RATIONAL APPROXIMANTS GENERATED BY PADE APPROXIMATION AND u-TRANSFORM

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This work is dedicated to **my parents**

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Abstract

The importance of summation of series lies in the abundance of their occurrence and their utility in all branches of applied mathematics. The usual approach for summation is to approximate it by some rational approximant. There are many methods for numerical computation of the rational approximants for the series. Almost all of them directly or indirectly use Pade approximants and u-transformation which are very simple, elegant as well as efficient routines. We studied convergence rates of the series by these methods. We have observed that u-transform is more accelerating in convergence than the other methods. We have chosen some representative positive and alternating series whose exact results are known and using the methods of Pade and u-approximation we have evaluated the corresponding approximants. Lastly we compared these calculated approximants with each other and with the exact/partial sum of the series. In order to put our observations on strong footings theoretical investigation on error estimation and error control of these approximants is required.

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Chapter 1

Introduction

There are many methods for accelerating the convergence of sequences and the subsequent evaluation of the limit of an infinite sequence (Ford and Sidi [1987]; Smith and Ford [1977, 1982]). These methods generally employ specific sequence-to-sequence transformations and belong, accordingly, to two broad classes; linear and non-linear. In a comparative study of a number of these methods, Smith and Ford [1977] have concluded that nonlinear methods are more general in scope than the linear ones. The nonlinear methods they have reviewed are all generalizations of Aitkenfs Δ^2(Aitken [1926]). A linear method may, however, be comparable in effectiveness in special circumstances, for example, when the parameters of the transformations are chosen suitably for specific sequences (Knopp [1951]), or when the method is exact on a certain class of sequences (Bauer [1965]). All methods rely on some scheme of suitably approximating an arbitrary sequence by another sequence that is more amenable to manipulation and whose nature, consequently, is incorporated into the method. Any method is able; therefore, to evaluate the limit of at least one class of sequences, most often the class whose terms are the successive partial sums of an infinite geometric series.

In their study Smith and Ford conclude that Levin′s u-transform (Levin [1973]) is " the best available across-the-board method " for accelerating the convergence of a very broad class of sequences. A particular sequence transform requires a finite number of terms of the sequence on which it is applied. This number is, therefore, a parameter of the transform. A given acceleration method refine its approximation procedure by progressively absorbing a greater number of terms of a sequence in the transform it employs. The number of significant digits in the final value increases, correspondingly, to a limit imposed by round-off errors and/or the effectiveness of the method. If the number of digits to which the evaluation of the limit is accurate in a given method decreases finally as more terms of a sequence are used, we call the method unstable. Levin's method is unstable, on this count, for positive series.

In all methods the accuracy of evaluation is usually checked against a known result or by noting the consistent appearance of certain number of digits. It would be more convenient if there existed an independent estimate of the error at each point of the calculation.

Accurate numerical evaluation of a function may often pose problems even if the function is known in closed form, as an integral or as a solution of a differential equation. Power series expansions are useful, but the question of convergence of such series is crucial. The series obtained may converge very slowly or may even turn out to be divergent or asymptotic. However, it is possible to ensure a uniform treatment in the efficient numerical evaluation of such widely different series by means of sequence transforms.

A sequence transform uses a finite number of terms of one sequence to generate each term of an auxiliary sequence. Such a primary sequence may be a sequence of numbers or a sequence of functions. The most widely used nonlinear sequence transforms are Aitkenfs Δ^2 -transform, Shankes' s e-transform, Wynn' s ϵ-transform and Levin ' s u-transform. A unified discussion of these transforms is found in ref. (Levin [1973]; Bender and Orszag [1985]; Ford and Sidi [1987]; Bhowmick et al. [1989]; Roy et al. [1992]). If the limit of the generated sequence is the same as that of the original sequence, the sequence transform is said to be regular.

It is well known that nonlinear sequence transforms are very effective accelerators of convergence on monotone and alternating sequences of numbers. Interestingly, they induce convergence in divergent sequences and hence are valid methods of summation.

When a nonlinear sequence transform is applied to the sequence of partial sums of a power series, it generates approximants in the form of rational functions. The representation of functions by rational approximants has been a major field of endeavor, especially for functions represented by divergent series expansions. Uses of the rational function representation of a function whose series expansion is known are too numerous to mention.

The Pade approximant has been used most frequently in tackling divergent series encountered in theoretical physics (Baker and Gammel [1970]), although the methods of Euler and Borel have also been used to some extent (Bender and Wu [1969]; Baker [1970]; Baker and Morris [1981]). It is well known that the nonlinear sequence transform ϵ is closely related to the Pade approximant. The superiority of the u-transform over the ϵ-transform in summing a wide class of convergent and divergent test sequences of numbers, both real and complex (Bhowmick et al. [1989]; Smith and Ford [1982]), lends encouragement to the conjecture that the former may also prove useful as a generator of rational approximants, at least for a certain class of power series. A recent comparison between the two methods made on a divergent perturbation series expansion for the excluded volume effect in the theory of polymer solutions extends support to this surmise (Bhowmick et al. [1989]; Bhattacharya et al. [1997]).

Almost any method of summation has a sequence transform at its core. A typical transform uses some finite sub-sequence of one sequence to generate each term of another. A divergent sequence may thereby be transformed into another with a non-infinite limit; the transform then produces a finite result and defines a method of summation. The method of Pade approximants in particular has been used extensively in the context of divergent series arising in physical theories, predominantly in the fields of cooperative phenomena and critical points (Baker and Gammel [1970]). The sequence transform $\epsilon_{2k}^{(n)}$ has been demonstrated to be closely related to the Pade table (Shanks [1995]). This transform, however, is only one within a family of nonlinear sequence transforms (Smith and Ford [1977]; Bhowmick et al. [1989]), the most promising member of which is believed to be the Levin u-transform (Levin [1973]). Where the power series coefficients are available for a function, as they are in the case of a perturbation expansion, these transforms effectively generate successive approximants in the form of rational polynomials (Schield [1961]; Bender and Wu [1969]; Sidi [1979]; Gerald [1980]).

Apart from the aspects mentioned above, the present work also extends the numerical precision of the work reported by Smith and Ford for both positive and alternating series (Weniger [1989]; Roy et al. [1992, 1996]).

This work is an outcome of investigations on how the u-approximants, i.e., the rational approximants obtained by applying the u-transform on power series, fare in comparison with Pade approximants for convergent and divergent series. The class of convergent series that we have worked on is as wide as that reported in Smith and Ford [1977].

The second chapter briefly touches on improvement of convergence, the Shanks transformation, summation of divergent series, Euler summation, Borel summation, Chebyshev polynomials etc. Chapter three introduces the method of Pade approximants, mostly for introducing the notation used in the rest of the work, the u-transform and the associated formulas for the generation of u-approximants. Chapter four is a comparative study of the u-approximants and Pade approximants on a number of test series. Finally in the conclusion we make some brief comments on the outcome of our research work.

Chapter 2

Review

In this chapter we briefly discuss mathematical preliminaries for study on improvement of convergence of a series with short mathematical examples

2.1 Improvement of Convergence

In this section we show how to speed up the convergence of slowly converging series. An example of such a series is $\sum_{k=0}^{\infty}(-z)^k$. Although this series converges for all $|z| < 1$, the convergence is very slow as z approaches the unit circle because the limit function $(1+z)^{-1}$ has a pole at $z = -1$. When z is near $+1$, the converges rate is affected by the distant pole at $z = -1$. The remainder R_n after n terms of the series is $(-z)^{n+1}/(1+z)$; R_n goes to zero as $n \to \infty$ for $|z| < 1$. Near $z = +1$ the remainder oscillates rapidly in sign (from odd to even n) and decays slowly. We will call such a term a transient because it resembles the transient behavior of a weakly damped harmonic oscillator, which undergoes many oscillations before coming to rest.

Another slowly converging series is the Taylor series for the function $A(z) = 1/[(z+1)(z+2)]$. The nth partial sum of this Taylor series is

$$\begin{aligned} A_n(z) &= \sum_{k=0}^{n}(-1)^k(1-\frac{1}{2^{k+1}})z^k \\ &= \frac{1}{(z+1)(z+1)} - \frac{(-z)^{n+1}}{z+1} + \frac{(-z/2)^{n+1}}{z+2} \end{aligned} \tag{2.1}$$

The poles of $A(z)$ at $z = -1$ and $z = -2$ affect the rate of convergence of $A_n(z)$ to $A(z)$. More than 1,500 terms of this series are necessary to evaluate $A(0.99)$ accurate to six decimal places. Yet the analytic structure of $A(z)$ is so simple that it would be very surprising if the first few terms did not contain enough information to compute $A(z)$ accurately. Indeed, there are several ways to accelerate the convergence of (2.1); one way is to perform a Shanks transformation.

2.1.1 The Shanks Transformation

A good way to improve the convergence rate of a sequence of partial sums (or of any sequence for that matter) is to eliminate its most pronounced transient behavior (i.e., to eliminate the term in the remainder which has the slowest decay to zero). Suppose the nth term in the sequence takes the form

$$A_n = A + \alpha q^n \tag{2.2}$$

with $|q| < 1$, so that $A_n \to A$ as $n \to \infty$. Here, the term αq^n is the transient. Since any member of this sequence depends on the three parameters A, α, and q, it follows that A can be determined from three terms of the sequence, say A_{n-1}, A_n, A_{n+1}: $A_{n-1} = A + \alpha q^{n-1}$, $A_n = A + \alpha q^n$, $A_{n+1} = A + \alpha q^{n+1}$. Solving this system of equations for A gives

$$A = \frac{A_{n+1}A_{n-1} - A_n^2}{A_{n+1} + A_{n-1} - 2A_n}$$

(If the denominator vanishes, then $A_n = A$ for all n.)

This formula is exact only if the sequence A_n has just one transient of the form in (2.2). Nontrivial sequences may have many transients, some of which oscillates in a very irregular fashion. Nevertheless, if the most pronounced has the form αq^n, $|q| < 1$, then the *nth* term in the sequence takes the form $A_n = A(n) + \alpha q^n$, where for large n, $A(n)$ is more slowly varying function of n than A_n. Let us suppose that $A(n)$ varies sufficiently slowly so that $A(n-1)$, $A(n)$ and $A(n+1)$ are all approximately equal. Then the above discussion motivates the nonlinear transformation,

$$S(A_n) = \frac{A_{n+1}A_{n-1} - A_n^2}{A_{n+1} + A_{n-1} - 2A_n}, \tag{2.3}$$

investigated in depth by Shanks. This transformation creates a new sequence $S(A_n)$ which often converges more rapidly than the old sequence A_n, even if the old sequence has more than one transient. The sequences $S^2(A_n) = S[S(A_N)]$, $S^3(A_n) = S\{S[S(A_N)]\}$, and so on, may be even more rapidly convergent.

2.2 Summation of Divergent Series

Perturbation methods commonly yield divergent series. A regular perturbation series converges only for those values of $|\epsilon|$ less than the radius of convergence. A singular perturbation series diverges for all values of $\epsilon \neq 0$, and even if the series is asymptotic, the value of ϵ may be too large to obtain much useful information.

