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ON THE ERROR IN PADE APPROXIMATIONS FOR FUNCTIONS DEFINED BY ST--ETC(U)
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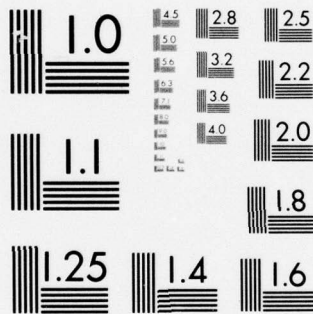
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analysis is applied to three important examples. Further, it is shown how to obtain the main diagonal Padé approximation. Extension to generalized Stieltjes integrals is indicated.

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On the Error in Padé Approximations for Functions
Defined by Stieltjes Integrals*

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I. Summary and Introduction

In a previous paper, the author derived an infinite series representation for the error in the Gaussian quadrature of

$$I = \int_a^b w(t)f(t,z)dt \quad \text{where } w(t) \text{ is the weight function and}$$

$f(t,z)$ is known. We suppose that $f(t,z)$ can be represented by an expansion in series of orthogonal polynomials $\{q_n(t)\}$ which is uniformly convergent in $[a,b]$. Thus, $f(t,z)$

$$= \sum_{n=0}^{\infty} c_n q_n(t), \quad c_n = h_n^{-1} \int_a^b w(t)q_n(t)f(t,z)dt. \quad \text{Then the error}$$

can be expressed in the form $\sum_{s=0}^{\infty} c_{2n+2+s} g_{2n+2+s}^{(n)}$ where the

$g_k^{(n)}$'s depend only on the properties of $q_n(t)$. Usually only one or two terms of the series are needed to achieve a realistic estimate of the error. Here asymptotic estimates for c_n for large n are employed. In the present paper, the error analysis is applied to the situation where $f(t,z) = (1+t/z)^{-1}$. In this instance, Gaussian quadrature of I and integrals simply

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related to I lead to approximations in z which occupy the $(n, n+r-1)$ positions of the Padé matrix table for I . Three important examples are treated. Two examples are generalized to the case where $f(t, z) = (1+t/z)^{-b}$.

II. Gaussian Quadrature

Let

$$I(z, a, b) = \int_a^b w(t) f(t, z) dt \quad (1)$$

where we suppose that $w(t)$ and $f(t, z)$ are integrable over the path a to b . We consider approximation of (1) by use of the Gaussian quadrature formula. To this end, let $\{q_n(t)\}$ be a system of orthogonal polynomials of the form

$$q_n(t) = \sum_{k=0}^n a_{k,n} t^k \quad (2)$$

such that

$$\int_a^b w(t) q_n(t) q_m(t) dt = h_n \delta_{mn}, \quad (3)$$

$$\delta_{mn} = 1 \quad \text{if } m = n, \text{ and}$$

$$\delta_{mn} = 0 \quad \text{if } m \neq n. \quad (4)$$

Let t_i be defined by

$$q_{n+1}(t_i) = 0, \quad i = 0, 1, \dots, n \quad (5)$$

and put

$$\lambda_{i,n} = \frac{A_n h_n}{q'_{n+1}(t_i) q_n(t_i)}, \quad A_n = \frac{a_{n+1,n+1}}{a_{n,n}}. \quad (6)$$

Following Luke [1], Gaussian quadrature of (1) leads to the formulation

$$I(z,a,b) = I_n(z,a,b) + E_n(z) , \quad (7)$$

$$I_n(z,a,b) = \sum_{i=0}^n \lambda_{i,n} f(t_i, z) \quad (8)$$

where $E_n(z)$ is the remainder which is zero if $f(t,z)$ is a polynomial in t of degree $\leq 2n+1$. Under the assumption that $f(t,z)$ can be expressed as an expansion in the polynomials $\{q_n(t)\}$ which is uniformly convergent in $[a,b]$, that is,

$$f(t,z) = \sum_{k=0}^{\infty} c_k q_k(t) , \quad (9)$$

$$c_k = h_k^{-1} \int_a^b w(t) q_k(t) f(t,z) dt , \quad (10)$$

then*

$$E_n(z) = \sum_{s=0}^{\infty} c_{2n+2+s} g_{2n+2+s}^{(n)} , \quad (11)$$

where

$$g_{2n+2}^{(n)} = \frac{h_{n+1}}{a_{0,0}} \prod_{k=0}^n \frac{A_{n+k+1}}{A_k} = \frac{a_{2n+2, 2n+2} h_{n+1}}{a_{n+1, n+1}^2} \quad (12)$$

and expressions for $g_{2n+2+s}^{(n)}$, $s > 0$, are detailed in the source cited. There explicit forms for $s = 0, 1, 2$ are derived for the classical orthogonal polynomials of Jacobi, Laguerre, Hermite and Bessel.

