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ON THE CONSTRUCTIVE RATIONAL APPROXIMATION OF CERTAIN ENTIRE FUNCTIONS

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ABSTRACT

We present a conjecture on the first order asymptotics of the polynomials forming multipoint Pade approximants to certain entire functions, including some of the form exp[polynomial]. The conjecture is very simple to state (see equation (5.4)), and leads to two inhomogeneous Hilbert problems on arcs, for which solutions are given. The conjecture is motivated and supported by a number of examples and previous results. An outline of a proof of the conjecture in a special case is provided.

1. INTRODUCTION

Having been stimulated by the question of the asymptotic behavior of the N-soliton solution of the non-linear Schrodinger equation [Mi98], we have generated some speculations about the first order (strong) asymptotic form of the polynomials in the $\left[m/n\right]$ multi-point Pade approximant (MPA) to certain entire functions as $m,n\to\infty$. We propose a compact characterization of the form which we speculate applies to a variety of cases. From the compact characterization we derive equations for the zero and first order approximations.

Sections 2, 3, and 4 describe previous work on special cases of MPA polynomials which points the way towards our conjecture. The main features of the previous results on PA polynomials are summarised in Appendix A. The conjecture is set out in Section 5 and some technical details of the solution of the required equations are given in Section 6.

We have derived an extension of the integral equation described in Section 4 that may perhaps be used to prove the conjecture in some cases, although it will need modification in the NLS case. This equation and some numerical tests which support the conjecture are not included in this version of the report.

We are concerned here with the formal approximation of a function $F(\lambda)$ of the complex variable λ by the ratio of polynomials $Q(\lambda), P(\lambda)$ of degrees m,n respectively. The polynomials are chosen with the help of prescribed interpolation points $\left\{\ \lambda_j,\ j=1,\ m+n+1\ \right\}$ in the extended complex plane by solving the equations

$$Q(\lambda_j)-F(\lambda_j)P(\lambda_j)=0,\quad j=1,n+m+1\ . \tag{1.1}$$

If say k of the points λ_j coincide at the point λ_1, then (1.1) is replaced at that point by

$$Q(\lambda) - F(\lambda)P(\lambda) = O((\lambda-\lambda_1)^{k+1}, \quad \lambda \to \lambda_1. \tag{1.2}$$

The MPA to $F(\lambda)$, the ratio $Q(\lambda)/P(\lambda)$, is sometimes called a rational interpolant or other names. If all the points of interpolation coincide at λ_1 the ratio is called the Pade approximant (PA) to $F(\lambda)$ at the point λ_1.

With $z = 1/\lambda$ define the function $f(z)$ and polynomials $q(z), p(z)$ of degrees m, n respectively, by

$$f(z) = F(\lambda), \quad q(z) = z^m Q(\lambda), \quad p(z) = z^n P(\lambda). \tag{1.3}$$

Denote by M the set $\{\mu_j, j = 1, n+m+1\}$, where $\mu_j = 1/\lambda_j$.

Suppose that $f(z)$ is single-valued and analytic outside a compact set V, with $V \cap \mathrm{M} = 0$. Then it is known and easy to show that $p(z)$ is a (generalized) orthogonal polynomial in the sense that

$$\int_\Gamma dz \omega(z) p(z) z^k = 0, \quad k = 1, n-1 \tag{1.4}$$

Here

$$\omega(z) = z^{m-n} f(z)/d(z) \tag{1.5}$$

with $d(z) = \prod_{k=1}^{n+m+1} (z - \mu_j)$, (1.6)

and Γ is a closed curve containing V but not containing any point of M. In the case of diagonal $(m = n)$ PAs about $z = \infty$, (1.5) reduces to

$$\omega(z) = f(z). \tag{1.7}$$

There is an explicit representation for a polynomial satisfying (1.4) which Szego in his book [Sz78] declares “is not suitable in general for derivation of properties of the polynomials in question”. Actually, as an aid to guessing the correct result, as we show below, the formula has proved to be very useful. The representation is

$$p(z) = const. \int_\Gamma dz_1 \ldots \int_\Gamma dz_n I \prod_{k=1}^{n} (z - z_k) \omega(z_k). \tag{1.8}$$

where

$$I = \prod_{i<j=1}^{n} (z_i - z_j)^2. \tag{1.9}$$

2. DIAGONAL PADE APPROXIMANTS TO FUNCTIONS WITH BRANCH POINTS

The asymptotic behavior of $q(z), p(z)$ as $n \to \infty$ for this simplest case of the family we are considering is reasonably well understood. Below we have chosen three simple examples to illustrate a number of properties that reappear in the later development.

