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CHAPTER 5

Best uniform and modified Padé approximants to probability densities in econometrics

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In this chapter, a new method of approximating the probability density functions (pdf's) of econometric estimators and test statistics is developed. It is shown that best uniform approximants to a general class of pdf's exist in the form of rational functions. A procedure for extracting the approximants is devised, based on modifying multiple-point Padé approximants to the distribution. The new approximation technique is very general and should be widely applicable in mathematical statistics and econometrics. It has the advantage, unlike the Edgeworth and saddlepoint approximations, of readily incorporating extraneous information on the distribution, even qualitative information. The new procedure is applied to a simple simultaneous-equations estimator, and it gives exceptionally accurate results even for tiny values of the concentration parameter.

1 Introduction

The idea of approximating small sample distributions, rather than extracting their exact mathematical forms, has a long history in statis-

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tics, and a number of different techniques have been explored. Kendall and Stuart (1969) gave an introductory survey of some of these techniques in their Chapters 6, 12, and 13. Approximations are clearly of importance in those cases in which mathematical difficulties have prevented the development of an exact theory. An example is provided by regression models with lagged endogenous variables as regressors, models that are of particular relevance in econometrics. Approximations to distributions are also useful in those cases in which the exact mathematical expressions are too complicated for numerical computations. Some examples of the latter have been discussed previously (Phillips, 1980a, 1980b).

Several authors have recently obtained approximations to the distribution of econometric estimators and test statistics based on asymptotic series. The approximations used in most of these studies have been based on the first few terms of Edgeworth-type asymptotic expansions of the distribution function (df) or probability density function (pdf) of the statistic under consideration. An alternative approach that can, when it is available, provide significant improvement on the Edgeworth approximation, particularly in tail areas, is based on the method of steepest descents in contour integration. This method leads to the saddlepoint approximation. Its use was systematically explored for the first time in statistics by Daniels (1954, 1956), and it has recently been the subject of renewed interest (Daniels, 1980; Durbin, 1980a, 1980b; Holly & Phillips, 1979; Phillips, 1978a, 1978b).

Both these methods of approximation are capable of representing the exact distribution to an acceptable degree of accuracy in certain parameter environments. This has been confirmed by the numerical evaluations of Anderson and Sawa (1973, 1979), Phillips (1977a, 1978a), and Holly and Phillips (1979). Moreover, the approximate distributions that have been obtained in the literature have already given valuable information concerning the small-sample behavior of competing estimators and the adequacy of asymptotic theory in simple simultaneous equations and dynamic models. However, given the current state of our knowledge, the use of either of these methods in practical econometric work to advise on the choice of estimator and improve inferential accuracy is bound to encounter difficulites, some of them major.

First of all, there are certain parameter environments in which the performance of the approximations is poor, sometimes a good deal worse than the asymptotic distribution (particularly in the case of the Edgeworth approximation). Unfortunately, the parameter environments for which this poor performance obtains are not at all unusual. As we might expect, given that the approximations are based on asymptotic

series, this problem tends to become more widespread when sample sizes are small. Some indication of the wayward nature of these approximations in certain parameter environments is already available (Phillips, 1977a, 1978a). Further documentation will be given in a companion article (Phillips, 1982).

Second, although general formulas for the Edgeworth approximation are now available (Phillips, 1977a; Sargan, 1976) and widely applicable, the saddlepoint technique is practicable only in specialized cases in which the characteristic function is available or simple integral formulas for the pdf can be used, such as in the case of ratios (Daniels, 1956), or in which there exists a set of sufficient statistics for the parameters to be estimated (Durbin, 1979b). No doubt progress will be made in tackling some of these latter difficulties, but in the meantime they remain a barrier to the general use of the procedure.

Another difficulty that can arise in the use of the saddlepoint technique is that for certain values of the argument of the pdf, singularities can occur within the strip of the imaginary axis containing the saddlepoint through which the path of integration is normally deformed. In such cases, this path of deformation is no longer permissible, and special techniques must be used to smooth the approximation past the singularity; the resulting approximants are called uniform asymptotic expansions. Uniform approximants typically are much more complicated in form than the saddlepoint approximation; an example has been given in Phillips (1978b). They are not always easy to extract, and further work will be required to splice them with the saddlepoint approximation, where it does exist, to cover the whole of the distribution.

Finally, it seems difficult to embody additional information on the distribution in question into these approximations. To take a simple example, in spite of the fact that the actual pdf is nonnegative and the df is monotonic, it is sometimes awkward to modify the Edgeworth approximations so that they share these properties. To take a more complicated example, often we know or can find the leading term in the series representation of the exact pdf (in many cases, without knowing the full expression for the pdf). Frequently this leading term has a simple algebraic form and is instrumental in determining the behavior of the exact distribution in certain domains, particularly the tails. Yet, even when this information is available, there seems to be no obvious way of building it into either the Edgeworth or the saddlepoint approximation. The resulting approximations, therefore, end up neglecting what is potentially very useful analytic information on the form of the distribution.

The purpose of this chapter is to introduce a new technique of ap-

proximating sampling distributions. The technique is quite general and should be widely applicable in mathematical statistics and econometrics. Unlike the Edgeworth and saddlepoint approximations, it has the advantage of readily incorporating extraneous information on the distribution, even qualitative information. Moreover, because the technique is not based on an asymptotic series expansion in terms of the sample size or concentration parameter, accurate approximations can be obtained even in very small samples. The technique should, therefore, be most useful in cases in which the Edgeworth and saddlepoint approximations run into difficulty. It turns out that the new approximation is close to the best uniform approximant in the class of certain rational functions. These approximants will be discussed and the class of rational functions to be used will be defined in Section 2. A general theory of best uniform approximation in the context of density approximation will be given in Sections 3 and 4. These sections will provide the theoretical basis for the new technique. Sections 5, 6, and 7 will describe the procedure and give the general formulas needed in applications. In Section 8 the method will be applied to a simple simultaneous-equations estimator, facilitating comparison between the new technique and existing techniques of approximation.

2 A general class of density functions and rational approximants

To fix ideas, we write the estimator or test statistic in which we are interested as θ_T. In what follows, we treat θ_T as a scalar, so that when dealing with estimators we are, in effect, concentrating on the marginal distribution of individual components of a complete vector of estimates. The characteristic function (cf) of θ_T is written as $\mathrm{cf}(s) = E(\exp(is\theta_T))$ and is assumed to be absolutely integrable. This implies that θ_T has a bounded continuous pdf given on inversion by

$$\text{(1)} \qquad \mathrm{pdf}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-isx} \mathrm{cf}(s)\, ds$$

Moreover, by the Riemann-Lebesgue lemma, it follows from equation (1) that $\mathrm{pdf}(x) \to 0$ as $x \to \pm\infty$. Thus the effect of the integrability requirement on $\mathrm{cf}(s)$ is to confine our attention to the class of densities covered by the following assumption.

Assumption 1: θ_T has a continuous pdf that tends to zero at the limits of its domain of definition $(\pm\infty)$.

Note that the boundedness of the pdf now follows from its continuity and behavior at $\pm\infty$. Assumption 1 covers a wide variety of densities arising in econometric work. It can, in fact, be extended to allow for certain types of discontinuity and singularity, but this complicates the development of the approximants that follows. Therefore, in this chapter we shall keep to the class of densities defined by Assumption 1. This is sufficiently general to include all the usual simultaneous-equations estimators and test statistics, as well as their extensions to models with lagged endogenous variables as regressors and autoregressive moving-average errors.

Having defined the class of density functions, the general problem of approximation takes the following form: For a particular density function $\text{pdf}(x)$, find an approximating function that depends on a finite number of parameters whose values are selected in such a way that the approximating function is as close, in some sense, as possible to the original density over its entire domain of definition. Once stated in this way, it is clear that there are two major components to the problem. The first is the form the approximating function should take. The second is the criterion of closeness of approximation to be used in selecting the best approximant. By a best approximant we mean the member (or members) of the given family of approximating functions whose closeness to the function $\text{pdf}(x)$ cannot be improved by use of any other member of the same family. Thus, the second problem clearly raises the further question whether or not there exists a best approximation to $\text{pdf}(x)$ in the given family of approximants. This question of existence will be the subject of the next section. We now define the class of approximating functions and the measure of approximation to be used in the rest of this chapter.

Definition: If $s(x)$ is a real continuous function satisfying $s(x)>0$ and $s(x)\to 0$ as $x\to\pm\infty$, then we define the class of rational approximating functions by

$$(2)\qquad R_{n,n}(x;s,\gamma) = s(x)\frac{P_n(x)}{Q_n(x)} = s(x)\frac{a_0 + a_1x + \cdots + a_nx^n}{b_0 + b_1x + \cdots + b_nx^n} \quad (-\infty < x < \infty)$$

where (i) the numerator and denominator are reduced to their lowest degree by the cancellation of identical factors, (ii) n is an even integer, and (iii) $\gamma' = (a_0a_1, \ldots, a_n, b_0, b_1, \ldots, b_n) \in \Gamma$, the parameter space, which is defined as the following subspace of $(2n+2)$-dimensional Euclidean space

$$\Gamma = \left\{ \gamma : \sum_{i=0}^{n} b_i^2 = 1, \ \ Q_n(x) > 0 \ \text{ for all } \ x \in (-\infty, \infty) \right\}$$

The condition $\sum_{i=0}^{n} b_i^2 = 1$ on the parameter space Γ is a normalization that eliminates the redundancy in the coefficients of the rational function (2). Other normalizations, such as $b_0 = 1$ or $b_n = 1$, are possible and may be more useful in applications. In fact, we shall later use the normalization $b_0 = 1$ in the application of Section 8, but the present definition of Γ is retained for the theoretical development.

The condition $Q_n(x) > 0$ ensures that the rational fractions of equation (2) have no poles on the real line and are therefore compatible with the class of density functions to be approximated. Because this is possible only when n is an even integer, we have introduced this requirement explicitly under condition (ii). On the other hand, when the density function we wish to approximate is nonzero on part, rather than all, of the real axis, it is clear that this requirement may be relaxed. Moreover, if singularities in the density function do occur on the real axis, we may remove the condition $Q_n(x) > 0$. If the position of the singularity is known, this can be incorporated directly into equation (2); otherwise, it must be approximated, and for certain values of n it may not be captured by the approximation, although whether or not this occurs will depend on the technique used to construct the approximation.

We might consider working with the somewhat wider class of rational functions for which the numerator and denominator polynomials are not necessarily of the same degree. In certain applications it may seem appropriate to make such a generalization of the class of approximants, and the theory we shall develop can be modified to take this generalization into account. However, there are various reasons why we do not choose to work with the more general class in developing our theory. The first is that the coefficient function $s(x)$ frequently will be constructed so that it captures the behavior of the exact pdf(x) as x approaches the limits of its domain. A rational fraction of equal degree is then immediately compatible with this behavior. The second is that when the numerator and denominator are of the same degree, modifications to the coefficients that are designed to avoid unwanted zeros and poles in the final approximant are easier to make. That this is of particular importance will be seen in Section 4, where the practical procedure we develop for obtaining a good approximant of the type in equation (2) is based on modifying multiple-point Padé approximants, which in crude form frequently possess zeros and poles that need to be removed in order to improve the approximation over the whole real line. Finally, numerical experience with rational function approximations in applied

mathematics (Hart, 1968; Meinardus, 1967) suggests that rational fractions with numerator and denominator of equal or nearly equal degrees tend, on the whole, to give better approximations than those for which the degrees differ markedly. Taking an extreme case for comparison, polynomial approximations usually become unsatisfactory when it is necessary to approximate a function over a wide interval. Moreover, they lack the capacity to turn corners sharply and then go straight for long periods, particularly in a direction almost parallel to the horizontal axis. It is useful for a density function approximant to be capable of capturing these properties. An important feature of rational fraction approximations is that even low-degree fractions of the type in equation (2) are flexible enough to assume this behavior. This is endorsed by the large number of numerical results with rational approximants reported by Hastings (1955) and Hart (1968). It will also be confirmed in our own application of the technique reported in Section 5.

In order to develop a theory for the goodness of approximation based on members of the class (2), we introduce a norm to measure the error in the approximation. We shall use the uniform norm (also known as the Tchebycheff or L_∞ norm) defined as

$$\|f(x)\| = \sup_{x \in (-\infty, \infty)} |f(x)| \tag{3}$$

If we now let $f(x) = \mathrm{pdf}(x) - R_{n,n}(x; s, \gamma)$ denote the approximation error, our problem is, for a given value of n and a given function $s(x)$, to find a value of γ that minimizes the maximum error. At this value of γ, $R_{n,n}(x; s, \gamma)$ is then called a best uniform (or Tchebycheff) approximation to $\mathrm{pdf}(x)$.

Other choices of norm are certainly possible and will generally lead to different best approximations, where they exist. However, for accurately approximating $\mathrm{pdf}(x)$ over a wide interval, the choice of the uniform norm seems very appropriate.

