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Legendre Padé approximants and their application in potential scattering

A K Common and T Stacey

Mathematical Institute, Cornwallis Building, University of Kent, Canterbury, Kent CT2 7NF, UK

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Abstract. A generalisation of Padé approximants to Legendre series expansions, previously introduced for series when the coefficients are those of a series of Stieltjes, is extended to the case of more general series. Convergence and other useful properties are described. Comparison with other types of 'Legendre Padé approximants' is made using examples of scattering amplitudes in potential scattering. It is found that the approximants defined here give better results than the other types. Finally the scattering amplitude for the repulsive inverse square potential $V=\lambda/r^2$ is evaluated using the above approximants and the approach to the classical limit as $\lambda\to\infty$ investigated.

1. Introduction

Padé approximants have proved very useful in the evaluation of functions which have power series expansions (for a general survey see Baker 1975), even if these series are only 'formal' in the sense that they converge only at the origin. In many situations, especially in scattering theory it is more usual to expand a function $f(z)$ as a Legendre series

$$f(z)=\sum_{l=0}^{\infty} f_l P_l(z). \tag{1.1}$$

In practice it will usually only be possible to evaluate the first few coefficients of this series. It would be useful if one could define approximants to $f(z)$, in terms of these coefficients in analogy to the Padé approximants to the corresponding power series

$$g(w)=\sum_{l=0}^{\infty} f_l(-w)^l. \tag{1.2}$$

In a previous work (Common 1969) one of the authors did this for the case when $g(w)$ is a 'series of Stieltjes'. Our aim here is to extend these results to more general series. The first step is to show in § 2 how $f(z)$ may be written as the integral of $g(w)$ over a certain contour with a certain weight (depending on z as well as w), even when one or both of the series (1.1) and (1.2) is only 'formal'.

The approximants to $f(z)$ are defined in § 3. It is shown that if $f^{\mathrm{L}}_{n+j/n}(z)$ is the approximant corresponding to the $[n+j/j]$ Padé approximant to $g(w)$, being constructed from the first $2n+j+1$ coefficients of the series, then

$$f(z)-f^{\mathrm{L}}_{n+j/n}(z)=\mathrm{O}(P_{2n+j+1}(z)), \tag{1.3}$$

a property completely analogous to the defining property of the ordinary Padé approximant. We also prove that sequences of $f^{L}_{n+j/n}(z)$ converge to $f(z)$ if corresponding sequences of Padé approximants converge to $g(w)$ in certain domains.

Alternative definitions of 'Legendre Padé approximants' have been given by Holdeman (1969) and Fleischer (1973). Although convergence theorems have not been proved, numerical examples do indicate that they approximate the Legendre series quite well.

In § 4 we will compare the numerical results obtained by Fleischer (1973), with those obtained by using our approximants for the same example. It will be found that on the whole our approximants give better convergence. This is also true when we apply them to evaluating the scattering amplitude for the potential $V(r)=\lambda/r^2$ with $\lambda>0$. Here the comparison is made with the results of Corbella *et al* (1976). This example is particularly interesting since it has been shown that in the limit as the strength λ of the potential tends to infinity, the above scattering amplitude tends to its classical limit (Kayser 1974). In fact our numerical results indicate that even for values of $\lambda \simeq 3$, the scattering amplitude is close to this limit.

In § 5 examples are discussed which show how the singularities of our approximants try to simulate the singularities of the exact function in much the same way as the poles of the Padé approximant simulate the corresponding singularities of the power series.

Finally in § 6, we summarise the results of this work and discuss briefly further developments which will be described in a following paper (Common and Stacey 1978).

2. Legendre series related to power series

It is well known (Kinoshita *et al* 1964) that if the power series

$$g(w)=\sum_{l=0}^{\infty} f_l(-w)^l \tag{2.1}$$

converges in the open disc $|w|<r$ which we denote by C_r and if $r>1$, then the corresponding Legendre series

$$f(z)=\sum_{l=0}^{\infty} f_l P_l(z) \tag{2.2}$$

converges in the domain $\{z\,|\,z=\frac{1}{2}(w+w^{-1}),\ w\in C_r\cap F\}$ where F is the domain $|w|>1$. The above domain of convergence is the elliptical disc E_r with foci at ±1 and having semi-major axis $\frac{1}{2}(r+r^{-1})$. The two functions $g(w)$ and $f(z)$ are holomorphic in their respective domains of convergence. The following result connects the two functions.

Theorem 2.1.

$$f(z)=\frac{1}{2\pi \mathrm{i}}\int_{\Gamma} K(z,w)g(w)\,\mathrm{d}w \tag{2.3}$$

where $K(z,w)=(1+2zw+w^2)^{-1/2}$ and the branch is chosen such that $wK(z,w)\to 1$ as $|w|\to\infty$. Γ here is a closed contour lying completely inside C_r encircling in the positive direction the branch cut P_+P_- of $K(z,w)$ joining the respective branch points

$w = -z \pm (z^2-1)^{1/2}$ as indicated in figure 1. If $g(w)$, as well as being holomorphic in C_r, is continuous in $C_r \cup \partial C_r$ where ∂C_r is the boundary of C_r, then Γ may be replaced in (2.3) by ∂C_r.