It is discouraging to discover that a perturbation series diverges, especially if the terms in the series have been painstakingly computed. Clearly a naive summation of a divergent series by simply adding up the first N terms is silly because it gives a partial sum which gets further from the actual " sum " of the series as $N \to \infty$. By comparison, the indirect summation methods we shall introduce here again require as input the first N terms in the series, but the output is an approximant which converges the " sum " of the series as $N \to \infty$.

Thus, whenever summation methods apply, they provide the reward for investing one 's time in perturbative calculations; even if the perturbation series diverges and whatever the size of ϵ, the more terms one computes, the closer one can approximate the exact answer. Our purpose here is merely to induce the proper frame of mind by showing that there are special kinds of divergent series whose sums can actually be defined.

2.2.1 Euler Summation

If a series $\sum_{n=0}^{\infty} a_n$ is algebraically divergent (the terms blow up like some power of n), then the series

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \tag{2.4}$$

converges for all $|x| < 1$. The Euler sum S of $\sum_{n=0}^{\infty} a_n$ is defined as $S \equiv lim_{x \to 1^-} f(x)$ whenever the limit exists.

2.2.2 Borel Summation

If the coefficients a_n in the series $\sum_{n=0}^{\infty} a_n$ grow faster than a power of n [$a_n \sim 2^n$ or $a_n \sim (n!)^{1/2}$, for example], then Euler summation is not applicable because $\sum_{n=0}^{\infty} a_n x^n$ diverges for x near 1. However, this power series may still have meaning as an asymptotic series.

Suppose

$$\phi(x) = \sum_{n=0}^{\infty} \frac{a_n x^n}{n!} \tag{2.5}$$

converges for sufficiently small x and that

$$B(x) \equiv \int_0^{\infty} e^{-t} \phi(xt) dt \tag{2.6}$$

exists. If we expand the integral $B(x) = \int_0^{\infty} e^{-t/x} \phi(t) dt/x$ for small x by substituting the series (2.5) and integrating term by term [this is justified by Watsonfs lemma in Bender and Orszag [1985], then

$$B(x) \sim \sum_{n=0}^{\infty} \frac{a_n}{n!} \int_0^{\infty} e^{-t/x} t^n \frac{dt}{x} = \sum_{n=0}^{\infty} a_n x^n, x \to 0^+ \tag{2.7}$$

By construction, the series in (2.7) is asymptotic to $B(x)$ as $x \to 0^+$.

The asymptotic series diverges, but since the function $B(x)$ exists it makes sense to $define$ the Borel sum of $\sum_{n=0}^{\infty} a_n x^n$ as $B(x)$ and in particular to define the sum of $\sum_{n=0}^{\infty} a_n$ as $B(1)$.

Example: *Borel summation. The series* $\sum_{n=0}^{\infty} (-1)^n n!$ *diverges but* $\phi(x) = \sum_{n=0}^{\infty} (-x)^n$ *converges for* $|x| \leq 1$ *to* $(1+x)^{-1}$. *Thus, the Borel sum of* $\sum_{n=0}^{\infty} (-x)^n n!$ *is* $B(x) = \int_0^{\infty} [e^{-t}/(1+xt)] dt$ *and the Borel sum of* $\sum_{n=0}^{\infty} (-1)^n n!$ *is* $B(1) = \int_0^{\infty} [e^{-t}/(1+t)] dt$.

2.2.3 Generalized Borel Summation

Generalized Borel summation is an iterated version of Borel summation. The series $\sum_{n=0}^{\infty} a_n$ is generalized Borel summable if

$$\phi(x) = \sum_{n=0}^{\infty} \frac{a_n}{(n!)^k} x^n \tag{2.8}$$

converges for sufficiently small x and for some positive integer k. Then, when the multiple integral converges, we define the generalized Borel sum of $\sum_{n=0}^{\infty} a_n x^n$ to be

$$B(x) \equiv \int_0^{\infty} \cdots \int_0^{\infty} dt_1 dt_2 \cdots dt_k e^{-t_1-t_2-\cdots-t_k} \phi(xt_1t_2\cdots t_k), \tag{2.9}$$

and, in particular, the sum $\sum_0^{\infty} a_n$ to be $B(1)$.

2.3 Chebyshev Polynomials

We turn now to the problem of representing a function with minimum error. This is a central problem in the software development of digital computers because it is more economical to compute the values of the common functions using an efficient approximation than to store a table of values and employ interpolation techniques. Since digital computers are essentially only the arithmetic devices, the most elaborate function they can compute is a rational function, a ratio of polynomials. We will hence restrict our discussion to representation of functions by polynomials or rational functions.

One way to approximate a function by a polynomial is to use a truncated Taylor series. This is not the best way, in most cases. In order to study better ways, we need to introduce the Chebyshev polynomials.

The familiar Taylor-series expansion represents the function with very small error near the point of expansion, but the error increases rapidly (proportional to a power) as we employ it at points further away. In a digital computer, we have no control over where in an interval the approximation will be based, so the Taylor series is not usually appropriate. We would prefer to trade some its excessive precision at the centre of the interval to reduce the errors at the ends.

We can do this while still expressing functions as polynomials by the use of Chebyshev polynomials. The first few of these are:

$$
\begin{aligned}
T_0(x) &= 1, \\
T_1(x) &= x, \\
T_2(x) &= 2x^2 - 1, \\
T_3(x) &= 4x^3 - 3x, \\
T_4(x) &= 8x^4 - 8x^2 + 1, \\
T_5(x) &= 16x^5 - 20x^3 + 5x, \\
T_6(x) &= 32x^6 - 48x^4 + 18x^2 - 1, \\
T_7(x) &= 64x^7 - 112x^5 + 56x^3 - 7x, \\
T_8(x) &= 128x^8 - 256x^6 + 160x^4 - 32x^2 + 1, \\
T_9(x) &= 256x^9 - 576x^7 + 432x^5 - 120x^3 + 9x, \\
T_{10}(x) &= 512x^{10} - 1280x^8 + 1120x^6 - 400x^4 + 50x^2 - 1,
\end{aligned} \tag{2.10}
$$

The number of this series of polynomials can be generated from the two-term recursion formula

$$
T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad T_0(x) = 1, \quad T_1(x) = x \tag{2.11}
$$

2.4 Approximation of Functions with Economized Power Series

We are now ready to use Chebyshev polynomials to "economize" a power series. Consider the Maclaurin series for e^x:

$$
e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \frac{x^5}{120} + \frac{x^6}{720} \cdots
$$

If we would like to use a truncated series to approximated e^x on the interval $[0, 1]$ with a precision of 0.001, we will have to retain terms through that in x^6, since the error after the term in x^5 will be more than $1/720$. Suppose we subtract

$$
\left(\frac{1}{720}\right)\left(\frac{T_6}{32}\right)
$$

from the truncated series. We note from Eq. (2.9) that this will exactly cancel the x^6 term and at the same time make adjustments in other coefficients of the Maclaurin series. Since the maximum value of T_6 on the interval $[0, 1]$ is unity, this will change the sum of the truncated series by only

$$\frac{1}{720} . \frac{1}{32} < 0.00005$$

which is small with respect to our required precision of 0.001. Performing the calculations, we have

$$\begin{aligned} e^x &= 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \frac{x^5}{120} + \frac{x^6}{720} - \frac{1}{720}\left(\frac{1}{32}\right)\left(32x^6 - 48x^4 + 18x^2 - 1\right) \\ &= 1.000043 + x + 0.499219x^2 + \frac{x^3}{6} + 0.043750x^4 + \frac{x^5}{120} \end{aligned} \tag{2.12}$$

This gives a fifth-degree polynomial that approximates e^x on $[0, 1]$ almost as well as the sixth degree one derived from the Maclaurin series. (The actual maximum error of the fifth-degree expression is 0.000270; for the sixth-degree expression it is 0.000226). We hence have "economized" the power series in that we get nearly the same precision with fewer terms.

In the next section we discuss some methods which are available for approximation other than u-transform in [Bhowmick et al. [1989]].

2.5 The Δ^2 transform

This is derived by approximating the remainder after the nth partial sum of a series whose first term is a_{n+1} and common ratio is ρ_{n+1}. Thus, we have

$$\begin{aligned} S &= S_n + g_n \Delta S_n \\ &= S_n + \frac{a_{n+1}}{1 - a_{n+2}/a_{n+1}} \end{aligned}$$

i.e.

$$S = S_n - (\Delta S_n)^2 / \Delta^2 S_n \tag{2.13}$$

Clearly the Δ^2 transform sums a geometric series exactly.

Alternatively, this transform can be obtained by demanding in

$$S = S_n + g_n \Delta S_n \tag{2.14}$$

that

$$\Delta g_n = \Delta((S - S_n)/\Delta S_n) = 0 \tag{2.15}$$

We should really write g_{1n} for g_n and T_{1n} for S in the above relations. here, and subsequently, we write g_n for its approximation g_{kn} to simplify the notation.

From equation (2.15), then, g_n is a constant (c, say) and the relation (2.15) is equivalent to a relation on $\{S_n\}$ given by

$$S_{n+2} + c_1 S_{n+1} + c_0 S_n = 0,$$

where c_1 and c_0 are simply related to c, with

$$1 + c_1 + c_0 = 0$$

The method, therefore, is exact if $\{S_n\}$ satisfy a homogeneous linear difference equation of the second order with constant coefficients. It is well known that the partial sums of a geometric series satisfy such a relation. Hence this is another way of saying that the Δ^2 transform uses the geometric series as a template for the remainder.

2.5.1 The ϵ transform

We can write the Δ^2 transform which follows from (2.14) and (2.15) as

$$T_{1n} = \frac{\Delta(S_n/\Delta S_n)}{\Delta(1/\Delta S_n)}$$

Now, $\Delta(S_n/\Delta S_n) = S_{n+1}\Delta(1/\Delta S_n) + 1$.

Hence,

$$T_{1n} = S_{n+1} + 1/\Delta(1/\Delta S_n). \tag{2.16}$$

Introduce here the variables

$$\begin{aligned} \epsilon_0^{(n)} &= S_n, \\ \epsilon_1^{(n)} &= 1/\Delta S_n = 1/\Delta\epsilon_0^{(n)}, \\ \epsilon_{-1}^{(n)} &= 0, \quad \epsilon_2^{(n)} = T_{1n} \end{aligned}$$

Then we have

$$\epsilon_1^{(n)} = \epsilon_{-1}^{(n+1)} + 1/\Delta\epsilon_0^{(n)},$$

and from Eq. (2.16)

$$\epsilon_2^{(n)} = \epsilon_0^{(n+1)} + 1/\Delta\epsilon_1^{(n)},$$

This can be generalized as

$$\epsilon_{k+1}^{(n)} = \epsilon_{k-1}^{(n+1)} + 1/\Delta\epsilon_k^{(n)}, \quad k = 0, 1, ...,$$

Collected together, the transform

$$\begin{aligned}
\epsilon_1^{(n)} &= 0, \quad \epsilon_0^{(n)} = S_n, \\
\epsilon_{k+1}^{(n)} &= \epsilon_{k-1}^{(n+1)} + 1/\Delta\epsilon_k^{(n)}, \quad k = 0, 1, ...,
\end{aligned} \tag{2.17}$$

is called the ϵ transform.

