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Frequency Fitting of Rational Approximations to the Exponential Function

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Abstract. Rational approximations to the exponential function are considered. Let $R = P/Q$, $\deg P = \deg Q = n$, $R(z) = \exp(z) + \mathcal{O}(z^{2n-1})$ and $R(\pm iT) = \exp(\pm iT)$ for a given positive number T. We show that this approximation is A-acceptable if and only if T belongs to one of intervals, whose endpoints are related to zeros of certain Bessel functions. The existence of this type of approximation and its connection to diagonal Padé approximations is studied. Approximations which interpolate the exponential on the imaginary axis are important in the numerical analysis of highly-oscillatory ordinary differential systems.

1. Introduction. The study of rational approximations to the exponential function plays a central role within the framework of the numerical analysis of stiff ordinary differential equations.

Let R be a rational function, $R = P/Q$, $\deg P = m$, $\deg Q = n$, $Q(0) = 1$. R is said to be of order p if

$$R(z) = e^z + \mathcal{O}(z^{p+1})$$

and A-acceptable if $|R(z)| \leqslant 1$ for every complex z such that $\operatorname{Re} z \leqslant 0$. These concepts are important, because of their relation to order and stability of numerical schemes for stiff equations.

It is well known that the maximal attainable order is $m + n$, in which case we have the classical Padé approximations to $\exp(z)$. The A-acceptability of these approximations has been studied extensively and the proof that A-acceptability is attained just for $m \leqslant n \leqslant m + 2$ was given by Wanner, Hairer and Nørsett [8].

It is useful for some practical purposes to relax the order conditions at the origin and to use the ensuing degrees of freedom to interpolate the exponential at some other points. In this context Liniger and Willoughby [5] introduced the concept of *exponential fitting* of order p at $z = z_0$, namely that $R(z) = \exp(z) + \mathcal{O}(|z - z_0|^{p+1})$. In their paper they discussed the cases $1 \leqslant m \leqslant n \leqslant 2$, and considered either up to two real, negative, fitting points or a conjugate pair of fitting points with negative real parts. The case of exponential fitting to real, negative, points has also lately been studied by Iserles and Powell [3]. The main result of [3] is that exponential fitting at more than two negative points results in non A-acceptable approximations.

The purpose of this paper is to investigate the *frequency fitting*, namely exponential fitting at conjugate, pure imaginary points. We restrict ourselves to $m = n$ and order $2n - 2$ at the origin. Frequency fitting is important within the framework of

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numerical solution of highly oscillatory equations. The case $1 \leqslant n \leqslant 2$ has already been studied by Lambert [4], as well as in the path-breaking paper of Liniger and Willoughby [5].

We show that, while fitting at $z_0 = \pm iT$, as T varies from zero to infinity, intervals of A-acceptability and non A-acceptability occur. The endpoints of these intervals are related to zeros of spherical Bessel functions of the first kind.

In a later paper we hope to analyse the more complicated case of fitting at two conjugate points z_0 and $\bar{z}_0$, with $\operatorname{Re} z_0 < 0$. Our motivation is to characterize all the A-acceptable approximations which use all their coefficients to fit the exponential in $\{z \in \mathbf{C}\colon \operatorname{Re} z \leqslant 0\}$.

2. Frequency Fitting. As already mentioned in the introduction we set $m = n$ and demand order $2n - 2$ at the origin. The general form of such approximations is given by Nørsett [6] and Ehle and Picel [2],

$$(2.1)\quad R_n(z; \alpha, \beta) = \frac{(1-\alpha-\beta)P_{n/n}(z) + \alpha P_{(n-1)/n}(z) + \beta P_{(n-2)/n}(z)}{(1-\alpha-\beta)Q_{n/n}(z) + \alpha Q_{(n-1)/n}(z) + \beta Q_{(n-2)/n}(z)},$$

where α and β are arbitrary constants and $P_{m/n}$ and $Q_{m/n}$ are the numerator and the denominator, respectively, of the Padé approximation $R_{m/n}$,

$$P_{m/n}(z) := \sum_{k=0}^{m} \frac{(n+m-k)!}{(n+m)!}\binom{m}{k} z^k, \quad Q_{m/n}(z) := P_{n/m}(-z).$$

The exponential fitting of R_n at z_0 and $\bar{z}_0$ gives two linear equations for the determination of the parameters α and β, namely

$$(2.2)\qquad R_n(z_0; \alpha, \beta) = e^{z_0}, \quad R(\bar{z}_0; \alpha, \beta) = e^{\bar{z}_0}.$$

Note that, if a solution to (2.2) exists, it is necessarily real.

This pair of equations can be reformulated, by using the relation (2.1), as

$$(2.3)\quad \begin{bmatrix} \psi_{n/n}(z_0) - \psi_{(n-1)/n}(z_0); & \psi_{n/n}(z_0) - \psi_{(n-2)/n}(z_0) \\ \psi_{n/n}(\bar{z}_0) - \psi_{(n-1)/n}(\bar{z}_0); & \psi_{n/n}(\bar{z}_0) - \psi_{(n-2)/n}(\bar{z}_0) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \psi_{n/n}(z_0) \\ \psi_{n/n}(\bar{z}_0) \end{bmatrix},$$

where

$$\psi_{m/n}(z) := Q_{m/n}(z)e^z - P_{m/n}(z).$$

The determinant $D_n(z_0)$ of the system (2.3) is

$$D_n(z_0) = 2i \operatorname{Im}\{[\psi_{n/n}(z_0) - \psi_{(n-1)/n}(z_0)][\psi_{(n-1)/n}(\bar{z}_0) - \psi_{(n-2)/n}(\bar{z}_0)]\}.$$