*In references [1,4], the n superscript notation on $g_{2n+2+s}^{(n)}$ was omitted. It should be noted, for example, that the formula for g_{k+1} is not necessarily that for g_k with k replaced by $k+1$. Here we have added the superscript notation to alert the reader to this situation.

We also have

$$E_n(z) = \frac{h_{n+1} \left. \frac{d^{2n+2} f(t,z)}{dt^{2n+2}} \right|_{t=\theta}}{(2n+2)! a_{n+1,n+1}^2}, \quad a < \theta < b, \quad (13)$$

and clearly $E_n(z) \equiv 0$ if $f(t,z)$ is a polynomial in t of degree $\leq 2n+1$.

III. Padé Approximations

Let

$$F(z) = \sum_{k=0}^{\infty} v_k z^k. \quad (14)$$

Let $P_m(z)$ and $Q_n(z)$ be polynomials in z of degree m and n , respectively, such that

$$Q_n(z)F(z) - P_m(z) = O(z^{m+n+1}). \quad (15)$$

Then $P_m(z)/Q_n(z)$ is the Padé approximation to $F(z)$ which occupies the (n,m) position in the Padé matrix table. If $m = n$, we have the main diagonal entries and if $m = n-1$, we have the first subdiagonal entries. For further information on Padé approximations with references and numerous examples, see [2,3]*. See also references [6-9] ahead.

*In [2], the first subdiagonal approximants are said to occupy the $(n-1,n)$ positions in the Padé matrix table in contradistinction to the present notation $(n,n-1)$. Also in [3, pp.493,494] there are a few (obvious) typographical errors.

IV. Application to Stieltjes Integrals

In this section, we apply the results of Sections 2 and 3 to the situation where

$$f(t, z) = (1 + t/z)^{-1}. \quad (16)$$

In this event,

$$I_n(z, a, b) = \sum_{i=0}^n \frac{\lambda_{i,n}}{1+t_i/z} = \frac{\text{polynomial in } z^{-1} \text{ of degree } n}{\text{polynomial in } z^{-1} \text{ of degree } n+1}, \quad (17)$$

$$E_n(z) = \frac{zh_{n+1}}{a_{n+1,n+1}^2(z+\xi)^{2n+3}} = O(z^{-2n-2}), \quad a < \xi < b. \quad (18)$$

It follows that $I_n(z, a, b)$ is the first subdiagonal Padé approximation to $I(z, a, b)$ where $f(t, z)$ is given by (16). Notice that if a and b are real and z is positive, then $E_n(z)$ is also positive.

We now show how to get the main diagonal Padé approximation. From (16),

$$f(t, z) = 1 - \frac{t}{z}(1 + \frac{t}{z})^{-1}, \quad (19)$$

and so

$$I(z, a, b) = \int_a^b w(t)dt - z^{-1}I^*(z, a, b),$$

$$I^*(z, a, b) = \int_a^b tw(t)(1 + t/z)^{-1}dt. \quad (20)$$

We apply our basic quadrature procedure to $I^*(z, a, b)$. In effect, this is a generalization of Gaussian quadrature for (1)

and (16) with an additional abscissa $t = 0$, which goes by the name Radau. For a discussion of generalized Gaussian quadrature with arbitrary additional abscissae, see Luke, Ting and Kemp [2]. For quadrature of (20), let

$$p_n(t) = \sum_{k=0}^n b_{k,n} t^k, \quad (21)$$

$$\int_a^b tw(t)p_n(t)p_m(t)dt = j_n \delta_{mn}, \quad (22)$$

$$p_n(u_i) = 0, \quad i = 0, 1, \dots, n, \quad (23)$$

$$\gamma_{i,n} = \frac{F_n j_n}{p'_{n+1}(u_i)p_n(u_i)}, \quad F_n = \frac{b_{n+1,n+1}}{b_{n,n}}. \quad (24)$$