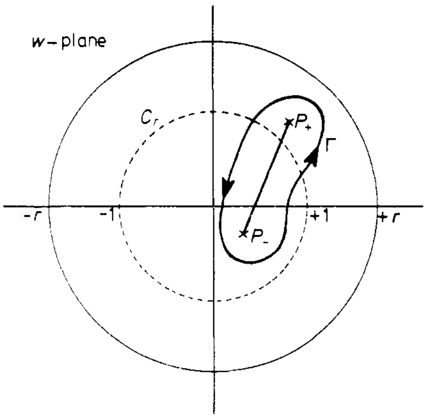

Figure 1. The domain C_r and the integration path Γ in the w-plane.

Proof. The power series expansion for $g(w)$ is valid for all $w \in \Gamma$. Hence

$$\begin{aligned}\frac{1}{2\pi \mathrm{i}}\int_\Gamma K(z,w)g(w)\,\mathrm{d}w \\ &= \frac{1}{2\pi \mathrm{i}}\int_\Gamma K(z,w)\Big(\sum_{l=0}^{\infty} f_l(-w)^l\Big)\,\mathrm{d}w = \frac{1}{2\pi \mathrm{i}}\Big(\sum_{l=0}^{\infty}(-1)^l f_l \int_\Gamma w^l K(z,w)\,\mathrm{d}w\Big) \\ &= \sum_{l=0}^{\infty} f_l \int_0^{\pi} [z+(z^2-1)^{1/2}\cos v]^l\,\mathrm{d}v = \sum_{l=0}^{\infty} f_l P_l(z) = f(z).\end{aligned} \tag{2.4}$$

Here we have evaluated the integrals over Γ by collapsing it around the cut of K and using the discontinuity of K across its cut. It may happen that the domain of holomorphy of $g(w)$ is not a disc C_r but a simply connected domain C, (which may or may not contain the disc C_r), such that if $w \in C \cap F$ then $w^{-1} \in C$ and these two points can be joined by a contour lying completely within C. A typical example is illustrated in figure 2.

We may define $f(z)$ again by (2.3), where the cut of $K(z, w)$ is taken along a straight line joining $w = -z \pm (z^2-1)^{1/2}$ when this lies completely inside C as when these branch points $P_\pm$ are situated as indicated in figure 2. When the branch points are of the type $Q_\pm$ then the cut γ of $K(z, w)$ is to be curved so that it remains completely inside C, the domain of holomorphy of $g(w)$. In either case from the assumed properties of C, and since $[-z+(z^2-1)^{1/2}]^{-1} = [-z-(z^2-1)^{1/2}]$, it is possible to arrange the cut of $K(z, w)$ and also Γ to lie completely inside C.

The following theorem may then be proved.

Theorem 2.2. Let E be the domain $\{z \mid z = \frac{1}{2}(w+w^{-1}),\ w \in C \cap F\}$. Then if $g(w)$ is

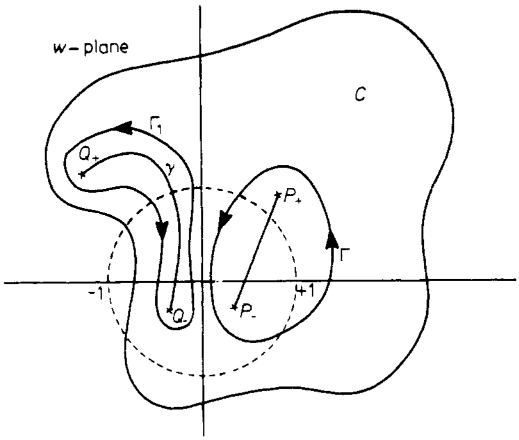

Figure 2. The domain C and integration paths Γ, Γ_1 in the w-plane with the corresponding cuts of $K(z, w)$.

holomorphic in C,

$$f(z) \equiv \frac{1}{2\pi i} \int_{\Gamma} K(z, w) g(w)\, dw \tag{2.5}$$

is holomorphic for $z \in E$ where Γ is chosen as above and is 'formally' at least equal to the Legendre series $\Sigma_{l=0}^{\infty} f_l P_l(z)$. If $g(w)$ is as well continuous in $C \cup \partial C$, then

$$f(z) = \frac{1}{2\pi i} \int_{\partial C} K(z, w) g(w)\, dw. \tag{2.6}$$

Proof. For all $z \in E$, Γ may be continuously deformed so that $K(z, w)$ is a holomorphic function of z for all $w \in \Gamma$. Hence $f(z)$ defined by (2.5) is holomorphic for all $z \in E$. For fixed $z \in E$, $K(z, w)g(w)$ is holomorphic in the domain between Γ and ∂C and is continuous in this domain and on the boundary. Hence

$$\int_{\partial C} K(z, w) g(w)\, dw = \int_{\Gamma} K(z, w) g(w)\, dw$$

and (2.6) follows.

If the power series (2.1) for $g(w)$ is substituted in (2.6) and the order of summation and integration interchanged, then as previously we obtain the Legendre series expansion (2.2) for $f(z)$. However, since the power series to $g(w)$ will not necessarily converge for all $w \in \partial C$, the corresponding Legendre series will not necessarily converge to $f(z)$. In those cases when the series does not converge, we say that $f(z)$ is only 'formally' equal to it.