By using the fundamental, readily verifiable relations

$$(2.4)\quad \psi_{m/n}(z) = \frac{m}{n+m}\psi_{(m-1)/n}(z) + \frac{n}{n+m}\psi_{m/(n-1)}(z),$$

$$(2.5)\quad \psi_{m/n}(z) = \psi_{(m-1)/(n+1)}(z) + \frac{1}{m+n} z\psi_{(m-1)/n}(z),$$

$$(2.6)\quad \psi_{m/n}(z) = \psi_{(m-1)/n}(z) + \frac{n}{(m+n)(m+n-1)} z\psi_{(m-1)/(n-1)}(z),$$

we find

$$(2.7)\quad D_n(z) = \frac{n}{2(n-1)(2n-1)^2}|z|^2 i\,\mathrm{Im}\{\psi_{(n-1)/(n-1)}(z)\psi_{(n-2)/(n-1)}(\bar{z})\}.$$

Furthermore, whenever $D_n(z_0) \neq 0$,

$$(2.8)\quad \begin{aligned} \alpha = \alpha_n(z_0) &= -2i\frac{\mathrm{Im}\{\psi_{n/n}(z_0)\psi_{(n-2)/n}(\bar{z}_0)\}}{D_n(z_0)}, \\ \beta = \beta_n(z_0) &= 2i\frac{\mathrm{Im}\{\psi_{n/n}(z_0)\psi_{(n-1)/n}(\bar{z}_0)\}}{D_n(z_0)}. \end{aligned}$$

This leads to our first conclusion:

THEOREM 1. *The exponential fitting to* z_0 *and* $\bar{z}_0$ *is possible whenever* $\mathrm{Im}\{\psi_{(n-1)/(n-1)}(z_0)\psi_{(n-2)/(n-1)}(\bar{z}_0)\} \neq 0$. *The coefficients* α *and* β *are real and given by the formulae* (2.8). $\square$

Let $z_0 = iT$, $T \in \mathbf{R}$. It is well known that $R_{n/n}$ is symmetric, namely

$$|R_{n/n}(iy)| \equiv 1$$

for all real y. It is natural to expect R_n to retain this property, when α and β are given by (2.8). To prove that this is indeed the case we need the following results:

LEMMA 2.

$$\alpha_n(z) + \frac{2n-1}{n-1}\beta_n(z) = \frac{2ni}{n-1}\mathrm{Im}\{\psi_{n/n}(z)\psi_{(n-1)/(n-1)}(\bar{z})\}/D_n(z).$$

Proof. From (2.8)

$$\begin{aligned} &\alpha_n(z) + \frac{2n-1}{n-1}\beta_n(z) \\ &\quad = 2i\,\mathrm{Im}\left\{\psi_{n/n}(z)\left[\frac{2n-1}{n-1}\psi_{(n-1)/n}(\bar{z}) - \psi_{(n-2)/n}(z)\right]\right\}/D_n(z). \end{aligned}$$

The desired result follows by (2.4). $\square$

LEMMA 3. *If* $T \in \mathbf{R}$, *then* $\mathrm{Im}\{\psi_{n/n}(iT)\psi_{(n-1)/(n-1)}(-iT)\} \equiv 0$.

Proof. The relation $P_{n/n}(z) = Q_{n/n}(-z)$ yields

$$\begin{aligned} \psi_{n/n}(z) &= Q_{n/n}(z)e^z - P_{n/n}(z) = P_{n/n}(-z)e^z - Q_{n/n}(-z) \\ &= -e^z\left[Q_{n/n}(-z)e^{-z} - P_{n/n}(-z)\right] = -e^z\psi_{n/n}(-z). \end{aligned}$$

Therefore

$$\psi_{n/n}(z)\psi_{(n-1)/(n-1)}(\bar{z}) = \left(-e^z\psi_{n/n}(-z)\right)\left(-e^{\bar{z}}\psi_{(n-1)/(n-1)}(-\bar{z})\right)$$

and

$$\mathrm{Im}\{\psi_{n/n}(z)\psi_{(n-1)/(n-1)}(\bar{z})\} = e^{2\mathrm{Re}\,z}\,\mathrm{Im}\{\psi_{n/n}(-z)\psi_{(n-1)/(n-1)}(-\bar{z})\}.$$

When $z = iT$ this gives

$$\mathrm{Im}\{\psi_{n/n}(iT)\psi_{(n-1)/(n-1)}(-iT)\} = \mathrm{Im}\,\overline{\{\psi_{n/n}(iT)\psi_{(n-1)/(n-1)}(-iT)\}}$$

and, consequently, $\mathrm{Im}\{\psi_{n/n}(iT)\psi_{(n-1)/(n-1)}(-iT)\} = 0$. $\square$

THEOREM 4. *Let $z_0 = iT$, $T \in \mathbf{R}$, and α, β be given by* (2.8). *Then R_n is a symmetric function and*

$$R_n(z; \alpha_n(iT), \beta_n(iT)) = R_n^*(z; \gamma_n(T))$$
$$= \frac{(1-\gamma_n(T))P_{n/n}(z) + \gamma_n(T)P_{(n-1)/(n-1)}(z)}{(1-\gamma_n(T))Q_{n/n}(z) + \gamma_n(T)Q_{(n-1)/(n-1)}(z)},$$

where

$$\gamma_n(T) = -\frac{n}{n-1}\beta_n(iT).$$

Proof. By the symmetry between $P_{n/n}$ and $Q_{n/n}$, it is sufficient to consider the numerator only. From Ehle and Picel [2]

$$P_{(n-2)/n}(z) = P_{(n-1)/n}(z) - \frac{n}{2n-1}P_{(n-1)/(n-1)}(z).$$

Therefore

$$(1-\alpha-\beta)P_{n/n}(z) + \alpha P_{(n-1)/n}(z) + \beta P_{(n-2)/n}(z)$$
$$= (1-\alpha-\beta)P_{n/n}(z) - \frac{n}{n-1}\beta P_{(n-1)/(n-1)}(z)$$
$$+ \left(\alpha + \frac{2n-1}{n-1}\beta\right)P_{(n-1)/n}(z).$$