Example 2.1 Two branch points [Nuun]

Assume that the branch points are at $z = \pm 1$, and that $f(z)$ has a representation of the form

$$f(z) = \int_{\Omega} dt \sigma(t)(t^2 - 1)^{1/2}(t - z)^{-1} \tag{2.1}$$

where Ω is an arc joining $-1,1$, and $\sigma(z)$ is analytic where required. Assume for simplicity that $\sigma(z)$ is non-zero on the line segment $[-1,1]$. It appears that the process that determines $q(z), p(z)$, which in this case is the equations

$$q(z) - f(z)p(z) = O(z^{-n-1}),\ z \to \infty\,, \tag{2.2}$$

is 'designed' so that $q(z)/p(z)$ approximates $f(z)$ as 'well' as possible. The function being approximated is not single-valued but the approximation is. It turns out that approximation simulates a cut, an arc joining $-1,1$, by distributing the zeros of $q(z), p(z)$ close to the arc for large n. This is 'better' than making $f(z)$ single-valued by using a connected set of positive area containing $-1,1$.

The 'designer' may be a physicist since the location of the chosen arc, which we call S, is found by solving a two-dimensional electrostatic equilibrium problem. Suppose that the limit density of zeros of $p(z)$ is $\rho(z)$, real, positive and normalized to unity, and define the function $\psi(z)$ by

$$\psi(z) = \int_{S} |dt| \rho(t)(t - z)^{-1}\,. \tag{2.3}$$

The electric field $\vec{E}(z)$ due to the charge $\rho(z)$ has components $E_x = \operatorname{Re}\psi(z),\ E_y = -\operatorname{Im}\psi(z)$. The arc S and the density $\rho(z)$ are characterized by the conditions on S that the normal force on the charge at z due to the remaining charge be zero, and that there is no tangential force on the charge, which gives

$$\psi(z)^{+} + \psi(z)^{-} = 0, \quad z \in S\,. \tag{2.4}$$

Thus the charge is in equilibrium on a flexible conducting wire that is itself in a position of unstable equilibrium.

It is easy and instructive to solve (2.4) using the techniques described by Muskhelishvili [Mu53]. Define $y(z) = (z^2 - 1)^{1/2}$, single-valued on S and approaching z as $z \to \infty$. Then (2.4) gives

$$[y(z)\psi(z)]^{+} = [y(z)\psi(z)]^{-}, \quad z \in S \tag{2.5}$$

which means that $y(z)\psi(z)$ must be entire, in fact -1, since $\psi(z)+1/z \to 0$, $z \to \infty$. Hence $\psi(z) = -y(z)^{-1}$, from which it follows that

$$\rho(z) = -(2\pi i)^{-1}\left[y(z)^{+}\right]^{-1}, \quad z \in S. \tag{2.6}$$

and, since $\rho(z)$ is real, that S is the line interval $[-1,1]$.

Now define

$$\phi(z) = \int_S |dt|\rho(t)\log(z-t) \tag{2.7}$$

so that $\frac{d\phi(z)}{dz} = -\psi(z)$. Considering that

$$\log(p(z)) = \exp(n\sum_{j=1}\log(z-t_j), \tag{2.8}$$

where $\{t_j\}$ are the zeros of $p(z)$,it is not surprising to find that

$$\log(p(z)) = n\phi(z) + h(z) + O(n^{-1}), \quad z \to \infty \quad \text{for } z \notin S, \tag{2.9}$$

where $h(z)$ is independent of n.

We call the term $n\phi(z)$ in (2.9) the zero order term in the asymptotic expansion, and the combination $n\phi(z)+h(z)$ the first order term. Note that only the real part of $n\phi(z)$ is of any significance in zero order, since the addition of an integer multiple of $2\pi i$ does not change $p(z)$. If we define $\chi_2(z)$ by $\chi_2(z) = \exp(n\phi(z)+h(z))$ it turns out that $\chi_2(z)$ may be characterized as the solution of the equation

$$\chi_2(z)^{+}\chi_2(z)^{-} = \sigma(z)^{-1}, \quad z \in S \tag{2.10}$$

which is analytic outside S, approaches z^n as $z \to \infty$, and has an appropriate behavior near $z = \pm 1$. The function $\chi_3(z)$ that approximates $q(z)$ to first order away from S is given by $\chi_3(z) = f(z)\chi_2(z)$.