Then

$$I(z, a, b) = I_n^*(z, a, b) + V_n(z), \quad (25)$$

$$\begin{aligned} I_n^*(z, a, b) &= \int_a^b w(t)dt - \frac{1}{z} \sum_{i=0}^n \frac{\gamma_{i,n}}{1+u_i/z} \\ &= \frac{\text{polynomial in } z^{-1} \text{ of degree } n+1}{\text{polynomial in } z^{-1} \text{ of degree } n+1}, \end{aligned} \quad (26)$$

where $V_n(z)$ is the remainder and

$$V_n(z) = - \frac{j_{n+1}}{b_{n+1,n+1}^2 (z+\phi)^{2n+3}} = O(z^{-2n-3}),$$

$$a < \phi < b. \quad (27)$$

Thus, $I_n^*(z, a, b)$ is the main diagonal Padé approximation to $I_n(z, a, b)$. If a and b are real and z is positive, then

$$V_n(z) < I(z, a, b) < E_n(z). \quad (28)$$

Since

$$(1+t/z)^{-1} = \sum_{k=0}^r (-)^k (t/z)^k + (-)^r (t/z)^r (1+t/z)^{-1}, \quad (29)$$

$$I(z, a, b) = \sum_{k=0}^{r-1} (-)^k z^{-k} \int_a^b t^k w(t) dt + \{(-)^r / z^r\} \int_a^b t^r w(t) (1+t/z)^{-1} dt, \quad (30)$$

Gaussian quadrature of the integral in (30) leads to an approximation which occupies the $(n, n+r-1)$ position in the Padé matrix table.

That Gaussian quadrature of Stieltjes integrals leads to Padé approximations is rather well known. Indeed it goes back to Stieltjes [5]. In recent times, Padé approximations of Stieltjes integrals via Gaussian quadrature together with error analyses have been considered by a number of writers. We make no attempt to give a complete bibliography, but see Allen et al [6,7], Chui [8], Karlsson and Sydow [9] and the references noted in these sources. There is an extensive literature on Gaussian quadrature for general integrals which we do not quote. In this connection, see Davis and Rabinowitz [10] and Donaldson and Elliott [11]. The latter is especially valuable as it develops a unified approach to quadrature formulas with the error expressed as a contour integral from which asymptotic estimates of the error can be deduced. Our approach differs from all other authors in that we study the error in Padé approximations by use of (11). We now turn to three examples.

V. Examples

We treat three cases for which considerable information is known about their Padé approximations. In what follows, we make free use of notations and ideas found in my books [2,3].

In each situation we treat the first subdiagonal Padé approximation only.

Example 1. Consider

$${}_2F_1(1, a; c-1/z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 \frac{t^{a-1}(1-t)^{c-a-1}}{(1+t/z)} dt, \quad (31)$$

$$R(c) > R(a) > 0, \quad |\arg(1+1/z)| < \pi.$$

We have [2, v.2, p.31],

$$(1+t/z)^{-1} = \sum_{n=0}^{\infty} c_n(z) R_n^{(\alpha, \beta)}(t), \quad \alpha = c-a-1, \quad \beta = a-1, \quad (32)$$

$$c_n(z) = \frac{n!(-)^n}{z^n(n+\lambda)_n} {}_2F_1\left(\begin{matrix} n+\beta+1, n+1 \\ 2n+\lambda+1 \end{matrix} \middle| -1/z \right), \quad \lambda = \alpha+\beta+1 = c-1, \quad (33)$$

where $R_n^{(\alpha, \beta)}(t)$ is the shifted Jacobi polynomial. From [2, v.1, p.237],

$$c_n(z) = \frac{(-)^n 2^{3-\lambda} z^{(n\pi)} \frac{1}{2} e^{-\xi(n+1)} (1+e^{-\xi})^{\lambda-\beta-3/2}}{(1-e^{-\xi})^{\frac{1}{2}-\beta}} \{1 + O(n^{-1})\}, \quad (34)$$

$$e^{-\xi} = 2z + 1 \mp 2(z^2+z)^{\frac{1}{2}} \quad (35)$$

where $\mp$ sign is chosen so that $|e^{-\xi}| < 1$. This is possible for all z except $-1 \leq z \leq 0$. From [1],