2.5.2 The θ transform

In order to proceed with the generalization of the Δ^2 transform, we may now demand instead of (2.15) that

$$\Delta^2 g_n = 0 \tag{2.18}$$

using Eq. (2.18) in (2.14) we get

$$T_{2n} = \frac{\Delta^2(S_n/\Delta S_n)}{\Delta^2(1/\Delta S_n)} \tag{2.19}$$

Now

$$\Delta^2(S_n/\Delta S_n) = \Delta\{S_{n+1}\Delta(1/\Delta S_n)\}$$

Therefore, if we define

$$\begin{aligned}
\theta_{-1}^{(n)} &= 0, \quad \theta_0^{(n)} = S_n, \\
\theta_1^{(n)} &= 1/\Delta S_n = 1/\Delta\theta_0^{(n)}, \quad \theta_2^{(n)} = T_{2n}
\end{aligned}$$

we have from Eq. (2.19)

$$
\begin{aligned}
\theta_1^{(n)} &= \theta_{-1}^{n+1} + 1/\Delta\theta_0^{(n)}, \\
\theta_2^{(n)} &= \Delta(\theta_0^{n+1}\Delta\theta_1^{(n)})/\Delta^2\theta_1^{(n)}
\end{aligned}
$$

The above two relations can be generalized as

$$
\begin{aligned}
\theta_{2k+1}^{(n)} &= \theta_{2k-1}^{(n+1)} + 1/\Delta\theta_{2k}^{(n)}, \\
\theta_{2k+2}^{(n)} &= \Delta(\theta_{2k}^{(n+1)}\Delta\theta_{2k+1}^{(n)})/\Delta^2\theta_{2k+1}^{(n)} \\
&= \theta_{2k+1}^{(n)} + \frac{\Delta\theta_{2k}^{(n+1)}\Delta\theta_{2k+1}^{(n+1)}}{\Delta^2\theta_{2k+1}^{(n)}}
\end{aligned}
\tag{2.20}
$$

This is the θ transform of Brenziski [1971]. Here also only the even order transforms are meaningful.

However, in our investigation we will concentrate our attention only on the Pade and u-approximation and work then out in details. This is the object of the next chapter.

Chapter 3

Method of Pade and u-Approximation

We have seen that expansion of a function in terms of Chebyshev polynomials gives a power-series expansion that is much more efficient on the interval (-1, 1) than the Maclaurin expansion. In this application, we measure efficiency by the computer time required to evaluate the function, plus some consideration of storage requirements for the constants. Since the arithmetic operations of a computer can directly evaluate only polynomials, we limit our discussion on more efficient approximations to rational functions, which are the ratios of two polynomials.

3.1 Approximation with Rational Functions

Our discussion of methods of finding efficient rational approximations will be elementary and introductory only. Obtaining truly best approximations is a difficult subject. In this present stage of development it is as much art as science, and requires successive approximations form a "suitably close" intial approximation. Our study will serve to introduce some of the ideas and procedures used.

We start with a discussion of Pade approximations. Suppose we wish to represent a function as the quotient of two polynomials:

$$f(x) = R_N(x) = \frac{a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n}{b_0 + b_1 x + b_2 x^2 + \cdots + b_m x^m}, N = n + m.$$

The constant term in the denominator can be taken as unity without loss of generality, since we can always convert to this form by dividing numerator and denominator by b_0. The constant b_0 will generally not be zero, for, in that case, the fraction would be undefined at $x = 0$. The most useful of the Pade approximations are those with the degree of numerator equal to, or one greater than, the degree of the denominator. Note that the number of constants in $R_N(x)$ is $N + 1 = n + m + 1$.

The Pade approximations are related to Maclaurin expansions in that the coefficients are determined in a similar fashion to make $f(x)$ and $R_N(x)$ agree at $x = 0$ and also to make the first N derivatives agree at $x = 0$.

We begin with Maclaurin series for $f(x)$ (we use only terms through x^N) and write

$$f(x) - R_N(x) \quad = \quad (c_0 + c_1x + c_2x^2 + \cdots + c_Nx^N) - \frac{a_0 + a_1x + \cdots + a_nx^n}{b_0 + b_1x + \cdots + b_mx^m} \tag{3.1}$$

The coefficient c_i are $f^{(i)}(0)/(i!)$ of the Maclaurin expansion. Now if $f(x) = R_N(x)$ at $x = 0$, the numerator of Eq. (3.1) must have no constant term. Hence

$$c_0 - a_0 = 0 \tag{3.2}$$

In order for the first N derivatives of $f(x)$ and $R_N(x)$ to be equal at $x = 0$, the coefficients of the power of x up to and including x^N in the numerator must all be zero also. This gives N additional equations for the $a's$ and $b's$. The first

n of these involves $a's$, the rest only $b's$ and $c's$:

$$\begin{aligned}
b_1 + c_1 - a_1 &= 0, \\
b_2c_0 + b_1c_1 + c_2 - a_2 &= 0, \\
b_3c_0 + b_2c_1 + b_1c_2 + c_3 - a_3 &= 0, \\
&\vdots \\
b_mc_{n-m} + b_{m-1}c_{n-m+1} + \cdots + c_n - a_n &= 0, \\
b_mc_{n-m+1} + b_{m-1}c_{n-m+2} + \cdots + c_{n+1} &= 0, \\
b_mc_{n-m+2} + b_{m-1}c_{n-m+3} + \cdots + c_{n+2} &= 0, \\
&\vdots \\
b_mc_{N-m} + b_{m-1}c_{N-m+1} + \cdots + c_N &= 0,
\end{aligned} \tag{3.3}$$

Note that, in each equation, the sum of the subscripts on the factors of each product is the same, and is equal to the exponent of the x-term in the numerator. The $N+1$ equations of Eqs. (3.2) and (3.4) give the required coefficients of the Pade approximation. We illustrate this by an example.

Example: Find the rational approximants of $arctanx$ for $N = 9$. Use in the numerator a polynomial of degree five.

The maclaurin series through x^9 is

$$arctanx = x - \frac{1}{3}x^3 + \frac{1}{5}x^5 - \frac{1}{7}x^7 + \frac{1}{9}x^9 \tag{3.4}$$

We form, analogously to Eq. (3.1),

$$f(x) - R_9(x) \quad = \quad (x - \frac{1}{3}x^3 + \frac{1}{5}x^5 - \frac{1}{7}x^7 + \frac{1}{9}x^9) - \frac{a_0 + a_1x + \cdots + a_5x^5}{b_0 + b_1x + \cdots + b_4x^4} \tag{3.5}$$

Making coefficients through that of x^9 in the numerator equal to zero, we get

$$\begin{aligned}
a_0 &= 0, \\
a_1 &= 1, \\
a_2 &= b_1, \\
a_3 &= -\frac{1}{3} + b_2, \\
a_4 &= -\frac{1}{3}b_1 + b_3, \\
a_5 &= \frac{1}{5} - \frac{1}{3}b_2 + b_4, \\
& \frac{1}{5}b_1 - \frac{1}{3}b_3 = 0, \\
& \frac{1}{7} + \frac{1}{5}b_2 - \frac{1}{3}b_4 = 0, \\
& -\frac{1}{7}b_1 + \frac{1}{5}b_3 = 0, \\
& \frac{1}{9} - \frac{1}{7}b_2 + \frac{1}{5}b_4 = 0.
\end{aligned}$$

Solving first the last four equations for the $b's$, and then getting the $a's$, we have

$$a_0 = 0, a_1 = 1, a_2 = 0, a_3 = \frac{7}{9}, a_4 = 0, a_5 = \frac{64}{945}$$

$$b_1 = 0, b_2 = \frac{10}{9}, b_3 = 0, b_4 = \frac{5}{21}$$

A rational function which approximates $arctanx$ is then

$$arctanx = \frac{x + \frac{7}{9}x^3 + \frac{64}{945}x^5}{1 + \frac{10}{9}x^2 + \frac{5}{21}x^4} \tag{3.6}$$

Before we discuss better approximations in the form of rational functions, remarks on the amount of effort required for the computation using Eq. (3.6) are in order. If we implement the equation in a computer as it stands, we would, of course, use the constants in decimal form, and we would evaluate the polynomials in nested form:

$$Numerator = [(0.0677x^2 + 0.7778)x^2 + 1]x,$$

$$Denominator = (0.2381x^2 + 1.1111)x^2 + 1$$

Since additions and subtractions are generally much faster than multiplications or divisions, we generally neglect them in a count of operations. We have then three multiplications for the numerator, two for the denominator, plus one to get x^2, and one division, for a total of seven operations.

3.2 Pade Summation

When a power series representation of a function diverges, it indicates the presence of singularities. The divergence of the series reflects the inability of a polynomial to approximate a function adequately near a singularity. The basic idea of summation theory is to represent $f(z)$, the function in question, by a convergent expression. In Euler summation this expression is the limit of a convergent series, while in Borel summation this expression is the limit of convergent integral.

The difficulty with Euler and Borel summation is that *all* of the terms of the divergent series must be known exactly before the "sum" can be found even approximately. In realistic perturbation problems only a few terms of a perturbation series can be calculated before a state of exhaustion is reached. Therefore, a summation algorithm is needed which requires as input only a finite number of terms of a divergent series. Then, as each new term is computed, it is immediately folded in with the others to give a new and improved estimate of the exact sum of the divergent series. A well-known summation method having this property is called Pade summation.

3.2.1 Generalized Pade Summation

The Pade methods that we have introduced here could be called "one-point" Pade methods because the approximants are constructed by comparing them with a power series about a particular point. However, the function in question may have been investigated in the vicinity of two or more points. For example, its large ϵ as well as its small ϵ dependences may have been determined perturbatively. One may wish to incorporate information from all these expansions in a single sequence of Pade approximants. The numerical results are sometimes impressive.

Suppose $f(z)$ has the asymptotic expansions

$$f(z) \sim \sum_{n=0}^{\infty} a_n (z - z_0)^n, z \to z_0, \tag{3.7}$$

$$f(z) \sim \sum_{n=0}^{\infty} b_n (z - z_1)^n, z \to z_1, \tag{3.8}$$

in the neighborhoods of the distinct points z_0 and z_1, respectively. A two-point Pade approximant to $f(z)$ is a rational function $F(z) = R_N(z)/S_M(z)$ where $S_M(0) = 1$. $R_N(z)$ and $S_M(z)$ are polynomials of degrees N and M, respectively, whose $(N + M + 1)$ are arbitrary coefficients are chosen to make the first J terms $(0 \leq J \leq N + M + 1)$ of the Taylor series expansion of $F(z)$ about z_0 agree with Eq. (3.7) and the first K terms of the Taylor series expansion of $F(z)$ about z_1 agree with (3.8), where $J + K = N + M + 1$. The formulation of the general equations for the coefficients of the polynomials $R_N(z)$ and $S_N(z)$, as well as the development of efficient numerical techniques for their solution.

