BULL. AUSTRAL. MATH. SOC. VOL. II (1974), 63-69.

Padé approximation and gaussian quadrature

G.D. Allen, C.K. Chui, W.R. Madych, F.J. Narcowich, and P.W. Smith

For certain types of formal power series, including the series of Stieltjes, we prove that the [n, n+j], $j \ge -1$, Padé approximants coincide with certain gaussian quadrature formulae and hence, convergence of these approximants follows immediately.

1. Introduction

In recent years the subject of Padé approximation of formal power series has aroused great interest among physicists as a tool for approximation and summability. One of the advantages of the method is that it seems to give good approximations to poorly behaved functions (which frequently occur in Physics). Another advantage is that it is calculable. For these reasons, this subject has also interested many mathematicians; namely, Franzen [5], Gragg [6], Pommerenke [8], Wallin [11], and others.

Our attention in this note is directed toward Stieltjes and other related series. Stieltjes series include many divergent perturbation series arising in quantum physics (for example, see [7]). These series were first investigated in relation to analytic continued fractions by T.J. Stieltjes and the study of Padé approximants was first undertaken by G. Frobenius.

Received 29 March 1974.

In our previous papers [1], [3], we investigated these series using systems of orthogonal polynomials and consequently derived a method of computation for the Padé approximants which is conceptually simple and numerically effective. The main contribution there is the variational approach to this subject which gives explicit formulas and error estimates.

In this note we observe that, in fact, the [n, n-1] Padé approximant of a formal power series arising from an integral of the form

(1.1)
$$f(z) = \int_{-\infty}^{\infty} \frac{d\psi(t)}{1-zt} ,$$

(where $d\psi(t)$ belongs to a class of not necessarily positive measures) and the gaussian quadratures of an integral related to (1.1) are identical! Therefore, convergence of the [n, n-1] approximants, and hence, by a simple transformation (*cf.* [3]) the [n, n+j], $j \ge -1$, approximants, to f is immediate. To the best of our knowledge, aside from our previous papers mentioned above, the only other proof of convergence is quite long and difficult, and convergence to f(z) is not obtained (see Baker [4]).

2. Pade approximation and gaussian quadrature

The Padé approximant is defined for an arbitrary formal power series,

(2.1)
$$f(z) = a_0 + a_1 z + a_2 z^2 + \dots,$$

as in [2]. (See also Wall [10].) That is, let

$$Q(z) = q_0 + q_1 z + q_2 z^2 + \dots + q_n z^n$$
,

and

$$P(z) = p_0 + p_1 z + \dots + p_m z^m$$

be polynomials of degrees no greater than n and m respectively. We wish to determine the constants q_0, \ldots, q_n and p_0, \ldots, p_m so that the resulting formal power series satisfies

$$f(z)Q(z) - P(z) = d_{m+n+1}z^{m+n+1} + \dots$$

This requires that the constants p_i and q_i satisfy

$$\sum_{j=0}^{l} a_{l-j}q_{j} - p_{l} = 0 , \quad l = 0, 1, \dots, m ,$$

$$\sum_{j=0}^{n} a_{l-j}q_{j} = 0 , \quad l = m+1, \dots, m+n ,$$

where we set $a_j = 0$ for j < 0. A rank argument shows that this system always has nontrivial solutions. Then [n, m](z) = P(z)/Q(z) is called the [n, m] Padé approximant to the formal series f(z) in (2.1). For details, together with the complete structure of all the Padé approximants, we refer the reader to [2]. Note that if $q_0 \neq 0$, then this definition is equivalent to the condition $f(z) - P(z)/Q(z) = c_1 z^{m+n+1} + c_2 z^{m+n+2} + \dots$

A Stieltjes series is a formal power series $a_0 + a_1 z + \dots$ generated by the integral

(2.2)
$$f(z) = \int_0^\infty \frac{d\phi(t)}{1-zt} ,$$

where $d\phi$ is a positive measure with an infinite support and the coefficients a_0, a_1, \ldots are the moments of the positive measure $d\phi$:

$$a_{j} = \int_{0}^{\infty} t^{j} d\phi(t)$$
, $j = 0, 1, ...$

Let $\{L_n(t)\}$ be the orthonormal set of polynomials with positive leading coefficients generated by the measure $d\phi$.

THEOREM 1. The [n, n-1] Padé approximant of the Stieltjes series $a_0 + a_1 z + \dots$ of

$$f(z) = \int_0^\infty \frac{1}{1-zt} \, d\varphi(t)$$

is given by the gaussian quadrature

$$Q_n\left(\frac{1}{1-zt}\right) = \sum_{j=1}^n \frac{\alpha_{n,j}}{1-zx_{n,j}} ,$$

where

(i) the x_{n,j}, j = 1, ..., n, are the zeros of L_n(t), and
(ii) the a_{n,j}, j = 1, ..., n, are the corresponding gaussian weights.