The above results may be obtained by a straightforward extension of the methods used by Szego [Sz78] in the case when $\rho(z)$ is real, positive on S.

<u>Example 2.2 Four branch points</u>

This example is close to those treated by Dumas in his 1908 thesis [Du08]. Define $X(z)$ by

$$X(z) = \prod_{j=1}^{4}(z-b_j) \tag{2.11}$$

where $b_1,..,b_4$ are distinct points in the complex plane. Let R: $y^2 = X(z)$ be a two-sheeted Riemann surface with sheet 1 such that $y(\infty^{(1)}) \sim z^2, z \to \infty$. Suppose that $f(z) = 1 + y(z)^{-1}$, which defines a meromorphic function on R. Define another meromorphic function $r(z)$ by

$$r(z) = f(z)p(z) - q(z), \tag{2.12}$$

which on account of (2.2) has a zero of order $n+1$ at $\infty^{(1)}$.

Because we can write

$$r(z^{(2)}) = r(z^{(1)}) - 2y(z^{(1)})^{-1}p(z) \tag{2.13}$$

it follows that $r(z)$ has poles only at $(\infty^{(2)})^{n-2}, b_1,..,b_4$ and zeros at $(\infty^{(1)})^{n+1}$. The function $r(z)$ must have one more zero, say at $c \in R$, since a meromorphic function has the same number of zeros as poles. The Jacobi inversion theorem shows that c is unique. By writing (2.12) for $z = z^{(1)}, z^{(2)}$ and solving for $p(z)$ we find

$$p(z) = K_2(z^{(1)}) + K_2(z^{(2)}), \tag{2.14}$$

here

$$K_2(z) = y(z)r(z)/2, \; z \in R. \tag{2.15}$$

It follows that $K_2(z)$ has poles at $(\infty^{(2)})^n$ and zeros at $(\infty^{(1)})^{n-1}, c$.

The above information is enough, as Dumas[Du08] showed (see Nuttall [Nu84b] for a more accessible treatment), to obtain exact explicit formulas for $r(z), q(z), p(z)$ in terms of Weierstrass ζ and σ functions, and to determine the asymptotic the form of the polynomials and location of their zeros.

We now restate the Dumas results in a language similar to that of the previous example. It is found as $n \to \infty$ that all but at most one of the zeros of $q(z), p(z)$ approach a set S, which now consists of two arcs each joining a different pair of branch points. We now suppose that the two sheets of R are joined at the arcs of S. If c is on sheet 2, $q(z), p(z)$ will each have a zero close to c. We give the name 'Dumas zeros' to zeros of $r(z), q(z), p(z)$ that are related to c.

There is again a function $\psi(z)$, obtained by solving (2.4), from which can be obtained the location of S and the density $\rho(z)$. In this case we have

$$\psi(z) = -(z-a)X(z)^{-1/2} \tag{2.15}$$

with a determined by the conditions

$$\mathrm{Re}\int_{b_1}^{b_2} dz\psi(z) = \mathrm{Re}\int_{b_1}^{b_3} dz\psi(z) = 0. \tag{2.16}$$

Integrating $\psi(z)$ gives the function $\phi(z)$ which tells us the zero order asymptotic behavior (away from c and S) of $q(z), p(z)$ via

$$\log(|p(z)|) = n\operatorname{Re}\phi(z) + O(1), \quad z \notin S, c, \tag{2.17}$$

where $\operatorname{Re}\phi(z) > 0, \quad z \notin S$. Dumas also shows that

$$\log(|r(z^{(1)})|) = -n\operatorname{Re}\phi(z) + O(1), \quad z \notin S, c. \tag{2.18}$$

We can describe the asymptotic behavior of $r(z), p(z), q(z)$ by introducing functions $\chi_1(z), \chi_2(z), \chi_3(z)$, analytic in the z-plane cut along S, defined by

$$\chi_1(z) = r(z^{(1)}); \quad \chi_2(z) = K_2(z^{(2)}); \quad \chi_3(z) = f(z^{(1)})\chi_2(z), \quad z \notin S \tag{2.19}$$

which are the first order approximations to $r(z), p(z), q(z)$ respectively away from S. The functions $\{\chi_j(z)\}$ may be characterized as the functions analytic away from S which satisfy the equations

$$\chi_3(z) = f(z\ )\chi_2(z), \quad z \notin S, \tag{2.20}$$

$$f(z)^{\mp}\chi_2(z)^{\pm} - \chi_3(z)^{\pm} = \chi_1(z)^{\mp}, \quad z \in S, \tag{2.21}$$

with $\chi_1(z) = O(z^{-n-1}); \quad \chi_2(z), \chi_3(z) = O(z^n), \quad z \to \infty$, and behave appropriately at the ends of S.

