

The application of Padé approximants to Wiener–Hopf factorization

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The key step in the solution of a Wiener–Hopf equation is the decomposition of the Fourier transform of the kernel, which is a function of a complex variable, α say, into a product of two terms. One is singularity and zero free in an upper region of the α -plane, and the other singularity and zero free in an overlapping lower region. Each product factor can be expressed in terms of a Cauchy-type integral formula, but this form presents difficulties due to the speed of its evaluation and numerical problems caused by singularities near the integration contour. Other representations are available in special cases, for instance an infinite product form for meromorphic functions, but not in general. To overcome these problems, several approximate methods for decomposing the transformed kernels have been suggested. However, whilst these offer simple explicit expressions, their forms tend to have been derived in an ad hoc fashion and to date have only mediocre accuracy (of order one per cent or so).

A new method for approximating Wiener–Hopf kernels is offered in this article which employs Padé approximants. These have the advantage of offering very simple approximate factors of Fourier transformed kernels which are found to be extremely accurate for modest computational effort. Further, the derivation of the factors is algorithmic and therefore requires little effort, and the Padé number is a convenient parameter with which to reduce errors to within set target values. The paper demonstrates the efficacy of the approach on several model kernels, and numerical results presented herein confirm theoretical predictions regarding convergence to the exact results, etc. The relationship between the present method and earlier approximate schemes is discussed.

1. Introduction

The Wiener–Hopf technique (Noble, 1988) has proved remarkably useful in solving an enormous variety of model problems in a wide range of branches of physics and engineering. These areas cover fracture mechanics (Atkinson, 1977) through wave diffraction (electromagnetic (Carlson & Heins, 1947a,b); acoustic (Rawlins, 1975); water (Abrahams & Wickham, 1991)) to geophysical problems (Hsieh & Buchwald, 1985) to name but a few. The method offers an exact solution to a class of integral equations formed by application of Fourier (or other) transforms to physical boundary-value problems which have two-part boundary conditions on an infinite line. It has much wider applicability than to just two-part boundary problems when employed in an asymptotic solution scheme; then the ‘inner’ or ‘outer’ problem geometries often simplify to allow the application of this technique (Keller, 1953; Abrahams & Wickham, 1992).

This article will address a crucial step in the Wiener–Hopf technique and for brevity

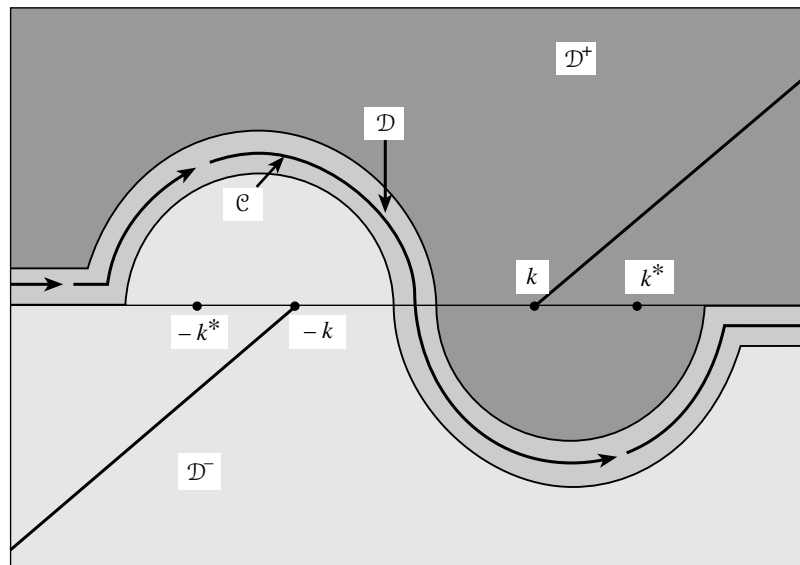


FIG. 1. Typical singularities of a Wiener–Hopf kernel, $K(\alpha)$, and its strip of analyticity, \mathcal{D} . The regions \mathcal{D}^\pm are the extensions of \mathcal{D} into the upper, lower half-planes respectively.

will not cover the complete procedure from Fourier transformation of the boundary-value problem to the solution. The reader is referred to the book by Noble (1988) or any of the articles cited above for a description of the scheme. The point at issue here is the factorization in the complex plane of the Fourier symbol, or Fourier transform of the kernel appearing in the Wiener–Hopf integral equation. Referring to this quantity here and henceforth merely as the kernel, $K(\alpha)$, for brevity, it has singularities in the complex transform plane, α say, which are related to key elements of the physical problem. The kernel is arranged to be singularity and zero free in a strip of the complex α -plane running from $-\infty$ to $+\infty$; the strip, of finite width, usually contains the real line at $\pm\infty$ but need not be straight sided, as shown in Fig. 1 with a typical singularity structure of kernel. Note that the final solution of a Wiener–Hopf problem is expressed as an inverse Fourier integral with integration path \mathcal{C} running, as shown, in this strip \mathcal{D} . To obtain this solution requires decomposition of the kernel into a product of two terms, one containing singularities in the region above the strip of analyticity, that is, it is zero and singularity free in the lower half-region (denoted by \mathcal{D}^- in Fig. 1) and the other zero and singularity free in \mathcal{D}^+ . The product factors for scalar kernels have an integral representation (2.3) if the kernel has reasonable behaviour at infinity (usually constant or smaller) and so the solution scheme can formally proceed without difficulty. However, in practice the integral representation of the factors often presents numerical difficulties due to singularities of the integrand encroaching the integration path. Also, the final solution of a Wiener–Hopf problem is often represented as a double integral containing these kernel factors, and so computations of such quantities are inevitably extremely slow. Specific examples displaying these problems can be found in Zhang & Abrahams (1995) and Abrahams & Lawrie (1995).

Matters relating to the efficient computation of kernel factors have been of concern for many years. As a consequence, alternative forms to the integral representation (2.3) have been sought; for example, infinite product representations for meromorphic kernels (Noble, 1988, p. 40) and finite integral forms such as can be found in Freund (1993, p. 88) or Abrahams & Lawrie (1995). The latter example is examined in Section 5. It transpires that the infinite product representation is often slowly convergent and so generally offers little advantage over the original Cauchy integral (2.3) (Lawrie & Abrahams, 1994). As an alternative route for computation Koiter (1954) proposed replacing a complicated kernel, $K(\alpha)$, with a simpler one, $K_0(\alpha)$, say, that takes values close to $K(\alpha)$ in the strip of analyticity \mathcal{D} . At that time it was the dearth of computational facilities, rather than matters of numerical inconvenience or speed which prompted such a procedure. Koiter chose $K_0(\alpha)$ such that it could be factored simply and explicitly, and demonstrated the method on various types of kernels. However, as Noble (1988) points out, the fact that $K_0(\alpha) \approx K(\alpha)$ for all $\alpha \in \mathcal{D}$ does not immediately imply that the product factors of the two kernels, zero and singularity free in \mathcal{D}^+ and \mathcal{D}^- respectively, are close to each other in the complex α -plane, or indeed even in their regions of analyticity. If the latter is not true then approximate kernel factorization is of no use!

This article is concerned with the introduction of a new scheme for generating approximate kernels with functions which have simple factorizations, and which offer computationally accurate and efficient means of solving the original Wiener–Hopf boundary-value problem. In Section 2, proof is given of the closeness of the product factors of $K_0(\alpha)$ to those of $K(\alpha)$ in their regions of regularity if $K_0(\alpha) \approx K(\alpha)$ for all $\alpha \in \mathcal{D}$ for a class of kernels. This justifies reappraisal of this longstanding topic. The proposed method employs Padé approximants which are ratios of polynomials, and has the advantage of offering a procedure in which the accuracy can generally be improved by simply increasing the order of the polynomials. Details of Padé approximants are given in Section 3; see also Baker (1975) and Baker & Graves-Morris (1996). However, in essence the key factor is that the polynomial coefficients are determined uniquely from the Taylor-series expansion at a point of regularity of the original kernel. Hence the locations of the zeros and poles are related, via the Padé approximants connection with the Taylor series, to the singularities of $K(\alpha)$. For the purposes of accurate Wiener–Hopf factorization, we further discuss two-point Padé approximants in this section. The new approach can be thought off as a generalization of Koiter’s original technique, and has the advantage that remarkably high accuracies can be achieved for the kernel factors, in their regions of analyticity, for modest effort. For example, Koiter achieved approximately one per cent accuracy for the kernel discussed in Section 6 whilst 10^{-7} per cent error is attainable for the more complicated kernel of Section 5.

The paper is constructed as follows. As mentioned above, Section 2 demonstrates that for kernels of concern in this article, a bound on the closeness of $K_0(\alpha)$ to $K(\alpha)$ for all $\alpha \in \mathcal{D}$ is sufficient to bound the error of the approximate kernel factors in their regions of analyticity. The following section introduces Padé approximants and briefly discusses convergence of Padé sequences. Rather than commence the demonstration of the new approach with Koiter’s original kernel, which in fact has some technical difficulties, it is more illustrative to discuss a simple kernel, such as that examined in Section 4. Following this, a kernel from a physically interesting problem is approximately factored in Section 5. Error calculations are given for both model kernels and their factors. Section 6

revisits Koiter's problem and demonstrates that generalizations of Padé approximations are possible and, as in this case, are sometimes superior to the standard approach. Concluding remarks are offered in Section 7.