In Common (1969), the case of a 'series of Stieltjes' was discussed, i.e.

$$g(w) = \int_0^{1/r} \frac{d\phi(u)}{1 + uw} \equiv \sum_{l=0}^{\infty} f_l (-w)^l \tag{2.7}$$

where $\phi(u)$ is a bounded non-decreasing function of u. Then $g(w)$ is holomorphic in the complex plane cut from $-r$ to $-\infty$ and the series (2.7) converges in C_r. Using the procedure above on this particular example it was then proved that for $r>1$,

$$f(z)=\frac{1}{2\pi i}\int_\Gamma K(z, w)g(w)\,dw=\sum_{l=0}^{\infty} f_l P_l(z) \tag{2.8}$$

is holomorphic in the complex z-plane cut from $\frac{1}{2}(r+r^{-1})$ to ∞ and the Legendre series converges to $f(z)$ in E_r.

When $0\leq r\leq 1$, $f(z)$ defined by the left-hand equality in (2.8) is holomorphic in the complex z-plane cut from 1 to ∞. However, in general the Legendre series obtained by substituting the power series expansion for $g(w)$ and then interchanging the order of summation and integration will not converge for any z in the cut plane. This is an example where $f(z)$ is only 'formally' equal to $\Sigma_{l=0}^{\infty} f_l P_l(z)$.

3. Legendre Padé approximants

In Common (1969), 'Legendre Padé approximants' were defined to the series of Stieltjes (2.7), and it was shown that sequences of such approximants converged to $g(w)$ in its domain of holomorphy. However, the definition does not really depend on the fact that $g(w)$ is a 'series of Stieltjes' and we can apply the method to any power series $g(w)$ and corresponding Legendre series $f(z)$.

Let us recall the definition of Padé approximants to $g(w)$.

Definition. The $[m/n]$ Padé approximant to $g(w)$ is a rational function $g_{m/n}(w)$ with numerator of degree m and denominator of degree n such that

$$g_{m/n}(w)\equiv\frac{\Sigma_{j=0}^{m} a_j w^j}{\Sigma_{k=0}^{n} b_k w^k}=g(w)+O(w^{m+n+1}) \tag{3.1}$$

with the normalisation $b_0=1$.

We will find it useful to consider the partial fraction expansion of 'diagonal' sequences

$$g_{n+j/n}(w)=\sum_{p=1}^{n}\frac{\alpha_p}{1+\sigma_p w}+\sum_{q=0}^{j}\beta_q(-w)^q \tag{3.2}$$

where j is a fixed integer. If j is negative then here and in the following discussion the second sum on the right-hand side of (3.2) is absent.

The defining relation (3.1) then requires

$$\begin{aligned}&\sum_{p=1}^{n}\alpha_p\sigma_p^r+\beta_r=f_r \qquad && r=0,1,\ldots,j\\ &\sum_{p=1}^{n}\alpha_p\sigma_p^r=f_r && r=j+1, j+2,\ldots,2n+j\end{aligned} \tag{3.3}$$

where the f_r are the coefficients in the power series expansion (1.2) of $g(w)$.

In our definition of 'Legendre Padé approximants' to the Legendre series (2.2) we use (2.3) in the following way.

Definition. The $[n+j/n]$ 'Legendre Padé approximant' to

$$f(z)=\frac{1}{2\pi i}\int_\Gamma K(z, w)g(w)\,dw \tag{3.4}$$

is

$$f^L_{n+j/n}(z)=\frac{1}{2\pi i}\int_\Gamma K(z, w)g_{n+j/n}(w)\,dw, \tag{3.5}$$

where $g_{n+j/n}(w)$ is the corresponding $[n+j/n]$ Padé approximant to $g(w)$ and Γ is taken sufficiently close to the cut of $K(z, w)$, so that it does not enclose any of the poles of the Padé approximant except those lying on the cut of $K(z, w)$. The cut of $K(z, w)$ may be adjusted so that in fact no poles of $g_{n+j/n}$ lie on it. An explicit representation for the 'Legendre Padé approximant' may be derived by by using the partial fraction expansion (3.2) for $g_{n+j/n}(w)$.

Theorem 3.1. For $n=0, 1, \ldots, j=0, \pm1, \pm2, \ldots,$

$$\begin{aligned} f^L_{n+j/n}(z) &= -\sum_{p=1}^{n}\frac{\alpha_p}{\sigma_p}K(z, -\sigma_p^{-1})+\sum_{q=0}^{j}\beta_q P_q(z) \\ &= \sum_{p=1}^{n}\frac{\alpha_p}{(1-2\sigma_p z+\sigma_p^2)^{1/2}}+\sum_{q=0}^{j}\beta_q P_q(z), \end{aligned} \tag{3.6}$$

where the branch of the square root is that which is real positive when the argument is real positive.