Proof. We note that

$$\frac{1}{1-zt} = 1 + zt + z^2t^2 + \ldots + z^{2n-1}t^{2n-1} + \frac{z^{2n}t^{2n}}{1-zt} .$$

It is known (cf. [9]) that $Q_n(t^j) = \int_0^\infty t^j d\phi(t) = a_j$, j = 0, ..., 2n-1. Hence, by the linearity of Q_n , we have

$$\begin{aligned} Q_n \bigg(\frac{1}{1-zt} \bigg) &= Q_n \big(1 + zt + \dots + z^{2n-1} t^{2n-1} \big) + Q_n \bigg(\frac{z^{2n} t^{2n}}{1-zt} \bigg) \\ &= \sum_{j=0}^{2n-1} a_j z^j + z^{2n} Q_n \bigg(\frac{t^{2n}}{1-zt} \bigg) \end{aligned}$$

As $z \rightarrow 0$, we see that

(2.4)
$$Q_n\left(\frac{1}{1-zt}\right) = \sum_{j=0}^{2n-1} a_j z^j + O(z^{2n}) .$$

Thus, this quadrature agrees with the formal powers up to the (2n-1)th term. Clearly, the formula (2.3) is a rational function with numerator and denominator of degrees n - 1 and n respectively, and the denominator does not vanish at the origin. Combining this fact with (2.4), we see that (2.3) is the [n, n-1] Padé approximant to the Stieltjes series of f. This completes the proof of the theorem.

Suppose now that we take for our domain of integration the whole real line, R, and that the positive measure $d\phi$ has infinite support and satisfies

(2.4)
$$\int_{R} t^{2k+1} d\phi = 0 , k = 0, 1, \dots$$

With these conditions, we have the following

COROLLARY. The [2n, 2n-1] Padé approximant of the formal power

series generated by $\int_R \frac{td\phi}{1-zt}$ is given by

(2.5)
$$Q_{2n+1}\left(\frac{t}{1-zt}\right) = \sum_{k=0}^{2n+1} \frac{\alpha_{2n+1,k}x_{2n+1,k}}{1-zx_{2n+1,k}}$$

where

- (i) the $x_{2n+1,k}$, k = 1, ..., 2n+1 are the zeros of the orthogonal polynomial L_{2n+1} (constructed with respect to $d\phi$), and
- (ii) the $\alpha_{2n+1,k}$, k = 1, ..., 2n+1, are the corresponding gaussian weights.

Furthermore, [2n+1, 2n](z) = [2n, 2n-1](z).

Proof. Note that the condition (2.4) implies that L_{2n+1} is an odd function, which in turn implies that one of the $x_{2n+1,j}$'s is zero. Thus (2.5) is in fact a rational function with numerator and denominator of degrees 2n - 1 and 2n respectively. The rest of the proof is identical to that of Theorem 1.

Finally, the relation [2n+1, 2n](z) = [2n, 2n-1](z) follows from the block structure of the Padé table (cf. [2]) and the fact that

$$f(z) - [2n, 2n-1](z) = O(z^{4n+1})$$
.

REMARKS. If $d\phi$ satisfies (2.4) and has compact support, then we can easily conclude, by taking the Fourier transform, that $d\phi$ is even, (that

is, if
$$a > b > 0$$
 then $\int_{-a}^{-b} d\phi = \int_{a}^{b} d\phi$).

3. Final remarks

It seems evident that underlying this theory there is a more general quadrature concept. Suppose that a measure $d\phi$ is given, which is not necessarily positive, and that there is a quadrature formula Q_n which is exact for polynomials of degree no greater than 2n - 1. That is,

$$Q_n(f) = \sum_{j=1}^n \alpha_{n,j} f(x_{n,j}) \doteq \int_R f(t) d\phi(t)$$

with

$$Q_n(t^j) = \int_R t^j d\phi(t) , \quad j = 0, \dots, 2n-1$$

Then it is easy to see that

$$Q_n\left(\frac{1}{1-zt}\right) = [n, n-1](z)$$

where [n, n-1](z) is the [n, n-1] Padé approximant to the formal power series generated by

$$\int_{R} \frac{d\phi(t)}{1-zt}$$

References

- [1] G.D. Allen, C.K. Chui, W.R. Madych, F.J. Narcowich, and P.W. Smith, "Padé approximants and orthogonal polynomials", Bull. Austral. Math. Soc. 10 (1974), 263-270.
- [2] G.D. Allen, C.K. Chui, W.R. Madych, F.J. Narcowich, and P.W. Smith,"On the structure of the Padé table", submitted.
- [3] G.D. Allen, C.K. Chui, W.R. Madych, F.J. Narcowich, and P.W. Smith, "Padé approximation of Stieltjes series", submitted.
- [4] George A. Baker, Jr, "The theory and application of the Padé approximant method", Advances in Theoretical Physics 1 (1965), 1-58.
- [5] N.R. Franzen, "Convergence of Padé approximants for a certain class of meromorphic functions", J. Approximation Theory 6 (1972), 264-271.
- [6] W.B. Gragg, "The Padé table and its relation to certain algorithms of numerical analysis", SIAM Rev. 14 (1972), 1-62.

- [7] J.J. Loeffel, A. Martin, and B. Simon and A.S. Wightman, "Padé approximants and the anharmonic oscillator", *Phys. Lett.* 30B (1969), 656-658.
- [8] Ch. Pommerenke, "Padé approximants and convergence in capacity", J. Math. Anal. Appl. 41 (1973), 775-780.
- [9] A.H. Stroud, Don Secrest, Gaussian quadrature formulae (Prentice-Hall, Englewood Cliffs, New Jersey, 1966).
- [10] H.S. Wall, Analytic theory of continued fractions (Van Nostrand, New York, Toronto, London, 1948).
- [11] H. Wallin, "The convergence of Padé approximants and the size of the power series coefficients", Applicable Anal. (to appear).

Department of Mathematics, Texas A&M University, College Station, Texas, USA.