2. Validation of approximate factorization

Suppose a scalar function of a complex variable α , say $K(\alpha)$, has arbitrary singularity structure but is analytic and zero free in some finite width strip, \mathcal{D} , which includes the real line as $|\alpha| \rightarrow \infty$; see Fig. 1. Without unreasonable loss of generality, it is also assumed that

$$K(\alpha) \rightarrow 1, \quad |\alpha| \rightarrow \infty, \alpha \in \mathcal{D}. \quad (2.1)$$

In practice (see for example Section 6), most Wiener–Hopf kernels of physical interest can be decomposed or multiplied by other functions to obtain this condition. Any scalar kernel which satisfies (2.1) can be written as

$$K(\alpha) = K^+(\alpha)K^-(\alpha), \quad (2.2)$$

where $K^+(\alpha)$, $K^-(\alpha)$ are the product factors of $K(\alpha)$ and are analytic and zero free in the overlapping regions \mathcal{D}^+ , \mathcal{D}^- , respectively, shown in Fig. 1. Cauchy's integral theorem is easily employed to obtain these factors; from Noble (1988, p. 16) it is found that

$$K^\pm(\alpha) = \exp \left\{ \frac{\pm 1}{2\pi i} \int_{\mathcal{C}} \frac{\log[K(\zeta)]d\zeta}{\zeta - \alpha} \right\}, \quad (2.3)$$

where \mathcal{C} runs from $\zeta = -\infty$ to $\zeta = +\infty$ in \mathcal{D} , and α lies above (below) the contour \mathcal{C} for $K^+(\alpha)$ ($K^-(\alpha)$).

Let us suppose for some reason that it is difficult to obtain $K^\pm(\alpha)$, the exact factors of $K(\alpha)$. Instead, a function $K_0(\alpha)$, which has the same strip of analyticity \mathcal{D} (and is also zero free there), has the known, and perhaps simple factors,

$$K_0(\alpha) = K_0^+(\alpha)K_0^-(\alpha), \quad (2.4)$$

where $K_0^\pm(\alpha)$ are again regular and zero free in $\mathcal{D}^\pm(\alpha)$. If the function $K_0(\alpha)$ is very close to $K(\alpha)$ *everywhere* in the strip \mathcal{D} , what can be concluded about the closeness of the product factor pairs $K^\pm(\alpha)$ and $K_0^\pm(\alpha)$ *in their respective regions of analyticity*? To answer this question, the following theorem is offered.

THEOREM 1 Two functions of α , $K(\alpha)$ and $K_0(\alpha)$, are analytic and zero free in the infinite strip \mathcal{D} (Fig. 1). They attain values close to each other in \mathcal{D} , viz.

$$K_0(\alpha) = K(\alpha)(1 + \varepsilon f(\alpha)), \quad \alpha \in \mathcal{D}, \quad (2.5)$$

where

$$0 < \varepsilon \ll 1, \quad \varepsilon \in \mathbb{R}, \quad (2.6)$$

$$|f(\alpha)|_{\max} = 1, \quad \alpha \in \mathcal{D}, \quad (2.7)$$

$$f(\alpha) \rightarrow C, \quad |C| \leq 1, \quad |\alpha| \rightarrow \infty, \alpha \in \mathcal{D}. \quad (2.8)$$

Then

$$K_0^\pm(\alpha) = K^\pm(\alpha)(1 + \varepsilon g^\pm(\alpha)), \quad \alpha \in \mathcal{D}^\pm, \quad (2.9)$$

where

$$g^\pm(\alpha) \text{ is a bounded function in } \mathcal{D}^\pm. \quad (2.10)$$

Further, if

$$f(\alpha) \rightarrow 0, \quad |\alpha| \rightarrow \infty, \alpha \in \mathcal{D}, \quad (2.11)$$

then

$$|g^\pm(\alpha)|_{\max \text{ over } \mathcal{D}^\pm} \text{ occurs in } \mathcal{D} \quad (2.12)$$

and

$$g^\pm(\alpha) \rightarrow 0, \quad |\alpha| \rightarrow \infty, \alpha \in \mathcal{D}^\pm. \quad (2.13)$$

Proof. Substituting the form (2.5) into the Cauchy integral representation (2.3) gives

$$K_0^\pm(\alpha) = \exp\left\{\frac{\pm 1}{2\pi i} \int_{\mathcal{C}} \frac{\log K_0(\zeta) d\zeta}{\zeta - \alpha}\right\} = \exp\left\{\frac{\pm 1}{2\pi i} \int_{\mathcal{C}} \frac{\log[K(\zeta)(1 + \varepsilon f(\zeta))] d\zeta}{\zeta - \alpha}\right\}, \quad (2.14)$$

defined for $\mathcal{C} \in \mathcal{D}$, $\pm\alpha$ lying above the contour \mathcal{C} . This can easily be written as

$$\exp\left\{\frac{\pm 1}{2\pi i} \int_{\mathcal{C}} \frac{\log K(\zeta) d\zeta}{\zeta - \alpha} \pm \frac{1}{2\pi i} \int_{\mathcal{C}} \log\left(\frac{1 + \varepsilon f(\zeta)}{1 + \varepsilon C}\right) \frac{d\zeta}{\zeta - \alpha} + \frac{1}{2} \log(1 + \varepsilon C)\right\}, \quad (2.15)$$

which, on expanding the logarithm of the second integrand, gives

$$K_0^\pm(\alpha) = (1 + \varepsilon C)^{\frac{1}{2}} K^\pm(\alpha) \exp\left\{\pm \sum_{n=1}^{\infty} \varepsilon^n I_n^\pm(\alpha)\right\}, \quad (2.16)$$

where

$$I_n^\pm(\alpha) = \frac{(-1)^n}{2\pi i} \int_{\mathcal{C}} \frac{\{C^n - f^n(\zeta)\}}{\zeta - \alpha} d\zeta, \quad \alpha \in \mathcal{D}^\pm, \pm\Im(\alpha) > \pm\Im(\zeta). \quad (2.17)$$

In view of the behaviour of $f(\alpha)$ in \mathcal{D} , (2.7), (2.8), every $I_n^\pm(\alpha)$ exists for all $\alpha \in \mathcal{D}^\pm$, and

$$I_n^\pm(\alpha) \rightarrow 0, \quad |\alpha| \rightarrow \infty, n \in \mathbb{N}, \alpha \in \mathcal{D}^\pm. \quad (2.18)$$

(In fact $I_n^\pm(\alpha) \sim O(1/\alpha)$, $|\alpha| \rightarrow \infty$, if $\int_{\mathcal{C}} (C^n - f^n(\zeta)) d\zeta$ exists.) Therefore from (2.16), it can be stated categorically that conditions (2.5)–(2.8), relating $K_0(\alpha)$ and $K(\alpha)$, imply that

$$K_0^\pm = K^\pm(\alpha) \left(1 + \varepsilon \left[\frac{1}{2}C \pm I_1^\pm(\alpha)\right] + O(\varepsilon^2)\right) \quad (2.19)$$

uniformly over all \mathcal{D}^\pm , which proves the result (2.9), viz.

$$g^\pm(\alpha) = \frac{1}{2}C \pm I_1^\pm(\alpha) + O(\varepsilon). \quad (2.20)$$

If the approximating kernel, $K_0(\alpha)$, is equal to $K(\alpha)$ at infinity, then $C \equiv 0$, and so $g^\pm(\alpha) \rightarrow 0$ as $|\alpha| \rightarrow \infty$ in \mathcal{D}^\pm . A complex function cannot have a maximum or minimum modulus within its domain of analyticity, and therefore for any given region of regularity the maximum modulus occurs at the boundary of such a domain. Hence, the maximum modulus of $g^\pm(\alpha)$ on \mathcal{D}^\pm occurs within the strip \mathcal{D} and *diminishes to zero* as α moves up or down into \mathcal{D}^\pm away from \mathcal{D} . \square

If $f(\alpha) \not\rightarrow 0$ as $|\alpha| \rightarrow \infty$, then the error function $g^\pm(\alpha)$ may attain a maximum modulus at a finite point within \mathcal{D} , or at the point at infinity. Whether C is zero or not, a significant advantage to the approximating scheme is that the error between $K^\pm(\alpha)$ and $K_0^\pm(\alpha)$ is smaller at interior points of \mathcal{D}^\pm than the maximum modulus error in \mathcal{D} . Therefore, a *sufficient* way of measuring the maximum error of the kernel factors in their respective domains of analyticity is to define the percentage error function

$$e(\alpha) = 100 \times \left| \frac{K_0(\alpha) - K(\alpha)}{K(\alpha)} \right|, \quad \alpha \in \mathcal{D}, \quad (2.21)$$

which from (2.5) is

$$e(\alpha) = 100\varepsilon|f(\alpha)|. \quad (2.22)$$

There is a good deal of arbitrariness in practice regarding the actual choice of \mathcal{D} , which does not need to be straight sided (as long as the singularities of $K(\alpha)$, $K_0(\alpha)$ all remain consistently either above or below the strip). For each choice of \mathcal{D} a different upper bound on the error will be attained. However, all choices of \mathcal{D} must yield the same solution to any given physical problem. Therefore, any particular \mathcal{D} will offer an error bound, which almost certainly will not be the minimum, or actual, error achieved in a solution for a specific choice of $K_0^\pm(\alpha)$. This is confirmed for examples tried here and elsewhere by the author; see also (Abrahams, 1996, 1997).