3 Best uniform approximation by rational functions

The theory of best uniform approximation of real continuous functions by rational fractions has a long history. One of the earliest discussions was undertaken by Tchebycheff (1859). Frobenius (1881) and Padé (1892) both systematically investigated the properties of a specialized class of rational approximants now known as Padé approximants (Section 4). In the complex domain, Runge (1885) (Rudin, 1974, Chapter 13) established the possibility of uniform approximation of analytic functions by rational fractions with preassigned poles. A general theory of

approximation in the complex domain by rational functions was developed in a treatise by Walsh (1965). Extensive modern treatments of the subject covering all the classical results on the approximation of real-valued functions are given in the volumes by Rice (1964) and Meinardus (1967). Because the theory in this literature, with the exception of the work of Walsh (1965), has been concerned with the approximation of functions that are defined over compact sets, this section will be devoted to the development of a theory that is applicable over the whole real line and is therefore directly relevant to the problem of density function approximation. Our treatment of the problem will be based on the framework laid out in Section 2 and will follow the lines of Rice (1964), particularly his Section 3.8.

To establish the existence of a best uniform approximant to a given $\mathrm{pdf}(x)$ in the class of rational fractions defined by equation (2), we need to show that there exists a set of parameters γ^* for which

$$\|R_{n,n}(x;s,\gamma^*) - \mathrm{pdf}(x)\| = \inf_{\gamma\in\Gamma} \|R_{n,n}(x;s,\gamma) - \mathrm{pdf}(x)\| = \rho, \quad \text{say} \tag{4}$$

Now, $0\leqslant\rho<\infty$, and we can find a sequence of rational fractions $\{R_{n,n}(x;s,\gamma^{(j)})\}$ for which

$$\rho_j = \|R_{n,n}(x;s,\gamma^{(j)}) - \mathrm{pdf}(x)\| \tag{5}$$

and

$$\lim_{j\to\infty} \rho_j = \rho \tag{6}$$

It remains to prove that the parameter sequence $\{\gamma^{(j)}\}$ has a convergent subsequence that converges to a set of finite parameters. If we call the latter γ^*, then it will follow from equation (6) that γ^* satisfies equation (4). As discussed by Rice (1964, pp. 26–7), the crucial part of the proof of existence is to demonstrate that the parameters lie in a compact set.[1] First, we show that we may restrict our attention to bounded subsets of Γ.

Definition: Condition E of Rice (1964, p. 27). The approximating function $R_{n,n}(x;s,\gamma)$ is said to satisfy condition E for the norm $\|\ \|$ if, given $M<\infty$, there is an $N<\infty$ such that

$$\|R_{n,n}(x;s,\gamma)\| \leqslant M$$

implies that

$$\max_i |\gamma_i| \leqslant N$$

where $\gamma = (\gamma_i)$.

In view of equations (5) and (6), there is an integer j_0 for which

$$\|R_{n,n}(x; s, \gamma^{(j)}) - \text{pdf}(x)\| \leqslant \rho + 1 \tag{7}$$

for all $j > j_0$. Moreover, from Assumption 1 it follows that there exists $K > 0$ for which $\|\text{pdf}(x)\| \leqslant K$, and, hence, using equation (7), we have the inequality

$$\|R_{n,n}(x; s, \gamma^{(j)})\| \leqslant K + \rho + 1 \tag{8}$$

We now verify that condition E holds for the approximating function $R_{n,n}(x; s, \gamma)$.

Lemma 1: The rational fraction $R_{n,n}(x; s, \gamma)$ defined by (2) satisfies condition E for the uniform norm (3).

Proof: We consider the set

$$\{\gamma : \|R_{n,n}(x; s, \gamma)\| \leqslant M, \quad M > 0\} \tag{9}$$

Because $\|R_{n,n}(x; s, \gamma)\| \leqslant M$ implies that, for a given number $L > 0$,

$$\max_{x \in [-L, L]} |R_{n,n}(x; s, \gamma)| \leqslant M$$

it follows that (9) lies in the set

$$\{\gamma : \max_{x \in [-L, L]} |R_{n,n}(x; s, \gamma)| \leqslant M\} \tag{10}$$

Now, for $x \in [-L, L]$, and taking $L > 1$, we have

$$\begin{aligned} |R_{n,n}(x; s, \gamma)| &\geqslant \frac{\min_{x \in [-L, L]} |s(x)|}{\max_{x \in [-L, L]} |Q_n(x)|} |P_n(x)| \\ &\geqslant \frac{s_L (L^2 - 1)^{1/2}}{(L^{2(n+1)} - 1)^{1/2}} |P_n(x)| \end{aligned} \tag{11}$$

where

$$s_L = \min_{x \in [-L, L]} |s(x)| > 0$$

Thus, when γ lies in the set (10), we have

$$\frac{M(L^{2(n+1)} - 1)^{1/2}}{s_L (L^2 - 1)^{1/2}} \geqslant \max_{x \in [-L, L]} |P_n(x)| = \max_{x \in [-L, L]} \left| \sum_{i=0}^{n} a_i x^i \right|$$

and the polynomial $\sum_{i=0}^{n} a_i x^i$ is bounded uniformly on the interval $[-L, L]$. It follows that the coefficient parameters a_i are also bounded. Moreover, $\sum_{i=0}^{n} b_i^2 = 1$, by definition, so that the parameter set (10) is bounded. By implication, the same is true for the set (9), and thus $R_{n,n}(x; s, \gamma)$ satisfies condition E for the uniform norm.

This lemma shows that we can confine our attention to bounded subsets of Γ in searching for a best approximant. Hence, for all $j \geqslant j_0$, the sequence $\{\gamma^{(j)}\}$ introduced earlier lies in a bounded subset of Γ. We may, therefore, select a subsequence that converges to the vector γ^*, say. If we reindex the subsequence, we can write for the individual components of γ the following: $\lim_{j\to\infty} a_i^{(j)} = a_i^*$ and $\lim_{j\to\infty} b_i^{(j)} = b_i^*$ for $i = 0, 1, \ldots, n$.

Now it is important to note that because Γ is not closed, γ^* may or may not lie in Γ. If $\gamma^* \in \Gamma$, then $R_{n,n}(x; s, \gamma^*)$ is a rational function of the form defined in (2) and, in view of (4), is therefore a best uniform approximant of $\mathrm{pdf}(x)$. But, if $\gamma^* \notin \Gamma$, then $R_{n,n}(x; s, \gamma^*)$ is the limit of a sequence of functions and is not necessarily a rational function itself. In fact, it may not even be continuous (we shall give an example later in this section). However, the limit function $R_{n,n}(x; s, \gamma^*)$ will differ from a rational function, $R'_{n,n}(x; s, \gamma^*)$, say, only at a finite number of points. And, in fact, $R'_{n,n}(x; s, \gamma^*)$ is a best uniform approximant to $\mathrm{pdf}(x)$ in the class defined by (2).

The problem discussed in the preceding paragraph arises because although the denominator polynomial $Q_n(x) = Q_n(x; \gamma) > 0$ for $\gamma \in \Gamma$, this no longer necessarily holds when γ does not lie in Γ. Because γ^* is a subsequential limit of elements of Γ, it follows that, in the limit, $Q_n^*(x) = Q_n(x; \gamma^*)$ can have, at most, n zeros. If we let $P_n^*(x) = P_n(x; \gamma^*)$ be the limit of the numerator polynomial as $\gamma^{(j)} \to \gamma^*$, it follows that there are, at most, n points where $R'_{n,n}(x; s, \gamma^*) = s(x)P_n^*(x)/Q_n^*(x)$ is undefined. At all other points we must have $R_{n,n}(x; s, \gamma^{(j)}) = R'_{n,n}(x; s, \gamma^*)$. Moreover, because $R'_{n,n}(x; s, \gamma^*) = \mathrm{pdf}(x) + \{R_{n,n}(x; s, \gamma^{(j)}) - \mathrm{pdf}(x)\} + \{R'_{n,n}(x; s, \gamma^*) - R_{n,n}(x; s, \gamma^{(j)})\}$, it follows from (7) that for $j \geqslant j_0$

$$|R'_{n,n}(x; s, \gamma^*)| \leqslant K + \rho + 1 + |R'_{n,n}(x; s, \gamma^*) - R_{n,n}(x; s, \gamma^{(j)})|$$

and allowing $j \to \infty$, we deduce that

$$|R'_{n,n}(x; s, \gamma^*)| \leqslant K + \rho + 1 \tag{12}$$

Hence, for all x other than zeros of $Q_n^*(x)$, we have the inequality

$$s(x)|P_n^*(x)| \leqslant (K + \rho + 1)Q_n^*(x) \tag{13}$$

By continuity, (13) holds also when $Q_n^*(x)=0$. Thus, any real zero of $Q_n^*(x)$ is also a zero of $P_n^*(x)$, because $s(x)>0$ for all finite x. We therefore eliminate by cancellation each linear factor of $Q_n^*(x)$ corresponding to a real root of $Q_n^*(x)=0$. We call the resulting rational fraction $R'_{n,n}(x;s,\gamma^*)$ and note that for all values of x other than zeros of $Q_n^*(x)$

$$R'_{n,n}(x;s,\gamma^*) = R_{n,n}(x;s,\gamma^*)$$

whereas at the zeros $\{x_k : k=1,\ldots,m\leqslant n\}$ of $Q_n^*(x)$

$$R'_{n,n}(x_k;s,\gamma^*) = \lim_{x\to x_k} R_{n,n}(x;s,\gamma^*)$$

Finally, we note that

$$\begin{aligned}\|R_{n,n}(x;s,\gamma^*) - \mathrm{pdf}(x)\| &= \sup_{x\in(-\infty,\infty)} |R_{n,n}(x;s,\gamma^*) - \mathrm{pdf}(x)| \\ &= \max\Bigg\{\sup_{\substack{x\in(-\infty,\infty)\\ x\neq x_k}} |R_{n,n}(x;s,\gamma^*) - \mathrm{pdf}(x)|, \\ &\qquad |R_{n,n}(x_k;s,\gamma^*) - \mathrm{pdf}(x_k)|, \\ &\qquad\qquad i=1,\ldots,m\Bigg\} \\ &\geqslant \sup_{x\in(-\infty,\infty)} |R'_{n,n}(x;s,\gamma^*) - \mathrm{pdf}(x)| \\ &= \|R'_{n,n}(x;s,\gamma^*) - \mathrm{pdf}(x)\|\end{aligned}$$

The rational function $R'_{n,n}(x;s,\gamma^*)$ is therefore a best uniform approximation of $\mathrm{pdf}(x)$, and we have proved the following theorem.

Theorem 1: Existence of a best uniform approximant. If $\mathrm{pdf}(x)$ satisfies Assumption 1 on $(-\infty,\infty)$, then there is a best uniform approximant to $\mathrm{pdf}(x)$ in the class of rational functions defined by (2).

To illustrate the problem that arises in the proof of this theorem because Γ is not closed, we consider the following density function of the Pareto distribution

$$\mathrm{pdf}(x) = \frac{ak^a}{x^{a+1}} \quad (a>0,\ x\geqslant k>0)$$

We consider the case in which $a=2$ and a class of rational approximants of the form (2) is being used with $s(x)=1/x$ $(x\geqslant k)$ and $n=4$. Now consider the sequence of approximants defined by

$$R_{4,4}(x;s,\gamma^{(j)}) = \left(\frac{2k^2}{x}\right) \times \frac{(1/(1+k^4) - 1/2j^2)^{1/2}x^2 - (k^4/(1+k^4) - 1/2j^2)^{1/2}}{(1/(1+k^4) - 1/2j^2)^{1/2}x^4 - (k^4/(1+k^4) - 1/2j^2)^{1/2}x^2 + 1/j}$$

Thus,

$$\gamma^{(j)'} = \left[-\left(\frac{k^4}{1+k^4} - \frac{1}{2j^2}\right)^{1/2}, 0, \left(\frac{1}{1+k^4} - \frac{1}{2j^2}\right)^{1/2}, 0, 0; \frac{1}{j}, 0, -\left(\frac{k^4}{1+k^4} - \frac{1}{2j^2}\right)^{1/2}, 0, \left(\frac{1}{1+k^4} - \frac{1}{2j^2}\right)^{1/2}\right]$$

and, as $j \to \infty$,

$$\gamma^{(j)'} \to \gamma^{*\prime} = \left[-\left(\frac{k^4}{1+k^4}\right)^{1/2}, 0, \left(\frac{1}{1+k^4}\right)^{1/2}, 0, 0; 0, 0, -\left(\frac{k^4}{1+k^4}\right)^{1/2}, 0, \left(\frac{1}{1+k^4}\right)^{1/2}\right]$$

The limiting function is then

$$R_{4,4}(x;s,\gamma^*) = \begin{cases} 2k^2/x^3 & \text{for } x > k \\ 0 & \text{for } x = k \end{cases}$$

which is not a rational function, nor is it continuous on the interval $[k,\infty)$. However,

$$R'_{4,4}(x;s,\gamma^*) = \frac{2k^2}{x^3} \quad (x \geqslant k)$$

is rational and continuous and is clearly the best uniform approximant to $\mathrm{pdf}(x)$ on $[k,\infty)$.

4 A convergence theorem

As the degree of the best approximating rational fraction increases, the error $E(n,s) = \|\mathrm{pdf}(x) - R'_{n,n}(x;s,\gamma^*)\|$ must be at least as small. In fact, as Theorem 3 will show, $E(n,s) \to 0$ as $n \to \infty$, so that the best approximant $R'_{n,n}(x;s,\gamma^*)$ converges to $\mathrm{pdf}(x)$ as $n \to \infty$. It follows that for any choice of density function satisfying Assumption 1, there is an arbitrarily close rational approximant. In this sense, the rational fractions of the class defined by equation (2) are dense in the set of density functions that satisfy Assumption 1.