$$\begin{aligned} g_{2n+2}^{(n)} &= \frac{\Gamma(n+\alpha+2)\Gamma(n+\beta+2)\Gamma(n+\lambda+1)(n+1)!\Gamma(4n+\lambda+4)}{\{\Gamma(2n+\lambda+2)\}^2 \Gamma(2n+\lambda+3)(2n+2)!} \\ &= 2^{-\lambda} (\pi/2n)^{\frac{1}{2}} \{1 + O(n^{-1})\}, \end{aligned} \quad (36)$$

$$\frac{g_{2n+3}^{(n)}}{g_{2n+2}^{(n)}} = - \frac{2(\alpha-\beta)(n+1)(n+2)(4n+\lambda+4)}{(2n+\lambda+1)(2n+\lambda+3)((2n+3))} = -(\alpha-\beta)\{1 + O(n^{-1})\}.$$

We suppose that $g_{2n+2+r}^{(n)}/g_{2n+2}^{(n)} = h(\alpha, \beta)\{1 + O(n^{-1})\}$ uniformly for all $r \geq 1$ where $h(\alpha, \beta)$ depends only on α and β . For the special cases $\alpha = \pm\beta$, we have verified this for $r = 2$. But

proof of the general situation seems elusive. From (11) and (34)-(36), we find with

$$F_n(z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} E_n(z), \quad (37)$$

$$F_n(z) = \frac{\Gamma(\lambda+1)\pi z e^{-\xi(2n+3)} (1+e^{-\xi})^{\alpha-\frac{1}{2}}}{\Gamma(\alpha+1)\Gamma(\beta+1)2^{2\lambda-3}(1-e^{-\xi})^{\frac{1}{2}-\beta}} \{1 + O(n^{-1})\} \\ \times \{1 + (\alpha-\beta)e^{-\xi} + A(\alpha, \beta, \xi) + O(n^{-1})\}, \quad (38)$$

where $A(\alpha, \beta, \xi)$ depends only on α, β and ξ and is $O(e^{-2\xi})$. From [2, v.2, p.173] (there put $a = 1, \sigma = \beta + 1, \rho = \lambda$ and to conform to the present notation, replace n by $n + 1$), we have

$$R_{n+1}(z) = \frac{\Gamma(\lambda+1)\pi z^{\beta+1} e^{-\xi(2n+3+\beta)} (1+e^{-\xi})^{2\alpha}}{\Gamma(\alpha+1)\Gamma(\beta+1)2^{2\alpha-1}} \{1 + O(n^{-1})\}. \quad (39)$$

Neglecting $O(n^{-1})$ terms, we have

$$\frac{F_n(z)}{R_{n+1}(z)} = \frac{\{1 + (\alpha-\beta)e^{-\xi} + A(\alpha, \beta, \xi)\}}{(4ze^{-\xi})^\beta (1+e^{-\xi})^{\alpha+\frac{1}{2}} (1-e^{-\xi})^{\frac{1}{2}-\beta}}. \quad (40)$$

If z is sufficiently large so that $e^{-\xi}$ is sufficiently small, then

$$\frac{F_n(z)}{R_{n+1}(z)} = \frac{\{1 + (\alpha-\beta)e^{-\xi} + A(\alpha, \beta, \xi)\}}{\{1 + (\alpha-\beta)e^{-\xi} + \frac{1}{2}e^{-2\xi}\{(\alpha-\beta)^2 - \lambda\} + O(e^{-3\xi})\}}, \quad (41)$$

and so within the limitations noted, the two different error analyses give the same result.