3. Padé approximants

3.1 Standard approximation

As discussed earlier, great savings in both programming effort and computation time can be achieved if a complicated kernel is replaced by a simple one which has an explicit factorization. Perhaps the best approximating kernels are those which contain only poles and zeros, as these are trivial to factorize and have direct usage for matrix kernels (see Section 7). For this reason Padé approximants will be employed, but they also have several qualities which make them particularly attractive in this context. First the procedure for determining them is algorithmic and secondly the accuracy of a Padé approximant representation can, in practice, be increased almost indefinitely. For completeness the basic properties of Padé approximants are written here, but details can be found in Baker (1975) and Baker & Graves-Morris (1996). An $[N/M]$ approximant of a function $f(\alpha)$ is written

$$f(\alpha) \approx \frac{P_N(\alpha)}{Q_M(\alpha)}, \quad (3.1)$$

where

$$P_N(\alpha) = a_0 + a_1\alpha + a_2\alpha^2 + \dots + a_N\alpha^N, \tag{3.2}$$

$$Q_M(\alpha) = 1 + b_1\alpha + b_2\alpha^2 + \dots + b_M\alpha^M. \tag{3.3}$$

The coefficients a_n, b_n are determined from the Taylor-series expansion of $f(\alpha)$ at any regular point. Without loss of generality the expansion point is taken as $\alpha = 0$, so

$$f(\alpha) = \sum_{n=0}^{\infty} c_n\alpha^n, \tag{3.4}$$

where c_n are known. From the algebraic system

$$\frac{P_N(\alpha)}{Q_M(\alpha)} + O(\alpha^{N+M+1}) = \sum_{n=0}^{\infty} c_n\alpha^n, \tag{3.5}$$

the coefficients of $\alpha^{N+1}, \alpha^{N+2}, \dots, \alpha^{N+M}$ directly yield the coefficients

$$\begin{pmatrix} b_M \\ b_{M-1} \\ \vdots \\ b_1 \end{pmatrix} = - \begin{pmatrix} c_{N-M+1} & c_{N-M+2} & \cdots & c_N \\ c_{N-M+2} & c_{N-M+3} & \cdots & c_{N+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_N & c_{N+1} & \cdots & c_{N+M+1} \end{pmatrix}^{-1} \begin{pmatrix} c_{N+1} \\ c_{N+2} \\ \vdots \\ c_{N+M} \end{pmatrix}, \tag{3.6}$$

where $c_n \equiv 0$ for $n < 0$. If the inverse matrix of c_n elements does not exist then the particular $[N/M]$ approximant is not defined. Once the b_n are found, then the remaining equations ($\alpha^0, \dots, \alpha^N$) yield the a_n coefficients.

For the purposes of this article, where $K(\alpha)$ is chosen to have constant behaviour as $|\alpha| \rightarrow \infty$ in \mathcal{D} , the approximants $[N/N]$ are employed, with successive N values improving the accuracy. Clearly the ratio of two polynomials is trivial to factorize into a product of two terms, one with zeros and poles in \mathcal{D}^+ , $K_N^-(\alpha)$, and the other with zeros and poles in \mathcal{D}^- , $K_N^+(\alpha)$. The invariance property of approximants (see Baker, 1975) can ensure that the level of approximation is uniform everywhere away from the singularities. This is a significant improvement over the Taylor-series expansion from which they are derived, and allows them to satisfy the criterion (2.5). Finally, the unique selection of the Padé coefficients ensures that spurious poles and zeros do not occur in \mathcal{D} ; in fact they usually lie near or on the singularities of $K(\alpha)$. The ratio of two polynomials of N th order can be seen to be a natural extension of Koiter’s method for kernel replacement (Koiter, 1954). He, however, chose values for the coefficients of his second-order polynomials by trial and error. This is not desirable at all as, in practice, it is extremely difficult for even moderate sized polynomials to control the stability of the location of the poles and zeros. Thus, it is found that the error cannot be contained within reasonable limits in \mathcal{D} as singularities tend to encroach on the strip.

There is one aspect of standard Padé approximants which is not particularly useful for the present application. For reasons concerning the relation between the growth of the kernel factors at infinity and the edge behaviour in physical models (Noble, 1988) we

would like the approximant kernel to tend to the exact value as $|\alpha| \rightarrow \infty$ in \mathcal{D} . However, as the approximant coefficients are chosen to agree with a truncated series expansion of the exact function $K(\alpha)$, at one finite point (usually $\alpha = 0$) the Padé approximant will not be exactly correct at the point at infinity. From (3.1)–(3.3), for $N = M$, it will take the value a_N/b_N which for large N is very close to but not equal to unity. This can be overcome by normalizing the approximant or by introducing two-point Padé approximants.

3.2 Two-point approximants

A rational function approximation can easily be obtained which agrees with a function up to arbitrary terms in its series expansion at two, or indeed any finite number of, points. For example, suppose a function $f(\alpha)$ has the behaviour

$$f(\alpha) \approx \sum_{n=0}^R d_n (\alpha - \alpha_1)^n \quad (3.7)$$

in the neighbourhood of α_1 , and

$$f(\alpha) \approx \sum_{n=0}^S e_n (\alpha - \alpha_2)^n \quad (3.8)$$

around α_2 . If we require an approximant representation (3.1) then the coefficients are defined uniquely, if the $[N/M]$ approximant exists, by equating coefficients of

$$\frac{P_N(\alpha)}{Q_M(\alpha)} + O((\alpha - \alpha_1)^{R+1}) = \sum_{n=0}^R d_n (\alpha - \alpha_1)^n \quad (3.9)$$

and

$$\frac{P_N(\alpha)}{Q_M(\alpha)} + O((\alpha - \alpha_2)^{S+1}) = \sum_{n=0}^S e_n (\alpha - \alpha_2)^n, \quad (3.10)$$

where $M + N = R + S + 1$.

There appears to be little theory in the literature on the relative accuracies of multi-point Padé approximants (Baker & Graves-Morris, 1996), but trial and error indicates that they do seem a good representation for functions in a strip. In particular, we usually require a good approximation at points in the vicinity of the origin and at infinity; in which case it is particularly simple to generate. If an expansion about the point at infinity yields

$$f(\alpha) = \sum_{n=0}^R d_n \alpha^{-n} + O(\alpha^{-R-1}) \quad (3.11)$$

for some integer R and given coefficients d_n , then a Padé approximant of the difference function can be generated from this equation. That is, the quantity

$$\alpha^R f(\alpha) - \sum_{n=0}^R d_n \alpha^{R-n} \quad (3.12)$$

is $O(\alpha^{-1})$ as $\alpha \rightarrow \infty$ and has a Taylor-series expansion

$$\sum_{n=0}^{\infty} c_n \alpha^n \quad (3.13)$$

about the origin. Hence, with this definition of the c_n and the behaviour at infinity, equation (3.5) yields an $[N/N + 1]$ approximant. This gives the final form:

$$f(\alpha) \approx \sum_{n=0}^R d_n \alpha^{-n} + \frac{P_N(\alpha)}{\alpha^R Q_{N+1}(\alpha)} = \frac{R_{N+1}(\alpha)}{S_{N+1}(\alpha)}, \quad (3.14)$$

where $R_{N+1}(\alpha)$ and $S_{N+1}(\alpha)$ are polynomials of degree $N + 1$ and it is required that $N \geq (R - 2)/2$. Varying the value of R for a given N alters the rate of convergence of the approximate function to the actual one at infinity and at the origin; that is, increasing R improves the behaviour at infinity but decreases the rate of convergence at the origin, and vice-versa. In practice, minimizing the maximum error in \mathcal{D} , that is, the value of ε , usually requires numerical experiment over a range of R values.

As a final note for this section, single and multi-point Padé approximants are still useful when the expansion point(s) are not regular, that is, when the expansion is not a Taylor series. As will be seen in later examples, this is often the case with the point at infinity in Wiener–Hopf kernels. If, at α_1 say, the function has a series in integer powers up to some term with a fractional or irrational higher-order exponent, then the procedure employed above is still valid as long as R (3.7) or (3.11) is less than the first non-integer term. The following sections include examples which clearly demonstrate the efficacy of the present method.

3.3 A note on convergence

For most practical purposes it is sufficient to have an error bound on the approximant kernel, and hence an idea of the accuracy of the final solution to any given boundary-value problem. Quantity (2.21) offers such a bound for any given Padé approximant representation of the kernel factors. However, what can be said in general regarding the error of approximant factors in their regions of regularity as the Padé numbers N , M increase? It would be expected that the accuracy improves as the numbers of poles and zeros of the approximant increases, and this is usually borne out by numerical experiment (see the following sections). Unfortunately it is not possible in general to prove that, in the limit as a $N \rightarrow \infty$, $M \rightarrow \infty$, a sequence of Padé approximants converges to the value of the original function at a point of regularity of that function. The issue of convergence of Padé sequences is a major area of study in the subject, and various details and theorems on the topic can be found in Baker & Graves-Morris (1996). The example in the next section is one of the few cases in which convergence can be proved everywhere in α away from branch-line discontinuities.