Meinardus (1967) proved a related theorem on the convergence of rational fractions to a continuous function over a bounded interval.[2]

Theorem 2: The real-valued function $f(x)$ is continuous and nonnegative over the interval $[-1,1]$ and is approximated by

$$R_{m,n}(x) = \frac{P_m(x)}{Q_n(x)} \tag{14}$$

where $P_m(x)$ and $Q_n(x)$ are polynomials with real coefficients and $Q_n(x) > 0$ for $x \in [-1,1]$.

$$E_{m,n}(f) = \inf_{R_{m,n} \in V_{m,n}} \|f - R_{m,n}\|$$

where $V_{m,n}$ is the set of all rational functions, as in (14). Then

$$\lim_{n+m\to\infty} E_{m,n}(f) = 0$$

independent of the manner in which we pass to the limit.

Proof: Meinardus (1967, pp. 158–60).

Theorem 3: If $\text{pdf}(x)$ satisfies Assumption 1 on $(-\infty, \infty)$ and

$$E(n,s) = \|\text{pdf}(x) - R'_{n,n}(x; s, \gamma^*)\|$$

where $R'_{n,n}(x; s, \gamma^*)$ is the best uniform approximant to $\text{pdf}(x)$ in the class of rational fractions defined by (2), then

$$\lim_{n\to\infty} E(n,s) = 0$$

Proof: Let $\epsilon > 0$ be arbitrarily small. Then, by Assumption 1 and the definition of $R_{n,n}(x; s, \gamma)$, there exists an $L > 0$ and large enough n for which

$$\sup_{|x|>L} |\text{pdf}(x) - R'_{n,n}(x; s, \gamma^*)| < \epsilon$$

Now,

$$\|\text{pdf}(x) - R'_{n,n}(x; s, \gamma^*)\| = \max\left\{ \max_{x\in[-L,L]} |\text{pdf}(x) - R'_{n,n}(x; s, \gamma^*)|, \sup_{|x|>L} |\text{pdf}(x) - R'_{n,n}(x; s, \gamma^*)| \right\}$$

$$= \max\left\{ \max_{x\in[-L,L]} |\mathrm{pdf}(x) - R'_{n,n}(x;s,\gamma^*)|, \epsilon \right\}$$

It only remains to show that there is an n_0 for which $n > n_0$ implies that

$$\max_{x\in[-L,L]} |\mathrm{pdf}(x) - R'_{n,n}(x;s,\gamma^*)| < \epsilon \tag{15}$$

For then, because ϵ is arbitrarily small, we can approximate $\mathrm{pdf}(x)$ by $R'_{n,n}(x;s,\gamma^*)$ over the whole real line as closely as we please for sufficiently large n. Hence, $E(n,s) \to 0$ as $n \to \infty$.

In fact, equation (15) follows from Theorem 2. We need only transform $x = Ly$ with $-1 \leqslant y \leqslant 1$, and setting

$$R'_{n,n}(x;s,\gamma^*) = s(Ly)\frac{P'_n(Ly)}{Q'_n(Ly)} = \bar{s}(y)\frac{\bar{P}'_n(y)}{\bar{Q}'_n(y)}$$

$$\mathrm{pdf}(x) = \mathrm{pdf}(Ly) = \overline{\mathrm{pdf}}(y)$$

we have

$$\max_{x\in[-L,L]} |\mathrm{pdf}(x) - R'_{n,n}(x)| = \max_{y\in[-1,1]} \bar{s}(y)\left| \frac{\overline{\mathrm{pdf}}(y)}{\bar{s}(y)} - \frac{\bar{P}'_n(y)}{\bar{Q}'_n(y)} \right|$$

Because $\overline{\mathrm{pdf}}(y)/\bar{s}(y)$ is continuous and nonnegative over $[-1,1]$, it follows by Theorem 2 that equation (15) holds for n sufficiently large.

5 Local expansions for densities

The theory of the last two sections shows that for a given pdf in the class defined by Assumption 1 there exists a best rational fraction approximant of the type (2) and that, as we increase the degree of the approximant, this converges to $\mathrm{pdf}(x)$ over the entire real axis. In any practical situation, of course, we will need to prescribe the degree of the approximant to be used and attempt to find the best approximant in the given class. This normally requires numerical methods, and the algorithms discussed in the literature (Meinardus, 1967, pp. 170–1; Rice, 1964, Chapter 6) rely on knowledge of the true function values at a grid of points as well as, in certain cases, the function derivatives. This seems too much to expect in an econometric context, where, even in those cases in which the exact density function is known in analytic form, numerical computations often are impossible because of convergence problems with the multiple series representation of the density or the inadequate tabulations of the special polynomials that appear in the analytic expressions.

We are therefore left with the problem of how, in a given situation, to

get close to the best approximant in the class (2) without having to rely on arbitrary evaluations of the exact distribution. The solution we present to this problem in this and succeeding sections of this chapter is based on the idea of using the local behavior of the true density in the body of the distribution and in the tails to construct a global approximation of the form (2). In principle, the procedure we develop for moving from local to global density approximations can be based on knowledge of local behavior at an arbitrary set of points. But, in practice, it will be sufficient to use information concerning the local behavior of the density in the tails and around the center of the distribution. The application we consider in Section 8 will show that this information is sufficient to secure excellent global approximations to rather complicated density functions, even with rational fractions of lower degree.

The local behavior of density functions can take the form of expansions about the value of the function at a certain point or perhaps estimates of the function values obtained from Monte Carlo simulations. We shall deal with the case in which some analytic information from local expansions is available; at the same time, it should be clear how the procedure we develop can also be used to accommodate Monte Carlo evidence.

Our present analytic knowledge of the exact distribution of a variety of econometric estimators and test statistics shows that there exists an asymptotic expansion of the density function in ascending powers of x^{-1} as the argument x approaches the limits of its domain ($\pm\infty$ or $+\infty$). In general, we can write the expansion about infinity in the form

$$\text{(16)} \qquad \text{pdf}(x) \sim t(|x|)\{\alpha_0 + \alpha_1/x + \alpha_2/x^2 + \alpha_3/x^3 + \alpha_4/x^4 \ldots\}$$

as $x \to \pm\infty$. The coefficient function $t(|x|) \to 0$ as $|x| \to \infty$ and, in the case of most of the common simultaneous-equations estimators, is of the form $t(|x|) = |x|^{-k}$, where $k \geq 2$. Thus, in the case of the two-stage least-squares estimator, $k = l + 2$, where l is the degree of overidentification in the equation being estimated. An expansion of the type (16) was developed by Sargan and Mikhail (1971) for the instrumental variable estimator and was used by Sargan (1981) in the analysis of Monte Carlo estimates of moments that do not exist.

At points $\{d_i : i = 1, \ldots, I\}$, where pdf$(x)$ is continuously differentiable to an appropriate order, we have the Taylor expansions

$$\text{(17)} \qquad \begin{aligned} \text{pdf}(x) = {} & \beta_{i0} + \beta_{i1}(x - d_i) + \beta_{i2}(x - d_i)^2 + \beta_{i3}(x - d_i)^3 \\ & + \beta_{i4}(x - d_i)^4 + \cdots \quad (i = 1, \ldots, I) \end{aligned}$$

In a number of cases we also have the analytic form of the leading term in the series representation of the density. If we denote this leading term

by $w(x)$, then it will be useful to consider extensions of the expansion (17) that take the form

$$\text{(18)} \qquad \text{pdf}(x) = w(x)\{\beta_{i0} + \beta_{i1}(x - d_i) + \beta_{i2}(x - d_i)^2 + \beta_{i3}(x - d_i)^3 + \beta_{i4}(x - d_i)^4 + \cdots\}$$

There are two obvious choices of the points d_i: (i) the origin, particularly for certain test statistics like the t ratio; (ii) the true value of the relevant parameter, when $\text{pdf}(x)$ refers to the marginal distribution of a certain estimator.

Although expansions such as (16) and (17) usually produce good approximations only in the immediate neighborhood of the point of expansion, they can be used to construct approximations that perform well outside the immediate locality of the approximation while retaining the good behavior of the original expansions within the locality. With reference to (17), the fourth-degree polynomial in x may yield a good approximation to $\text{pdf}(x)$ in a neighborhood of the point d_i, but in most cases its performance will rapidly deteriorate outside of this neighborhood, and it will be quite inadequate as an approximation on the tails. On the other hand, the coefficients β_{i1} in the expansion (17) usually contain information that can produce greatly improved approximations outside the range in which expansion (17) itself is immediately useful. That this is so is demonstrated by the extensive practical experience with Padé approximants in the applied mathematics literature. These approximants are rational fractions for which the corresponding Taylor series matches the Taylor-series expansion of a given function to as many powers as possible. In the present context, we can refer to the following example used by Baker (1975):

$$\text{(19)} \qquad f(x) = \left(\frac{1+2x}{1+x}\right)^{1/2} = 1 + \frac{1}{2}x - \frac{5}{8}x^2 + \frac{13}{16}x^3 - \frac{141}{128}x^4 + \cdots$$

The Taylor series for $f(x)$ in (19) has radius of convergence equal to $1/2$. Yet as x becomes large, $f(x)$ is a well-behaved function that tends to $\sqrt{2}$ as $x \to \infty$. Using only the first three coefficients 1, $1/2$, $-5/8$ in (18), we construct the Padé approximant

$$\text{(20)} \qquad \frac{1 + (7/4)x}{1 + (5/4)x} = 1 + \frac{1}{2}x - \frac{5}{8}x^2 + \frac{25}{32}x^3 + \cdots$$

This has the same Taylor-series expansion about the origin as $f(x)$ to $O(x^2)$, and it tends to $7/5 = 1.4$ as $x \to \infty$. Thus, using only three coefficients in a local expansion about the origin, the Padé approximation (19) provides an approximation at infinity to $f(x)$ that differs at the second

decimal place. Even within the radius of convergence of the Taylor expansion, expansion (20) outperforms the Taylor expansion. For instance, at $x=1/4$, $f(x)=1.0954451$, and the first three terms of the Taylor expansion give 1.0859375, whereas expansion (20) yields 1.0952381, providing accuracy to at least another decimal place.

This example suggests that Padé approximants can have the useful property of accelerating the convergence of a given power series within its circle of convergence, while at the same time considerably extending the domain over which truncated series expansions can give useful results. These features make Padé approximants attractive for constructing first-step rational fraction approximations from the information embodied in purely local density expansions such as (16), (17), or (18). Section 6 will be devoted to the algebraic details of this construction and will give the appropriate formulas.

Because the coefficients in the local expansions are needed in the construction of rational fraction approximants, we shall now give an analytic procedure for extracting local density expansions such as (16) and (17). It will be useful first to make explicit the general form of the characteristic function.

Assumption 2: (i) The characteristic function $\mathrm{cf}(s)$ has the general form

$$\mathrm{cf}(s) = \mathrm{cf}_1(s) + \mathrm{cf}_2(s) + \mathrm{cf}_3(s) \tag{21}$$

where

$$\mathrm{cf}_1(s) = e^{i\eta s} \sum_{m=0}^{M-1} p_m (is)^m$$

$$\mathrm{cf}_2(s) = e^{i\eta s} |s|^{\mu} \sum_{k=0}^{K} \sum_{l=0}^{L(k)} q_{kl} |s|^k (\ln|s|)^l,$$

$$\mu \geqslant M; \quad L(k) = 0 \quad \text{or} \quad 1 \quad \text{for all } k$$

$\mathrm{cf}_3^{(j)}(s)$ is absolutely integrable over every finite interval for $j = 0, 1, \ldots, N$, where N is the smallest integer greater than or equal to $\mu+K+1$ and $\mathrm{cf}^{(N)}(s)$ is well-behaved at infinity (Lighthill, 1958, p. 49).

(ii) The behavior of $\mathrm{cf}(s)$ as $s \to 0$ is given by the asymptotic series expansion

$$\mathrm{cf}(s) \sim e^{i\eta s} \left\{ \sum_{m=0}^{M-1} p_m (is)^m + |s|^{\mu} \sum_{k=0}^{\infty} \sum_{l=0}^{L(k)} q_{ke} |s|^k (\ln|s|)^l \right\}$$

This assumption is sufficiently general to include a very wide class of distributions and should apply to most econometric estimators and test statistics in both classical and nonclassical (including dynamic-model)

situations. The first component of the characteristic function $\mathrm{cf}_1(s)$ is analytic and ensures that integral moments will exist to order $M-1$ if this is an even integer and $M-2$ if $M-1$ is odd (Lukacs, 1970). In cases in which the distribution does not possess all its moments, the second component, $\mathrm{cf}_2(s)$, of (21) is important in the local behavior of $\mathrm{cf}(s)$ in the neighborhood of the origin and is, as we shall show later, instrumental in determining the form of the tails of $\mathrm{pdf}(x)$.

We start with the following two basic results that relate the tail behavior of density functions to the regularity properties of the characteristic function. They follow without difficulty from the standard discussions on this subject in the literature (Feller, 1971; Lukacs, 1970), but they also demonstrate that we need to go somewhat further to extract a tail expansion of the form (16).