Example 2. We consider the complementary incomplete gamma function

$$\Gamma(v, z) = \frac{e^{-z} z^{v-1}}{\Gamma(1-v)} \int_0^\infty \frac{e^{-t} t^{-v} dt}{(1+t/z)}. \quad (42)$$

Considerable information on the main diagonal and first sub-diagonal Padé approximations are known. See [2,3] where asymptotic results are given to show that these approximations converge, although the convergence is rather slow. Formally, at

least, we have [2, v.2, p.18],

$$(1+t/z)^{-1} = \sum_{n=0}^{\infty} k_n(z) L_n^{(-v)}(t), \quad (43)$$

$$k_n(z) = \{\Gamma(n+1-v)\}^{-1} G_{1,2}^{2,1} \left(z \middle| \begin{matrix} 1-n \\ 1-v, 1 \end{matrix} \right) = n! z^{1-v} U(n+1-v; 1-v; z), \quad (44)$$

$$L_n^{(-v)}(t) = \{(1-v)_n/n!\} {}_1F_1(-n; 1-v; t). \quad (45)$$

Here (45) is the generalized Laguerre polynomial. From [2, v.1, p.264],

$$L_n^{(-v)}(t) = \frac{(nt)^{\frac{1}{2}v - \frac{1}{4}} e^{t/2}}{\pi^{\frac{1}{2}} n^v} \{1 + O(n^{-1})\} \\ \times \cos\{2(nt)^{\frac{1}{2}} + \pi(\frac{1}{2}v - \frac{1}{4}) + O(n^{-\frac{1}{2}})\}, \quad (46)$$

with t fixed and $n \rightarrow \infty$. Also from [2, v.2, p.200] or from the work of Wimp [12],

$$k_n(z) = (\pi z)^{\frac{1}{2}} (n/z)^{\frac{1}{2}v - \frac{1}{4}} e^{z/2} \exp\{-2(nz)^{\frac{1}{2}}\} \{1 + O(n^{-\frac{1}{2}})\}, \\ z \text{ fixed, } |\arg z| \leq \pi - \epsilon, \epsilon > 0, n \rightarrow \infty. \quad (47)$$

Thus under the conditions stated

$$L_n^{(-v)}(t) k_n(z) = n^{-\frac{1}{2}} O(\exp\{-2(nz)^{\frac{1}{2}}\}), \quad (48)$$

and so (43) converges, though the convergence is rather slow. However, the convergence is not uniform in $0 \leq t \leq \infty$ as can be deduced from a known asymptotic expansion for the generalized Laguerre polynomial for large n which holds uniformly for large t . See Wyman [13]. Hence for the example (42), our method of error analysis fails.

Example 3. We now consider a form related to the incomplete gamma function,

$${}_1F_1(1; \lambda+1; -z) = \{\Gamma(\lambda+1)/2\pi i\} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{p} p^{-\lambda-1} (1+z/p)^{-1} dp, \quad (48)$$

$$\gamma > 0, R(\lambda) > -1, |\arg(1+z/\gamma)| < \pi. \quad (49)$$

This example is important since it illustrates use of Gaussian quadrature and our technique of error analysis for the inversion of Laplace transforms. From [2, v.2, p.7], we have

$$(1+z/p)^{-1} = \sum_{n=0}^{\infty} v_n(z) R_n(\lambda, p), \quad (50)$$

$$v_n(z) = \{z^n u_n(z)/(n+\lambda)_n\}, \quad u_n(z) = e^{-z} {}_1F_1(n+\lambda; 2n+\lambda+1; z); \quad (51)$$

$$R_n(\lambda, p) = {}_2F_0(-n, n+\lambda; p^{-1}), \quad (52)$$

The latter is called a Bessel polynomial and for properties of same needed in our present study, see [1, 2, 3]. From Luke [14], we have

$$u_n(z) = e^{-z} e^{z(n+\lambda)/(2n+\lambda+1)} \left\{ 1 + \frac{z^2(n+1)(n+\lambda)}{2(2n+\lambda+2)(2n+\lambda+1)} + O(n^{-3}) \right\}. \quad (53)$$

From [1],

$$\begin{aligned} g_{2n+2}^{(n)} &= \frac{(-)^{n+1} \Gamma(n+\lambda+1) (n+1)! \Gamma(4n+\lambda+4)}{\{\Gamma(2n+\lambda+2)\}^2 \Gamma(2n+\lambda+3)} \\ &= (-)^{n+1} 2^{2n-\lambda+3/2} n^{-\lambda} \{1 + O(n^{-1})\}, \end{aligned} \quad (54)$$

$$\frac{g_{2n+3}^{(n)}}{g_{2n+2}^{(n)}} = - \frac{4(n+1)^2(4n+\lambda+4)}{(2n+\lambda+1)(2n+\lambda+3)} = -4n\{1 + O(n^{-1})\}. \quad (55)$$