3.3 Pade Approximation

The idea of Pade summation is to replace a power series $\sum a_n x^n$ by a sequence of rational functions (a rational function is a ratio of two polynomials) of the form

$$P_M^N(x) = \frac{\sum_{n=0}^{N} A_n x^n}{\sum_{n=0}^{M} B_n x^n}, \tag{3.9}$$

where we choose $B_0 = 1$ without loss of generality. We choose the remaining $(M+N+1)$ coefficients $A_0, A_1, ..., A_N, B_1, B_2, ..., B_M$, so that the first $(M+N+1)$ terms in the Taylor series expansion of $P_M^N(x)$ match the first $(M + N + 1)$ terms of the power series $\sum_{n=0}^{\infty} a_n x^n$. The resulting rational function $P_M^N(x)$ is called a Pade approximant.

We will see that constructing $P_M^N(x)$ is very useful. If $\sum a_n x^n$ is a power series representation of the function $f(x)$, then in many instances $P_M^N(x) \to f(x)$ as $N, M \to \infty$, even if $\sum a_n x^n$ is a divergent series. Usually we consider only the convergence of the Pade sequences $P_0^j, P_1^{1+j}, P_2^{2+j}, P_3^{3+j}, \cdots$ having $N = M + J$

with J fixed and $M \to \infty$. The special sequence $J = 0$ is called the diagonal sequence.

Example: *Computation of* $p_1^0(x)$. To compute p_1^0 we expand this approximant in a Taylor series: $P_1^0 = A_0/(1 + B_1 x) = A_0 - A_0 B_1 x + O(x^2)$. Comparing this series with the first two terms in the power series representation of $f(x) = \sum_{n=0}^{\infty} a_n x^n$ gives two equations : $a_0 = A_0, a_1 = -A_0 B_1$. Thus, $P_1^0(x) = a_0/(1 - xa_1/a_0)$.

The full power series representation of a function need not be known to construct a Pade approximant - just the first $M + N + 1$ terms. Since Pade approximants involve only algebraic operations, they are more convenient for computational purposes than Borel summation, which requires one to integrate over an infinite range the analytic continuation of a function defined by a power series. In fact, the general Pade approximant can be expressed in terms of determinants.

The Pade approximant $P_M^N(x)$ is determined by a simple sequence of matrix operations. The coefficients $B_1, ..., B_M$ in the denominator may be computed by solving the matrix equation in (Bender and Orszag [1985])

$$\mathbf{a} \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_M \end{bmatrix} = - \begin{bmatrix} a_{N+1} \\ a_{N+2} \\ \vdots \\ a_{N+M} \end{bmatrix} \tag{3.10}$$

where $\mathbf{a}$ is an $M \times M$ matrix with entries $a_{ij} = a_{N+i-j} \quad (1 \leq i, j \leq M)$. Then the coefficients $A_0, A_1, ..., A_N$ in the numerator are given by

$$A_n = \sum_{j=0}^{n} a_{n-j} B_j, \quad 0 \leq n \leq N \tag{3.11}$$

where $B_j = 0$ for $j > M$. Equations (3.10) and (3.11) are derived by equating coefficients of $1, x, ..., x^{N+M}$

$$\sum_{j=0}^{N+M} a_j x^j \sum_{k=0}^{M} B_k x^K - \sum_{n=0}^{N} A_n x^n = O(x^{N+M+1}), \quad x \to 0 \tag{3.12}$$

which is just a restatement of the definition of Pade approximants.

3.4 The Method of Pade Approximation

For the power series expansion of a function $f(x)$ of the real variable x,

$$f(x) = \sum_{n=0}^{\infty} a_n x^n, \tag{3.13}$$

the sequence $\{S_n\}$ of the partial sums of this series is given by

$$S_n = \sum_{k=0}^{n-1} a_k x^k, \quad n = 1, 2, ... \tag{3.14}$$

The Pade approximant $[M, N]$ of $f(x)$ is the uniquely determined rational function defined by

$$[M, N] = \frac{P_M(x)}{Q_N(x)}, \tag{3.15}$$

where $P_M(x)$ and $Q_N(x)$ are polynomials in x of degree M and N, respectively, such that for any pair of integers (M, N). So we can write the equation of Pade approximant as follows:

$$P_M^N(x) = \frac{\sum_{n=0}^{N} A_n x^n}{\sum_{n=0}^{M} B_n x^n} \tag{3.16}$$

where A_n and B_n are the coefficients of the polynomials in the numerator and denominator of the Pade approximants, respectively.

In order to calculate the Pade approximants of some test series, we first have proceed as follows:

i) We have calculated the term a_i of given test series.
ii) Using these terms we have formed $M \times N$ matrix $\mathbf{a}$ by the relation $a_{ij} = a_{N+i-j}$, where $1 \leq i, j \leq M$
iii) It has been used to solve the matrix equation

$$\mathbf{a} \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_M \end{bmatrix} = - \begin{bmatrix} a_{N+1} \\ a_{N+2} \\ \vdots \\ a_{N+M} \end{bmatrix} \tag{3.17}$$

to determined $B_1, B_2, B_3, ..., B_M$. Notice that we have always chosen $B_0 = 1$.

After we have computed the coefficients of denominator i.e., $B_1, B_2, B_3, ..., B_M$, then we have calculated the coefficient of numerator A_n using the coefficient of denominator B_n and the coefficient of the given test series i.e. using the relation

$$A_n = \sum_{j=0}^{n} a_{n-j} B_j, \quad where \;\; 0 \leq n \leq N \tag{3.18}$$

where $B_j = 0$ for $j > M$ and a_{n-j} is the term of the given series.

After calculating the coefficient of numerators and denominators then we have calculated the total sum of the numerator using the coefficient of numerator and putting the value of x in the relation

$$\sum_{n=0}^{N} A_n x^n$$

After that we have calculated the total sum of the denominator using the coefficient of the denominator and putting the value of x in the relation

$$\sum_{n=0}^{M} B_n x^n$$

Finally, Pade approximants is obtained by substituting the value of numerator and denominator in the formula (3.16) of Pade approximant which is given above.

3.5 The u-transform

Let $\{S_n, n = 1, 2, ...\}$ be an infinite sequence of real numbers tending to a limit S. Define an associated sequence $\{g_n\}$ such that

$$S = S_n + g_n \Delta S_n, \tag{3.19}$$

where Δ is the usual forward difference operator defined by (Schield [1961]; Gerald [1980])

$$\Delta^0 S_n = S_n$$

,

$$\Delta^{k+1} S_n = \Delta^k S_{n+1} - \Delta^k S_n, k = 1, 2, ...$$

If $\{S_n\}$ is, in particular, the sequence formed by the successive partial sums of some infinite series with terms $\{a_n\}$ then

$$\Delta S_n = a_{n+1}$$

Also, $\{S_n\}$ may, in particular, be defined by the sequence of Partial sums of a power series, i.e., as

$$S_n = \sum_{k=0}^{n-1} a_k z^k, \quad n = 1, 2, ... \tag{3.20}$$

where $\{a_k\}$ is the sequence of the coefficients in the perturbation expansion.

Hence, if $\{g_n\}$ can be expressed in terms of $\{S_n\}$, S can be evaluated. In the general case, the term g_n depends on all the terms in the infinite sequence $\{S_i, i = n, n+1, n+2, ...\}$. A class of techniques for accelerating the convergence of sequences consists in assuming that each term g_n is a function of only $(k+1)$ corresponding terms in $\{S_n\}$. We thus define the sequence of approximations to $\{g_n\}$ as

$$g_{kn}(S_n) = g_{kn}(S_n, \rho_{n+1}, \cdots \rho_{n+k}),$$

where,

$$\rho_n = a_{n+1}/a_n = \Delta S_n / \Delta S_{n-1}.$$

If g_{kn} is used as an approximation to g_n, we then have a corresponding approximation T_{kn} for S obtained by the sequence transform

$$T_{kn} = S_n + g_{kn} \Delta S_n \tag{3.21}$$

The nth term of the transformed sequence is defined in terms of $(k+1)$ terms of the original sequence, beginning from the nth term. We call this an approximation of order k. If the transform is regular or limit preserving, in addition to being accelerating, then a further application would be useful in evaluating S. Thus using the transform iteratively we have,

$$T_{kn}^{\mu+1} = T_{kn}^{\mu} + g_{kn}^{\mu} \Delta T_{kn}^{\mu}, \tag{3.22}$$

$$T^0_{kn} = S_n, g^\mu_{kn} = g^\mu_{kn}(\Delta T^\mu_{kn}), \tag{3.23}$$

where μ is the order of iteration and T^μ_{kn} is the sequence obtained in the μth iteration of the transform.

The sequence transforms to be described attempt in some sense to simulate the approach to the limit by a given sequence. A certain transform and its iterates can be said to accelerate the convergence of a sequence if

$$|r'_n|/|r_n| \to 0 \;\; as \;\; n \to \infty$$

where,

$$r_n = S - S_n, \quad r'_n = S - T_{kn}.$$

Stated more simply, the limit can be evaluated to some desired accuracy by the transform using a rather small number of terms of the original sequence.

For completeness of study we note that a sequence transformation is linear if

(i) $T_{kn}(\{cS_n\}) = cT_{kn}(\{S_n\})$,

(ii) $T_{kn}(\{S_n + S'_n\}) = T_{kn}(\{S_n\}) + T_{kn}(\{S'_n\})$,
where c is a constant.

Thus the best approximation to g_n seems to be a linear expression in n corresponding to $\Delta^2 g_n = 0$. Further refinement can be achieved by adding terms in $1/n$ and its higher powers. To this end, we write

$$g_n = \alpha n + \sum_{i=0}^{k-2} \alpha_i n^{-i} = p_{k-1}/n^{k-2}, \tag{3.24}$$

where p_{k-1} is a polynomial of degree $(k-1)$ in n. Then

$$\Delta^k(p_{k-1}) = \Delta^k(n^{k-2} g_{kn}) = 0$$

using this in (3.22) and (3.23) we have

$$T_{kn} = \frac{\Delta^k (n^{k-2} S_n / \Delta S_n)}{\Delta^k (n^{k-2} / \Delta S_n)}, \tag{3.25}$$

This transform is known as Levin's u-transform given by

$$u_{kn}(\{S_n\}) = \frac{\Delta^k (n^{k-2} S_n / \Delta S_n)}{\Delta^k (n^{k-2} / \Delta S_n)}, \quad k, n = 1, 2, ..., \tag{3.26}$$

which can be recast in the form

$$\begin{aligned} u_{kn}(\{S_n\}) &= \frac{N_k(z)}{D_k(z)} \\ &= \frac{\sum_{j=0}^{k} v_{knj} S_{n+j} S_{n+j} / \Delta S_{n+j-1}}{\sum_{j=0}^{k} v_{knj} S_{n+j} 1 / \Delta S_{n+j-1}} \\ \Rightarrow u_{kn}(\{S_n\}) &= \frac{\sum_{j=0}^{n+k-1} z^i \sum_{j=0}^{k} w_{knj} a_{j-i}}{\sum_{j=0}^{k} w_{knj} z^i} \end{aligned} \tag{3.27}$$

where

$$v_{knj} = (-1)^j \frac{k!}{j!(k-j)!} (n+j)^{k-2},$$

$$w_{knj} = (-1)^j \frac{k!}{j!(k-j)!} \frac{(n+k-j)^{k-2}}{a_{n+k-j-1}},$$

and $a_i = 0$ for $i < 0$.

Thus u_{kn} represents a table of rational functions, each element of which is obtained from $n + k$ terms of the original sequence $\{S_n\}$ and is an approximant of the function $f(z)$.