4. Kernel with finite branch cuts

The first example is mainly illustrative, as it does not have a direct physical application. However, it is closely associated with matrix kernel factorization for problems in acoustics

and elasticity (Abrahams, 1996, 1997) and is therefore of more than purely academic interest. The kernel

$$K(\alpha) = \left(\frac{\alpha^2 + 1}{\alpha^2 + k^2} \right)^{1/2}, \quad k > 1, \quad (4.1)$$

has finite branch cuts between i and ki , and $-i$ to $-ki$, and if the strip \mathcal{D} encloses the real line, then by inspection

$$K^\pm(\alpha) = \left(\frac{\alpha \pm i}{\alpha \pm ik} \right)^{1/2}, \quad K^+(\alpha) = K^-(-\alpha). \quad (4.2)$$

The choice of Riemann surface for the cut plane has $K(0) = 1/k$. The Taylor-series expansion of (4.1) about $\alpha = 0$ can be used (3.5) to deduce the $[N/N]$ approximant. For each N , the standard Padé approximant will be exactly correct at $\alpha = 0$, but will have a small error at ∞ . To make the approximate kernel exact as $|\alpha| \rightarrow \infty$, we can follow the procedure set out in Section 3.2 and subtract off the constant at infinity (that is, we take $R = 0$ in (3.11)). Then, from (4.1)

$$K(\alpha) - 1 = O(\alpha^{-2}), \quad |\alpha| \rightarrow \infty \quad (4.3)$$

and so we can determine its Padé approximant in the form

$$K_{N+2}(\alpha) = 1 + \frac{P_N(\alpha)}{Q_{N+2}(\alpha)}, \quad N \geq 0. \quad (4.4)$$

Note that this is different from (3.14), with an $N + 2$ polynomial in the denominator, because $K(\alpha)$ is an even function of α . Hence N must be chosen to be even and replacing $N + 2$ by N in the above expression gives

$$K_N(\alpha) = K_N^+(\alpha)K_N^-(\alpha) = \frac{Q_N(\alpha) + P_{N-2}(\alpha)}{Q_N(\alpha)} = \frac{R_N(\alpha)}{S_N(\alpha)}, \quad N \geq 2, \quad (4.5)$$

where

$$K_N^\pm(\alpha) = \prod_{j=1}^{N/2} \left(\frac{\alpha \pm ip_j}{\alpha \pm iq_j} \right). \quad (4.6)$$

The zeros and poles of these functions lie along the imaginary line segments $1 < p_1 < p_2 \cdots < p_{N/2} < k$, $1 < q_1 < q_2 \cdots < q_{N/2} < k$, and are trivial to find by factorizing $R_N(\alpha)$, $S_N(\alpha)$ respectively.

The percentage error function (2.21), used here as

$$e_N(\alpha) = 100 |K_N(\alpha)/K(\alpha) - 1|, \quad \alpha \in \mathcal{D}, \quad (4.7)$$

is plotted in Fig. 2 along the positive real line (the function $e_N(\alpha)$ is symmetric in α) for the N values shown and $k = 4$. The ordinate is given on a logarithmic scale because of the significant reduction in error as N increases, and this clearly indicates the very

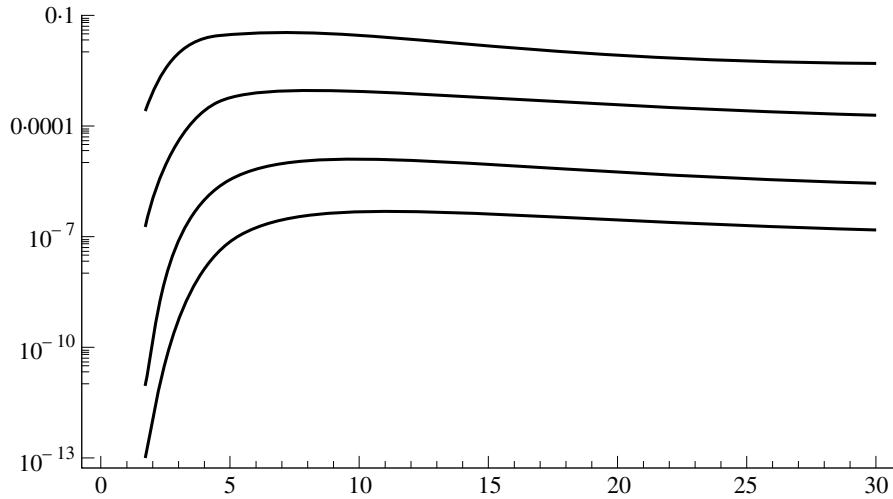


FIG. 2. The percentage error $e_N(\alpha)$ (4.7) plotted on a logarithmic scale along the positive real axis for $N = 10, 16, 24, 30, k = 4$. The curves are ordered sequentially top to bottom (largest to smallest error) as the Padé number N increases.

high accuracies achievable. To confirm the theorem of Section 2, relating the error of approximation of $K(\alpha)$ to that of the product factors $K^\pm(\alpha)$, the function

$$e_N^+(\alpha) = 100 |K_N^+(\alpha)/K^+(\alpha) - 1|, \quad (4.8)$$

which is the percentage error between the approximate and exact plus factors, is also plotted. In Fig. 3 it is shown by the solid curves for positive real values of α , and the dashed curves are the percentage error (4.8) given along the positive imaginary axis. As expected (see comments above (2.21)) the maximum modulus of the error (4.8) for every N is seen to be greater along the real line (that is, in \mathcal{D}) than in the interior of the domain \mathcal{D}^+ .

Note that all the errors in Figs 2 and 3 are sufficiently small for the approximate kernel factor to be indistinguishable from the exact one. A Padé number of 40 say, corresponds to 20 poles and zeros replacing each finite branch cut of $K(\alpha)$, and takes a few seconds of computer time to calculate using, say, the built-in Padé approximant routine in MATHEMATICA. The error can be diminished to a considerable extent before either computation time or inversion of the large square matrix in (3.6) becomes a problem.

4.1 Convergence

The remarkable accuracy of the approximant shown in Figs 2, 3, and the apparent convergence with increasing N , suggests that the representations in (4.6) do indeed yield the exact value of $K^\pm(\alpha)$ in \mathcal{D}^\pm as $N \rightarrow \infty$. For this simple function this can be proved, and for ease of exposition we here discuss only single rather than multipoint Padé approximants, defined by the Taylor-series expansion about the origin alone. We can take

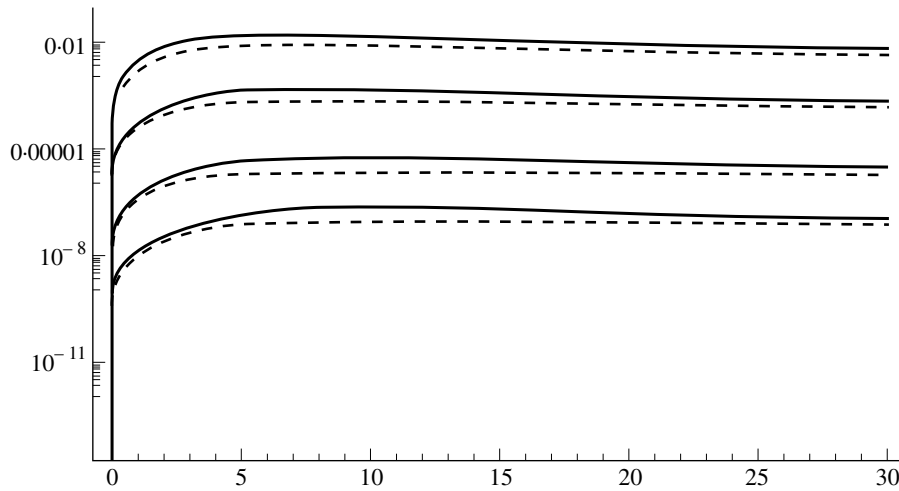


FIG. 3. The percentage error $e_N^+(\alpha)$ (solid line) and $e_N^+(i\alpha)$ (dashed line) (4.8) plotted on a logarithmic scale for positive real values of α with (from top to bottom as shown) $N = 10, 16, 24, 30$, and $k = 4$.

$K^+(\alpha)$, (4.2), and transform it via

$$\alpha = \frac{-iz}{(z + 1 - 1/k)} \tag{4.9}$$

which maps the upper half of the α -plane to the disk of radius and centre

$$\frac{k-1}{2k}, \quad \left(\frac{1-k}{2k}, 0 \right) \tag{4.10}$$

respectively in the z -plane, and the branch points

$$\alpha = -ik \Leftrightarrow z = -1, \quad \alpha = -i \Leftrightarrow z = \infty. \tag{4.11}$$

So,

$$K^+(\alpha(z)) = F(z) = \frac{1}{k^{1/2}(z+1)^{1/2}} \tag{4.12}$$

which is a single-valued function if we make a single cut from $z = -1$ to ∞ along the negative real line. The Taylor-series expansion about the origin is

$$F(z) = \frac{1}{k^{1/2}} \sum_{j=0}^{\infty} f_j (-z)^j, \tag{4.13}$$

where

$$f_0 = 1, f_1 = \frac{1}{2}, f_2 = \frac{3}{8}, \dots, \quad f_j > 0 \forall j. \tag{4.14}$$

Such a function, with strictly positive decreasing values of f_j , can be expressed as a Stieltjes integral (Baker & Graves-Morris, 1996) from which many results follow. An

important point is that one can *prove* that the zeros and poles of the $[N/M]$ approximant lie on the cut, that is, on the negative real axis for $z < -1$, and so the disk of convergence (of unit radius) of (4.13) is also free of singularities for all Padé approximants. From this and other results, it can be deduced that sequences, including paradiagonal ones $[N + J/N]$, J fixed with $N \rightarrow \infty$ in integer steps, converge to $F(z)$ for z inside the unit circle. The invariance property, that Padé approximants are preserved under transformations of the form $a\alpha/(\alpha + b)$ (a, b constants), allows us to deduce therefore that sequences of Padé approximants in the α -plane converge to $K^+(\alpha)$ in \mathcal{D}^+ , as the image of \mathcal{D}^+ lies entirely within the unit disk. It can be shown by different choices of maps (4.9), which transform different parts of the α -plane to the unit disk, that in fact every point off the branch cut on the negative imaginary axis between $-i$ and $-ik$ gives convergence of Padé sequences to $K^+(\alpha)$ as $N, M \rightarrow \infty$.