Let $\alpha = \alpha_n(iT)$, $\beta = \beta_n(iT)$. Then, by Lemmas 2 and 3,

$$\alpha + \frac{2n-1}{n-1}\beta = 0.$$

The proof follows. □

The main conclusion to be drawn from Theorem 4 is that, from now on, we can study the rational function R_n^* with respect to existence, i.e. $D_n(iT) \neq 0$, and A-acceptability. Moreover, since $|R_n^*(iy, \gamma_n(T))| \equiv 1$ for every $y \in \mathbf{R}$, the approximation is A-acceptable if and only if it is analytic in the complex left half plane—in other words, if all its poles are in $\mathbf{C}^{(+)} = \{z \in \mathbf{C}\colon \operatorname{Re} z > 0\}$.

3. The Behavior of the Frequency-Fitted Approximation. As we have already stated, the approximation R_n^* exists whenever $D_n(iT) \neq 0$. The definition of γ_n implies that this happens when $\gamma_n(T)$ is bounded.

It is helpful to derive another expression for $\gamma_n(T)$: by definition

$$R_n^*(\pm iT, \gamma_n(T)) = e^{\pm iT}.$$

Solving for γ_n, we obtain from (2.9)

$$\gamma_n(T) = \frac{\psi_{n/n}(iT)}{\psi_{n/n}(iT) - \psi_{(n-1)/(n-1)}(iT)}. \tag{3.1}$$

For $n \geqslant 2$ we know from Ehle and Picel [2] that

$$\psi_{n/n}(z) = \psi_{(n-1)/(n-1)}(z) + \frac{1}{4(2n-1)(2n-3)}z^2\psi_{(n-2)/(n-2)}(z). \tag{3.2}$$

Hence (3.1) gives

$$\gamma_n(T) = -\frac{4(2n-1)(2n-3)}{T^2}\frac{\psi_{n/n}(iT)}{\psi_{(n-2)/(n-2)}(iT)}. \tag{3.3}$$

Let $r_1^{(n)} < r_r^{(n)} < \cdots$ denote all the roots of the equation $\psi_{n/n}(iT) = 0$, $T > 0$, i.e. the "natural" interpolation points of the nth diagonal Padé aproximation along the open upper imaginary half-axis. It is easy to see that there exists an infinite number of such points.

LEMMA 5. *$\gamma_n(T)$ is unbounded if and only if $T = \pm r_k^{(n-2)}$ for some $k \geqslant 1$.*

Proof. By (3.3), if $T = r_k^{(n-2)}$ then $\gamma_n(T)$ becomes unbounded. If $T = -r_k^{(n-2)}$, then the same follows by $\gamma_n(T) = \gamma_n(-T)$. Finally, if $T = 0$ then $\gamma_n(T) = 0$, because $\psi_{m/m}(iT) = \mathcal{O}(T^{2m+1})$ for every $m \geqslant 0$. An inspection of (3.3) shows that no other values of T might give unboundedness. □

Let us split $P_{n/n}$ into a sum of even and odd polynomials, i.e. $P_{n/n}(z) = E_n(z^2) + zU_n(z^2)$. By symmetry $Q_{n/n}(z) = E_n(z^2) - zU_n(z^2)$ and

$$(3.4)\quad \begin{aligned}\psi_{n/n}(iT) &= \left(E_n(-T^2) - iTU_n(-T^2)\right)e^{iT} - \left(E_n(-T^2) + iTU_n(-T^2)\right)\\ &= 2ie^{iT/2}\left(E_n(-T^2)\sin\frac{T}{2} - TU_n(-T^2)\cos\frac{T}{2}\right).\end{aligned}$$

Let

$$(3.5)\qquad r_n(T) := E_n(-T^2)\sin\frac{T}{2} - TU_n(-T^2)\cos\frac{T}{2}.$$

Then from (3.1)

$$(3.6)\qquad \gamma_n(T) = \frac{r_n(T)}{r_n(T) - r_{n-1}(T)}.$$

Furthermore, it is obvious from (3.4) and (3.5) that, for $T > 0$, the zeros of $r_n(T)$ are exactly $\{r_k^{(n)}\}_{k=1}^{\infty}$.

Example. By considering the explicit expression for $R_{n/n}$, it is easily obtained that

$$E_0(x) = 1,\quad U_0(x) = 0,\quad r_0(T) = \sin\frac{T}{2};$$

$$E_1(x) = 1,\quad U_1(x) = \frac{1}{2},\quad r_1(T) = \sin\frac{T}{2} - \frac{1}{2}T\cos\frac{T}{2};$$

$$E_2(x) = 1 + \frac{1}{12}x,\quad U_2(x) = \frac{1}{2},\quad r_2(T) = \left(1 - \frac{1}{12}T^2\right)\sin\frac{T}{2} - \frac{1}{2}T\cos\frac{T}{2};$$

$$E_3(x) = 1 + \frac{1}{10}x,\quad U_3(x) = \frac{1}{2} + \frac{1}{120}x,$$

$$r_3(T) = \left(1 - \frac{1}{10}T^2\right)\sin\frac{T}{2} - \left(\frac{1}{2}T - \frac{1}{120}T^3\right)\cos\frac{T}{2}.$$

The zeros of r_n are the positive solutions of the nonlinear equation

$$\frac{TU_n(-T^2)}{E_n(-T^2)} = \operatorname{tg}\frac{T}{2}.$$

The geometrical picture of these equations is presented in Figure 1.