Proof. Consider the integral around the contour illustrated in figure 3 made up of four parts, Γ, Γ_2, Γ_1 and Γ_3. Since by construction there are no poles of $g_{n+j/n}(w)$ in the region enclosed by Γ, the large contour may be made to enclose all the poles of $g_{n+j/j}(w)$ by taking Γ_1 sufficiently large. In that case by the residue theorem

$$\frac{1}{2\pi i}\int_{\Gamma+\Gamma_2+\Gamma_1+\Gamma_3} K(z, w)\Big(g_{n/n+j}(w)-\sum_{q=0}^{j}\beta_q(-w)^q\Big)\,dw=-\sum_{p=1}^{n}\frac{\alpha_p}{\sigma_p}K\Big(z, -\frac{1}{\sigma_p}\Big) \tag{3.7}$$

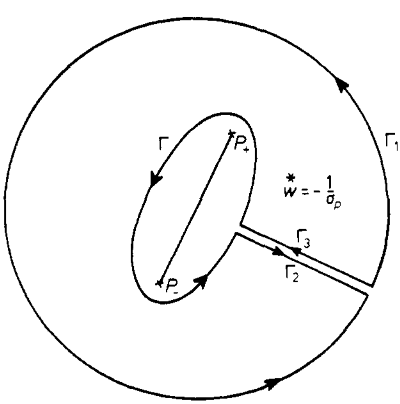

Figure 3. The contour for evaluating $f^L_{n+j/n}(z)$ and a specimen pole of $g(w)$.

On the left-hand side the integrals over Γ_3, Γ_2 cancel and by expanding Γ_1 to infinity the integral over this contour also vanishes. Hence

$$f^{L}_{n+j/n}(z)=\frac{1}{2\pi i}\int_{\Gamma} K(z,w)\Big(g_{n+j/n}(w)-\sum_{q=0}^{j}\beta_q(-w)^q\Big)\,dw$$
$$+\frac{1}{2\pi i}\int_{\Gamma} K(z,w)\sum_{q=0}^{j}\beta_q(-w)^q\,dw$$
$$=-\sum_{p=1}^{n}\frac{\alpha_p}{\sigma_p}K\Big(z,-\frac{1}{\sigma_p}\Big)+\sum_{q=0}^{j}\beta_q P_q(z).$$

The representation (3.6) of our approximants shows that they are closely related to 'generalised Padé approximants' whose properties have been described by Baker (1975, chapter 19). In fact when $g(w)$ is a 'series of Stieltjes', our approximants are identical to the above approximants as may be seen from the expressions (3.11) for the exact function $f(z)$ and (3.6) for $f^{L}_{n+j/n}(z)$.

An interesting property of our approximants which was not discussed previously is an anology of the defining property (3.1) of the Padé approximant $g_{n+j/n}(z)$.

Theorem 3.2.

$$f^{L}_{n+j/n}(z)=f(z)+O(P_{2n+j+1}(z)). \tag{3.8}$$

Proof. Using the standard expansion for $(1-2\sigma_p z+\sigma_p^2)^{-1/2}$ in (3.6), and the relations (3.3),

$$f^{L}_{n+j/n}(z)=\sum_{p=1}^{n}\alpha_p\sum_{l=0}^{\infty}\sigma_p^l P_l(z)+\sum_{q=0}^{j}\beta_q P_q(z)$$
$$=\sum_{l=0}^{j}\Big(\sum_{p=1}^{n}\alpha_p\sigma_p^l+\beta_l\Big)P_l(z)+\sum_{l=j+1}^{2n+j}P_l(z)\sum_{p=1}^{n}\alpha_p\sigma_p^l+O(P_{2n+j+1}(z))$$
$$=\sum_{l=0}^{j}f_lP_l(z)+\sum_{l=j+1}^{2n+j}f_lP_l(z)+O(P_{2n+j+1}(z))$$
$$=f(z)+O(P_{2n+j+1}(z)). \tag{3.9}$$

Alternative methods of defining 'Legendre Padé approximants' give approximants which have the property (3.8) in analogy to the Padé approximants. However, our method has the advantage that if the Padé approximants converge uniformly to $g(w)$ in a domain with the required properties then our approximant $f^{L}_{n+j/n}(z)$ will converge uniformly to $f(z)$ in a corresponding domain in the complex z-plane.

Theorem 3.3. Suppose that C is a simply connected domain in the complex w-plane such that if $w\in C\cap F$ (where F is the domain $|w|>1$) then $w^{-1}\in C$ and these two points can be joined by a contour lying completely within C.

If the Padé approximants $g_{n+j/n}(w)\to g(w)$ uniformly in C as $n\to\infty$ for fixed $j=0,\pm1,\pm2,\ldots$, then $f^{L}_{n+j/n}(z)\to f(z)$ uniformly in the domain E, $\{z\,|\,z=\frac{1}{2}(w+w^{-1}),\ w\in C\cap F\}$ where $f(z)$ is the function whose Legendre series expansion (2.2) has the same coefficients as the power series expansion (2.1) of $g(z)$.