Lemma 2: If the distribution with density $\mathrm{pdf}(x)$ and characteristic function $\mathrm{cf}(s)$ has finite $(M-1)$th absolute moment, then $\mathrm{cf}(s)$ is $M-1$ times continuously differentiable and the derivatives $\mathrm{cf}^{(n)}(s) \to 0$ as $s \to \pm\infty$ for each $n=0,1,\ldots,M-1$.

Proof: The first statement follows by dominated convergence from the existence of the $(M-1)$th absolute moment. The behavior of the derivatives at $\pm\infty$ follows from the representation

$$\mathrm{cf}^{(n)}(s) = \int_{-\infty}^{\infty} e^{isx}(ix)^n \mathrm{pdf}(x)\, dx$$

and, because $(ix)^n \mathrm{pdf}(x)$ is absolutely integrable on $(-\infty,\infty)$, the Riemann–Lebesgue lemma ensures that $\mathrm{cf}^{(n)}(s) \to 0$ as $s \to \pm\infty$ for each $n=0,1,\ldots,M-1$.

Lemma 3: If $\mathrm{cf}(s)$ is $M-1$ times continuously differentiable, if $\mathrm{cf}^{(n)}(s) \to 0$ as $s \to \pm\infty$, and if $\mathrm{cf}^{(n)}(s)$ is absolutely integrable for each $n=0,1,\ldots,M-1$, then

$$\mathrm{pdf}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-isx}\mathrm{cf}(s)\, ds$$

$$= \frac{(ix)^{-M+1}}{2\pi} \int_{-\infty}^{\infty} e^{-isx}\mathrm{cf}^{(M-1)}(s)\, ds = 0(x^{-M+1})$$

as $x \to \infty$.

Proof: Erdélyi (1956, p. 47). Lemma 3 shows that $\text{pdf}(x) \to 0$ as $x \to \pm\infty$ at least as fast as x^{-M+1}; but this is, in general, not a very sharp result, for if the $(M-1)$th absolute moment of the distribution exists and $\text{pdf}(x)$ satisfies Assumption 1, then we would expect that $\text{pdf}(x) = O(x^{-M-\delta})$ for some $\delta > 0$. For example, in the case of the Cauchy distribution, $\text{cf}(s) = e^{-|s|}$, and Lemma 3 demonstrates that $\text{pdf}(x) = 0(1)$, whereas, in fact, $\text{pdf}(x) = O(x^{-2})$. Thus, Lemmas 2 and 3 are not very helpful in providing local expansions about infinity of the form (16).

However, a sharper result that does lead directly to the asymptotic expansion (16) can be obtained from the more explicit representation of the characteristic function (21) and the theory of Fourier transforms of generalized functions and their asymptotic expansions (Jones, 1966; Lighthill, 1958).

Theorem 4: If the distribution with density $\text{pdf}(x)$ and characteristic function $\text{cf}(s)$ satisfies Assumptions 1 and 2, then $\text{pdf}(x)$ has the following asymptotic expansion as $|x| \to \infty$:

$$\text{pdf}(x) = \frac{1}{\pi |x|^{\mu+1}} \sum_{r=0}^{K} \Bigg[\sum_{k+l=r} c_{kl} (\text{sgn}(x))^k + \sum_{\substack{k+l+m=r \\ m \geq 1}} c_{klm} (\text{sgn}(x))^k + \sum_{k+l=r} d_{kl} \ln|x| (\text{sgn}(x))^k \Bigg] x^{-r} + 0(|x|^{-N})$$

where the coefficients c_{kl}, c_{klm}, and d_{kl} in this expansion are defined by equations (26) and (27), which follow, and N is the least integer $\geq \mu + k + 1$.

Proof: This is based on the theory of asymptotic expansions of Fourier transforms as developed by Lighthill (1958) and Jones (1966).

We shall use the notation $\text{ft}_i(x)$ to denote the inverse Fourier transform of $\text{cf}_i(s)$. Now, because the functions $\text{cf}_i(s)$ for $i = 1, 2$ do not lie in $L(-\infty, \infty)$, the $\text{ft}_i(x)$ cannot be defined in the usual way but do exist as generalized functions. In particular, the $\text{cf}_i(s)$ can be defined as generalized functions, because there exists a $G > 0$ for which $(1+s^2)^{-G} \text{cf}_i(s) \in L(-\infty, \infty)$ (Lighthill, 1958, p. 21). The $\text{ft}_i(x)$ are then defined as the generalized functions obtained as the inverse Fourier transforms of the generalized functions $\text{cf}_i(s)$ (Lighthill, 1958, p. 18).

Starting with $\text{cf}_1(s)$, we write

$$\text{cf}_1(s) = \lim_{t \to 0+} e^{i\eta s} \sum_{m=0}^{M-1} p_m e^{-|s|t} (is)^m$$

and then, by definition,

$$\begin{aligned}
\mathrm{ft}_1(x) &= \lim_{t\to 0+}\left\{\frac{1}{2\pi}\sum_{m=0}^{M-1} p_m \int_{-\infty}^{\infty} e^{-isx}e^{i\eta s}e^{-|s|t}(is)^m\,ds\right\} \\
&= \frac{1}{2\pi}\sum_{m=0}^{M-1} p_m(-1)^m \lim_{t\to 0+}\left\{\frac{d^m}{dx^m}\int_{-\infty}^{\infty} e^{-i(x-\eta)s}e^{-|s|t}\,ds\right\} \\
&= \frac{1}{2\pi}\sum_{m=0}^{M-1} p_m(-1)^m \lim_{t\to 0+}\left\{\frac{d^m}{dx^m}\left[\int_0^{\infty} e^{[-i(x-\eta)-t]s}\,ds\right.\right. \\
&\qquad\left.\left. + \int_0^{\infty} e^{[i(x-\eta)-t]s}\,ds\right]\right\} \qquad (22) \\
&= \frac{1}{2\pi}\sum_{m=0}^{M-1} p_m(-1)^m \delta^{(m)}(x-\eta)
\end{aligned}$$

where $\delta(y)$ is the Dirac delta function and $\delta^{(m)}(y)$ is its mth derivative. We deduce the asymptotic behavior of $\mathrm{ft}_1(x)$ as $x\to\infty$ immediately from (22) as

$$\mathrm{ft}_1(x) = 0(x^{-k}) \qquad (23)$$

for any value of $k>0$.

The second component is

$$\begin{aligned}
\mathrm{cf}_2(s) &= e^{i\eta s}\sum_{k=0}^{K}\{q_{k0}|s|^{\mu+k} + q_{k1}|s|^{\mu+k}\ln|s|\} \\
&= e^{i\eta s}\sum_{k=0}^{K}\left[\left(q_{k0} + q_{k1}\frac{\partial}{\partial\alpha}\right)|s|^{\alpha}\right]_{\alpha=\mu+k} \\
&= \lim_{t\to 0+} e^{i\eta s}\sum_{k=0}^{K}\left[\left(q_{k0} + q_{k1}\frac{\partial}{\partial\alpha}\right)|s|^{\alpha}e^{-|s|t}\right]_{\alpha=\mu+k}
\end{aligned}$$

On inversion, we obtain

$$\begin{aligned}
\mathrm{ft}_2(x) &= \lim_{t\to 0+}\left\{\frac{1}{2\pi}\sum_{k=0}^{K}\left[\left(q_{k0}+q_{k1}\frac{\partial}{\partial\alpha}\right)\int_{-\infty}^{\infty} e^{-isx}e^{i\eta s}e^{-|s|t}|s|^{\alpha}\,ds\right]_{\alpha=\mu+k}\right\} \\
&= \lim_{t\to 0+}\left\{\frac{1}{2\pi}\sum_{k=0}^{K}\left[\left(q_{k0}+q_{k1}\frac{\partial}{\partial\alpha}\right)\right.\right.
\end{aligned}$$

$$\times\left(\int_0^\infty e^{-(iy+t)s}s^\alpha\,ds+\int_0^\infty e^{-(-iy+t)s}s^\alpha\,ds\right)\Bigg]_{\substack{\alpha=\mu+k\\ y=x-\eta}}\Bigg\}$$

$$=\frac{1}{2\pi}\sum_{k=0}^{K}\Bigg[\left(q_{k0}+q_{k1}\frac{\partial}{\partial\alpha}\right)\times\left(\lim_{t\to 0+}\Gamma(\alpha+1)\{(t+iy)^{-\alpha-1}+(t-iy)^{-\alpha-1}\}\right)\Bigg]_{\substack{\alpha=\mu+k\\ y=x-\eta}}$$

$$=\frac{1}{2\pi}\sum_{k=0}^{K}\Bigg[\left(q_{k0}+q_{k1}\frac{\partial}{\partial\alpha}\right)\Gamma(\alpha+1)|y|^{-\alpha-1}\times\{e^{-(i\pi/2)\,\mathrm{sgn}(y)(\alpha+1)}+e^{(i\pi/2)\,\mathrm{sgn}(y)(\alpha+1)}\}\Bigg]_{\substack{\alpha=\mu+k\\ y=x-\eta}}$$

$$=\frac{1}{2\pi}\sum_{k=0}^{K}\Bigg[\left(q_{k0}+q_{k1}\frac{\partial}{\partial\alpha}\right)\times 2\Gamma(\alpha+1)\cos\{\tfrac{1}{2}\pi(\alpha+1)\}|y|^{-\alpha-1}\Bigg]_{\substack{\alpha=\mu+k\\ y=x-\eta}}$$

$$=\frac{1}{\pi}\sum_{k=0}^{K}\Bigg[\Gamma(\alpha+1)\cos\{\tfrac{1}{2}\pi(\alpha+1)\}\times\{q_{k0}+(\psi'(\alpha+1)-\tfrac{1}{2}\pi\tan\{\tfrac{1}{2}\pi(\alpha+1)\}-\ln|y|)q_{k1}\}\times|y|^{-(\alpha+1)}\Bigg]_{\substack{\alpha=\mu+k\\ y=x-\eta}}$$

where $\psi'(z)=\Gamma'(z)/\Gamma(z)$, the logarithmic derivative of the Gamma function. Thus, the asymptotic behavior of $\mathrm{ft}_2(x)$ as $x\to\infty$ is given by the series

$$\mathrm{ft}_2(x)=\frac{1}{\pi}\sum_{k=0}^{K}\sum_{l=0}^{\infty}\Bigg[\Gamma(\alpha+1)\cos\{\tfrac{1}{2}\pi(\alpha+1)\}\times\Bigg\{q_{k0}+\Bigg(\psi'(\alpha+1)-\tfrac{1}{2}\pi\tan\{\tfrac{1}{2}\pi(\alpha+1)\}-\ln|x|+\sum_{m=1}^{\infty}\frac{1}{m}\left(\frac{\eta}{x}\right)^m\Bigg)q_{k1}\Bigg\}\tag{24}$$

$$\times \frac{(\alpha+1)_l}{l!}\left(\frac{\eta}{x}\right)^l |x|^{-(\alpha+1)}\Big]_{\alpha=\mu+k}$$

where $(\alpha+1)_l=\Gamma(\alpha+1+l)/\Gamma(\alpha+1)$.

The third component of the characteristic function is $\mathrm{cf}_3(s)$. Now, $\mathrm{ft}_3(x)$ is the inverse Fourier transform of $\mathrm{cf}_3(s)$, so that $(-ix)^N \mathrm{ft}_3(x)$ has the inverse Fourier transform $\mathrm{cf}_3^{(N)}(s)$. By Theorem 18 of Lighthill (1958, p. 49), it now follows that $(-ix)^N \mathrm{ft}_3(x)=O(1)$ as $x\to\infty$. This last result, together with equations (23) and (24), implies that as $|x|\to\infty$,

$$\mathrm{pdf}(x) = \mathrm{ft}_1(x) + \mathrm{ft}_2(x) + \mathrm{ft}_3(x)$$

$$(25)\quad = \frac{1}{\pi|x|^{\mu+1}}\sum_{k=0}^{K}|x|^{-k}\left[q'_{k0} + q'_{k1}\left\{\sum_{m=1}^{\infty}\frac{1}{m}\left(\frac{\eta}{x}\right)^m - \ln|x|\right\}\right] \times \sum_{l=0}^{\infty}\frac{(\mu+k+1)l}{l!}\left(\frac{\eta}{x}\right)^l + O(|x|^{-N})$$

$$(26)\quad = \frac{1}{\pi|x|^{\mu+1}}\sum_{r=0}^{K}\Bigg[\sum_{k+l=r}\frac{q'_{k0}(\mu+k+1)_l\eta^l}{l!}(\mathrm{sgn}(x))^k + \sum_{\substack{k+l+m=r\\ m\geqslant 1}}\frac{q'_{k1}(\mu+k+1)_l\eta^{l+m}}{l!m}(\mathrm{sgn}(x))^k - \sum_{k+l=r}\frac{q'_{k1}(\mu+k+1)_l\eta^l}{l!}\ln|x|(\mathrm{sgn}(x))^k\Bigg] \times x^{-r} + O(|x|^{-N})$$

where

$$q'_{k0} = \Gamma(\mu+k)\cos\{\tfrac{1}{2}\pi(\mu+k+1)\} \times \{q_{k0} + (\psi'(\mu+k+1) - \tfrac{1}{2}\pi\tan\{\tfrac{1}{2}\pi(\mu+k+1)\})q_{k1}\}$$

$$q'_{k1} = \Gamma(\mu+k)\cos\{\tfrac{1}{2}\pi(\mu+k+1)\}q_{k1}$$

and N is the least integer $\geqslant \mu+k+1$. We rewrite (26) in the form

$$(27)\quad \frac{1}{\pi|x|^{\mu+1}}\sum_{r=0}^{K}\Bigg[\sum_{k+l=r}c_{kl}(\mathrm{sgn}(x))^k + \sum_{\substack{k+l+m=r\\ m\geqslant 1}}c_{klm}(\mathrm{sgn}(x))^k - \sum_{k+l=r}d_{kl}\ln|x|(\mathrm{sgn}(x))^k\Bigg]x^{-r} + O(|x|^{-N})$$

and this establishes the result.