We now show that

$$f(z) - u_{kn} = \bigcirc(z^{n+k})$$

To establish this, making use of the symbol $P_n(z)$ to denote *any* polynomial in z of degree n. Thus

$$S_n = P_{n-1}(z)$$

Let us also assume that $a_i \neq 0$ for all $i > 0$. Then it follows that

$$
\begin{aligned}
\Rightarrow \Delta^i S_n &= \Delta^i(P_{n-1}(z)) \\
\Rightarrow \Delta^i S_n &= z^n(P_{n-1}(z))
\end{aligned} \tag{3.28}
$$

where $P_{n-1}(z)$ denote <u>*some*</u> polynomial in z of degree $(i-1)$.
and, for convenience, writing

$$
\begin{aligned}
b_n &= \frac{n^{k-2}}{a_{n-1}z^{n-1}}, \\
&= \Delta^i\left(\frac{n^{k-2}}{a_{n-1}z^{n-1}}\right), \\
&= \frac{\Delta^i(n^{k-2})}{\Delta^i(a_{n-1}z^{n-1})}, \\
\Rightarrow \Delta^i(b_n) &= \frac{P_i(z)}{z^{n-1}}
\end{aligned} \tag{3.29}
$$

Now, for two sequences $\{u_n\}$ and $\{v_n\}$ by using

$$\Delta(u_k v_k) = u_k \Delta v_k + v_{k+1} \Delta u_k$$

we have

$$\Delta^k(u_n v_n) = \sum_{j=0}^{k} \frac{k!}{j!(k-j)!} \Delta^{k-j} u_{n+j} \Delta^j v_n$$

and therefore,

$$
\begin{aligned}
\Delta^k(b_n S_n) &= \sum_{j=0}^{k-1} \frac{k!}{j!(k-j)!} \Delta^{k-j} S_{n+j} \Delta^j b_n + S_{n+k} \Delta^k b_n. \\
\Rightarrow \Delta^k(b_n S_n) &= z P_{k-1}(z) + S_{n+k} \Delta^k b_n
\end{aligned} \tag{3.30}
$$

Since each term inside the summation symbol is a polynomial of the same degree, i.e.,

$$
\begin{aligned}
\Delta^{k-j} S_{n+j} \Delta^j b_n &= z^{n+j} P_{k-j-1}(z) \frac{P_j(z)}{z^{n+j-1}} \\
&= z P_{k-1}(z)
\end{aligned}
$$

[since, $\Delta^i S_n = z^n P_{i-1}(z), \Delta^i b_n = \frac{P_i(z)}{z^{n-1}}$]
Hence,

$$
\begin{aligned}
u_{kn}(\{S_n\}) &= \frac{\Delta^k(b_n S_n)}{\Delta^k b_n} \\
&= \frac{zP_{k-1}(z) + S_{n+k}\Delta^k b_n}{\Delta^k b_n} \\
&= \frac{zP_{k-1}(z)}{\Delta^k b_n} + S_{n+k} \\
&= S_{n+k} + \frac{zP_{k-1}(z)}{\Delta^k b_n} \\
&= S_{n+k} + \frac{zP_{k-1}(z)}{P_k(z)/z^{n+k-1}} \\
\Rightarrow u_{kn}(\{S_n\}) &= S_{n+k} + z^{n+k}\frac{P_{k-1}(z)}{P_k(z)} \qquad (3.31)
\end{aligned}
$$

which completes the demonstration.

Incidentally, the right hand side of Eq. (3.31) brings into focus the extrapolative nature of the $u-$transform in its assessment of the limit of an infinite sequence. In this case, the "remainder" is clearly in the form of a rational function and can be obtained in closed form. Since it is evident from Eq. (3.27) that

$$u_{kn}(\{S_n\}) = \frac{P_{n+k-1}(z)}{P_k(z)}$$

(disregarding the exact cancellation of the coefficient of the highest power in the numerator), Eq. (3.29) can be rewritten as

$$u_{kn}(\{S_n\}) = S_{n+k} + z^{n+k}\frac{\sum_{j=0}^{k-1} r_{knj}z^j}{\sum_{j=0}^{k} w_{knj}z^j} \qquad (3.32)$$

where

$$r_{knj} = \sum_{i=j}^{k-1} w_{k,n,k+j-i}a_{n+i}.$$

When some a_i's vanish, suitable modifications in the above considerations may be made by correspondingly redefining $\{S_n\}$.

3.6 The Method of u-transformation

If $\{S_n, n = 1, 2, ...\}$ is the sequence of partial sums of a power series and Δ the forward difference operator (Schield [1961]; Gerald [1980]), i.e.,

$$\Delta^0 S_n = S_n$$

$$\Delta^{k+1} S_n = \Delta^k S_{n+1} - \Delta^k S_n, k = 1, 2, ...$$

the kth order $u-$transform is then defined by

$$u_{kn}(\{S_n\}) = \frac{\Delta^k (n^{k-2} S_n / \Delta S_n)}{\Delta^k (n^{k-2} / \Delta S_n)}, \quad k, n = 1, 2, ...,$$

which can be recast in the form

$$\begin{aligned} u_{kn}(\{S_n\}) &= \frac{N_k(z)}{D_k(z)} \\ &= \frac{\sum_{j=0}^{k} v_{knj} S_{n+j} S_{n+j} / \Delta S_{n+j-1}}{\sum_{j=0}^{k} v_{knj} S_{n+j} 1 / \Delta S_{n+j-1}} \\ &= \frac{\sum_{j=0}^{n+k-1} z^i \sum_{j=0}^{k} w_{knj} a_{j-i}}{\sum_{j=0}^{k} w_{knj} z^i} \end{aligned}$$

where

$$v_{knj} = (-1)^j \frac{k!}{j!(k-j)!} (n+j)^{k-2},$$

$$w_{knj} = (-1)^j \frac{k!}{j!(k-j)!} \frac{(n+k-j)^{k-2}}{a_{n+k-j-1}},$$

and $a_i = 0$ for $i < 0$.

Thus u_{kn} represents a table of rational functions, each element of which is obtained from $n + k$ terms of the original sequence $\{S_n\}$ and is an approximant of the function $f(z)$.

To calculate the $u-$approximants of a test series we have followed the following steps:

(i.) Calculate the coefficient of the given series i.e., a_i where $0 \leq i \leq n$

(ii.) Calculate w_{knj} from the relation

$$w_{knj} = (-1)^j \frac{k!}{j!(k-j)!} \frac{n+k-j^{k-2}}{a_{n+k-j-1}},$$

(iii.) Calculate the sum of one part of the numerator i.e., $\sum_{i=0}^{\infty} w_{kni} a_{j-i}$

(iv.) After calculating the above part the total sum of the numerator was obtained from the relation $\sum_{j=0}^{n+k-1} z^i \sum_{j=0}^{k} w_{knj} a_{j-i}$

(v.) Then calculate the total sum of the denominator of the $u-$approximants from the relation $\sum_{j=0}^{k} w_{knj} z^i$

(vi.) Finally we have calculated the $u-$approximants from definition (3.27) given above

3.7 Calculation of the $u-$approximants : an example

Here we discuss in some detail the explicit calculation of the approximant u_{31} for the series expansion of $\frac{1}{x} ln(1+x)$ (series 2 of Table 3.1) as an example. Thus, taking $n = 1$ and $k = 3$,

$$u_{31} = \frac{\sum_{j=0}^{3} x^j \sum_{i=0}^{3} w_{31i} a_{j-i}}{\sum_{j=0}^{3} w_{31j} x^j},$$

with

$$w_{31j} = (-1)^j \frac{3!}{j!(3-j)!} \frac{(4-j)}{a_{3-j}}$$

Now,

$$\begin{aligned}\frac{1}{x}ln(1+x) &= \frac{1}{x}(x-\frac{1}{2}x^2+\frac{1}{3}x^3-\frac{1}{4}x^4+\cdots) \\ &= (1-\frac{1}{2}x+\frac{1}{3}x^2-\frac{1}{4}x^3+\cdots)\end{aligned}$$

For this series

$$a_n = \frac{(-1)^n}{n+1},$$

so that

$$\begin{aligned}w_{310} &= (-1)^0\frac{3!}{0!(3-0)!}\frac{(4-0)}{a_{3-0}} \\ &= \frac{4}{a_3} \\ &= \frac{4}{-1/4} \\ &= -16\end{aligned}$$

$$\begin{aligned}w_{311} &= (-1)^1\frac{3!}{1!(3-1)!}\frac{(4-1)}{a_{3-1}} \\ &= -\frac{3.2.1}{1.2.1}\frac{3}{a_2} \\ &= -3\frac{3}{1/3} \\ &= -27\end{aligned}$$

$$\begin{aligned}w_{312} &= (-1)^2\frac{3!}{2!(3-2)!}\frac{(4-2)}{a_{3-2}} \\ &= \frac{3.2.1}{2.1.1}\frac{2}{a_1} \\ &= 3\frac{2}{-1/2} \\ &= -12\end{aligned}$$

$$\begin{aligned} w_{313} &= (-1)^3 \frac{3!}{3!(3-3)!}\frac{(4-3)}{a_{3-3}} \\ &= -\frac{3!}{3!0!}\frac{1}{a_0} \\ &= -\frac{1}{1} \\ &= -1 \end{aligned}$$

Now we calculate the numerator of the approximant u_{31}, taking

$$\begin{aligned} N_i &= \sum_{i=0}^{3} w_{31i} a_{j-i} \\ &= w_{310} a_{j-0} + w_{311} a_{j-1} + w_{312} a_{j-2} + w_{313} a_{j-3} \\ &= -16a_j - 27a_{j-1} - 12a_{j-2} - a_{j-3} \end{aligned}$$

Therefore,

$$\begin{aligned} N_3(x) &= \sum_{j=0}^{3} x^j(-16a_j - 27a_{j-1} - 12a_{j-2} - a_{j-3}) \\ &= -16a_0 + x(-16a_1 - 27a_0) + x^2(-16a_2 - 27a_1 - 12a_0) \\ &\quad +x^3(-16a_3 - 27a_2 - 12a - 1 - a_0) \\ &= -16(1) + x\{-16(-1/2) - 27(1)\} + x^2\{-16(1/3) - 27(-1/2) - 12(1)\} \\ &\quad +x^3\{-16(-1/4) - 27(1/3) - 12(-1/2) - 1\} \\ &= -16 - 19x - \frac{23}{6}x^2 \end{aligned}$$

[since, $a_i = 0$ for $i < 0$]

Again, we calculate the denominator of the approximant u_{31}, taking,

$$\begin{aligned} D_3(x) &= \sum_{j=0}^{3} w_{31j} x^j \\ &= w_{310}x^0 + w_{311}x^1 + w_{312}x^2 + w_{313}x^0 3 \\ &= -16 - 27x - 12x^2 - x^3 \end{aligned}$$