Proof. By definition

$$f^{\mathrm{L}}_{n+j/n}(z)=\frac{1}{2\pi \mathrm{i}}\int_\Gamma K(z,w)g_{n+j/n}(w)\,\mathrm{d}w$$

and for all $z\in E$ we may choose Γ to lie completely inside C. Then since $g_{n+j/n}(w)$ converges uniformly to $g(w)$ for $w\in C$,

$$\lim_{n\to\infty} f^{\mathrm{L}}_{n+j/n}(z)$$

$$=\frac{1}{2\pi\mathrm{i}}\int_\Gamma K(z,w)\lim_{n\to\infty} g_{n+j/n}(w)\,\mathrm{d}w \qquad j=0,\pm1,\pm2,\dots$$

$$=\frac{1}{2\pi\mathrm{i}}\int_\Gamma K(z,w)g(w)\,\mathrm{d}w=f(z). \tag{3.10}$$

The convergence is uniform for $z\in E$.

The special case when $g(w)$ is a 'series of Stieltjes',

$$g(w)=\int_0^{1/r}\frac{\mathrm{d}\phi(u)}{1+uw}$$

was considered previously (Common 1969). It was shown that the sequences $f^{\mathrm{L}}_{n/n+j}$ of approximants to

$$f(z)=\frac{1}{2\pi\mathrm{i}}\int_\Gamma K(z,w)g(w)\,\mathrm{d}w=\int_0^{1/r}\frac{\mathrm{d}\phi(u)}{(1-2uz+u^2)^{1/2}} \tag{3.11}$$

converge uniformly for fixed $j\geqslant -1$ as $n\to\infty$ in any finite closed region of the complex plane cut from $\frac{1}{2}(r+r^{-1})$ to ∞ when $r>1$ and cut from 1 to ∞ when $0\leqslant r\leqslant 1$ so long as $\Sigma_{n=0}^{\infty}(f_n)^{-1/(2n+1)}$ diverges. This result is equivalent to theorem (3.3) for this particular type of series. It often happens that one wishes to deal with a Legendre series.

$$f(z)=\sum_{l=0}^{\infty}(2l+1)f_lP_l(z). \tag{3.12}$$

The corresponding power series is

$$h(z)\equiv\sum_{l=0}^{\infty}(2l+1)f_l(-z)^l=\left(g(z)+2z\frac{\mathrm{d}g}{\mathrm{d}z}\right). \tag{3.13}$$

Again we may derive the relation

$$f(z)=\frac{1}{2\pi\mathrm{i}}\int_\Gamma K(z,w)\left(g(w)+2w\frac{\mathrm{d}g}{\mathrm{d}w}\right)\mathrm{d}w, \tag{3.14}$$

and show that $f(z)$ indeed has the Legendre series expansion (3.12) which again may be only 'formal'. The 'Legendre Padé approximants' in this case are defined to be

$$f^{\mathrm{L}}_{n+j/n}(z)=\frac{1}{2\pi\mathrm{i}}\int_\Gamma K(z,w)\left(g_{n+j/n}(w)+2w\frac{\mathrm{d}g_{n+j/n}(w)}{\mathrm{d}w}\right)\mathrm{d}w.$$

On using the partial fraction expansion (3.2) for $g_{n+j/n}(z)$, we find†

$$f^{\mathrm{L}}_{n+j/n}(z)=\sum_{p=1}^{n}\frac{\alpha_p(1-\sigma_p^2)}{(1-2z\sigma_p+\sigma_p^2)^{3/2}}+\sum_{q=0}^{j}(2q+1)\beta_qP_q(z) \tag{3.15}$$

† Let us remind the reader that if j is negative the second sum on the right-hand side of (3.15) is absent.

where again we take the branch of the square root which is positive when the argument is positive real.

It is straightforward to prove that these approximants again satisfy (3.8) and have the convergence properties given by theorem 3.3.

4. Comparison with other types of 'Legendre Padé approximants'

The defining equation for Padé approximants was given in § 3 and may be written

$$g(w)-\frac{p_m(w)}{q_n(w)}=\mathrm{O}(w^{n+m+1}). \tag{4.1}$$

where p_m is the numerator and q_n the denomintor of $g_{m/n}(w)$. This relation is equivalent to the requirement that

$$g(w)q_n(w)-p_m(w)=\mathrm{O}(w^{n+m+1}). \tag{4.2}$$

In the corresponding case of Legendre series $f(z)=\Sigma_{l=0}^{\infty} f_l P_l(z)$, Holdeman (1969) has defined the $[m/n]$ 'Legendre Padé approximant' to $f(z)$ to be given by the requirement analogous to (4.2), that

$$f(z)q_n(z)-p_m(z)=\mathrm{O}(P_{n+m+1}(z)) \tag{4.3}$$

where $q_n(z)=\Sigma_{r=0}^{n} b_r P_r(z)$ and $p_m(z)=\Sigma_{s=0}^{m} a_s P_s(z)$ are respectively the denominator and numerator of the approximant.

Alternatively Fleischer (1973) has suggested that the $q_n(z)$ and $p_m(z)$ can be determined by the requirement analogous to (4.1), i.e.

$$f(z)-\frac{p_m(z)}{q_n(z)}=\mathrm{O}(P_{n+m+1}(z)). \tag{4.4}$$

Unlike the case of ordinary Padé approximants, the 'Legendre Padé approximants' defined from (4.3) are different from those defined by (4.4). The former have been called 'linear' by Fleischer since (4.3) leads to a set of linear equations for the coefficients $\{a_s;\ s=0,\ldots,m\}$ and $\{b_r;\ r=0,1,\ldots,n\}$, while the latter have been called 'non-linear' since they lead to a set of non-linear equations for these coefficients. It is not guaranteed that the latter set of equations has a solution, but for the examples treated by Fleischer this indeed was the case and the 'non-linear approximants' gave better numerical results than the 'linear approximants'.

