right) \frac{t^i}{i!}\\ &= a_k + a_{k-1}t + \cdots + a_0 t^k.\end{aligned}$$

Thus

$$a_i = \left(1 - \frac{1}{k}\right) \cdots \left(1 - \frac{k-i-1}{k}\right) \frac{1}{(k-i)!}, \qquad i = 0, 1,..., k-2,$$

$$a_{k-1} = a_k = 1.$$

It must be notice that we have to study the convergence when k goes to infinity for a fixed subscript i. Thus

$$a_i t^{k-i} \leqslant \left(\frac{k-1}{k}\right)^{k-i-1} \frac{t^{k-i}}{(k-i)!}$$

and $\lim_{k\to\infty} a_i t^{k-i} = 0$ for $i = 0, 1,...$ and $\forall t \geqslant 0$ which ends the proof.

An interesting question about these approximations would be to study if the convergence has a geometric character like the approximations proposed in [17].

Let us now turn to the A-acceptability of these approximations. It seems difficult to know if these approximations are A-acceptable for every k. However, by applying Theorem 11, it is easy to see that the condition is satisfied for $k = 1, \dots, 4$. Thus, the following approximations to e^{-t} are A-acceptable:

$$\frac{1}{1+t}, \qquad \frac{1}{(1+t/2)^2}, \qquad \frac{1-t^2/6}{(1+t/3)^3}, \qquad \frac{1-t^2/8+t^3/48}{(1+t/4)^4}.$$

The same is true for the diagonal Padé-type approximants

$$\frac{1}{1+t}, \qquad \frac{1-t^2/4}{(1+t/2)^2} = \frac{1-t/2}{1+t/2} = [1/1]_f(t), \qquad \frac{1-t^2/6+t^3/27}{(1+t/3)^3}.$$

The following approximant is $(1 - t^2/8 + t^3/48 + t^4/256)/(1 + t/4)^4$. We get

$$|r(it)|^2 = 1 + \frac{t^6}{2304\,|\tilde{v}(it)|^2}$$

which shows that this approximant is not A-acceptable. The approximants given in [7] are not A-acceptable for $k = 2, \dots, 7$ because the constant term of the numerator is greater than 1.

Let us now describe the application of rational approximations to the Laplace transform inversion. Let f be the Laplace transform of g

$$f(t) = \int_0^\infty g(x)\, e^{-xt}\, dx.$$

If the series expansion of f is known, then a method due to Longman [10] for finding g consists in constructing some Padé approximant to f and inverting it. The Laplace transform inversion of a rational function needs either the partial fraction decomposition (that is the computation of the roots of the denominator) or a special trick due to Longman and Sharir [12] involving the summation of an infinite series.

The same can be done with Padé-type approximants instead of Padé approximants. The advantage will be the knowledge as well as the arbitrary choice of the poles. If the interpolating points are distinct, for example, then, as we saw in Theorem 1

$$\frac{\tilde{w}(t)}{\tilde{v}(t)} = \sum_{i=1}^{k} \frac{A_i^{(k)}}{1 - x_i t} = -\sum_{i=1}^{k} \frac{A_i^{(k)} x_i^{-1}}{t - x_i^{-1}} \qquad \text{with} \qquad A_i^{(k)} = w(x_i)/v'(x_i).$$

Thus the Laplace transform inversion of $\tilde{w}(t)/\tilde{v}(t)$ will immediately provide an approximation of g given by $-\sum_{i=1}^{k} A_i^{(k)} x_i^{-1} e^{x/x_i}$.

Let us show, by example, how this method works. If $tf(t) = e^{-t}$ then $g(x) = H(x - 1)$. We shall construct approximations to $tf(t)$ with the same degree k in the numerator and in the denominator, then we shall divide by t and finally invert.

We shall compare the Padé-type approximant for $k = 2$ with $x_1 = -1$, $x_2 = -1/3$ (formula 1), the Padé-type approximant with $x_1 = -1/4$, $x_2 = -1/3$ (formula 2) and the Padé approximant [1/1] (formula 3). We get

$$\text{formula 1:} \quad 1 - \tfrac{1}{4}e^{-x} - \tfrac{9}{4}e^{-3x},$$
$$\text{formula 2:} \quad 1 + 8e^{-4x} - 9e^{-3x},$$
$$\text{formula 3:} \quad 1 - 2e^{-2x}.$$

x	formula 1	formula 2	formula 3
0	−1.5	0.	−1.
0.5	0.3463	0.0745	0.2642
1.0	0.7960	0.6984	0.7293
1.5	0.9192	0.9198	0.9004
2.0	0.9606	0.9804	0.9634
2.5	0.9782	0.9954	0.9865

Let now $tf(t) = \exp(-t/(1 + at)^{1/2})$. If we invert the Padé-type approximant with $k = 2$, $x_1 = -1/4$ and $x_2 = -1/3$ we obtain, for $a = 0.1$

$$1 + 10.4e^{-4x} - 10.8e^{-3x}.$$

The numerical results can be compare with the method of Longman using Padé approximants [11]

x	(2/2)	Padé [2/2]	exact values
0	0.6	−0.8182	0
0.5	−0.0023	0.2675	0.0274
1.0	0.6528	0.7049	0.5475
1.5	0.9058	0.8811	0.9290
2.0	0.9767	0.9521	0.9944
2.5	0.9945	0.9807	0.9997

The results obtained by a Padé-type approximant using c_0, c_1, and c_2 are better than those obtained with a Padé approximant using $c_0, \ldots, c_4$.

4. Conclusions

In this paper a systematic way for obtaining rational approximations to formal power series has been studied. Many aspects of the problem have not been treated and numerous questions have no answer at the present time. For example, the algorithmic part has not been developed, the algebraic properties of the approximants remain to be studied as well as the existence of best interpolation points, etc. Approximatory quadrature methods should be similarly studied.

Some generalizations are of interest, the most important of which seems to be formal power series in several variables.

Note added in proofs. Recently many authors independently used special cases of Padé type approximants. They are: S. A. Gustafson, *Computing.* **21** (1978), 53–70; A. Iserles, *SIAM J. Num. Anal.* (to appear); E. V. Krishnamurthy *et al.*, *Proc. Indian Acad. Sci.* **819** (1975), 58–79; G. Lopes, *Soviet Math. Dokl.* **19** (1978), 425–428; S. P. Norsett, *Numer. Math.* **25** (1975), 39–56; A. Sidi, *Math. Comp.* (to appear); A. C. Smith, *Utilitas Math.* **13** (1978), 249–269.

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