Table 3.1: Test series and their $u-$approximants

No.	Test Series	numerators and Denominators
(1.)	$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$	$N_3(x) = 1 + \frac{1}{4}x$ $D_3(x) = 1 - \frac{3}{4}x + \frac{1}{4}x^2 - \frac{1}{24}x^3$
(2.)	$\frac{1}{x}ln(1+x)$ $= \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n+1}$	$N_3(x) = 16 + 19x + \frac{23}{6}x^2$ $D_3(x) = 16 + 27x + 12x^2 + x^3$
(3.)	$\int_0^{infty} \frac{e^{-t}}{1+xt}dt$ $= \sum_{n=0}^{\infty} n!(-x)^n$	$N_4(x) = 1 + \frac{231}{25}x + \frac{442}{25}x^2 + \frac{98}{25}x^3$ $D_4(x) = 1 + \frac{256}{25}x + \frac{648}{25}x^2 + \frac{348}{25}x^3 + \frac{24}{25}x^4$
(4.)	$\sqrt{2/\pi} \int_0^{\infty} \frac{e^{-t^2/2}}{1-x^2t^2}dt$ $= \sum_{n=0}^{\infty}(-1)^n \frac{(2n)!}{2^n n!}x^{2n}$	$N_4(x) = 1 + \frac{423}{25}x^2 + \frac{1517}{25}x^2 + \frac{759}{25}x^6$ $D_4(x) = 1 + \frac{448}{25}x^2 + \frac{378}{5}x^4 + \frac{336}{5}x^6 + \frac{21}{5}x^8$
(5.)	$\sqrt{\pi}/2erf(x)/x$ $= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{x^{2n}}{2n+1}$	$N_4(x) = 1 + \frac{37}{225}x^2 + \frac{23}{675}x^4 + \frac{4}{2625}x^6$ $D_4(x) = 1 + \frac{112}{225}x^2 + \frac{1}{10}x^4 + \frac{2}{225}x^6 + \frac{1}{5400}x^8$

Thus, we can write,

$$\begin{aligned} u_{31} &= \frac{N_3(x)}{D_3(x)} \\ &= \frac{-16 - 19x - \frac{23}{6}x^2}{-16 - 27x - 12x^2 - x^3} \\ &= \frac{16 + 19x + \frac{23}{6}x^2}{16 + 27x + 12x^2 + x^3}. \end{aligned}$$

Finally, putting the value of x in this relation we can get required approximation.

The table 3.1 is a list of some functions and the numerators and denominators of their respective $u-$approximants.

Chapter 4

Comparative Study of Pade and u-approximants on some test series

In this chapter we make a comparative study of Pade approximants (PAppxs) and $u-$approximants (uAppxs) calculated from the series expansions of some known functions. In the previous chapter the actual calculation of an $u-$approximant was given in some detail. Table 3.1 is a list of these functions and the numerators and denominators of their respective uAppxs. The numerical efficiency of these approximants in relation to PAppxs for these functions appear in tables 4.1, 4.2 and 4.3. The comparison of the actual functions with their PAppxs and uAppxs is shown in Figs. 4.1 to 4.5.

The use of the $u-$transform as a generator of approximants has not previously been investigated. Preliminary investigations on forming rational approximants with the $u-$transform indicate unambigously its capability to achieve better results than the Pade scheme. The $u-$transform has the considerable practical advantage of being simple in structure and is consequently easier to implement. *The definition is more direct and for a given number of terms used in the transform, the u-approximant requires less algebraic manipulations than the Pade scheme.*

Before considering the results it should be made clear that the number of terms of the power series required to obtain an aprroximant depends on the degree of both its denominator and the numerator. Thus direct computation of the Pade approximant $[M, N]$ requires $M+N+1$ partial sums of the power series, whereas any approximant $\{M, N\}$ given by the $u-$transform has the form $\{M, M-1\}$ and uses $M+1$ partial sums.

In all the examples $n=1$ in u_{kn} and for brevity we shall write u_k for u_{k1}.

4.1 Comparison of the Numerical Results

The actual values of the approximants and their errors $[error = abs(exactvalue - approximant)]$ are listed in Tables 4.1, 4.2 and 4.3 for exponential series e^x for $x = 1$, $x = 5$ and for logarithmic series $\frac{1}{x}ln(1+x)$ for $x = 1$. Here we have considered two series where one is positive series and the other is alternating. Below we discuss convergence rates and errors of $u-$approximants and Pade approximants separately. From Tables 4.1 through 4.3 we have taken different terms of series which indicates in the first column in each table and taking the accuracy upto five decimal places of the approximants. Everywhere we have observed that Pade approximants need more terms than the $u-$approximants of the original series. We have calculated error terms in exponential form which indicates in the last two columns in each table.

In table 4.1, we have taken 21 terms of the series which indicates in the first column. For calculating the required accuracy, Pade approximant needs minimum *eight* terms of the series whereas $u-$approximant needs *six* terms. We have observed that the error of $u-$approximants is more smaller than the Pade approximants. In table 4.2, we have taken 27 terms of the series which indicates in the first column. For calculating the required accuracy, Pade approximant needs minimum *nineteen* terms of the series whereas $u-$approximant needs only *thirteen* terms. We have observed that the error of $u-$approximants is much more smaller than the Pade approximants. Here we also observed that upto first seven terms Pade approximants gives unexpected result. In table 4.3, we have taken 18 terms of the series which indicates in the first column. For calculating the required accuracy, Pade approximant needs minimum *seven* terms of the series whereas $u-$approximants needs only *six* terms. We have observed that the error of $u-$approximants is more smaller than the Pade approximants upto fourteen terms. On the other hand the error of Pade approximant is more smaller than

Table 4.1: A comparison of the convergence rates of the Pade approximants and u-approximants to e^x at $x = 1$.

k	Exact Value	Pade Appxs $P_M^N(1)$	u-Appxs $u_k(\{S_n\})$	Error of u-Appxs.	Error of Pade Appxs.
0	2.71828	$P_0^0 = 1.00000$			1.71828
1	2.71828	$P_1^0 = \infty$	$u_1 = 0.00000$	2.7	∞
2	2.71828	$P_1^1 = 3.00000$	$u_2 = 2.00000$	7.2×10^{-1}	2.8×10^{-1}
3	2.71828	$P_2^1 = 2.66667$	$u_3 = 2.72727$	9.0×10^{-3}	5.2×10^{-2}
4	2.71828	$P_2^2 = 2.71429$	$u_4 = 2.71845$	1.6×10^{-4}	4.0×10^{-3}
5	2.71828	$P_3^2 = 2.71875$	$u_5 = 2.71828$	1.4×10^{-5}	4.7×10^{-4}
6	2.71828	$P_3^3 = 2.71831$	$u_6 = 2.71828$	4.5×10^{-9}	2.8×10^{-5}
7	2.71828	$P_4^3 = 2.71828$	$u_7 = 2.71828$	2.4×10^{-10}	2.3×10^{-6}
8	2.71828	$P_4^4 = 2.71828$	$u_8 = 2.71828$	2.7×10^{-12}	1.1×10^{-7}
9	2.71828	$P_5^4 = 2.71828$	$u_9 = 2.71828$	1.4×10^{-14}	6.7×10^{-9}
10	2.71828	$P_5^5 = 2.71828$	$u_{10} = 2.71828$	1.2×10^{-14}	2.8×10^{-10}
11	2.71828	$P_6^5 = 2.71828$	$u_{11} = 2.71828$	4.4×10^{-16}	1.4×10^{-11}
12	2.71828	$P_6^6 = 2.71828$	$u_{12} = 2.71828$	4.4×10^{-16}	4.8×10^{-13}
13	2.71828	$P_7^6 = 2.71828$	$u_{13} = 2.71828$	4.4×10^{-16}	2.0×10^{-14}
14	2.71828	$P_7^7 = 2.71828$	$u_{14} = 2.71828$	4.4×10^{-16}	8.9×10^{-16}
15	2.71828	$P_8^7 = 2.71828$	$u_{15} = 2.71828$	8.9×10^{-16}	4.4×10^{-16}
16	2.71828	$P_8^8 = 2.71828$	$u_{16} = 2.71828$	8.9×10^{-16}	4.4×10^{-16}
17	2.71828	$P_9^8 = 2.71828$	$u_{17} = 2.71828$	8.9×10^{-16}	4.4×10^{-16}
18	2.71828	$P_9^9 = 2.71828$	$u_{18} = 2.71828$	4.4×10^{-16}	4.4×10^{-16}
19	2.71828	$P_{10}^9 = 2.71828$	$u_{19} = 2.71828$	4.4×10^{-16}	4.4×10^{-16}
20	2.71828	$P_{10}^{10} = 2.71828$	$u_{20} = 2.71828$	4.4×10^{-16}	4.4×10^{-16}

Table 4.2: A comparison of the convergence rates of the Pade approximants and u-approximants to e^x at $x = 5$.

k	Exact Value	Pade Appxs $P_M^N(1)$	u-Appxs $u_k(\{S_n\})$	Error of u-Appxs.	Error of Pade Appxs.
0	148.41316	$P_0^0 = 1.00000$			147.41316
1	148.41316	$P_1^0 = -0.25000$	$u_1 = 0.44444$	1.5×10^2	1.5×10^2
2	148.41316	$P_1^1 = -2.33333$	$u_2 = 0.11765$	1.5×10^2	1.5×10^2
3	148.41316	$P_2^1 = 1.45455$	$u_3 = -1.11765$	1.5×10^2	1.5×10^2
4	148.41316	$P_2^2 = 9.57143$	$u_4 = 456.00000$	3.1×10^2	1.4×10^2
5	148.41316	$P_3^2 = -12.75000$	$u_5 = 108.50965$	4.0×10	1.6×10^2
6	148.41316	$P_3^3 = -169.00000$	$u_6 = 145.98121$	2.4	3.2×10^2
7	148.41316	$P_4^3 = 71.38462$	$u_7 = 148.51068$	9.8×10^{-2}	7.7×10
8	148.41316	$P_4^4 = 128.61905$	$u_8 = 148.42553$	1.2×10^{-2}	2.0×10
9	148.41316	$P_5^4 = 158.62097$	$u_9 = 148.41345$	2.9×10^{-4}	1.0×10
10	148.41316	$P_5^5 = 149.69688$	$u_{10} = 148.41315$	8.1×10^{-6}	1.3
11	148.41316	$P_6^5 = 148.00123$	$u_{11} = 148.41315$	4.5×10^{-6}	4.1×10^{-1}
12	148.41316	$P_6^6 = 148.36220$	$u_{12} = 148.41316$	2.4×10^{-6}	5.1×10^{-2}
13	148.41316	$P_7^6 = 148.42659$	$u_{13} = 148.41316$	5.3×10^{-8}	1.3×10^{-2}
14	148.41316	$P_7^7 = 148.41469$	$u_{14} = 148.41316$	1.6×10^{-7}	1.5×10^{-3}
15	148.41316	$P_8^7 = 148.41282$	$u_{15} = 148.41316$	1.9×10^{-7}	3.4×10^{-4}
16	148.41316	$P_8^8 = 148.41312$	$u_{16} = 148.41316$	1.0×10^{-7}	3.6×10^{-5}
17	148.41316	$P_9^8 = 148.41317$	$u_{17} = 148.41316$	5.5×10^{-8}	6.8×10^{-6}
18	148.41316	$P_9^9 = 148.41316$	$u_{18} = 148.41316$	2.8×10^{-8}	6.7×10^{-7}
19	148.41316	$P_{10}^9 = 148.41316$	$u_{19} = 148.41316$	4.0×10^{-9}	1.1×10^{-7}
20	148.41316	$P_{10}^{10} = 148.41316$	$u_{20} = 148.41316$	2.0×10^{-9}	1.0×10^{-8}
21	148.41316	$P_{11}^{10} = 148.41316$	$u_{21} = 148.41316$	2.9×10^{-10}	1.5×10^{-9}
22	148.41316	$P_{11}^{11} = 148.41316$	$u_{22} = 148.41316$	1.2×10^{-10}	1.2×10^{-10}
23	148.41316	$P_{12}^{11} = 148.41316$	$u_{23} = 148.41316$	2.2×10^{-11}	1.9×10^{-11}
24	148.41316	$P_{12}^{12} = 148.41316$	$u_{24} = 148.41316$	8.2×10^{-12}	3.4×10^{-12}
25	148.41316	$P_{13}^{12} = 148.41316$	$u_{25} = 148.41316$	3.0×10^{-12}	9.7×10^{-13}
26	148.41316	$P_{13}^{13} = 148.41316$	$u_{26} = 148.41316$	7.4×10^{-13}	2.4×10^{-12}