An example considered by the above author was the function

$$\begin{aligned} f(z)&=\ln\left(\frac{1-az}{1-a}\right)\\ &=\left(Q_0\left(\frac{1}{a}\right)+Q_1\left(\frac{1}{a}\right)\right)P_0(z)+\sum_{l=1}^{\infty}\left(Q_{l+1}\left(\frac{1}{a}\right)-Q_{l-1}\left(\frac{1}{a}\right)\right)P_l(z). \end{aligned} \tag{4.5}$$

This function is holomorphic in the complex z-plane cut from $1/a$ to ∞ and the particular value $1/a=1{\cdot}816$ was used. Using the f_l up to and including $l=6$, the [2/2] 'linear' approximant and the [3/3] 'non-linear' can be evaluated. In table 1 the values of these approximants (as taken from Fleischer 1973) are given in the third and fourth column for various real values of z. From these same coefficients we may evaluate our approximant $f^{\mathrm{L}}_{3/3}(z)$, the results being given in the fifth column while for

Table 1. Approximants to ln $[(1-az)/(1-a)]$.

z	Partial sum	Linear approximant	Non-linear approximant	$f^{L}_{3/3}(z)$	$f(z)$
−3·5		1·865	1·872 7	1·873 1	1·873 4
−1·75	1·42	1·473 5	1·474 13	1·474 15	1·474 156
−1·0	1·237 97	1·238 06	1·238 078 3	1·238 078 36	1·238 078 42
−0·5	1·042 62	1·042 655	1·042 653 57	1·042 653 61	1·042 653 64
0·0	0·799 537	0·799 521	0·799 527 67	0·799 527 62	0·799 527 58
0·5	0·477 65	0·477 65	0·477 627 52	0·477 627 54	0·477 627 55
1·0	0·000 20	0·000 18	0·000 001 3	0·000 000 6	0·0
1·5	−0·854	−0·907	−0·942	−0·945	−0·947
1·75	−1·57	−1·90	−2·24	−2·33	−2·51

comparison in the last column of table 1 we give the exact values of $f(z)$ and in the second column give the partial sum of the series.

It will be seen that the partial sum is a quite reasonable approximation well inside the convergence domain of the series, but is no use near the cut of $f(z)$ or outside this domain. The three types of 'Legendre Padé approximants' give better results, and the best approximation is given by our approximant $f^{L}_{3/3}(z)$.

Another interesting application of the 'linear Legendre approximants' has been made by Corbella *et al* (1976) who have used them to sum the partial wave expansion of the scattering amplitude for a repulsive inverse square potential. Potentials of this type are involved in elastic e–H scattering, near the inelastic threshold (Geltman 1969) and sometimes hundreds of terms are needed to get good estimates for the scattering amplitude.

The partial wave expansion for the potential $V=\lambda r^{-2}$ with $\lambda>0$ may be obtained explicitly (Cobella *et al* 1976) and is

$$f(\cos\theta)=\frac{1}{k}\sum_{l=0}^{\infty} f_l P_l(\cos\theta) \tag{4.6}$$

where

$$f_l=(2l+1)\,\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l$$

and

$$\delta_l=\frac{\pi}{2}\left[l+\tfrac{1}{2}-\left((l+\tfrac{1}{2})^2+\frac{\lambda}{\hbar^2}\right)^{1/2}\right]. \tag{4.7}$$

Also $\hbar k$ is the momentum of the scattered particles which are taken to be of unit mass. Corbella *et al* (1976) evaluated the 'diagonal' linear approximants

$$\{m/m\}=\frac{\sum_{s=0}^{m} a_s P_s(z)}{\sum_{r=0}^{m} b_r P_r(z)} \tag{4.8}$$

defined by the requirement (4.3), for various values of $z=\cos\theta$ and m, taking $\lambda=\hbar^2$ and $k=10$. It should be noted that the first $(3m+1)$ coefficients of the partial wave series are needed to construct this approximant, whilst we only need $(2m+1)$ coefficients to construct our corresponding approximant $f^{L}_{m/m}(z)$. The above authors found for the values of z considered that to obtain a 10% relative accuracy for $|f(\theta)|^2$

Table 2. Approximants to the scattering amplitude for potential $V(r)=\lambda r^{-2}$.