This is the place to mention that $TU_n(-T^2)/E_n(-T^2)$ is the nth Padé approximation to $\operatorname{tg}(T/2)$. The proof follows at once from the definition of U_n and E_n and from the invariance theorem for Padé approximations [1, p. 113].

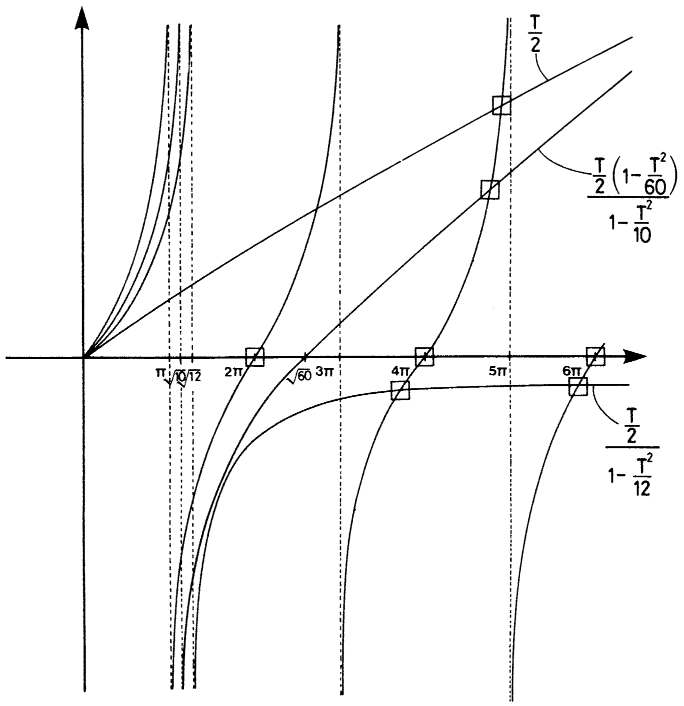

FIGURE 1
The functions present in $r_n(T)$, $n = 0, 1, 2, 3$.
The zeros of $r_n(T)$ are indicated by '$\square$'.

There are three sets of special values of T which are important to the present work, namely the zeros of $\gamma_n(T)$, the roots of the equation $\gamma_n(T) = 1$ and the points where $\gamma_n(T)$ becomes unbounded. A simple examination of (3.6) shows that $R_n^*(z; 0) = R_{n/n}(z)$ and $R_n^*(z; 1) = R_{(n-1)/(n-1)}(z)$, while (3.3) yields that $\lim_{|\gamma|\to\infty} R_n^*(z, \gamma) = R_{(n-2)/(n-2)}(iT)$. The pattern of passage of $\gamma_n(T)$ through the different special values, as a function of T, is central to the understanding of the approximation.

Example. Let $n = 2$. Then

$$\gamma_2(T) = -12\frac{\left(1 - \frac{1}{12}T^2\right)\operatorname{tg}\frac{T}{2} - \frac{1}{2}T}{T^2 \operatorname{tg}\frac{T}{2}}.$$

This expression is similar to a formula of Liniger and Willoughby [5]. By simple calculation

$$\gamma_2'(T) = -\frac{12}{T^3\operatorname{tg}^2\frac{T}{2}}\left[\frac{1}{4}\left(1 + \operatorname{tg}^2\frac{T}{2}\right)T^2 + \frac{1}{2}T\operatorname{tg}\frac{T}{2} - 2\operatorname{tg}^2\frac{T}{2}\right]$$

and $\gamma_2'(T) < 0$ for $T > 0$. Figure 2 illustrates the shape of $\gamma_2(T)$. It will be proved later that the pattern of passage of γ_2 through the special values is typical.

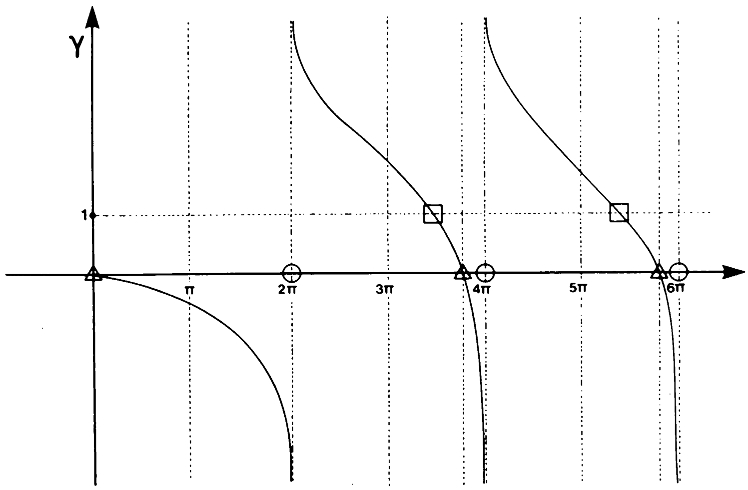

FIGURE 2. $\gamma_2(T)$, $T > 0$

□: $\gamma(T) = 1$

○: $|\gamma(T)| = \infty$

△: $\gamma(T) = 0$

LEMMA 6.

$$r_n(T) = \frac{(-1)^n n! 2^{2n}}{(2n)!} \sum_{k=n}^{\infty} \frac{(-1)^k}{(2k+1)!} \frac{k!}{(k-n)!} \left(\frac{1}{2}T\right)^{2k+1}.$$