Table 4.3: A comparison of the convergence rates of the Pade approximants and u-approximants to $\frac{1}{x}ln(1+x)$ at $x=1$.

k	Exact Value	Pade Appxs $P_M^N(1)$	u-Appxs $u_k(\{S_n\})$	Error of u-Appxs.	Error of Pade Appxs.
0	0.69315	$P_0^0 = 1.00000$			3.1×10^{-1}
1	0.69315	$P_1^0 = 0.66667$	$u_1 = 0.75000$	5.7×10^{-2}	2.6×10^{-2}
2	0.69315	$P_1^1 = 0.70000$	$u_2 = 0.68750$	5.6×10^{-3}	6.9×10^{-3}
3	0.69315	$P_2^1 = 0.69231$	$u_3 = 0.69345$	3.1×10^{-4}	8.4×10^{-4}
4	0.69315	$P_2^2 = 0.69333$	$u_4 = 0.69314$	4.8×10^{-6}	1.9×10^{-4}
5	0.69315	$P_3^2 = 0.69312$	$u_5 = 0.69315$	5.9×10^{-7}	2.5×10^{-5}
6	0.69315	$P_3^3 = 0.69315$	$u_6 = 0.69315$	4.9×10^{-8}	5.3×10^{-6}
7	0.69315	$P_4^3 = 0.69315$	$u_7 = 0.69315$	1.1×10^{-9}	7.6×10^{-7}
8	0.69315	$P_4^4 = 0.69315$	$u_8 = 0.69315$	9.2×10^{-11}	1.5×10^{-7}
9	0.69315	$P_5^4 = 0.69315$	$u_9 = 0.69315$	8.8×10^{-12}	2.3×10^{-8}
10	0.69315	$P_5^5 = 0.69315$	$u_{10} = 0.69315$	3.8×10^{-10}	4.4×10^{-9}
11	0.69315	$P_6^5 = 0.69315$	$u_{11} = 0.69315$	3.6×10^{-10}	6.7×10^{-10}
12	0.69315	$P_6^6 = 0.69315$	$u_{12} = 0.69315$	4.1×10^{-10}	1.3×10^{-10}
13	0.69315	$P_7^6 = 0.69315$	$u_{13} = 0.69315$	1.2×10^{-11}	2.0×10^{-11}
14	0.69315	$P_7^7 = 0.69315$	$u_{14} = 0.69315$	1.3×10^{-11}	3.7×10^{-12}
15	0.69315	$P_8^7 = 0.69315$	$u_{15} = 0.69315$	4.6×10^{-10}	5.9×10^{-13}
16	0.69315	$P_8^8 = 0.69315$	$u_{16} = 0.69315$	5.9×10^{-10}	1.1×10^{-13}
17	0.69315	$P_9^8 = 0.69315$	$u_{17} = 0.69315$	7.5×10^{-10}	1.7×10^{-14}

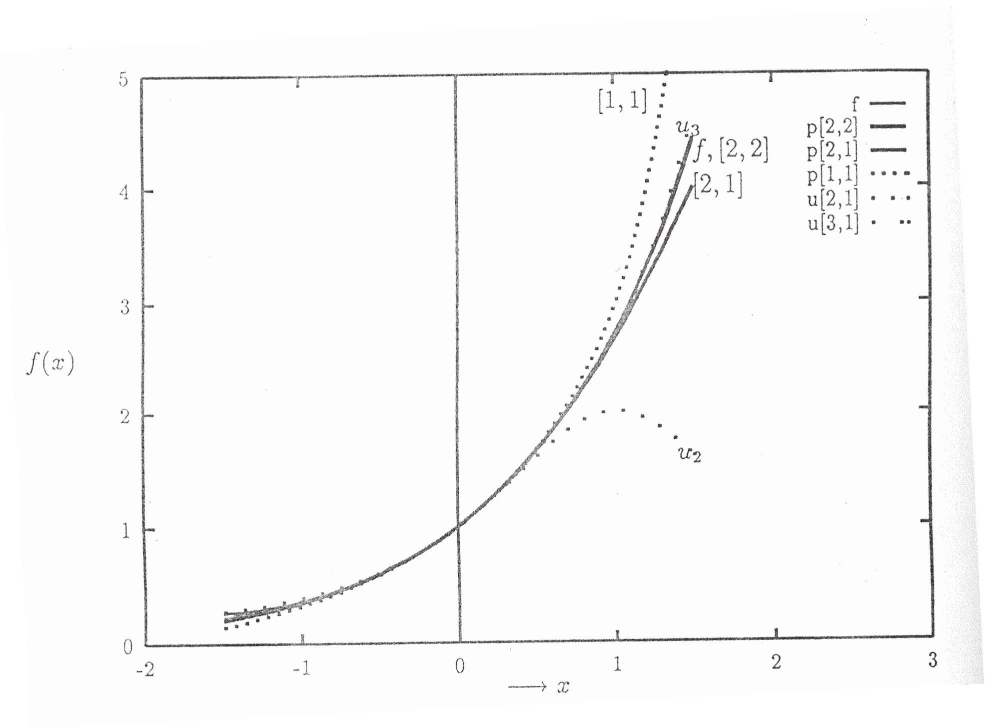

Figure 4.1: Rational approximants for $f(x) = e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$.

the $u-$approximant in the rest of three terms. From overall study we conclude that uAppxs is better representation than the PAppxs for the same number of terms of the series.

4.2 Comparison of the Graphical Representation

Now we make a comparative study of Pade approximants (PAppxs) and u-approximants (uAppxs) with the exact value and/or partial sum as follows.

Case 1: Taking $f(x) = e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$.

The first example is on approximating e^x in the interval $(-\infty, \infty)$. It is well known that in binary arithmetic the problem can be reduced to one of approximating e^x in the finite interval $(-ln2, ln2)$, or approximately $(-0.7, 0.7)$. Figure 4.1 shows the different approximants along with the actual function. It is seen that u_3 represents the function well over almost the entire range $(-1.5, 1.5)$ and is a better representation than the $[2,2]$PAppxs. For calculation of u_3, only four terms of the original series as input we used, whereas to compute $[2,2]$ five terms of the original series are essential. Here we have calculated the exact value of the original series and compared with the different approximants in the given figure 4.1[1]. On the other hand we have observed that u_2 is more divergent than the $[1,1]$PAppxs beyond the range $(-0.7, 0.7)$ which uses the same number of terms. Also it is seen that $[2,1]$PAppxs represents the function well over almost the entire range $(-1.5, 1.5)$ and is therefore, a better representation than u_2 whereas $[2,1]$PAppxs uses the four terms and u_2 uses the three terms of the original series respectively. We thus conclude that $u-$approximants is better representation than the Pade approximants in the given range. The straddling property of PAppxs is not present here as the exponential series is not a Stieltjes series. However, the higher PAppxs approaches the true limit.

Case 2: Taking $f(x) = \frac{1}{x}ln(1+x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n+1}$

The second example is on approximating $\frac{1}{x}ln(1+x)$ in the whole range. Figure 4.2 shows the different approximants along with the actual function. Now, the given series for $\frac{1}{x}ln(1+x)$ converges very slowly for $x < 1$ and diverges for $x > 1$. It is seen that u_3 and $[2,1]$PAppxs represents the function well over almost the entire range $(-1, 2.5)$ and is a better representation than the other approximants, where uses the same number of terms of the given series i.e., needs only four terms. Here we have calculated the exact value of the original series and compared with the different approximants in the given figure 4.2. On the other hand it is seen that for u_2 represents the fucntion well over almost the entire range $(-1, 2.5)$ and is a better representation than the $[1,1]$PAppxs for the same number of terms. Here we have used the exct value of the original series. In

[1]Notice that in figure 4.1, we have calculated the exact value instead of partial sum of actual function. Also we have denoted the exact value by f which used in figure.

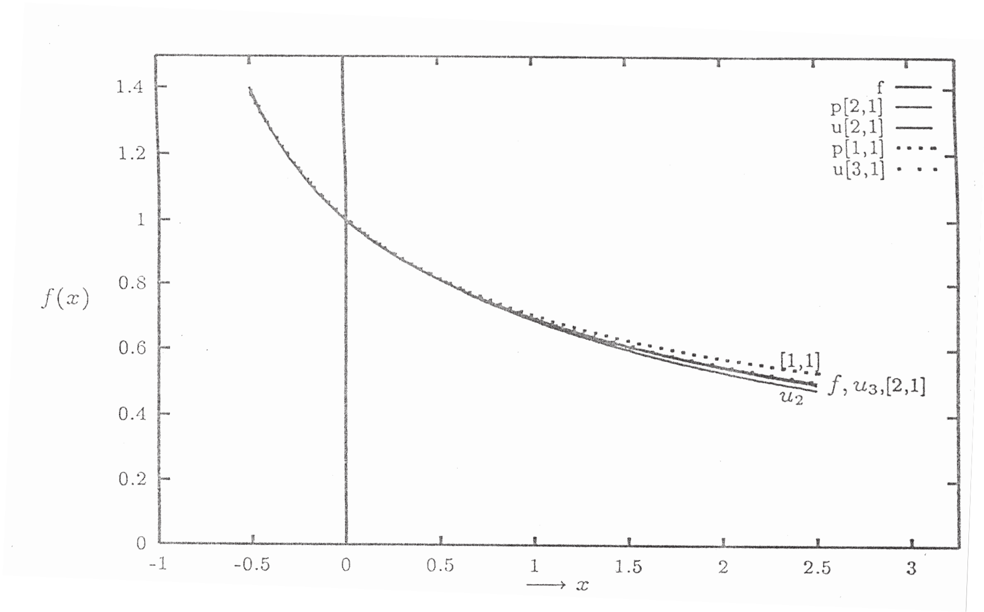

Figure 4.2: Rational approximants for $f(x) = \frac{1}{x}ln(1+x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n+1}$

the figure 4.2[1], f indicates the exact value of the original series. A glance at figure 4.2 confirms that u_3 reproduces the function $\frac{1}{x}ln(1+x)$ over the range $(-1, 2.5)$, i.e., beyond the radius of convergence of the series. Overall we can conclude that $u-$approximants is better representation than the Pade approximants.