Number of coefficients	$\theta=4°$				$\theta=18°$				$\theta=58°$			
	$\mathrm{Re} f^{L}_{m/m}$	$\mathrm{Im} f^{L}_{m/m}$	$\mathrm{Re}\{m/m\}$	$\mathrm{Im}\{m/m\}$	$\mathrm{Re} f^{L}_{m/m}$	$\mathrm{Im} f^{L}_{m/m}$	$\mathrm{Re}\{m/m\}$	$\mathrm{Im}\{m/m\}$	$\mathrm{Re} f^{L}_{m/m}$	$\mathrm{Im} f^{L}_{m/m}$	$\mathrm{Re}\{m/m\}$	$\mathrm{Im}\{m/m\}$
3	0·21	0·64			−0·21	0·33			−0·0386	0·078		
5	−1·96	0·83			−0·330	0·202			−0·03831	0·0821		
7	−2·02	0·48	−1·26	0·10	−0·3373	0·1969	−0·37	0·22	−0·03823	0·08196	−0·03817	0·0815
9	−2·049	0·41			−0·3370	0·1982			−0·03824	0·08197		
11	−2·059	0·385			−0·3368	0·1983			−0·03824	0·08197		
13	−2·063	0·3780	−2·12	0·32	−0·3368	0·1983	−0·3364	0·1985			−0·03824	0·08197
15	−2·064	0·3769										
17	−2·064	0·3773										
19	−2·064	0·3775	−2·20	0·40			−0·3367	0·1982			−0·03824	0·08197
21	−2·064	0·3776										
23	−2·064	0·3774										
25	−2·064	0·3779	−2·12	0·40			−0·3368	0·1983				
27	−2·064	0·3779										
29	−2·064	0·3780										
31	−2·064	0·3778	−2·085	0·389								
33	−2·064	0·3780										
35	−2·064	0·3780										
37			−2·063	0·389								
39												
41												
43			−2·066	0·380								
45												
47												
$f(\cos\theta)$			−2·064	0·3780			−0·3368	0·1983			−0·03824	0·08197

only about 20 terms of the partial wave series were needed when the approximants $\{m/m\}$ were used as compared with about 2000 terms of the series if summed directly.

In table 2 we compare the above results, with those obtained from $f^{\mathrm{L}}_{m/m}(z)$ using the same number of coefficients. In the last row are given the 'exact' values of $f(\cos\theta)$, which were in fact obtained by summing directly the partial waves series and taking more and more terms until stability was obtained. It will be seen that our approximants given appreciably better results than the 'linear' approximants, and in many cases only half the number of coefficients is needed to given comparable accuracy.

The classical cross section for scattering by the inverse square potential is linear in the strength of the potential, while from the Born approximation to the quantum mechanical amplitude one might expect it to be quadratic. Kayser (1974) has discussed this apparent contradiction by showing that for the conditions under which quantum scattering becomes classical, the Born approximation is not valid. His result is essentially that the classical limit is approached as λ becomes large, whilst the power series in λ for the scattering amplitude converges and hence the Born approximation can be used only when $|\mu\lambda| < \hbar^2/4$ where μ is the mass of the particle being scattered. It is interesting to see how quickly the classical limit is reached as λ is increased above these values.

We have therefore used our approximants to calculate $f^{\mathrm{L}}_{m/m}(\cos\theta)$ and hence

$$\frac{\mathrm{d}\sigma_{m/m}(\cos\theta)}{\mathrm{d}\Omega} \equiv |f^{\mathrm{L}}_{m/m}(\cos\theta)|^2 \tag{4.9}$$

and compared with the classical cross section†

$$\frac{\mathrm{d}\sigma_{\mathrm{cl}}}{\mathrm{d}\Omega} = \frac{\lambda}{\pi k^2}\left(1-\frac{\theta}{\pi}\right)\left[\left(\frac{\theta}{\pi}\right)^2\left(2-\frac{\theta}{\pi}\right)^2 \sin\theta\right]^{-1} \tag{4.10}$$

for various values of λ and for $\theta = 18°, 180°$.

The results are given in table 3 and it will be seen that as λ is increased higher-order approximants are needed to get equivalent accuracy. Assuming that the highest approximant in each column gives a close approximant to the quantum mechanical

Table 3. $\mathrm{d}\sigma_{m/m}(\cos\theta)/\mathrm{d}\Omega$ corresponding to potential $V(r) = \lambda r^{-2}$ for a selection of coupling strengths and scattering angles θ.

θ	m \ λ	0·1	0·2	1	3	10	30	100
18°	4	0·236	1·89	15·28	74·3			
	5	0·236	1·89	15·27	74·0	269	40	
	10					264	769·6	823
	15					264	769·5	2540
	$\mathrm{d}\sigma_{\mathrm{cl}}/\mathrm{d}\Omega$	2·57	7·70	25·7	77·0	257	770·4	2568
180°	4	0·004	0·024	0·100	0·301			
	5	0·004	0·024	0·100	0·301	1·010	3·4	
	10					1·010	3·04	
	15					1·010	3·04	
	$\mathrm{d}\sigma_{\mathrm{cl}}/\mathrm{d}\Omega$	0·010	0·030	0·101	0·304	1·013	3·04	

† In units where $\hbar = \mu = 1$.

cross section for the given value of λ, we see that this is close to the classical amplitude for $\lambda \geqslant 3$ near the forward direction and for $\lambda \geqslant 1$ in the backward direction. So the classical limit is obtained for quite moderate values of λ.

5. The singularities of the Legendre Padé approximants

It is a well known property that the singularities (poles) of the Padé approximants to a function $g(w)$ in practice try to give a representation of the singularities of $g(w)$ by lying close to these singularities. So the Padé approximants tend to have no poles well inside domains of analyticity of $g(w)$, except for spurious pole-zero pairs.