Proof. It is easy to see from (3.2) and (3.5) that

$$r_n(T) = r_{n-1}(T) - \frac{1}{4(2n-1)(2n-3)} T^2 r_{n-2}(T).$$

This three-term recurrence relation, in conjunction with

$$r_0(T) = \sin\frac{T}{2} = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \left(\frac{1}{2}T\right)^{2k+1},$$

$$r_1(T) = \sin\frac{T}{2} - \frac{1}{2}T\cos\frac{T}{2} = -2\sum_{k=1}^{\infty} \frac{(-1)^k k}{(2k+1)!} \left(\frac{1}{2}T\right)^{2k+1},$$

determines the r_n's for every $n \geqslant 0$. The proof is completed by a simple induction argument. □

LEMMA 7.

$$r_n(T) = \frac{\sqrt{2}}{2} \frac{n!}{(2n)!} \sqrt{\pi} \left(\frac{T}{2}\right)^{n+1/2} J_{n+1/2}\left(\frac{T}{2}\right),$$

where $J_{n+1/2}$ is the nth spherical Bessel function of the first kind.

Proof. By Lemma 6

$$r_n(T) = \frac{n!2^{2n}}{(2n)!}\left(\frac{1}{2}T\right)^{2n+1} \sum_{k=0}^{\infty} (-1)^k \frac{(n+k)!}{k!\,(2n+2k+1)!}\left(\frac{T}{2}\right)^{2k}$$

$$= \frac{1}{2}\frac{n!}{(2n)!\left(\frac{1}{2}\right)_{n+1}}\left(\frac{1}{2}T\right)^{2n+1} {}_0F_1\left[\begin{matrix} -, \\ n+\frac{3}{2}, \end{matrix} \quad -\frac{1}{16}T^2\right].$$

The proof follows by the definition of Bessel functions of the first kind [7, p. 108]. □

We investigate now the sign of $\gamma_n'(T)$. By (3.6)

$$(3.7)\quad \operatorname{sgn}\gamma_n'(T) = \operatorname{sgn}(r_{n-1}'(T)r_n(T) - r_{n-1}(T)r_n'(T))$$
$$= \operatorname{sgn}\left\{\frac{1}{2}T\left(J_{n+1/2}\left(\frac{T}{2}\right)J_{n-1/2}'\left(\frac{T}{2}\right) - J_{n+1/2}'\left(\frac{T}{2}\right)J_{n-1/2}\left(\frac{T}{2}\right)\right)\right.$$
$$\left. -J_{n+1/2}\left(\frac{T}{2}\right)J_{n-1/2}\left(\frac{T}{2}\right)\right\}.$$

By [7, p. 111]

$$\frac{1}{2}TJ_{n-1/2}'\left(\frac{T}{2}\right) = -\frac{1}{2}TJ_{n+1/2}\left(\frac{T}{2}\right) + \left(n-\frac{1}{2}\right)J_{n-1/2}\left(\frac{T}{2}\right);$$
$$\frac{1}{2}TJ_{n+1/2}'\left(\frac{T}{2}\right) = \frac{1}{2}TJ_{n-1/2}\left(\frac{T}{2}\right) - \left(n+\frac{1}{2}\right)J_{n+1/2}\left(\frac{T}{2}\right).$$

Therefore, (3.7) gives

LEMMA 8.

$$\operatorname{sgn}\gamma_n'(T) = \operatorname{sgn}\left\{-\frac{1}{2}T\left(J_{n-1/2}^2\left(\frac{T}{2}\right) + J_{n+1/2}^2\left(\frac{T}{2}\right)\right)\right.$$
$$\left. + (2n-1)J_{n-1/2}\left(\frac{T}{2}\right)J_{n+1/2}\left(\frac{T}{2}\right)\right\}. \quad \square$$

An immediate conclusion from the last lemma is that $\gamma_n'(T) < 0$ for $T \geqslant 2(2n-1)$, because

$$-\frac{1}{2}T\left(J_{n-1/2}^2\left(\frac{T}{2}\right) + J_{n+1/2}^2\left(\frac{T}{2}\right)\right) + (2n-1)J_{n-1/2}\left(\frac{T}{2}\right)J_{n+1/2}\left(\frac{T}{2}\right)$$
$$= -\ (2n-1)\left(J_{n+1/2}\left(\frac{T}{2}\right) - J_{n-1/2}\left(\frac{T}{2}\right)\right)^2$$
$$-\left(\frac{1}{2}T - 2n + 1\right)\left(J_{n+1/2}^2\left(\frac{T}{2}\right) + J_{n-1/2}^2\left(\frac{T}{2}\right)\right) < 0.$$

Moreover, by [7, p. 121]

$$J_\alpha(z)J_\beta(z) = \frac{\left(\frac{1}{2}z\right)^{\alpha+\beta}}{\Gamma(\alpha+1)\Gamma(\beta+1)}\,{}_2F_3\left[\begin{matrix} \frac{1}{2}(\alpha+\beta+1),\ \frac{1}{2}(\alpha+\beta+2); \\ \alpha+1,\ \beta+1,\ \alpha+\beta+1; \end{matrix} \quad -z^2\right].$$