Case 3: Taking $f(x) = \int_0^{\infty} \frac{e^{-t}}{1+xt}dt = \sum_{n=0}^{\infty} n!(-x)^n$.

The third example is on approximating $\int_0^{\infty} \frac{e^{-t}}{1+xt}dt$ in the whole range. Series 3 is a divergent Stieltjes series and is obtained by expanding as an infinite power series in t, the function

$$f(x) = \int_A^B \frac{\rho(t)}{1+xt}dt,$$

where $\rho(t)$, t and x are real, and each of the limits A and B $(B > A)$ may be finite or infinite. Taking $\rho(t) = e^{-t}$, the range of integration $(0, \infty)$ and expanding $(1+xt)^{-1}$ one gets Euler's famous series (series 3 of table 3.1). Figure

[1]Notice that in figure 4.2, we have calculated the exact value instead of partial sum of actual function. Also we have denoted the exact value by f which used in figure.

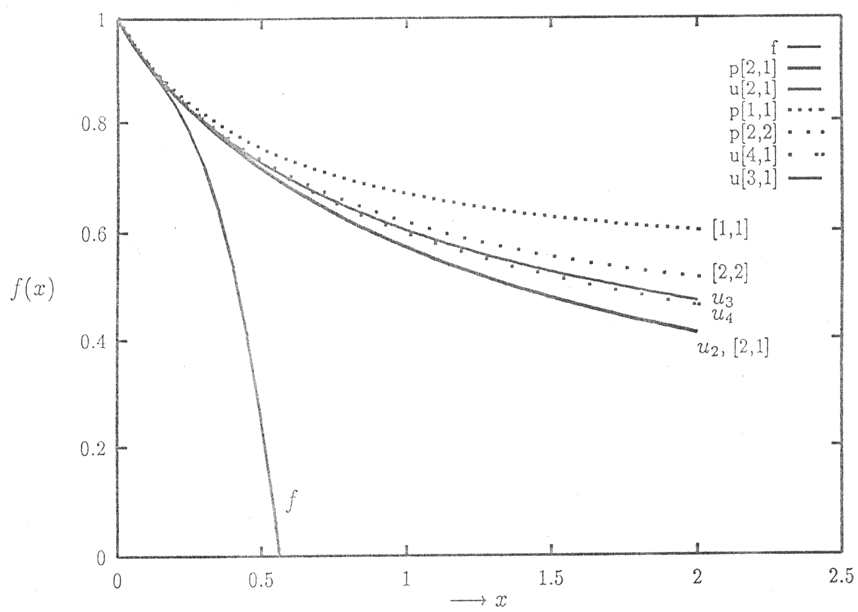

Figure 4.3: Rational approximants for $f(x) = \int_0^\infty \frac{e^{-t}}{1+xt}dt = \sum_{n=0}^\infty n!(-x)^n$.

4.3 shows the different approximants along with the partial sum. It is seen that u_2 and $[2,1]$PAppxs reproduce the same approximants over the interval $(0,2)$, whereas u_2 needs only three terms of the series and $[2,1]$PAppxs needs four terms of the series i.e., one term more than the uAppxs. It is observed that u_3 and u_4 represent the functions well over almost the entire range $(0,2)$ and are better representation than $[2,2]$PAppxs and $[1,1]$PAppxs. Here we use the partial sum of only four terms of the series. The given series is an alternating series, so the partial sums oscilate. In the figure 4.3, f indicates the partial sum upto four terms.

Case 4: Taking $f(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{e^{-t^2/2}}{1-x^2t^2}dt = \sum_{n=0}^\infty (-1)^n \frac{(2n)!}{2^n n!} x^{2n}$.

The fourth example is on approximating $\sqrt{\frac{2}{\pi}} \int_0^\infty \frac{e^{-t^2/2}}{1-x^2t^2}dt$ over the interval $(-\infty, +\infty)$. Series 4 is a divergent Stieltjes series and is obtained by expanding as an infinite power series in x, the function

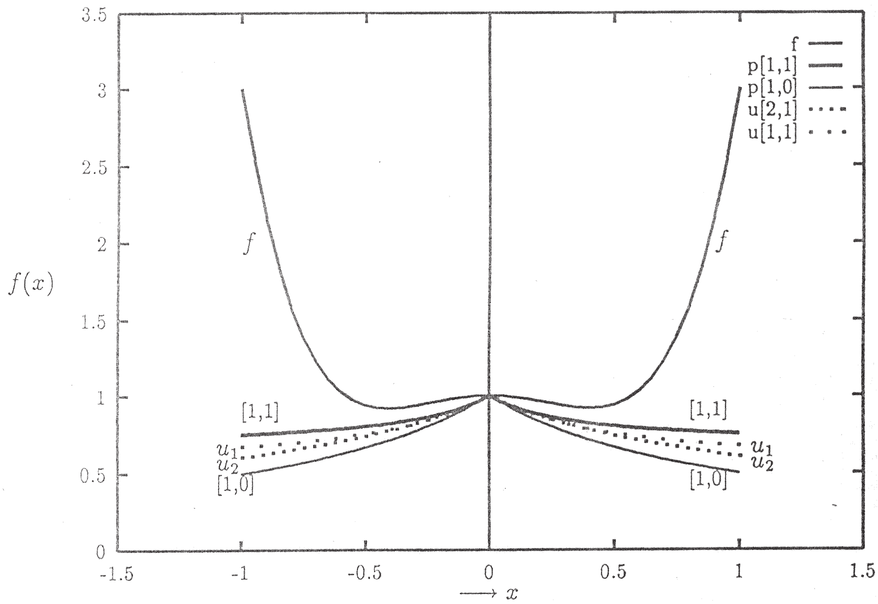

Figure 4.4: Rational approximants for $f(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{e^{-t^2/2}}{1-x^2t^2} dt = \sum_{n=0}^{\infty}(-1)^n \frac{(2n)!}{2^n n!} x^{2n}$.

$$\sqrt{\frac{2}{\pi}} \int_A^B \frac{\rho(t)}{1-x^2t^2} dt,$$

where $\rho(t)$, t and x are real, and each of the limits A and B $(B > A)$ may be finite or infinite. If $\rho(t)$ is an even function of t and the domain of integration $(-\infty, +\infty)$, we can rewrite the integral as

$$f(x) = 2 \int_0^\infty \frac{\rho(t)}{1-x^2t^2} dt.$$

To get series 4 of table 3.1 (in the previous chapter), we take $\rho(t) = \sqrt{\frac{2}{\pi}} e^{-t^2/2}$. The PAppxs $[M, M]$ and $[M, M-1]$ for this case are teh approximants of a special case of Gauss's continued fraction. These approximants bound the exact value from above and below. Figure 4.4 shows the different approximants along with the partial sum. It is seen that u_2 and u_1 are reproduces the different approximants over the range $(-1, 1)$. It is also observed that these two approximants are bounded by the other two Pade approximants $[1, 1]$PAppxs and $[1, 0]$PAppxs. It is decided that u_1 and u_2 represents the functions well over almost the entire

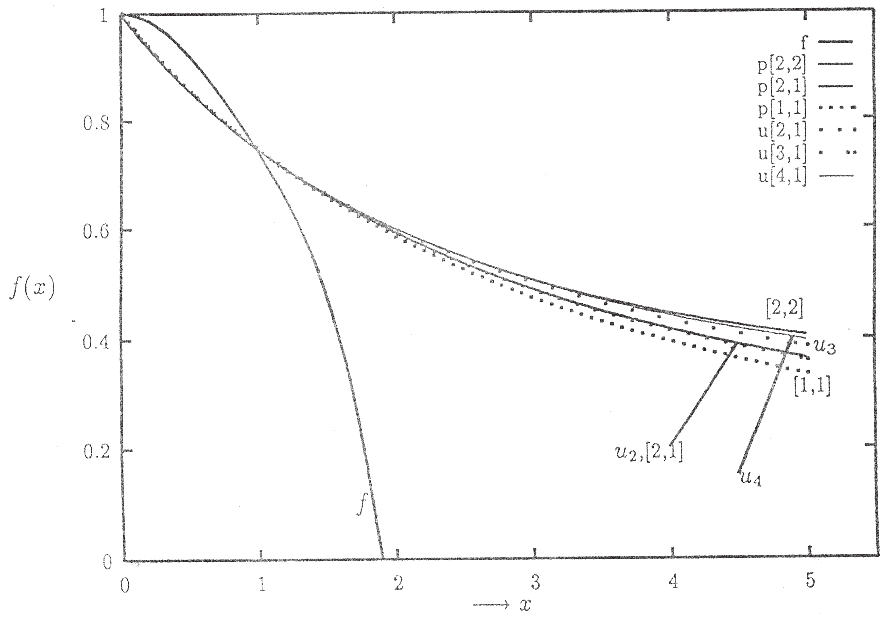

Figure 4.5: Rational approximants for $f(x) = \sqrt{\pi}/2erf(x)/x = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{x^{2n}}{2n+1}$.

range $(-1, 1)$ and the better representations than $[1, 1]$PAppxs and $[1, 0]$PAppxs. Here we use the partial sum of only three terms of the original series. The given series is an alternating series, so the partial sum oscilate. In the figure 4.4, f indicates the partial sum upto three terms.

Case 5. Taking $f(x) = \sqrt{\pi}/2erf(x)/x = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{x^{2n}}{2n+1}$.

Finally we have considered the function $\sqrt{\pi}/2erf(x)/x$ over the interval $(-\infty, +\infty)$. The figure 4.5 shows the different approximants indicated by different lines along with the partial sum. It is seen that u_2 and $[2, 1]$PAppxs represent the function closely well over almost the entire range $(0, 5)$. Here we observe that u_2 needs three terms and $[2, 1]$PAppxs needs four terms of the series. It is also seen that u_3 and u_4 substitute the function well over almost the entire range $(0, 5)$ and are better approximation than $[2, 2]$PAppxs and $[1, 1]$PAppxs. Also we observed that PAppxs needs more terms than the uAppxs of the original series. Here we used the partial sum of only four terms of the series. The given series is an alternating series, so the partial sum oscilate. In the figure 4.5, f indicates the partial sum upto four terms.

It is apparent from the comparison of the two kinds of approximants for these representative convergent and divergent series that, for a given number of terms as input, the uAppxs are, on the whole, significantly better.

Finally, from the above observation we conclude that for the cases we have considered $u-$approximants is the better representation than the Pade approximants.

Conclusions and Discussion

In our work we have established a new method of finding rational approximants of a function from its series expansion by applying the u-transform. We have developed the theory, algorithm and program for approximation of a function by u-transform. We have also reproduced the well-established Pade Approximant for these functions. The new approximants have been compared with the corresponding Pade approximants on some test functions. Given a fixed number of terms of a power series as input, we found that the u-approximant is better representation than the Pade approximant for a wide class of test series. However, the present method is unable to reproduce the poles of a function with the same facility as the Pade approximant but if it is known that a function has only poles and no zeros in a given interval, then the reciprocal of the series can be used to generate the reciprocal of the desired approximant. In certain cases a regrouping of the terms of a given series and the application of the u-transform on the groups separately produces better results. These conclusions are consistent with those reported previously on sequence of numbers.

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