From the discussion in §§ 2, 3 especially, the representation

$$f(z)=\frac{1}{2\pi i}\int_{\Gamma} K(z, w)g(w)\,dw \tag{2.3}$$

for the Legendre series $f(z)$ corresponding to the power series, and from the defining relation for our approximants, i.e.

$$f^{L}_{n+j/n}(z)=\frac{1}{2\pi i}\int_{\Gamma} K(z, w)g_{n+j/n}(w)\,dw, \tag{3.5}$$

we would then expect the singularities of our approximants, which are branch cuts, to approximate the singularities of the exact function $f(z)$.

In practice, this does turn out to be a generally held property of our approximants. For example, in Common and Stacey (1978), we will consider the Coulomb scattering amplitude (Landau and Lifshitz 1958),

$$f_c(z)=-\frac{2^{i/k}}{k^2}(1-z)^{-1-i/k}\frac{\Gamma(1+i/k)}{\Gamma(1-i/k)} \tag{5.1}$$

where $\hbar k$ is the momentum of the scattered particles and z is the cosine of the scattering angle. This amplitude has the partial wave expansion

$$f_c(z)=\sum_{l=0}^{\infty}(2l+1)\,e^{i\delta_l}\sin\delta_l P_l(z), \tag{5.2}$$

where

$$e^{2i\delta_l}=\frac{\Gamma(l+1+i/k)}{\Gamma(l+1-i/k)}. \tag{5.3}$$

To be precise the series on the right-hand side of (5.2) does not converge point-wise but does converge in the sense of a distribution (Taylor 1974).

The amplitude $f_c(z)$ is holomorphic in the complex z-plane cut from 1 to ∞. In table 4, we give the branch point singularities $z_p=\frac{1}{2}(\sigma_p+\sigma_p^{-1})$ of the [6/6] 'Legendre Padé approximant' to $f_c(z)$. Corresponding to each point there is a branch cut along the line which is the set of points,

$$\{z(\lambda);\, z(\lambda)=\tfrac{1}{2}(\sigma_p+\lambda/\sigma_p),\, \lambda\geqslant 1\}.$$

It will be seen that the singularities do represent the cut of $f_c(z)$ along the positive real axis. Also in table 4 are given the strengths α_p of the branch cuts of the approximant, and it will be seen that the last branch point which is furthest away from the real axis gives a weak singularity.

Table 4. Branch points and strengths of the cuts of the [6/6] Legendre Padé approximant to the Coulomb scattering amplitude.

$\frac{1}{2}(\sigma_p+\sigma_p^{-1})$	α_p
0·999 86 − 0·000 02i	−3·0 + 0·4i
1·000 05 − 0·000 000i	+2·8 − 0·5i
1·01 − 0·000 5i	$O(10^{-1})$
1·14 − 0·002i	$O(10^{-2})$
1·69 − 0·008i	$O(10^{-2})$
4·7 − 0·4i	$O(10^{-3})$

Another amplitude treated by Corbella *et al* (1976) is that corresponding to the delta-shell potential

$$V=-\frac{g}{a}\delta(r-a).$$

In that case the scattering amplitude $f(z)$ and the corresponding power series $g(w)$ are entire functions, i.e. have no singularities excapt at ∞. For such functions the poles of the Padé approximants migrate to infinity as the order of the approximant increases, and in a similar way we find that the branch points of our Legendre Padé approximants to $f(z)$ also migrate to infinity.

Finally, when $g(w)$ is a 'series of Stieltjes' the poles of its Padé approximants all lie precisely on the cut of $g(w)$. We will show that our approximants to the corresponding Legendre series $f(z)$ have a similar property. Let

$$g(w)=\int_0^{1/r}\frac{d\phi(u)}{1+uz}$$

where $\phi(u)$ has the usual properties. As the poles of $g_{n+j/n}(w)$ lie on $[0, 1/r]$ it follows from (3.2) that

$$0\leqslant\sigma_p\leqslant 1/r \qquad p=1,2,\ldots,n. \tag{5.4}$$

The cuts of the corresponding approximant $f^{L}_{n+j/n}(z)$ run along the real axis from $z_p=\frac{1}{2}(\sigma_p+\sigma_p^{-1})$ to ∞. It is straightforward to prove using (5.4) that these cuts are contained in the cut of $f(z)$ which runs from $\frac{1}{2}(r+r^{-1})$ to infinity when $r\geqslant 1$ and from one to infinity when $0\leqslant r\leqslant 1$.

6. Conclusions

We believe that our 'Legendre Padé approximants' defined in § 3 form a simple and natural generation of ordinary Padé approximants. In the previous sections we have shown that the two types of approximant have many properties in common, and have in particular corresponding domains of convergence.

In the numerical examples presented here, our approximants usually gave better results than the other types of 'Legendre Padé approximants' discussed in Fleischer (1973). The latter type have the big drawback that no convergence theorems have been proved for them.

In a following paper (Common and Stacey 1978) we will continue the study of convergence theorems for our approximants. We will prove that for a variety of potentials including the very important Coulomb potential, our approximants to the scattering amplitude converge in the domain of holomorphy of this amplitude.

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