Unfortunately, convergence results of the type shown here cannot be deduced in general. It explains, and indeed seems to prove, the rapid convergence of the approximant matrix factors to the exact decompositions for the particular examples discussed in Abrahams (1996, 1997). It also justifies the particular approach taken by the author (Abrahams, 1998) to approximate the non-commutative matrix kernel factors for Khrapkov matrices with exponential growth at infinity. An example where convergence to the exact factors as $N \rightarrow \infty$ cannot be proven is the kernel arising in a Stokes flow problem discussed by Abrahams & Davis (2000).

5. Elastic plate kernel

5.1 Fluid loaded semi-infinite plate

The previous section demonstrated the success of the method in achieving high accuracies, albeit for a simple kernel. As a second, and more physically important example, we examine the following:

$$K(\alpha) = \alpha^4 - \mu^4 - \tau/\gamma(\alpha), \quad (5.1)$$

where

$$\gamma(\alpha) = (\alpha^2 - k^2)^{1/2} \quad (5.2)$$

is the usual square-root function found in scalar diffraction problems, and k, μ and τ are positive real constants. The function $\gamma(\alpha)$ is made single valued by cutting the α -plane from $+k$ to $+\infty$ (in \mathcal{D}_+) and $-k$ to $-\infty$ (in \mathcal{D}_-) and choosing $\gamma(0) = -ik$. This kernel arises in the study of scattering of sound waves by a semi-infinite thin elastic plate joined to a semi-infinite rigid screen (Cannell, 1976), where k is the acoustic wavenumber, μ is determined by the plate properties and τ is a measure of the relative dominance of fluid (occupying the half-space above the two-part barrier) over plate vibrations. The kernel has simple zeros on the real line, at $\pm k^*$ say, which correspond to unattenuated fluid coupled plate waves which can be supported by the structure. The complex roots give rise to plate waves which propagate with attenuation; that is, leaky waves.

The strip of analyticity \mathcal{D} for the Wiener–Hopf equation is usually made finitely thick by allowing k to be slightly complex (with small positive imaginary part). This moves the

branch points and $\pm k^*$ off the real line, and the Cauchy integrals (2.7) defining the product factors run between them along the real line. However, as $\Im(k) \rightarrow 0$, the singularities move on to the contour path, and we usually require the function value α to take real values also. This makes a direct numerical determination of (2.7) both delicate and slow as the singularities on the path must be removed. A more complex kernel exhibiting these same difficulties is numerically evaluated in Zhang & Abrahams (1995).

The problems associated with (5.1) suggest that an alternative factorization method is to be preferred, and Padé approximants can certainly be employed. However, we have chosen to examine the fluid loaded elastic plate kernel here because there is, in fact, an alternative form to the exact representation (2.3) for the product factors to which the approximant expression can be compared. This is a product of finite integrals, found by performing integration by parts on (2.5), differentiating with respect to α , splitting the integrand into partial fraction form, integrating with respect to ζ and finally integrating with respect to α . Omitting these workings here, the reader is referred to the paper by Abrahams & Lawrie (1995) for such details and also to an alternative derivation using Maliuzhinets's functions and difference equations. The factorization takes the form

$$K^+(-k \sin s) = \frac{4k^2}{M^{10}(\pi/2) \sin[\frac{1}{2}(s - \pi/2)]} \prod_{j=1}^5 M(s - X_j + \pi)M(s + X_j), \quad (5.3)$$

where the transformation $\alpha = -k \sin s$ is chosen to map the upper (lower) half of the α -plane into $-3\pi/2 \leq \Re(s) \leq -\pi/2, \Im(s) > 0$ ($\Im(s) < 0$), the X_j are the five distinct roots of

$$\sin^5(X_j) - 2 \sin^3(X_j) + (1 - \mu^4/k^4) \sin(X_j) + i\tau/k^5 = 0 \quad (5.4)$$

lying in $0 \leq \Re(X) < \pi/2, \Im(X) < 0$ and $-\pi < \Re(X) \leq \pi/2, \Im(X) \geq 0$, and

$$M(s) = \exp\left(\frac{1}{4\pi} \int_0^s \frac{2u - \pi \sin u}{\cos u} du\right). \quad (5.5)$$

We now compare the exact factorization of the elastic kernel (5.3) with the factorization of the two-point Padé approximant of (5.1). Section 3 discussed the derivation of such approximants for functions which behave as unity at infinity. Here we relax that condition, which was introduced purely for ease of mathematical exposition, and write

$$K_N(\alpha) = \frac{R_{N+4}(\alpha)}{S_N(\alpha)} \quad (5.6)$$

for some Padé number N in view of the $O(\alpha^4)$ growth in (5.1). Note that $K(\alpha)$ is even in α and so $R_{N+4}(\alpha)$ and $S_N(\alpha)$ must only contain even powers of α . We insist that the first three terms in the even expansion for large $|\alpha|$ of $K_N(\alpha)$ agree with those of the exact kernel:

$$K(\alpha) \sim \alpha^4 + 0 \times \alpha^2 - \mu^4 + O(|\alpha|^{-1}). \quad (5.7)$$

To achieve this in a simple fashion, the terms are found following (3.14) from

$$\frac{R_{N+4}(\alpha)}{S_N(\alpha)} = \alpha^4 - \mu^4 - \frac{P_{N-2}(\alpha)}{Q_N(\alpha)}, \quad N \geq 2, \quad (5.8)$$

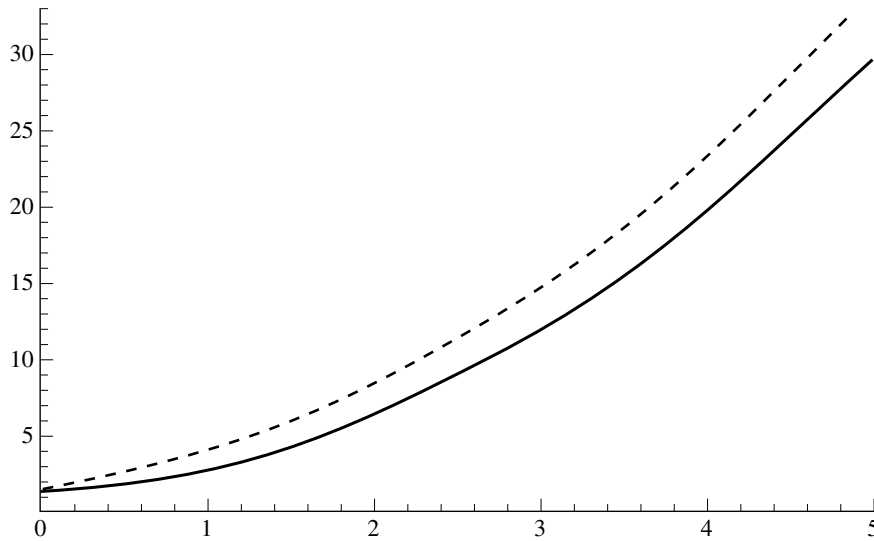


FIG. 4. Plot of the exact form of $K_N^+(\alpha)$ (solid line) and $K_N^+(i\alpha)$ (dashed line), see (5.3), together with their [40/40] two-point Padé approximations (5.6) plotted over $0 < \alpha < 5$ for $N = 40$, and typical values $\mu = 0.5$, $\tau = 2, k = 1$.

where the $[N - 2/N]$ Padé approximant is given by

$$\frac{P_{N-2}(\alpha)}{Q_N(\alpha)} \approx \frac{\tau}{\gamma(\alpha)}, \quad N \geq 2. \tag{5.9}$$

The factorization of $K_N(\alpha)$ is now straightforward. As before the $[N - 2/N]$ approximant of (5.9) is found by a standard algorithm, such as (3.5), (3.6). Substituting this into (5.8) and re-expressing over a common denominator yields the two polynomials $R_{N+4}(\alpha), S_N(\alpha)$. These are factored, again using a polynomial solver, and the simple zeros and poles separated into those in upper and lower half-planes. For the kernel (5.1), and the physical constraints on the associated boundary-value problem from which it is derived, the strip \mathcal{D} and upper and lower regions are as defined in Fig. 1. Note that the strip has to be deformed around the branch points and poles on the real lines. Figure 4 compares the exact factorization $K^+(\alpha)$ of (5.1), analytic in the upper-half plane, with that computed by (5.6) for $N = 40$. The solid line shows the absolute values plotted along the positive real axis, and the dashed lines are for imaginary values. The fit between *exact* and approximate factors is visually excellent in both cases; that is, the exact and approximate curves are indistinguishable. This is borne out by the percentage error plots, $e_N^+(\alpha)$ (4.8), comparing the exact value of $K^+(\alpha)$ (5.3) against the approximant, which are illustrated in Fig. 5 for $N = 8, 16, 24, 32, 40, 60$. Again the solid lines indicate values of α along the positive real line, and dashed refer to α on the positive imaginary axis. Increasing the Padé number yields significant diminution of error, with values of 10^{-7} per cent ($N = 60$) easy to achieve. The selection of a two-point approximant again ensures that the error goes to zero at infinity as well as at the origin.