To illustrate the use of Theorem 4, we take the simple example of the Cauchy distribution with $\mathrm{cf}(s)=e^{-s}$. In this case

$$\mathrm{cf}_1(s) = 1$$

$$\mathrm{cf}_2(s) = |s| \sum_{k=0}^{K} \frac{(-1)^{k+1}}{(k+1)!} |s|^k$$

$$\mathrm{cf}_3(s) = \frac{|s|^{k+2}}{(k+2)!} e^{-\theta|s|} \quad (0<\theta<1)$$

and we deduce from (26), by setting $\mu=1$, $\eta=0$, and $q_{k1}=0$, that

$$\begin{aligned}\mathrm{pdf}(x) &= \frac{1}{\pi x^2} \sum_{r=0}^{K} \frac{(-1)^{r+1}\Gamma(r-2)\cos\{\frac{1}{2}\pi(r+2)\}}{(r+1)!} \\ &\quad \times (\mathrm{sgn}(x))^r x^{-r} + O(|x|^{-K-2}) \\ &= \frac{1}{\pi x^2} \sum_{r=0}^{K} (-1)^{r+1} \cos\{\tfrac{1}{2}\pi(r+2)\} |x|^{-r}\end{aligned}$$

Now, $\cos\{\frac{1}{2}\pi(r+2)\}$ equals $(-1)^{1/2(r+1)}$ when r is an even integer and equals zero when r is odd. Hence, setting $r=2n$ and $K=2$, we have

$$\mathrm{pdf}(x) = \frac{1}{\pi x^2} \sum_{n=0}^{N} (-1)^n (x^2)^{-n} + O((x^2)^{-(N+1)})$$

This expansion can be verified directly from the density function $\mathrm{pdf}(x)=[\pi(1+x^2)]^{-1}$ itself.

Theorem 5: If $s^N \mathrm{cf}(s)$ is absolutely integrable over $(-\infty,\infty)$, then the local expansion of $\mathrm{pdf}(x)$ about the point $x=d_i$ is given by

$$\mathrm{pdf}(x) = \sum_{j=0}^{N-1} \beta_{ij}(x-d_i)^j + O(x-d_i)^N \tag{28}$$

where

$$\beta_{ij} = \frac{1}{2\pi j!} \int_{-\infty}^{\infty} (-is)^j \exp(-isd_i)\,\mathrm{cf}(s)\,ds \quad (j=0,1,\ldots,N-1)$$

Proof: Because $s^N \mathrm{cf}(s) \in L(-\infty,\infty)$, we expand the exponential e^{-isx} in the inversion formula

$$\mathrm{pdf}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-isx}\,\mathrm{cf}(s)\,ds$$

about the point $x=d_i$ and integrate term by term, giving

$$\frac{1}{2\pi j!}\sum_{j=0}^{N-1}\int_{-\infty}^{\infty}(-is)^j\exp(-isd_i)\,\mathrm{cf}(s)\,ds(x-d_i)^j$$

$$+\frac{1}{2\pi N!}\int_{-\infty}^{\infty}(-is)^N\exp(-is\tilde{d}_i)\,\mathrm{cf}(s)\,ds(x-d_i)^N$$

where $\tilde{d}_i$ lies on the line segment connecting x and d_i.

Local expansions of the type discussed in this section for the tails and the body of the distribution can also be extracted under similar conditions for the distribution function. These expansions will be useful in the development of a corresponding theory of global approximation for the distribution function rather than the density, and they will be discussed in a later paper. Expansions of this type have already been given for many of the common distributions in the statistical literature (Zelen & Severo, 1965).

6 Multiple-point Padé approximants

As discussed in the previous section, Padé approximants can be used to improve the convergence properties of local Taylor expansions, and they have the additional useful property that they frequently extend the domain over which these local expansions provide good approximations. This section will show how Padé approximants can be derived from the local density expansions (16) and (17). These approximants will provide a preliminary set of rational fractions. They can then be used directly as approximations to $\mathrm{pdf}(x)$ or modified so that they belong to the class of rational fractions (2) and have satisfactory global behavior. The question of modifying the preliminary rational fractions will be taken up in Section 7.

We start by writing the density function in the form

$$\mathrm{pdf}(x)=s(x)\,\mathrm{pdf}_s(x)\quad(-\infty<x<\infty) \tag{29}$$

where $s(x)$ is a real continuous function satisfying $s(x)>0$ over the entire real axis and $s(x)\to 0$ as $x\to\pm\infty$. This representation of $\mathrm{pdf}(x)$ reconciles with the class of rational fractions defined in (2) and allows us to accommodate information about the coefficient functions $t(|x|)$ and $w(x)$ that appear in the local density expansions (16) and (18). In many cases, $s(x)$ will represent the leading term in the multiple series representation of the density $\mathrm{pdf}(x)$, and in such cases $s(x)$ usually will be identical with $t(|x|)$ and $w(x)$. When this leading term in the density is

unknown, a suitable alternative will be to set $s(x)=t(|x|)$ directly or some modified form of $t(|x|)$ that has the same asymptotic behavior but that is well behaved elsewhere on the real axis. If necessary, the expansion (18) can then be adjusted to take account of this modification so that (17) will be correct to the same number of terms.

If we write the local expansions of $\mathrm{pdf}_s(x)$ in the form

$$\mathrm{pdf}_s(x) \sim \alpha_0 + \alpha_1 x^{-1} + \alpha_2 x^{-2} + \alpha_3 x^{-3} + \alpha_4 x^{-4} + \cdots \quad (x \to \pm\infty) \tag{30}$$

$$\mathrm{pdf}_s(x) \sim \beta_{i0} + \beta_{i1}(x-d_i) + \beta_{i2}(x-d_i)^2 + \beta_{i3}(x-d_i)^3 + \beta_{i4}(x-d_i)^4 + \cdots \quad (i=1,\ldots,I), \quad x \to d_i \tag{31}$$

our problem is to construct a rational fraction of the form

$$[n/n] = \frac{P_n(x)}{Q_n(x)} = \frac{a_0 + a_1 x + \cdots + a_n x^n}{b_0 + b_1 x + \cdots + b_n x^n} \tag{32}$$

(n = an even integer)

which has the same local behavior as (30) and (31) and to as high an order as possible. Such a rational fraction is called a multiple-point Padé approximant, and these have been discussed by Baker (1975, Chapter 8).[3]

The equations that define (32) can best be introduced by considering the approximant based on the Taylor series about a single point. We take the case of (31), with $d_i=0$, and normalize (32) by setting $b_0=1$. This normalization ensures that $Q_n(0)=1>0$, so that the $[n/n]$ approximant will not have a pole at the origin, this now being the point of expansion of the Taylor series (31). The coefficients of $[n/n]$ are now determined by the equation

$$\mathrm{pdf}_s(x)Q_n(x) - P_n(x) = O(x^{2n+1}) \tag{33}$$

Explicitly, we have the relations

$$\begin{aligned}
&\beta_{i0} && && && && && && = a_0\\
&\beta_{i1} && + \beta_{i0}b_1 && && && && && = a_1\\
&\beta_{i2} && + \beta_{i1}b_1 && + \beta_{i0}b_2 && && && && = a_2\\
&\beta_{i3} && + \beta_{i2}b_1 && + \beta_{i1}b_2 && + \beta_{i0}b_3 && && && = a_3\\
&\cdots && \cdots && \cdots && \cdots && \cdots && \cdots && \cdots\\
&\beta_{in} && + \beta_{in-1}b_1 && + \beta_{in-2}b_2 && + \beta_{in-3}b_3 && + \cdots && + \beta_{i0}b_n && = a_n\\
&\beta_{in+1} && + \beta_{in}b_1 && + \beta_{in-1}b_2 && + \beta_{in-2}b_3 && + \cdots && + \beta_{i1}b_n && = 0\\
&\cdots && \cdots && \cdots && \cdots && \cdots && \cdots && \cdots\\
&\beta_{i2n} && + \beta_{i2n-1} && + \beta_{i2n-2}b_2 && + \beta_{i2n-3}b_3 && + \cdots && + \beta_{in}b_n && = 0
\end{aligned} \tag{34}$$

which comprise $2n+1$ equations in the $2n+1$ required coefficients of $[n/n]$, namely, $\{a_0, a_1, \ldots, a_n; b_1, \ldots, b_n\}$. Baker (1975)[4] has proved that although a solution to (34) does not necessarily exist for all positive integers n, there is an infinite subsequence $\{n_j\}$ for which the Padé approximant $[n_j/n_j]$ exists for any formal power series with $\beta_{i0} \neq 0$. Further, when the approximant $[n/n]$ exists, it is unique.[5]

We see by inspection of (34) that in order to compute the coefficients of $[n/n]$ we need the coefficients in the local expansion (31) to order $2n$. Even for low values of n this is likely to become prohibitive quite quickly when dealing with the distribution of an econometric statistic because of the increasing difficulty in extracting higher-order coefficients and the complications of the resulting formulas. Moreover, in view of the smoothness of most density functions, in practice there will be little advantage to be gained from increasing the order of contact at a particular point past $n=3$ or 4. In many cases, $n=2$ will be sufficient to provide a highly satisfactory local density approximant.[6]

Multiple-point expansions provide an excellent means of reducing the order of contact at individual points to within manageable limits while extending the domain over which the final approximant will perform well. Thus, a two-point Padé approximant $[n/n]$ might be based on the first $n+1$ equations of (34), which require local expansion coefficients up to β_{in} and a corresponding set of n equations with expansion coefficients up to order $n-1$ for a point other than the origin. These equations will then yield an approximant with contact of order n at the origin and $n-1$ at the second point.

If one of the points of local expansion is infinity, then the equations take on a slightly different form. In this case, rather than (33), we require

$$\text{(35)} \qquad \text{pdf}_s(x)Q_n(x) - P_n(x) = O(x^{-2n-1})$$

as $x \to \infty$. We then have the following explicit relations from (30), (32), and (35)

$$\text{(36)} \qquad \begin{array}{lllll}
\alpha_0 b_n & & & & = a_n \\
\alpha_1 b_n & + \alpha_0 b_{n-1} & & & = a_{n-1} \\
\alpha_2 b_n & + \alpha_1 b_{n-1} & + \alpha_0 b_{n-2} & & = a_{n-2} \\
\cdot & \cdot \quad \cdot & \cdot \quad \cdot & \cdots \quad \cdot \quad \cdot & \cdot \\
\alpha_n b_n & + \alpha_{n-1} b_{n-1} & + \alpha_{n-2} b_{n-2} & + \cdots + \alpha_0 & = a_0 \\
\alpha_{n+1} b_n & + \alpha_n b_{n-1} & + \alpha_{n-1} b_{n-2} & + \cdots + \alpha_1 & = 0 \\
\cdot & \cdot \quad \cdot & \cdot \quad \cdot & \cdots \quad \cdot \quad \cdot & \cdot \\
\alpha_{2n} b_n & + \alpha_{2n-1} b_{n-1} & + \alpha_{2n-2} b_{n-2} & + \cdots \quad \cdot \quad \cdot & = 0
\end{array}$$

As with (34), this is a system of $2n+1$ equations in the same number of unknown coefficients.