From (51) and (53),

$$\frac{v_{2n+3}}{v_{2n+2}} = \frac{z(2n+\lambda+2)e^{z(1-\lambda)/(4n+\lambda+5)(4n+\lambda+7)}}{(4n+\lambda+4)(4n+\lambda+5)} \{1 + O(z^2/n^2)\}. \quad (56)$$

We suppose that

$$\frac{g_{2n+2+r}^{(n)} v_{2n+2+r}}{g_{2n+2}^{(n)} v_{2n+2}} = f_{r,n} \{1 + O(n^{-1})\},$$

$$f_{r,n} = \frac{(-)^r}{r!} \left(\frac{z(2n+\lambda+2)}{4n+\lambda+5} \right)^r, \quad (57)$$

uniformly in r , $r \geq 1$. This is true for $r = 1$ in view of (55,56). Using a result in [1], we can verify (57) when $\lambda = 1$ for $r = 1, 2$. However, proof of the general statement appears elusive. If $U_n(z)$ is the error in the first subdiagonal Padé approximation for the left hand side of (49), then from (11), (51-54) and (57), we find

$$U_n(z) = \frac{(-)^{n+1} \pi \Gamma(\lambda+1) z^{2n+2} e^{-z} \Gamma(n+\lambda+1) (n+1)! \{1+O(n^{-1})\}}{2^{4n+2\lambda+3} \Gamma(n+1+\lambda/2) \{\Gamma(n+3/2+\lambda/2)\}^2 \Gamma(n+2+\lambda/2)}, \quad (58)$$

since

$$e^{z(2n+\lambda+2)/(4n+\lambda+5)} \sum_{r=0}^{\infty} f_{r,n} = 1, \quad (59)$$

and (58) is precisely the result given in [2, v.2, p.191], where to conform to our present notation, we must replace n and v by $n+1$ and λ respectively, and set $a = 1$.

VI Extension to Generalized Stieltjes Integrals

It is of interest to indicate an extension of the above analyses to the case where

$$f(t, z) = (1 + t/z)^{-b} \quad (60)$$

where b is arbitrary so long as the integral (1) has meaning. Then/in the quadrature formula (8), the summation part holds save that $f(t_i, z)$ is now computed from (60), since the weights $\lambda_{i,n}$ are independent of b . Now in the expression for the error, see (7), (11), (12) and [1], the coefficients c_k depend on b , but

but the coefficients $g_{2n+2+s}^{(n)}$ depend only on the system of orthogonal polynomials and so are independent of b . The expansion (60) in series of shifted Jacobi polynomials and in series of Bessel polynomials after the manner of the corresponding expansions for $b = 1$ as in Examples 1 and 3, respectively, are readily deduced from results given in the cited references. With such data in hand, (38) and (58) are easily generalized.

For a generalization of Example 1, we have

$${}_2F_1(a, b; c; -1/z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 \frac{t^{a-1}(1-t)^{c-a-1}}{(1+t/z)^b} dt, \quad (61)$$

valid under the same conditions as for (31).

Let $F_n(z, b)$ be the error in the Gaussian approximation for (61) such that when $b = 1$ we get the error in the first subdiagonal Padé approximation, see (38). Then under the same assumptions which led to (38), we find

$$F_n(z, b)/F_n(z, 1) = \{\Gamma(b)\}^{-1} \{2z(z^2+z)^{-1/2}\}^{b-1} \{1 + O(n^{-1})\}. \quad (62)$$

Similarly, for a generalization of Example 3, we have

$${}_1F_1(b; \lambda+1; -z) = \{\Gamma(\lambda+1)/2\pi i\} \int_{\gamma-i\infty}^{\gamma+i\infty} e^p p^{-\lambda-1} (1+z/p)^{-b} dp, \quad (63)$$

valid under the same conditions as for (49). Now let $U_n(z, b)$ be the error in the Gaussian approximation for (63) such that when $b = 1$, we obtain the error in the first subdiagonal Padé approximation, see (58). Then under the same assumptions which led to (58), we get

$$U_n(z, b)/U_n(z, 1) = \{(2n)^{b-1}/\Gamma(b)\} \{1 + O(n^{-1})\}. \quad (64)$$

In each example, the dependence of the error on b is quite weak.

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