There are three observations which can be drawn from this example. First, the accuracy

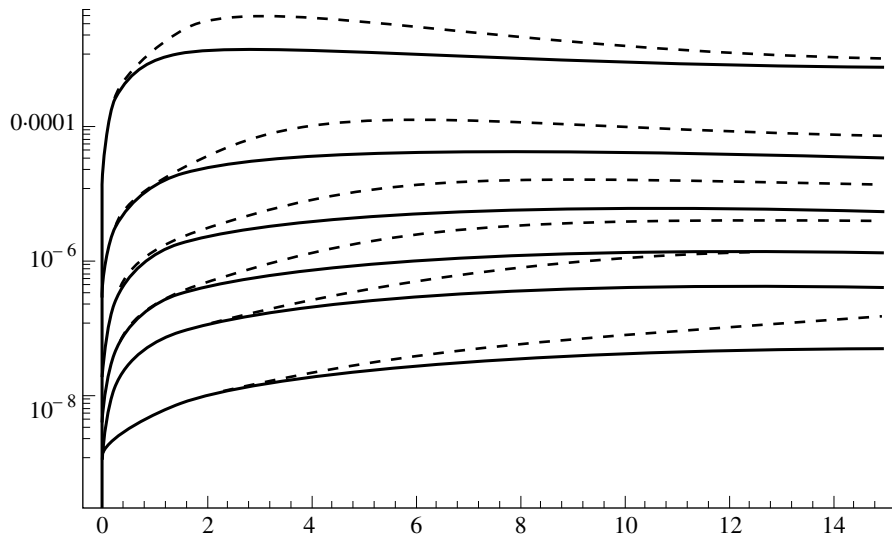


FIG. 5. The percentage error $e_N^+(\alpha)$ (solid line) and $e_N^+(i\alpha)$ (dashed line) (4.8) for the elastic plate kernel factor (5.3). Plotted on a logarithmic scale for positive real values of α with (from top to bottom as shown) $N = 8, 16, 24, 32, 40, 60$, and material constants as in Fig. 4.

is very good *even though the point at infinity is not regular*. This confirms what was stated in Section 3, that multi-point approximants can be employed at locations for which a function does not possess a Taylor-series expansion. As long as a finite number of leading terms in the expansion have integer powers then the procedure will be likely to succeed. The second point to contemplate is the real difference between the *exact* and approximate functions. Although (5.3) is exact, its evaluation requires a numerical solution procedure, such as quadrature or the trapezoidal method. This means that the so-called *exact* results are numerically approximate also, and for very small errors it is therefore valid to question from which expression the major component of this discrepancy occurs. As well as consideration of the error in computing the exact solution, the author is currently addressing the question of whether a high Padé number approximant can, in this case, be considered exact in the limited sense illustrated in Section 4.1. As a final point, it is clear that the approximant representation of the kernel factors is simple both to determine, and to employ computationally. This is in contrast to most exact factors; although (5.3) is relatively straightforward here, in general $K^\pm(\alpha)$ are very messy and slow to compute. The last point is illustrated in the following section by employing a slight variant of (5.1).

5.2 *Semi-infinite plate immersed in two differing fluids*

The above example kernel, whilst being complicated, had a simple finite integral representation with which to compare the Padé approximant expression. As an example to show that the approximation technique is still easy to apply even when no simple exact factorization forms are available, we offer the following generalization of the above model. This is the case of a semi-infinite elastic plate, joined to a rigid baffle, and immersed in

compressible fluids of different material properties on either side of the structure. The kernel, modified from (5.1), can be shown to be

$$K(\alpha) = \alpha^4 - \mu^4 - \tau_1/\gamma_1(\alpha) - \tau_2/\gamma_2(\alpha), \tag{5.10}$$

where

$$\gamma_j(\alpha) = (\alpha^2 - k_j^2)^{1/2}, \quad j = 1, 2, \tag{5.11}$$

k_1 and k_2 are the acoustic wavenumbers for the fluid above and below the plate respectively, μ is the constant given above, and τ_1, τ_2 are constants proportional to the mean densities of upper, lower fluids respectively. As above, the functions $\gamma_j(\alpha)$ are made single-valued by cutting the α -plane from $\pm k_j$ to $\pm\infty$ in $\mathcal{D}_\pm, j = 1, 2$, with $\gamma_j(0) = -ik_j, j = 1, 2$. This kernel does not have a representation in terms of simple Maliuzhinets-type integrals and so an exact evaluation of the product factors will prove both numerically cumbersome and time consuming. The approximant factors, by contrast, are simple in form and efficient to compute. Indeed, once the Padé approximant of the root functions has been determined, that is,

$$\frac{P_{N-2}(\alpha)}{Q_N(\alpha)} \approx \frac{\tau_1}{\gamma_1(\alpha)} + \frac{\tau_2}{\gamma_2(\alpha)}, \quad N \geq 2, \tag{5.12}$$

there is no practical difference between evaluating the two-fluid and single-fluid approximant kernel factors.

6. Limitations and extensions of the method; Koiter’s example

Koiter (1954) examined the issue of approximating the kernel

$$K(\alpha) = \frac{1}{\alpha} \tanh \alpha, \quad \alpha \in \mathcal{D}, \tag{6.1}$$

by

$$K_0(\alpha) = \frac{1}{(\alpha^2 + 1)^{1/2}}, \quad \alpha \in \mathcal{D} \tag{6.2}$$

in the straight strip, \mathcal{D} , containing the real line. They agree to within about nine per cent on the real line, and so to increase the accuracy he suggested modifying $K_0(\alpha)$ as

$$K_0(\alpha) = \frac{1}{(\alpha^2 + 1)^{1/2}} \frac{\alpha^4 + C\alpha^2 + D}{\alpha^4 + E\alpha^2 + D}. \tag{6.3}$$

Koiter used trial and error to find C, D, E in order to improve the accuracy. By a suitable choice he managed to achieve a fit between (6.1) and (6.3) of better than one per cent. As mentioned previously, this is an unpredictable exercise as the poles and zeros move rapidly in the complex plane as the coefficients are varied. It is, in fact, almost impossible to improve the accuracy by this ad hoc approach for larger polynomials top and bottom. The new procedure outlined in this article allows the generalized polynomial ratios to be calculated without ambiguity, and with a greater level of accuracy.

It is interesting, as this article essentially offers an extension of Koiter's method, to examine how well Padé approximants generalize and improve upon the rational approximation on the right-hand side of (6.3). For convenience, it is useful to combine the square-root function into $K(\alpha)$, viz.

$$K(\alpha) = \frac{(\alpha^2 + 1)^{1/2}}{\alpha} \tanh \alpha, \quad (6.4)$$

for which

$$K(\alpha) \rightarrow 1, \quad |\alpha| \rightarrow \infty, \alpha \in \mathcal{D}, \quad (6.5)$$

and hence the two-part approximant is chosen, cf. (4.4), as

$$K_0(\alpha) = \frac{P_{N-2}(\alpha)}{Q_N(\alpha)} + 1, \quad N \text{ even}, \quad (6.6)$$

where $P_{N-2}(\alpha)/Q_N(\alpha)$ is the $[N-2/N]$ Padé approximant of $K(\alpha) - 1$ about $\alpha = 0$. This form ensures that $K_0(\alpha) \rightarrow K(\alpha)$ as $|\alpha| \rightarrow \infty$ in the strip. The series expansion of (6.4) contains only even powers of α , and hence the poles and zeros of (6.6) lie symmetrically with respect to the real line. Thus it is a simple matter, once $P_{N-2}(\alpha)$, $Q_N(\alpha)$ are found, to factorize $K_0(\alpha)$ into functions non-zero and pole free in overlapping half-planes, and which satisfy

$$K_0^+(\alpha) = K_0^-(-\alpha). \quad (6.7)$$

From the exact kernel (6.4) it is easy to show that the decomposition factors of $K(\alpha)$ are

$$K^\pm(\alpha) = \frac{e^{-i\pi/4} \Gamma(\frac{1}{2} - i\alpha/\pi)}{\sqrt{\pi} \Gamma(1 - i\alpha/\pi)} (i \pm \alpha)^{1/2}. \quad (6.8)$$

The absolute (percentage) error function which measures the deviation between exact and approximate kernel factors is, as before,

$$e_N^+(\alpha) = 100 |K_0^+(\alpha)/K^+(\alpha) - 1|. \quad (6.9)$$

Figure 6 gives $e_N^+(\alpha)$ along the positive real line, that is, in \mathcal{D} for the N values shown in the caption. As N increases the maximum error decreases initially although not particularly rapidly. However, at $N = 16$ the accuracy is poor and has a spike which indicates that the plus factor of the $[16/16]$ approximant has a pole and zero near the positive real axis. This is confirmed in Fig. 7 which illustrates the location of the singularities of the $[16/16]$ approximant of (6.4). Thereafter, the error continues to decrease with increasing N for the values chosen, but it is not uniform and other values of N can be found for which the error is again large. For $N = 28$ an approximate plus factor with error less than 0.002 per cent everywhere in the upper half of the α -plane is achieved. To obtain higher accuracy requires a check, for each N , that the poles and zeros are all located away from the real line. Also, as N becomes very large, the usual difficulties associated with Padé approximants are encountered (ill-conditioned matrices for real arithmetic or extremely