In the general case of expansions about arbitrary points d_i, as in (31), the equations that determine the coefficients take the form

$$\left\{\sum_{j=0}^{\infty}\beta_{ij}(x-d_i)^j\right\}Q_n(d_i+(x-d_i))-P_n(d_i+(x-d_i)) = O((x-d_i)^{2n+1}) \quad (i=1,\ldots,I) \tag{37}$$

If we write $y=x-d_i$ and expand $Q_n(d_i+y)$ and $P_n(d_i+y)$ as

$$Q_n(d_i+y)=\sum_{k=0}^{n}b_k(d_i+y)^k=\sum_{k=0}^{n}b_k^{(i)}y^k=Q_n^{(i)}(y)$$

$$P_n(d_i+y)=\sum_{k=0}^{n}a_k(d_i+y)^k=\sum_{k=0}^{n}a_k^{(i)}y^k=P_n^{(i)}(y)$$

we have

$$b^{(i)}=K^{(i)}b, \qquad a^{(i)}=K^{(i)}a \tag{38}$$

where

$$K^{(i)}=\begin{bmatrix} 1 & d_i & d_i^2 & d_i^3 & \cdots & d_i^n \\ 0 & 1 & 2d_i & 3d_i^2 & \cdots & \binom{n}{1}d_i^{n-1} \\ 0 & 0 & 1 & 3d_i & \cdots & \binom{n}{2}d_i^{n-2} \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}, \tag{39}$$

$$b^{(i)}=\begin{bmatrix} b_0^{(i)} \\ b_1^{(i)} \\ \cdot \\ \cdot \\ b_n^{(i)} \end{bmatrix}, \quad b=\begin{bmatrix} b_0 \\ b_1 \\ \cdot \\ \cdot \\ b_n \end{bmatrix}, \quad a^{(i)}=\begin{bmatrix} a_0^{(i)} \\ a_1^{(i)} \\ \cdot \\ \cdot \\ a_n^{(i)} \end{bmatrix}, \quad a=\begin{bmatrix} a_0 \\ a_1 \\ \cdot \\ \cdot \\ a_n \end{bmatrix}$$

and (37) becomes

$$\left(\sum_{j=0}^{\infty}\beta_{ij}y^j\right)Q_n^{(i)}(y)-P_n^{(i)}(y)=O(y^{2n+1}) \tag{40}$$

which is of the same form as (33) but in the transformed coefficients.

To work in terms of the original coefficients, we can use the transfor-

mation matrix $K^{(i)}$ in the case of the vector $a^{(i)}$, as in (38), but in view of the normalization on the vector b, we partition $K^{(i)}$ and b as follows

$$K^{(i)} = \left[\begin{array}{c|c} 1 & k^{(i)'} \\ \hline 0 & K_{22}^{(i)} \end{array}\right], \qquad k^{(i)'} = [d_i, d_i^2, d_i^3, \ldots, d_i^n]$$

$$b' = [b_0, b_*'] = [1, b_*']$$

We then have, from (38),

$$b_0^{(i)} = k^{(i)'} b_*, \qquad b_*^{(i)} = K_{22}^{(i)} b_*$$

We now define

$$G^{(i)} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ -\beta_{i0} & 0 & 0 & \cdots & 0 \\ -\beta_{i1} & -\beta_{i0} & 0 & \cdots & 0 \\ -\beta_{i2} & -\beta_{i1} & -\beta_{i0} & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ -\beta_{in-1} & -\beta_{in-2} & -\beta_{in-3} & \cdots & -\beta_{i0} \end{bmatrix}, \qquad g^{(i)} = \begin{bmatrix} \beta_{i0} \\ \beta_{i1} \\ \cdot \\ \cdot \\ \cdot \\ \beta_{in} \end{bmatrix}$$

The first $n+1$ equations of (34) can be written as

$$a + G^{(i)} b_* = g^{(i)}$$

or, in the general case of a local expansion about the point d_i (not necessarily the origin),

$$a^{(i)} + G^{(i)} b_*^{(i)} = g^{(i)} + g^{(i)} b_0^{(i)} \tag{41}$$

Transforming back to the original coefficients in the rational fraction, we get

$$K^{(i)} a + G^{(i)} K_{22}^{(i)} b_* = g^{(i)} + g^{(i)} k^{(i)'} b_*$$

or

$$K^{(i)} a + [G^{(i)} K_{22}^{(i)} - g^{(i)} k^{(i)'}] b_* = g^{(i)} \tag{42}$$

The system of equations (42) holds for each point of local expansion, that is, for $i=1, \ldots, I$ in our original notation (see equation (31)).

Note that as we have constructed (42) the system involves $n \times 1$ equations. In practice, it may be convenient to use fewer equations at each point, thus reducing the order of contact of the Padé approximant at each point and requiring less analytic information about the expansion coefficients. The procedure allows us to make up for this reduction in the number of equations at each point by increasing the number of

points we use in developing the approximant. This process has the additional advantage of improving the global nature of the final approximation.

In the general case we let $K^{(i)}$ be $(m_i+1)\times(n+1)$, $G^{(i)}$ be $(m_i+1)\times m_i$, $K_{22}^{(i)}$ be $m_i\times n$, $g^{(i)}$ be $(m_i+1)\times 1$, and $k^{(i)}$ be $n+1$. The complete system of equations that determine the coefficients in the $[n/n]$ Padé approximant are then based on (36) and (42) and take the following general form:

(43)

$$\begin{bmatrix} K^{(1)} & G^{(1)}K_{22}^{(1)} - g^{(1)}k^{(1)\prime} \\ \vdots & \vdots \\ K^{(I)} & G^{(I)}K_{22}^{(I)} - g^{(I)}k^{(I)\prime} \\ 0_{rx(n+1)} & \begin{matrix} -\alpha_{r+1} & -\alpha_{r+2} & \cdots & -\alpha_{n+r} \\ -\alpha_r & -\alpha_{r+1} & \cdots & -\alpha_{n+r-1} \\ \vdots & \vdots & \cdots & \vdots \\ -\alpha_2 & -\alpha_3 & \cdots & -\alpha_{n+1} \end{matrix} \\ I_{n+1} & \begin{matrix} -\alpha_1 & -\alpha_2 & \cdots & -\alpha_n \\ -\alpha_0 & -\alpha_1 & \cdots & -\alpha_{n-1} \\ 0 & -\alpha_0 & \cdots & -\alpha_{n-2} \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & -\alpha_0 \end{matrix} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \\ b_1 \\ b_2 \\ \\ \\ b_n \end{bmatrix} = \begin{bmatrix} g^{(1)} \\ \vdots \\ g^{(I)} \\ 0 \\ \vdots \\ 0 \\ -\alpha_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where $m_\infty = n+r+1$. In (43) we need to select I and the m_i and m_∞ in such a way that $\sum_{i=1}^{I} m_i + m_\infty \geqslant 2n+1$. In the final block of equations in (43) we shall often select $r=0$, so that $m_\infty \leqslant n+1$. As with the case of the local expansions (31) about the points d_i, this will reduce the number of final expansion coefficients that are required to solve for the $[n/n]$ Padé coefficients. In some cases (the application in Section 8 turns out to be such a case) we may have more than enough coefficients, so that $\sum m_i + m_\infty > 2n+1$, and we may neglect some equations of (43) to obtain a solution. When this happens, it would seem preferable to neglect those equations that refer to higher-order points of contact of the Padé approximant with the local expansions rather than those that refer to lower-order points of contact.

7 Modifying the Padé approximants

By solving (43) for the Padé coefficients, we obtain a preliminary rational fraction $[n/n]$ as in (32). This can be used to construct an approximation to pdf(x) of the form $s(x)[n/n] = s(x)P_n(x)/Q_n(x)$. In

some cases this will turn out to be a perfectly satisfactory approximant. In others, it will need to be modified to produce a good approximation to pdf(x) over a wide interval. This is because there is nothing in the procedure outlined in Section 6 that prevents the occurrence of zeros in the polynomial $Q_n(x)$ on the real axis. These zeros induce poles in the approximant and will need to be eliminated if the approximation is to perform well, unless the zeros appear in remote and irrelevant regions of the distribution. My experience to date suggests that the latter is not usually the case. The normal occurrence is for the procedure in Section 6 to produce a preliminary approximant with either no poles at all or a pair of poles, at least one of which lies within the main body of the distribution.

In addition to unwanted poles, the $[n/n]$ Padé approximant may become zero at a finite number of points on the real axis. Because we shall, in general, have pdf(x) >0 for all finite x, we shall normally wish to eliminate the zeros of the approximant unless they occur well outside the region of interest in the distribution.

When poles occur, they are typically found in the bridging region between the points of local density expansion used in (43) to construct the Padé approximant. This suggests that an obvious way of helping to remove unwanted poles is to introduce an additional point of local expansion in (43), perhaps at the price of reducing the order of contact at another point. However, there is no guarantee that this method will eliminate poles, and it has the disadvantage of requiring additional information about the distribution to be operational. The procedure we shall suggest later does not suffer from these disadvantages. It will eliminate the poles, and it is sufficiently flexible to allow for additional information about the distribution to be incorporated at the time of modification, if such information is available.

Before we outline the procedure, it may be worth mentioning that the occurrence of unwanted poles in Padé approximants is a long-standing problem. The presence of poles in the approximant is one of the reasons that it is difficult to prove general theorems about the convergence of Padé approximants to a given function as the degree of the approximant increases. Many of the general results that are available (Baker, 1975, Part II) concern the convergence of subsequences as $n \to \infty$. For an example of nonconvergence, we can cite the work of Chui (1976), who proved that in the general family of entire functions there exists a function for which the sequence of $[n/n]$ Padé approximants is divergent everywhere in the whole complex plane except at the origin.

The procedure we suggest for modifying Padé approximants so that they will be well behaved over the whole real axis is based on the follow-

ing simple idea. If zeros of the numerator and denominator polynomials $P_n(x)$ and $Q_n(x)$ occur on the real axis, they will occur in pairs, because n is even. We then replace the real roots of the associated quadratic equations by complex conjugate pairs in such a way that we preserve, as far as possible, the known behavior of the function at the points of local expansion. Various degrees of sophistication are possible in the practical application of this method. In fact, as we shall demonstrate in the application of Section 8, even crude adjustments that preserve only contact of order 1 at the points of local expansion seem to work remarkably well. After we have adjusted the coefficients in the Padé approximant so that $P_n(x) > 0$ and $Q_n(x) > 0$ throughout the real axis, we simply numerically integrate and rescale so that the area under the curve is unity.

Some of the principles involved in the method outlined in the preceding paragraph can be illustrated in the case of an approximant with $n=4$. Let the $[n/n]$ Padé approximant extracted by the procedure of Section 6 with points of local expansion at $x=0$ and $x^{-1}=0$ be given by

$$(44) \qquad [4/4](x) = \frac{\sum_{i=0}^{4} a_i x^i}{\sum_{i=0}^{4} b_i x^i} = \frac{a_4(x-\gamma_1)(x-\gamma_2)(x-\gamma)(x-\bar{\gamma})}{b_4(x-\delta_1)(x-\delta_2)(x-\delta)(x-\bar{\delta})}$$

where γ_1 and γ_2 denote real zeros of the numerator and δ_1 and δ_2 denote real zeros of the denominator; $(\gamma, \bar{\gamma})$ and $(\delta, \bar{\delta})$ are complex conjugate pairs. We start by rewriting (44) in the form

$$(45) \qquad [4/4](x) = \frac{a_4\{x^2 - (\gamma_1 + \gamma_2)x + \gamma_1\gamma_2\}(x-\gamma)(x-\bar{\gamma})}{b_4\{x^2 - (\delta_1 + \delta_2)x + \delta_1\delta_2\}(x-\delta)(x-\bar{\delta})}$$

We now propose to modify the coefficients of the quadratics in braces so that $[4/4](x) > 0$ for all real x, while retaining the same behavior as in (45) in the neighborhood of $x=0$ and $x^{-1}=0$. We therefore define the family of functions

$$(46) \qquad [4/4](x;\Theta) = \frac{a_4\{cx^2 + dx + e\}(x-\gamma)(x-\bar{\gamma})}{b_4\{fx^2 + gx + h\}(x-\delta)(x-\bar{\delta})}$$

where $\Theta' = (c, d, e, f, g, h)$ is a vector of real parameters to be chosen. To ensure equivalent local behavior in (45) and (46), we restrict our choice of Θ so that

(i) $\quad c/f = 1$

(ii) $\quad e/h = \gamma_1\gamma_2/\delta_1\delta_2$

Now, (i) will ensure that $[4/4](x;\Theta) \to a_4/b_4$ as $x \to \pm\infty$, and (ii) will ensure that $[4/4](x;\Theta) \to a_4\gamma_1\gamma_2|\gamma|^2/b_4\delta_1\delta_2|\delta|^2$ as $x \to 0$.

In most cases we find that the zeros (γ_1, γ_2) and (δ_1, δ_2) occur with the same sign patterns. This is because the zeros and singularities lie in the intervals between the points (here 0 and $\pm\infty$) of local expansion. If we take the case in which both $\gamma_1\gamma_2 > 0$ and $\delta_1\delta_2 > 0$, our task is then to raise f and h from their original values in (45) so that the discriminant $g^2 - 4fh < 0$. This will require proportional changes in c and e so that (i) and (ii) remain valid. Often these automatic changes in c and e will be sufficient to ensure that there are no zeros in (46). If they are not, some small adjustment in the value of d will normally suffice. There is an added advantage to adjusting the value of d, in that simple hand calculations will show what adjustments in this parameter will improve the order of contact of (46) at the points of local expansion while preserving the desired global behavior of $[4/4](x;\Theta) > 0$ for all x. Various other scenarios for parameter changes are possible, but those we have illustrated should indicate some of the relevant considerations and the ease with which they can be performed.

The family of rational fractions (46) based on Padé approximants have introduced extra flexibility in the approximating procedure. The idea is essentially to partially reparameterize a first-stage Padé approximant so that we can achieve good global behavior by sacrificing some degree of contact at the points of local expansion. But with the new family of approximating rational fractions (46), we have the opportunity to adjust the parameters to take account of any additional information about the distribution that has not already been used in the equations (43) that define the original coefficients (perhaps less precise information based on Monte Carlo work with the same distribution).