Therefore

$$J_{n-1/2}^2(z) = \frac{\left(\frac{1}{2}z\right)^{2n-1}}{\left(\Gamma\left(n+\frac{1}{2}\right)\right)^2} {}_1F_2\left[\begin{matrix} n; \\ n+\frac{1}{2}, 2n; \end{matrix} \; -z^2\right], \tag{3.8}$$

$$J_{n+1/2}^2(z) = \frac{\left(\frac{1}{2}z\right)^{2n+1}}{\left(\Gamma\left(n+\frac{3}{2}\right)\right)^2} {}_1F_2\left[\begin{matrix} n+1; \\ n+\frac{3}{2}, 2n+2; \end{matrix} \; -z^2\right],$$

$$J_{n-1/2}(z)J_{n+1/2}(z) = \frac{\left(\frac{1}{2}z\right)^{2n}}{\Gamma\left(n+\frac{3}{2}\right)\Gamma\left(n+\frac{1}{2}\right)} {}_1F_2\left[\begin{matrix} n+1; \\ n+\frac{3}{2}, 2n+1; \end{matrix} \; -z^2\right].$$

Let

$$\rho_n(z) := -z\left(J_{n-1/2}^2(z) + J_{n+1/2}^2(z)\right) + (2n-1)J_{n-1/2}(z)J_{n+1/2}(z). \tag{3.9}$$

By Lemma 8 $\operatorname{sgn} \gamma_n'(T) = \operatorname{sgn} \rho_n(\frac{1}{2}T)$. However, from (3.8) and (3.9) we obtain

$$\rho_n(z) = -\frac{z^{2n}}{2^{2n-1}\Gamma\left(n+\frac{1}{2}\right)\Gamma\left(n+\frac{3}{2}\right)} {}_1F_2\left[\begin{matrix} n; \\ 2n, n+\frac{3}{2}; \end{matrix} \; -z^2\right].$$

Therefore, for $T \geqslant 0$, $\operatorname{sgn} \gamma_n'(T) = -\operatorname{sgn} \sigma_n(\frac{1}{2}T)$, where

$$\sigma_n(z) := {}_1F_2\left[\begin{matrix} n; \\ 2n, n+\frac{3}{2}; \end{matrix} \; -z^2\right]. \tag{3.10}$$

LEMMA 9. *If $\sigma_{n+2}(x) \geqslant 0$, then $\sigma_n(x) \geqslant 0$, whenever $x > 0$.*

Proof. By straightforward calculation

$$\sigma_n(x) = {}_1F_2\left[\begin{matrix} n+1; \\ 2n+2, n+\frac{3}{2}; \end{matrix} \; -x^2\right]$$

$$+ \frac{x^4}{(2n+1)(2n+3)^2(2n+5)} {}_1F_2\left[\begin{matrix} n+2; \\ 2n+4, n+\frac{7}{2}; \end{matrix} \; -x^2\right].$$

But, because of (3.8)

$${}_1F_2\left[\begin{matrix} n+1; \\ 2n+2, n+\frac{3}{2}; \end{matrix} \; -x^2\right] = \frac{\left(\Gamma\left(n+\frac{3}{2}\right)\right)^2}{\left(\frac{x}{2}\right)^{2n+1}} J_{n+1/2}^2(x) \geqslant 0,$$

and, by (3.10),

$${}_1F_2\left[\begin{matrix} n+2; \\ 2n+4, n+\frac{7}{2}; \end{matrix} \; -x^2\right] = \sigma_{n+2}(x).$$

Hence, if $x > 0$ and $\sigma_{n+2}(x)$ is nonnegative, so is $\sigma_n(x)$. $\square$

LEMMA 10. *For every* $T \geqslant 0$ *and* $n \geqslant 1$, $\gamma_n'(T) \leqslant 0$.

Proof. First, let $T > 1$. By Lemmas 8 and 9 it is sufficient to show that, for every such T, there exists $n_0 = n_0(T)$ such that $\gamma_n'(T) \leqslant 0$ for every $n \geqslant n_0$. But for $n \gg 0$ and T which is not an integer multiple of π, by (3.5) and considering the explicit expressions for E_n and U_n

$$r_{2n}(T) = (-1)^n \frac{(2n)!}{(4n)!} T^{2n} \sin \frac{T}{2}\left(1 + \mathcal{O}\left(\frac{1}{n}\right)\right);$$

$$r_{2n+1}(T) = (-1)^{n-1} \frac{(2n+1)!}{(4n+2)!} T^{2n+1} \cos \frac{T}{2}\left(1 + \mathcal{O}\left(\frac{1}{n}\right)\right).$$

Therefore

$$\begin{aligned}\gamma_{2n+1}'(T) &= -2(4n+1)\frac{\frac{1}{2}T\left(\operatorname{tg}^2 \frac{T}{2} + 1\right) - \operatorname{tg}\frac{T}{2}}{T^2} + \mathcal{O}(1)\\ &\leqslant -\frac{4n+1}{T^2}\left(\operatorname{tg}\frac{T}{2} - 1\right)^2 + \mathcal{O}(1) \leqslant 0\end{aligned}$$

for sufficiently large n. Furthermore,

$$\begin{aligned}\gamma_{2n}'(T) &= 2(4n-1)\frac{-\frac{1}{2}T\left(\operatorname{ctg}^2 \frac{T}{2} + 1\right) - \operatorname{ctg}\frac{T}{2}}{T^2} + \mathcal{O}(1)\\ &\leqslant -\frac{4n-1}{T^2}\left(\operatorname{ctg}\frac{T}{2} + 1\right)^2 + \mathcal{O}(1) \leqslant 0,\end{aligned}$$

where n is large enough.

If T is a multiple of π, the derivative of γ_n is nonnegative by continuity.