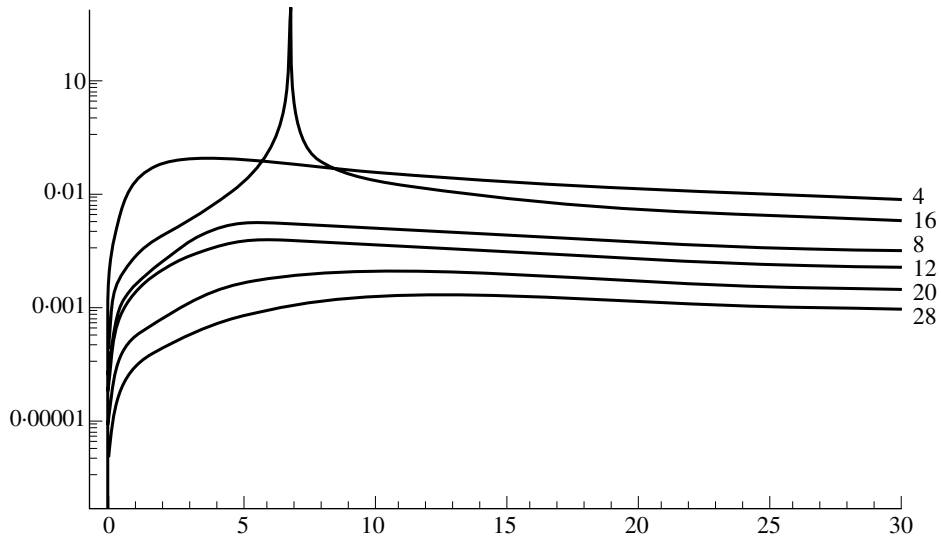


FIG. 6. The percentage error $e_N^+(\alpha)$ (6.9) of the approximant factor of Koiter's kernel (6.4). Plotted on a logarithmic scale for positive real values of α with $N = 4, 8, 12, 16, 20, 28$ as indicated.

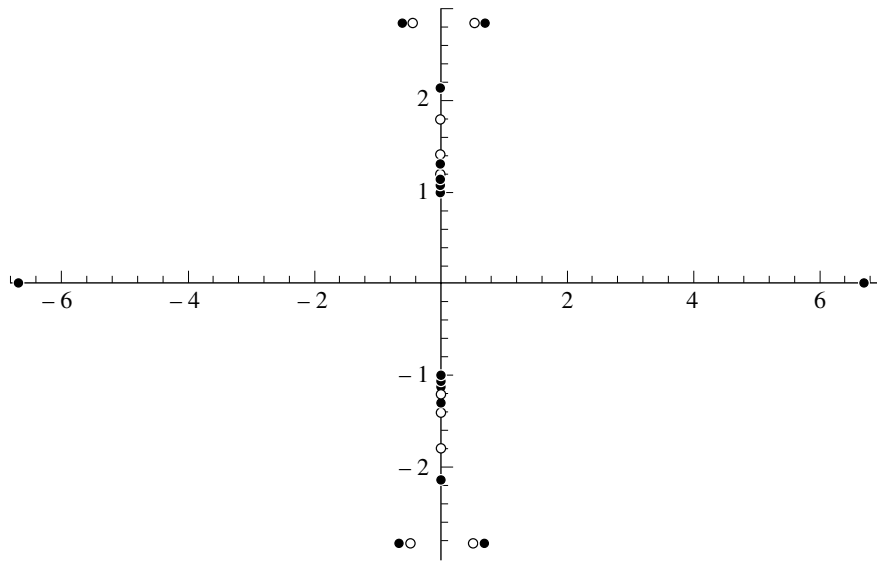


FIG. 7. The location of the poles (open circles) and zeros (closed circles) of the [16/16] approximant of Koiter's kernel (6.4). There are two zeros and two poles located close to the real line which accounts for the reduced accuracy of the approximant factorization at this Padé number.

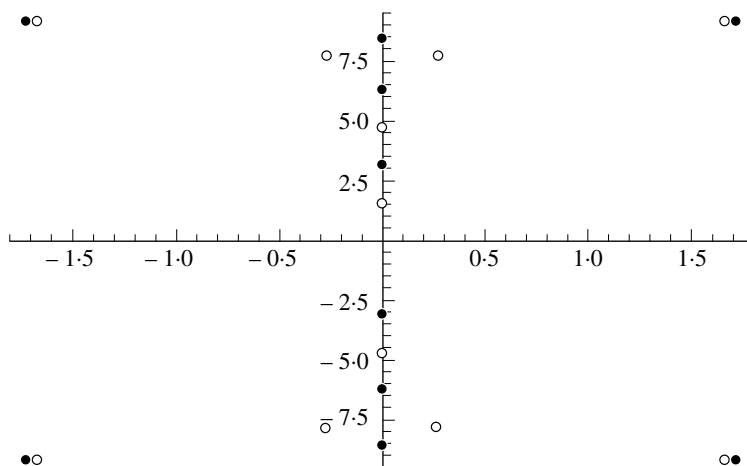


FIG. 8. The location of the branch points of the new approximation $K_0(\alpha)$ (defined in (6.11) with the chosen value of $N = 16$) to Koiter's kernel (6.1). Open circles signify zeros of $K_0(\alpha)$ and closed circles indicate where the function takes infinite values.

large and timely calculations for exact algebra, etc.). The level of accuracy found for $N = 28$ is probably satisfactory for most purposes but is not nearly as accurate as that found with earlier examples. So, the question is, why does the error diminish slowly if at all when N becomes very large? This has partly to do with the fact that the point at infinity is not regular; it is an accumulation point of a sequence of poles as well as a branch point. Unlike the kernel example (5.1) in Section 5.1, here the singularity at infinity is present at leading order and so there are no leading integer inverse powers of α (cf. 5.7). Further, the monotonic convergence displayed in earlier sections is clearly absent in this example because the pole and zero locations of the Padé approximants do not lie near the cut or pole sequences of the original function (6.4).

Once the problem is identified it is easy to offer an alternative approximate factorization procedure. Returning to the original kernel (6.1), clearly

$$K^2(\alpha) = \frac{1}{\alpha^2} \tanh^2 \alpha \tag{6.10}$$

is an even function of α and behaves as α^{-2} as $|\alpha| \rightarrow \infty$ in the strip \mathcal{D} . Hence, we can derive an $[N - 2/N]$ Padé approximation (derived from the expansion at the origin) of this new function:

$$K_0^2(\alpha) = \frac{R_{N-2}(\alpha)}{S_N(\alpha)}, \quad N \text{ even } \geq 0, \tag{6.11}$$

which contains $N - 2$ zeros and N poles which occupy both the upper and lower half-planes. Square-rooting this rational approximation gives $K_0(\alpha)$, with $N - 1$ branch points in the upper half-plane and $N - 1$ branch points in the lower half-plane. Thus, the approximate factors $K_0^\pm(\alpha)$ are now not rational functions but each contains $N - 1$ branch points (giving $(N - 2)/2$ finite cuts and one cut extending to infinity) in their respective half-planes; Fig. 8 illustrates the branch point locations of $K_0(\alpha)$ for $N = 16$. First, this

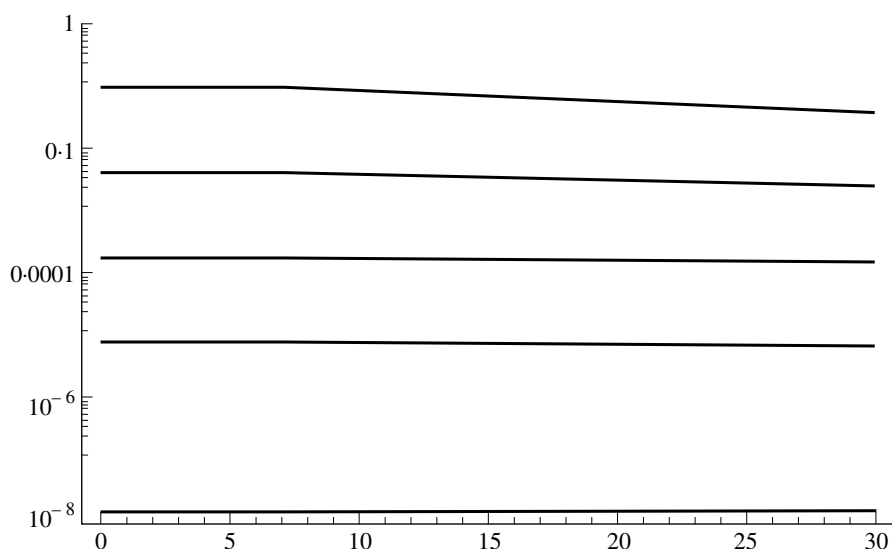


FIG. 9. The percentage error $e_N^+(\alpha)$ of the approximate factor (defined from (6.11) of the kernel given in (6.1)). Plotted on a logarithmic scale for positive real values of α with (from top to bottom as shown) $N = 4, 8, 12, 16, 20, 28$.

reveals that the singularities are well away from the real line which ensures accurate approximant factors. Indeed, by numerical experiment this appears to be the case for all N values. Secondly, it transpires that the branch points lying close to the imaginary axis all have very close neighbours, that is, they are double, and so act like poles or zeros rather than finite cuts. Their location, not surprisingly, is very close to the zeros and poles of $\tanh(z)$. Thus, the approximant factorization, in this form, closely mimics the original function, both in terms of the pole and zero locations and also with the inclusion of branch cuts approaching infinity which yield the $|\alpha|$ property of the function. The following figure, Fig. 9, demonstrates the percentage error (6.9) for the new kernel factor $K_0^+(\alpha)$ for the same Padé numbers as in Fig. 6. Clearly, for the reasons just discussed, substantial improvement has been achieved over the rational function approximation shown in Fig. 6. For example the error for $N = 28$ is now less than 1.6×10^{-8} per cent (cf. 0.002 per cent above), and it now appears to diminish extremely rapidly and monotonically with increasing N .