An obvious alternative procedure for modifying the Padé approximant (45), but one I have not yet tried in application, is to use splines to bridge the intervals in which singularities and zeros occur. This method may be particularly useful in cases in which zeros and singularities occur together in close proximity.

8 An application to a simultaneous-equations estimator

We consider the single structural equation

$$y_1 = \beta y_2 + Z_1\gamma_1 + u \tag{47}$$

where y_1 and y_2 are vectors of T observations on two endogenous variables, Z_1 is a $T \times K_1$ matrix of observations on K_1 exogenous variables, and u is a vector of random disturbances. The reduced-form equations for y_1 and y_2 are

$$(48) \qquad [y_1 \vdots y_2] = [Z_1 \vdots Z_2] \begin{bmatrix} \pi_{11} & \pi_{12} \\ \pi_{21} & \pi_{22} \end{bmatrix} + [v_1 \vdots v_2]$$

where Z_2 is a $T \times K_2$ matrix of observations of K_2 exogenous variables excluded from (47). We assume that the usual standardizing transformations have been carried out, so that (i) $T^{-1}Z'Z = I_K$, where $[Z = Z_1 \vdots Z_2]$, $k = k_1 + k_2$, and (ii) the rows of $[v_1 \vdots v_2]$ are independent and identically distributed normal vectors with zero mean and covariance matrix equal to the identity matrix. We also assume that (47) is identified so that $K_2 \geqslant 1$.

The two-stage least-squares estimator 2SLS of β in (47) is given by the ratio $\hat{\beta} = y_2' R y_1 / y_2' R y_2$, where $R = Z_2 Z_2'$. The exact density function of $\hat{\beta}$ is known to be the doubly infinite series (Richardson, 1968)

$$(49) \qquad \text{pdf}(x) = \frac{\exp[-(\mu^2/2)(1+\beta^2)]}{\beta(1/2, K_2/2)(1+x^2)^{(K_2+1)/2}} \sum_{j=0}^{\infty} \frac{[(K_2+1)/2]_j}{(K_2/2)_j \, j!} \times \left\{ \frac{\mu^2}{2} \frac{(1+\beta x)^2}{1+x^2} \right\}^j {}_1F_1\left(\frac{K_2 - 1}{2}, j + \frac{K_2}{2}; \frac{\mu^2 \beta^2}{2} \right)$$

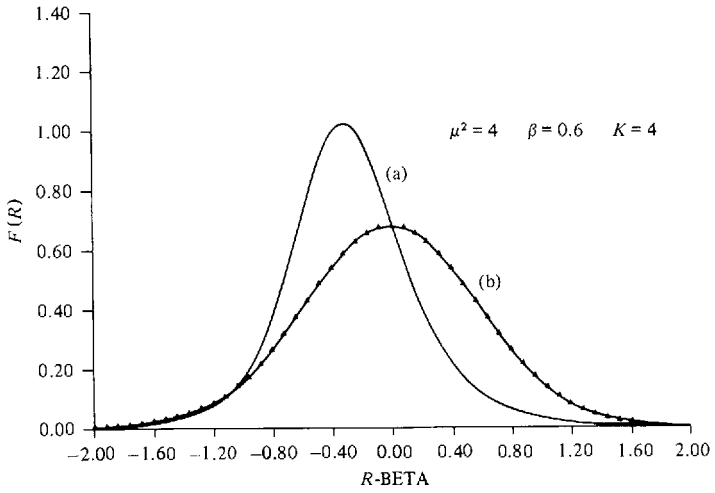
which depends on the three parameters β, K_2, and $\mu^2 = T\pi_{22}' \pi_{22}$.

The extensive tabulations of Anderson and Sawa (1979) show that (49) may be adequately approximated by the asymptotic normal only when μ^2 is very large; the size of μ^2 required for the asymptotic distribution to provide an adequate approximation is itself contingent on the size of β and K_2. Even for moderate values of β and K_2 the computations of Anderson and Sawa (1979) show that extremely large values of μ^2 (well over 1,000) are required to secure a satisfactory approximation.

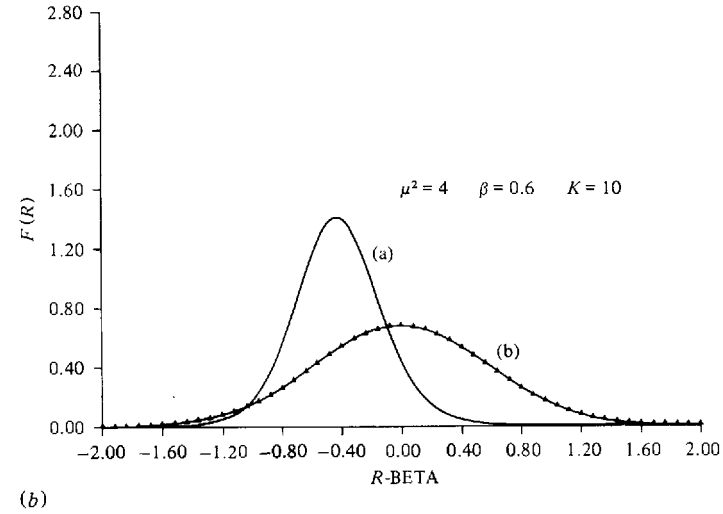
As discussed in the introduction, other approximations to (49) that perform satisfactorily for a range of parameter values are the Edgeworth (Anderson & Sawa, 1973, 1979) and saddlepoint (Holly & Phillips, 1979) approximations. But, when μ^2 is small, both these approximations become inadequate.

In Figures 5.1, 5.2, and 5.3 we illustrate the inadequacy of these three different methods of approximation in the case in which $\beta = 0.6$, $\mu^2 = 4.0$, and $K = 4, 10$. This is rather an extreme case in which μ^2 is very low (around the lower limit of μ^2 values found by Anderson and associates (1978) in their numerical computations of key parameters for actual econometric models). It has been chosen to test the adequacy of the new method of approximation discussed in the earlier sections of this chapter specifically in a case in which the existing methods break down.

Figures 5.4 to 5.8 detail the approximants obtained at each stage of the procedure outlined in the previous sections of this chapter.[7] In the



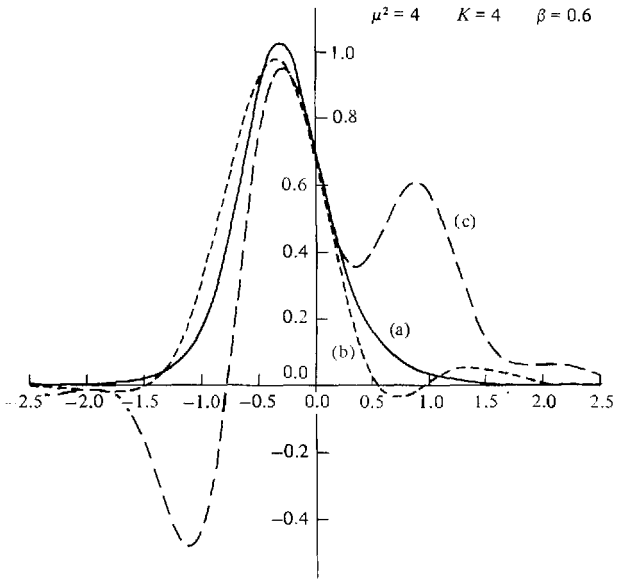
(a)



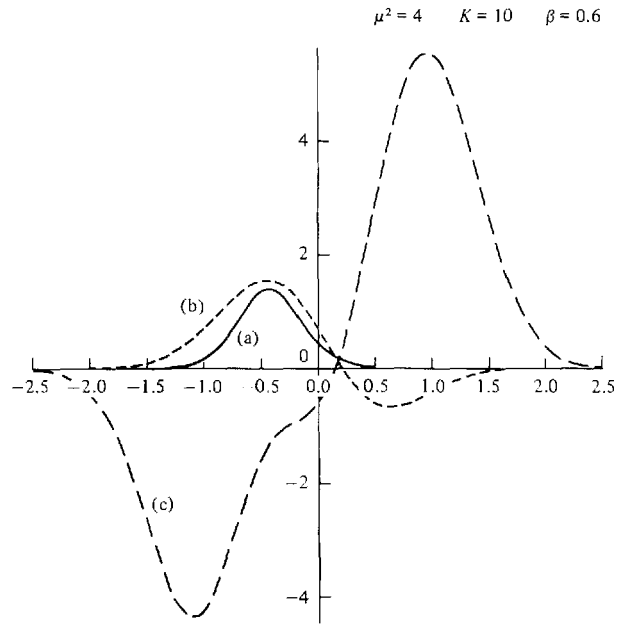
(b)

Figure 5.1. (*a*) Asymptotic normal approximation: (A) exact density; (B) asymptotic normal.
(*b*) Asymptotic normal approximation: (A) exact density; (B) asymptotic normal.

first stage of the procedure we need to select the coefficient function $s(x)$, as in equation (29). A crude choice would be $s(x) = [1 + |x|^{K_2+1}]^{-1}$, because this has the same asymptotic behavior as $|x|^{-(K_2+1)}$, which in this case is the coefficient function in the tail expansion (16), and because this function is also well behaved elsewhere on the real line. An

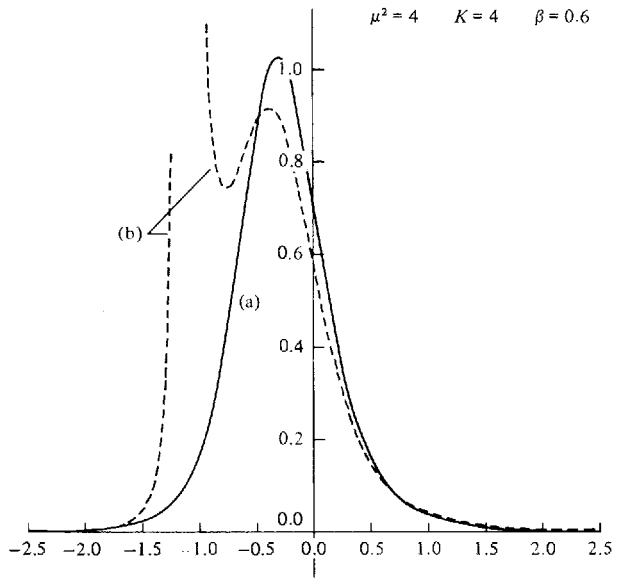


(*a*)

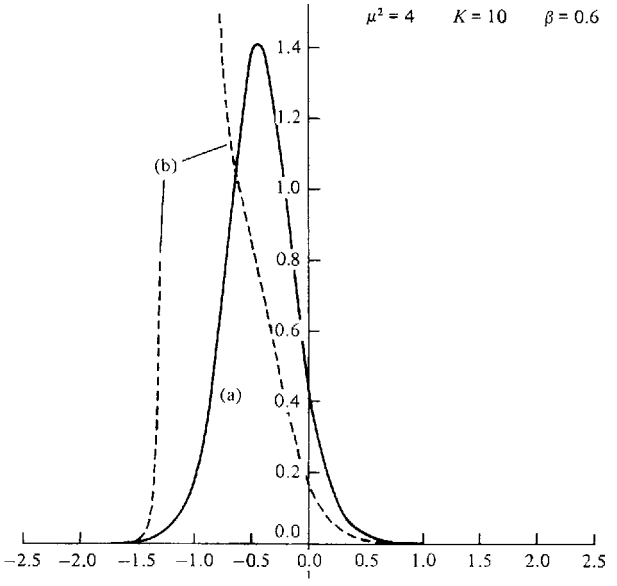


(*b*)

Figure 5.2. (*a*) Edgeworth approximation: (A) exact density; (B) $O(T^{-1/2})$; (C) $O(T^{-1})$.
(*b*) Edgeworth approximation: (A) exact density; (B) $O(T^{-1/2})$; (C) $O(T^{-1})$.



(*a*)



(*b*)

Figure 5.3. (*a*) Saddlepoint approximation: (A) exact density; (B) saddlepoint. (*b*) Saddlepoint approximation: (A) exact density; (B) saddlepoint.

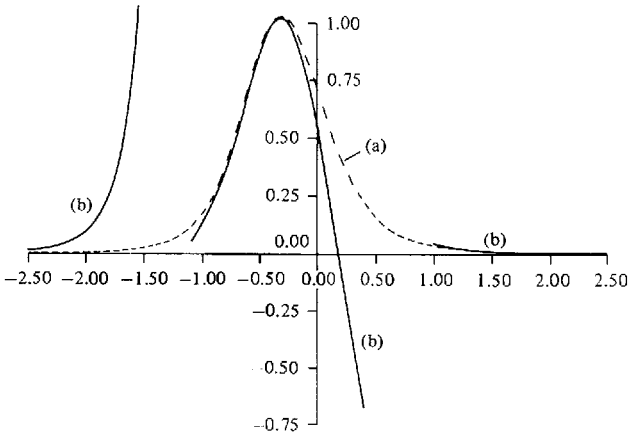


Figure 5.4. Local density approximations at the origin and in the tails to pdf(x): (A) exact density; (B) local approximations.