Finally, let $0 \leqslant T \leqslant 1$. We use (3.10) and separate the even-powered and the odd-powered parts of $\sigma_n(x)$:

$$\begin{aligned}\sigma_n(x) &= \sum_{k=0}^{\infty} \frac{(n)_{2k}}{(2k)!\,(2n)_{2k}(n+\frac{3}{2})_{2k}} x^{4k}\\ &\quad - \sum_{k=0}^{\infty} \frac{(n)_{2k+1}}{(2k+1)!\,(2n)_{2k+1}(n+\frac{3}{2})_{2k+1}} x^{4k+2}\\ &= \sum_{k=0}^{\infty} \frac{(n)_{2k}x^{4k}}{(2k+1)!\,(2n)_{2k+1}(n+\frac{3}{2})_{2k+1}}\\ &\quad \times \left\{(2k+1)(2n+2k)(n+\tfrac{3}{2}+2k) - x^2(n+2k)\right\}\\ &\geqslant \sum_{k=0}^{\infty} \frac{(n)_{2k}x^{4k}}{(2k+1)!\,(2n)_{2k}(n+\frac{3}{2})_{2k+1}} \left\{2(2k+1)(n+k) - x^2\right\}\\ &\geqslant (2n - x^2)\sum_{k=0}^{\infty} \frac{(n)_{2k}x^{4k}}{(2k+1)!(2n)_{2k}(n+\frac{3}{2})_{2k+1}} \geqslant 0\end{aligned}$$

whenever $0 \leqslant x \leqslant \sqrt{2n}$. But $\operatorname{sgn}\gamma_n'(T) = -\operatorname{sgn}\sigma_n(\frac{1}{2}T)$, and so $\gamma_n'(T) \leqslant 0$ for $0 \leqslant T \leqslant 2\sqrt{2n}$. □

We sum up the results of this section in the following theorem:

THEOREM 11. *The coefficient γ_n of R_n^* is a monotonically decreasing function of the fitting parameter T. R_n^* coincides with the diagonal approximation $R_{(n-j)/(n-j)}$, $0 \leqslant j \leqslant 2$, when $T > 0$ is a zero of the spherical Bessel function $J_{n-j+1/2}(\frac{1}{2}T)$. These zeros are arranged in the following order*:

$$0 < r_1^{(n-2)} < r_1^{(n-1)} < r_1^{(n)} < r_2^{(n-2)} < \cdots . \qquad \square$$

It ought to be mentioned that the interlacing property of the $r_j^{(m)}$'s, which is easily deduced from the inspection of the behavior of γ_n, can also be derived from the interlacing properties of the zeros of Bessel functions.

The values of the first $r_j^{(m)}$'s are displayed in Table I.

TABLE I. $r_n^{(i)}$, $0 \leqslant n \leqslant 6$, $1 \leqslant i \leqslant 4$

$n \backslash i$	1	2	3	4
0	6.2831853	12.5663706	18.8495559	25.1327412
1	8.9868189	15.4505037	21.8082433	28.1323878
2	11.5269184	18.1900227	24.6458819	31.0292060
3	13.9758640	20.8342371	27.3960463	33.8472426
4	16.3651229	23.4098143	30.0793294	36.6025119
5	18.7116242	25.9330603	32.7094193	39.3063042
6	21.0256708	28.4147849	35.2959497	41.9669261

4. *A*-Acceptability. In Nørsett [6] a necessary and sufficient condition for the A-acceptability of $R_n(z; \alpha, \beta)$ was given (Ehle and Picel [2] give a sufficient condition only). Of interest to us is the A-acceptability of $R_n^*(z; \gamma)$ in (2.9), which is a subclass of $R_n(z; \alpha, \beta)$ with

$$\gamma = -\frac{n}{n-1}\beta, \quad \alpha = -\frac{2n-1}{n-1}\beta.$$

By using Theorem 6 of Wanner, Hairer and Nørsett [8] we are able to prove

THEOREM 12. *The frequency-fitted rational approximation $R_n^*(z; \gamma)$ is A-acceptable if and only if $\gamma \leqslant 1$.*

Proof. If $\gamma \leqslant 1$ the A-acceptability follows by Theorem 6 of [8]. To see that $\gamma > 1$ gives no A-acceptability, we study the behavior of R_n^* as a function of γ. When $\gamma < 1$ R_n^* is A-acceptable and, because of symmetry of the numerator and the denominator about the pure imaginary axis, it has exactly n zeros in $\mathbf{C}^{(+)}$ and n poles in $\mathbf{C}^{(-)}$. When γ approaches 1 from below, a single zero and a single pole coalesce at the origin, as can be readily seen from (2.9). When γ has passed 1 the pole moves to the left and the zero to the right half-plane, respectively. This happens because both the numerator and the denominator of R_n^* are linear functions of γ. Hence, for $\gamma > 1$ R_n^* is not analytic in $\mathbf{C}^{(-)}$, and consequently cannot be A-acceptable.

It ought to be stressed that the pole in $\mathbf{C}^{(-)}$ cannot cross to $\mathbf{C}^{(+)}$ for $1 < \gamma < \infty$: by symmetry, during such crossing it must coalesce with a zero. In this case there is a common linear factor in the numerator and the denominator. The reduction of this factor and order conditions at the origin imply that R_n^* must coincide, for this particular γ, with $R_{(n-1)/(n-1)}$. But this is impossible, because $\gamma > 1$. $\square$