7. Concluding remarks

This article has demonstrated, by mathematical proof and by numerical evaluation of specific examples, that high accuracy can be achieved when approximating complicated kernel factors by simple ones. The approach leads to explicit kernel factors which are rapid to compute and which have none of the delicate numerical structure found with Cauchy integral representations. Padé approximants (usually two-point) can often be used directly as demonstrated in Sections 4 and 5, and in this form can be seen as algorithmic generalizations of Koiter's original (1954) method. However, as was shown

above, ironically on the very kernel proposed by Koiter himself, the straightforward approach is not always satisfactory, especially when the point at infinity is not regular. In that case each kernel factor is best approximated by a sequence of finite branch cuts plus one semi-infinite cut.

In Koiter's original article, two other kernels were examined. They were typical of those arising in elastostatic, or slow flow problems:

$$\frac{\sinh \alpha \cosh \alpha - \alpha}{2\alpha \sinh^2 \alpha}; \quad \frac{\sinh^2 \alpha - \alpha^2}{2\alpha(\sinh \alpha \cosh \alpha - \alpha)}. \quad (7.1)$$

Both are regular in a strip containing the real line and behave as $1/2|\alpha|$ as $\alpha \rightarrow \pm\infty$. Thus, they have the same behaviour at infinity as expression (6.1) and it can be expected that the scheme in Section 6 is applicable. That is, by squaring the kernels in (7.1), taking an $[N - 2/N]$ Padé approximant, and square-rooting, gives simple explicit approximate factors which are extremely accurate. Indeed errors as low as 10^{-7} per cent are typical, which questions the usual assumption that numerical integration on Cauchy integrals is the most accurate procedure. Further, the kernels in (7.1) are meromorphic and so the $K^\pm(\alpha)$ factors have an infinite product representation. However, these require truncation to evaluate and so will always contain errors usually at least as big as those of the Padé approximant unless very large numbers of terms in the product are included. Referring to the kernels in (7.1), Noble (1988, p. 162) has the following to say in regard to Koiter's approach '... an exact decomposition is possible by means of the infinite product theory, though the roots involved are complex. It seems to me that in this case the crude approximations provide an excellent method for obtaining a rough answer. But if an accurate answer is required it is doubtful whether a refined approximation ... is to be preferred to a straightforward though laborious solution based on the infinite product decomposition'. The purpose of this article has been to refute this assertion by clear demonstration of the efficacy of approximate factorization.

For completeness it is important to mention that other approximate factorization schemes have been offered in the literature. Kranzer & Radlow (1962, 1965) discussed the decomposition of kernels containing a small parameter, and were concerned with obtaining asymptotic expressions for the factors that were uniformly valid over values of $\alpha \in \mathcal{D}$. Jones (1990) employed the same idea on a matrix kernel arising from a problem in fluid/structure interaction; the full kernel has not been exactly solved to date but the simpler kernels arising within an asymptotic expansion can be decomposed by standard methods. Kranzer & Radlow's limited results have been extended recently by Crighton (2000), who proposes the use of matched asymptotic expansions: the strip \mathcal{D} is divided into the required number of asymptotically distinct but overlapping domains, and in each of these the kernel is appropriately approximated as the small parameter tends to zero. By this means a multiplicative composite can be formed, approximating the kernel uniformly in \mathcal{D} . Crighton illustrates the procedure with a number of examples taken from the field of aeroacoustics.

The most relevant alternative approximate scheme for the work herein is that proposed by Carrier (1959). He suggested approximating the kernel $K(\alpha)$ by a suitable simpler function $K_0(\alpha)$, one that can be factored explicitly, and which has enough arbitrary constants with which to 'fine-tune' the accuracy. The constants are then determined by

matching the area and a sufficient number of higher moments of the inverse Fourier transforms of both kernels. This is equivalent to the matching requirement

$$\frac{d^m K(\alpha)}{d\alpha^m} = \frac{d^m K_0(\alpha)}{d\alpha^m}, \tag{7.2}$$

which is applied on $\alpha = 0$ ($\alpha \in \mathcal{D}$) for $m = 0, 1, 2, \dots, M$, where $M + 1$ is the number of constants to be determined. In general the approximate kernel $K_0(\alpha)$ is not a Padé approximant, but the relationship between the moment matching conditions (7.2) and the work in previous sections is apparent. As an example of Carrier’s approach, Dahl & Frisk (1991) approximated the kernel

$$K(\alpha) = (\alpha^2 - k^2)^{1/2} + \eta, \tag{7.3}$$

where k, η are constants with positive real parts and the cuts of the root function are as given in Section 5, by the apparently arbitrary choice of

$$K_0(\alpha) = \frac{(\alpha^2 - k^2)^{1/2}(\alpha^2 + \eta^2 + k^2)}{(\alpha^2 + n^2k^2)^{1/2}} \frac{(\alpha^2 - k^2A_1^2)}{(\alpha^2 - k^2A_2^2)}. \tag{7.4}$$

As $K(\alpha)$ and $K_0(\alpha)$ are even functions, the m odd values of equation (7.2) are automatically satisfied. Thus, matching the $m = 0, 2$ moments for the kernels yields values for the constants A_1, A_2 in terms of the parameter n . This Dahl & Frisk choose by trial and error to yield reasonable approximation (less than five per cent error) between the branch cuts $|\alpha| < |k|$ on the real line. The error is worse for $|\alpha| > |k|$ on the real line but tends to zero at infinity. Clearly, by increasing the orders of the polynomials top and bottom of the second quotient of (7.4), the moment matching scheme is tantamount to obtaining successive single-point Padé representations of the function

$$\frac{(\alpha^2 + n^2k^2)^{1/2}((\alpha^2 - k^2)^{1/2} + \eta)}{(\alpha^2 - k^2)^{1/2}(\alpha^2 + \eta^2 + k^2)}. \tag{7.5}$$

Neither Koiter nor Carrier appeared to appreciate that the simple algorithmic device of Padé approximants for increasing accuracy to very high levels was available for such problems.

The final point to make in this article is to reiterate comments made in earlier sections regarding the importance of Padé approximants in matrix kernel decomposition. In general there is no method available for factorizing such kernels, because non-commutative factors cannot be derived from a sum decomposition. That is, if $K(\alpha)$ is a matrix, then we can define the sum factors:

$$g^\pm(\alpha) = \frac{\pm 1}{2\pi i} \int_C \frac{\log[K(\zeta)]d\zeta}{\zeta - \alpha} \tag{7.6}$$

as we would for a scalar, using the series expansion to define the matrix logarithm. However, unless $g^+(\alpha)$ and $g^-(\alpha)$ commute,

$$K(\alpha) = \exp[g^+(\alpha) + g^-(\alpha)] \neq \exp[g^+(\alpha)] \exp[g^-(\alpha)] \neq \exp[g^-(\alpha)] \exp[g^+(\alpha)] \tag{7.7}$$

and so a product decomposition cannot be achieved by this method. For a full discussion of matrix factorization, which details classes of kernels that do yield to analytical decomposition methods, the reader is referred to Abrahams (1997, 1998) and references cited therein. Kernels which have commutative factorizations (which can be written as (2.3)) are referred to as of Khrapkov form (Khrapkov, 1971). To obtain a general accurate approximate factorization method, the author introduced a new approach which is two-step. First the kernel is rearranged into a form for which a commutative (Khrapkov) factorization is performed. This separates the singularities into the requisite half-planes except for isolated singularities which stem from a single *scalar* function. For problems of interest to the author these singularities are branch cuts or poles (Abrahams, 1996, 1997; Abrahams & Davis, 2000) and the function is of polynomial growth or smaller at infinity. The offending singularities can be removed by replacing the scalar function by its Padé approximant representation, and eliminating the simple poles in the wrong half-planes of the kernel factors by pre- and post-multiplying by a suitable meromorphic matrix. This leads to an exact non-commutative decomposition of an approximate matrix kernel. As found in this article, numerical results suggest strong convergence to the exact matrix kernel factors as the Padé number is increased. So far, the author has examined several long-outstanding problems for which the scalar term in the kernel which requires approximation is reasonably simple, for example, $f(\alpha) = (\alpha^2 - 1)^{1/2}/(\alpha^2 - k^2)^{1/2}$ in Abrahams (1996, 1997); this is essentially the kernel discussed in Section 4. However, for more complicated problems (see, for example Abrahams & Davis, 2000), straightforward approaches are not so successful and so some of the extensions or developments suggested in this article for scalar kernels will be helpful in the matrix case also.

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