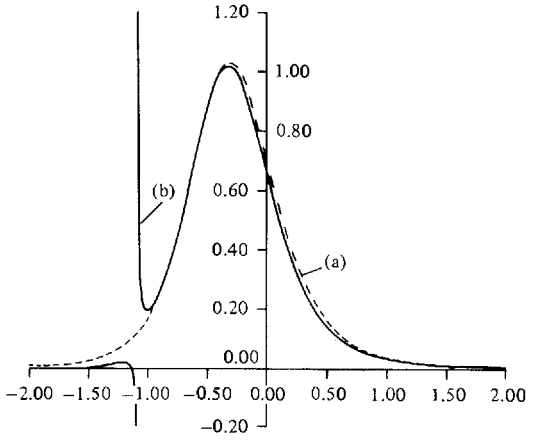


Figure 5.5. First-step [4/4] Padé approximant to pdf(x): (A) exact density; (B) Padé approximant.

alternative and better choice is the leading term in the density expansion (49), namely,

$$(50) \qquad s(x) = \left[B\left(\frac{1}{2}, \frac{K_2}{2}\right)(1 + x^2)^{(K_2+1)/2}\right]^{-1}$$

This is, in fact, the pdf of $\hat{\beta}$ under the null hypothesis that $\beta = 0$ and $\pi_{22} = 0$ (Basmann, 1974). As mentioned in the introduction, leading

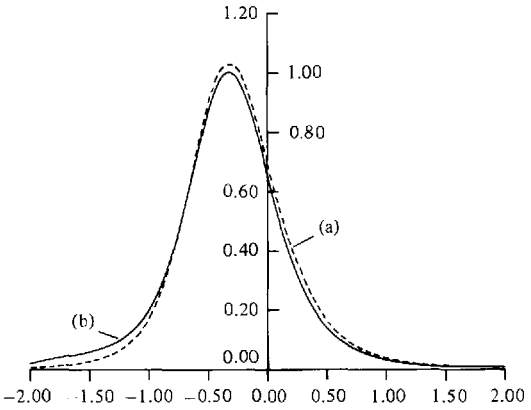


Figure 5.6. Modified Padé approximant to pdf(x); first change of coefficients: (A) exact density; (B) modified Padé approximants.

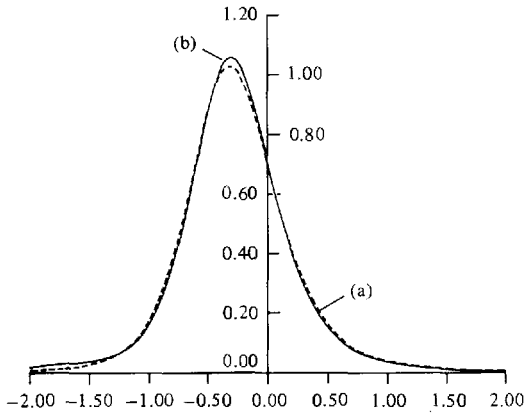


Figure 5.7. Modified Padé approximant to pdf(x); second change of coefficients: (A) exact density; (B) modified Padé approximant.

terms such as (50) in multiple series representations of density functions usually can be derived without much difficulty and often will be available even in cases in which an analytic form for the exact density has not been obtained. In the present case, a few elementary manipulations show that $\hat{\beta}$ takes the form of a standard normal variate divided by the square root of a chi square with K_2 degrees of freedom, with the numerator and denominator independent. The statistic $\hat{\beta}$ is therefore proportional to a t-variate with K_2 degrees of freedom, leading to a pdf of the form given by (50).

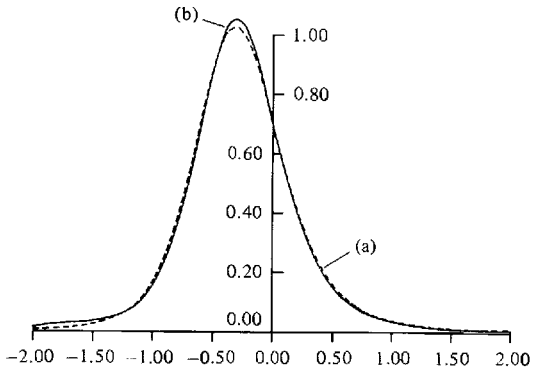


Figure 5.8. Modified Padé approximant to pdf(x) with renormalization: (A) exact density; (B) modified Padé approximant.

Writing $\text{pdf}(x) = s(x)\,\text{pdf}_s(x)$, as in (29), we then extract the local expansions (30) and (31) for $\text{pdf}_s(x)$. The expansions we use are for the tails $(x^{-1}=0)$ and the origin $(x=0)$. The coefficients that appear in (30) and (31) are given by

$$\alpha_0 = \sum_{j=0}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j\, j!} \left(\frac{\mu^2}{2}\right)^j W(K,j)$$

$$\alpha_1 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j 2\beta}{(K/2)_j (j-1)!} \left(\frac{\mu^2}{2}\right)^j W(K,j)$$

$$\alpha_2 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j (j-1)!} \left(\frac{\mu^2}{2}\right)^j [(2j-1)\beta^2 - 1] W(K,j)$$

$$\alpha_3 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j 2\beta}{(K/2)_j (j-1)!} \left(\frac{\mu^2}{2}\right)^j \left[\frac{(2j-1)(2j-2)}{3!}\beta^2 - j\right] W(K,j)$$

$$\alpha_4 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j (j-1)!} \left(\frac{\mu^2}{2}\right)^j \times \left[\frac{2(2j-1)(2j-2)(2j-4)}{4!}\beta^4 - j(2j-1)\beta^2 + \frac{(j+1)}{2}\right] W(K,j)$$

and

$$\beta_0 = \sum_{j=0}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j\, j!} \left(\frac{\mu^2\beta^2}{2}\right)^j W(K,j)$$

$$\beta_1 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j (j-1)!} \frac{\mu^{2j}\beta^{2j-1}}{2^{j-1}} W(K,j)$$

$$\beta_2 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j (j-1)!} \left(\frac{\mu^{2j}\beta^{2j-2}}{2^j}\right)(1-\beta^2) W(K,j)$$
$$+ \sum_{j=2}^{\infty} \frac{[(K+1)/2]2\beta^{-2}}{(K/2)_j (j-2)!} \left(\frac{\mu^2\beta^2}{2}\right)^j W(K,j)$$

$$\beta_3 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j (-j)}{(K/2)_j (j-1)!} \left(\frac{\mu^{2j}\beta^{2j-1}}{2^{j-1}}\right) W(K,j)$$

$$\beta_4 = \sum_{j=1}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j (j-1)!} \mu^{2j} \left[\frac{\beta^{2j}(j+1)}{2^{j+1}} - \frac{\beta^{2j-2} j}{2^j}\right] W(K,j)$$
$$+ \sum_{j=2}^{\infty} \frac{[(K+1)/2]_j}{(K/2)_j (j-2)!} \left(\frac{\mu^2}{2}\right)^j [\beta^{2j-2} j(j+1) + \tfrac{1}{2}\beta^{2j-4}] W(K,j)$$

where we have dropped the subscript on K_2 for convenience and where

$$W(K,j) = \exp[-\tfrac{1}{2}\mu^2(1+\beta^2)]\ {}_1F_1\left(\frac{K-1}{2}, j + \frac{K}{2}; \frac{\mu^2\beta^2}{2}\right)$$
$$= \exp(-\tfrac{1}{2}\mu^2)\ {}_1F_1\left(j + \tfrac{1}{2}, j + \frac{K}{2}; -\frac{\mu^2\beta^2}{2}\right)$$

by Kummer's transformation (Slater, 1960).

Figure 5.4 details the local density approximations to pdf(x) based on (30) and (31) with the coefficient function $s(x)$ as in (50). The approximations are good in the locality of the points of expansion, the origin, and the tails, but they start to deteriorate rapidly as we move out of the immediate vicinity. The right-hand tail expansion seems particularly good.

Figure 5.5 shows the [4/4] Padé approximant to the density (49). This has the form, in the notation of (44),

$$(51) \qquad R_{4,4}(x;s) = s(x)[4/4](x)$$
$$= s(x) \frac{a_4(x-\gamma_1)(x-\gamma_2)(x-\gamma)(x-\bar{\gamma})}{b_4(x-\delta_1)(x-\delta_2)(x-\delta)(x-\bar{\delta})}$$

where

$$a_4 = 4.533619 \qquad b_4 = 1.221628$$

$$\gamma_1 = -1.158240 \qquad \delta_1 = -3.567599$$

$$\gamma_2 = -0.537379 \qquad \delta_2 = -0.485485$$

$$\gamma, \bar{\gamma} = -2.133352 \pm 0.732053i \qquad \delta, \bar{\delta} = 0.310396 \pm 0.613123i$$

As a first step, approximant $R_{4,4}(x)$ is rather good, with problems occurring only in the left tail at the singularity $x=\delta_2$ (i.e., $x-\beta=\delta_2-\beta=-1.085485$ for $\beta=0.6$) and at the two zeros $x=\gamma_2, \gamma_1$ (note that the second pole occurs outside the region of immediate interest in the distribution).

The next stage in the procedure is to modify the Padé approximant (51) along the lines suggested in Section 7. We note that in the denominator the quadratic $x^2-(\delta_1+\delta_2)x+\delta_1\delta_2=x^2+4.05344x+1.7333$ has discriminant 9.497176. To remove the real zeros, we propose to replace this quadratic by

(52) $\quad 1.5x^2 + 4x + 3$

where we have raised the constant and the coefficient of x^2 and simply rounded the coefficient of x. According to the ideas outlined in Section 7, we now need to proportionately adjust the coefficient of x^2 and the constant term in one of the quadratics in the numerator. We select the quadratic $x^2-(\gamma_1+\gamma_2)x+\gamma_1\gamma_2 = x+1.695619x+0.622414$, which we need to modify in any case to remove the unwanted zeros of $R_{4,4}(x)$. Making the proportional adjustments recommended to this quadratic, we get $1.5x^2+1.695619x+1.077276$. This gives us the following modified Padé approximant after one change of coefficients:

$$(53) \quad R^{(a)}_{4,4}(x) = s(x) \times \frac{a_4\{1.5x^2+1.695619x+1.077276\}(x-\gamma)(x-\bar{\gamma})}{b_4\{1.5x^2+4x+3\}(x-\delta)(x-\bar{\delta})}$$

This function is graphed in Figure 5.6 against the exact density. We see that the singularity and zero problems have been eliminated, and the performance of the approximation is remarkably good. We note some reduction in the order of contact at the points of local expansion, particularly the origin (or, taking into account the change of origin on the graph, $x-\beta=-0.6$).

As suggested in Section 7, it is worthwhile to modify at least one of the remaining coefficients to improve the order of contact at the points of local expansion. Note that the success of this procedure can be measured against the original Padé approximant in the relevant locali-

ties; so we do not need a graph of the exact density to do so. Comparing the Padé and modified Padé approximants in Figures 5.5 and 5.6, it is clear that the order of contact of the modified Padé at the origin will be improved if we raise the derivative at this point ($x=0$, i.e., $x-\beta=-0.6$). This will be achieved by raising the coefficient of x in the quadratic in braces in the numerator of (53). We make a change in this coefficient from 1.69 to 2.0, giving the new modified Padé approximant

$$(54)\qquad R_{4,4}^{(b)}(x) = s(x) \times \frac{a_4\{1.5x^2+2.0x+1.077\}(x-\gamma)(x-\bar{\gamma})}{b_4\{1.5x^2+4x+3\}(x-\delta)(x-\bar{\delta})}$$

This function is graphed in Figure 5.7. Even with the rather crude adjustments we have made, (54) is really an exceptionally close approximation to the true density and is well behaved over the whole real axis. A final adjustment can be made by renormalizing so that the area under (54) is unity. The adjusted curve is shown in Figure 5.8.

9 Conclusion

This chapter has introduced a new technique of approximating probability density functions. The approximating functions belong to a family of rational fractions and are sufficiently flexible to produce good approximants to a very wide class of density functions. The theory developed in Sections 3 and 4 indicates that this family of rational fractions contains approximants that are best in a well-defined sense and that will perform well in reproducing the form of the exact density functions over the entire real axis. The practical procedure for finding good approximants in this family is based on the use of multiple-point Padé approximants to construct global approximations from purely local information about the density. These multiple-point Padé approximants are then modified to ensure that they have good global behavior and to incorporate any additional information that may be available concerning the density. The application in Section 8 to an already well-established test area for density approximations illustrates that the procedure can produce exceptionally good approximations even in cases in which existing methods break down. Further refinement of the ideas laid out in Section 7 on modifying the initial Padé approximant should lead to fine approximations that are very close to the best uniform approximants discussed in Sections 2 and 3.

NOTES

1 The compact set must obtain at least in this region of the overall parameter space Γ. We can, for example, exclude as irrelevant in terms of equation (4) those regions of Γ for which the parameters yield unbounded rational fractions.
2 The Weierstrass theorem (Meinardus, 1967, p. 7) established the same result for polynomial approximants.
3 This work and others (Baker & Gammel, 1970; Saff & Varga, 1977) have provided systematic coverage of the extensive literature on the theory of Padé approximants and their applications, particularly in mathematical physics.
4 Theorem 2.4 of Baker (1975).
5 Theorem 1.1 of Baker (1975).
6 These issues will be taken up at greater length in a later paper.
7 We deal specifically with the case $\mu^2=4$, $k=4$, $\beta=0.6$. Another paper will detail more fully some numerical experience with modified Padé approximants.

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