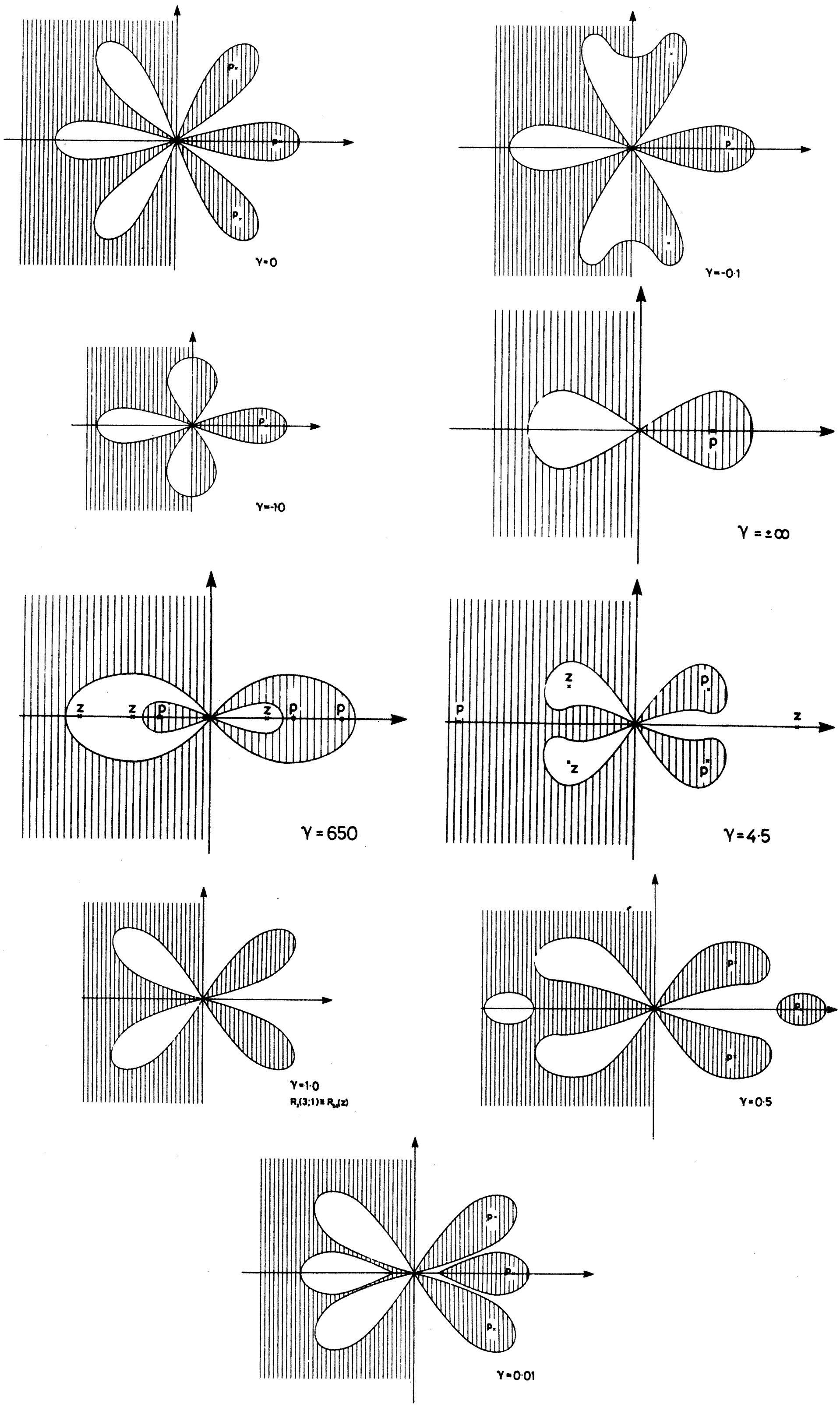

FIGURE 3

The behavior of the order-star of R_3^* as a function of γ.

By combining Theorems 11 and 12, we finally find

THEOREM 13. *The frequency fitted rational approximation $R_n^*(z;\gamma(T))$ is A-acceptable if and only if T belongs to one of the intervals $[r_j^{(n-1)}, r_{j+1}^{(n-2)}]$, $j = 0, 1, \ldots,$ where we set $r_0^{(n)} = 0$.* □

Let us as an illustration look at the order star and see how it changes as γ moves from 0 to $-\infty$ and then from $+\infty$ to 0 again.

Since we have

$$\psi_{m/m}(z) = (-1)^m\left(\frac{m!}{(2m+1)!}\right)^2 z^{2m+1} + \mathcal{O}(z^{2m+2})$$

we easily find

$$R_n^*(z;\gamma) = e^z + (-1)^n\gamma\left[\frac{(n-1)!}{(2n-1)!}\right]^2 z^{2n-1} + \mathcal{O}(z^{2n})$$

and

$$R_n^*(z;0) = e^z + (-1)^{n+1}\left[\frac{n!}{(2n+1)!}\right]^2 z^{2n+1} + \mathcal{O}(z^{2n+2}).$$

Without loss of generality, let us assume that n is odd, and even more so let $n = 3$. As γ moves from 0 to $-\infty$ and from $+\infty$ to 0 the situation is as given in Figure 3.

To conclude this paper, we show that the lack of A-acceptability can always be overcome by increasing n by one:

THEOREM 14. *If, for given $T > 0$, $R_n^*(z;\gamma(T))$ is not A-acceptable, then $R_{n+1}^*(z;\gamma(T))$ is A-acceptable.*

Proof. By Theorems 11 and 13, if $R_n^*(z,\gamma(T))$ is not A-acceptable then T belongs to an interval of the form $(r_m^{(n-2)}, r_m^{(n-1)})$, for some $m \geq 1$. By Theorem 11 $r_{m-1}^{(n)} < r_m^{(n-2)}$, and so $T \in [r_{m-1}^{(n)}, r_m^{(n-1)}]$. The A-acceptability of $R_{n+1}^*(z,\gamma_n(T))$ follows by Theorem 13. □

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