To solve (2.20), (2.21) first use (2.20) to eliminate $\chi_3(z)$ from (2.21), giving

$$((f(z)^+ - f(z)^-)\chi_2(z)^{\pm} = \mp\chi_1(z)^{\mp}, \quad z \in S. \tag{2.22}$$

Cross-multiplication shows that

$$\chi_1(z)\chi_2(z) = const.\, y(z)^{-1}(z-c) \tag{2.23}$$

for some choice of c, so that, with appropriate choice of normalization, $\chi_2(z)$ satisfies the equivalent of (2.10),

$$\chi_2(z)^+\chi_2(z)^- = \frac{z-c}{y(z)^+(f(z)^+ - f(z)^-)}, \quad z \in S \tag{2.24}$$

On taking logarithms (2.22) and similar equations reduce to an inhomogeneous Hilbert problem that may be solved using the techniques of Muskhelishvili [Mu53].

Example 2.3 Three branch points

Shortly before his death Laguerre [La85] was working without success on the asymptotics of diagonal PAs to a class of functions which included the example

$$f(z) = \prod_{j=1}^{3} (z - b_j)^{\nu_j} \tag{2.25}$$

where b_j, $j = 1,2,3$ are distinct, finite, noncollinear points in the complex plane and

$$\sum_{j=1}^{3} \nu_j = 0 . \tag{2.26}$$

With the help of a result of Stahl [St97], Nuttall [Nu86]was able to solve this problem, and we summarize the results. Again all the zeros of $q(z), p(z)$ but at most one approach a set S . This time we define

$$X(z) = \prod_{j=1}^{3} (z - b_j) \tag{2.27}$$

in terms of which $\psi(z)$ is given by

$$\psi(z) = -(z-a)^{1/2} X(z)^{-1/2} \tag{2.28}$$

where a is determined by

$$\mathrm{Re} \int_{b_1}^{b_2} dz(\psi(z)^+ - \psi(z)^-) = \mathrm{Re} \int_{b_1}^{b_3} dz(\psi(z)^+ - \psi(z)^-) = 0 . \tag{2.29}$$

In this case the Riemann surface needed to describe the asymptotics has the branch point a in addition to the branch points of the function being approximated. We call the point a a pseudo-branch point. Part of the solution is to find a from (2.29). This is a new Property which will reappear in extensions to entire functions. Otherwise the results are similar to Example 2.2.

3. MULTIPOINT PADE APPROXIMANTS TO ENTIRE FUNCTIONS

Our aim is to extend the theory summarized in Appendix A to the problem of MPAs to at least some entire functions (and possibly further). In this section we present some information that helps in formulating and supporting such an extension.

The cover of the proceedings of the Conference on Rational Approximation held in Tampa in 1976 [Sa77] suggests that progress in understanding our topic might be possible. It shows a plot of the poles and zeros of a non-diagonal PA to $\exp(\lambda)$ which lie close to two smooth arcs, one for the poles and one for the zeros, which meet at their ends to form a closed curve containing the origin. Such a pleasing picture strongly suggests that there is an underlying mathematical structure which could well be susceptible to analysis. Indeed there is, due to Saff and Varga [Sa77], as we summarize below, but we believe that the same reasoning could well apply to other cases where the structure is not yet known. The ability to compute such plots gives us a great advantage over Laguerre and his contemporaries.

Example 3.1 Pade approximants to the exponential function

The results of Saff and Varga apply to the non-diagonal case but for ease of explanation we consider only diagonal PAs. When $F(\lambda) = \exp(\lambda)$ and $m = n$ it may be shown that $Q(\lambda) = P(-\lambda)$ and that

$$Q(\lambda) = e^{\lambda/2}\lambda^{n}W_{0,\nu}(\lambda)\,, \tag{3.1}$$

where $\nu = n + \frac{1}{2}$ and $W_{0,\nu}(\lambda)$ is the Whittaker function of [Ol74] p. 260 which satisfies

$$\frac{d^2W}{d\lambda^2} = \left(\frac{1}{4} + \frac{\nu^2 - \frac{1}{4}}{\lambda^2}\right)W \;. \tag{3.2}$$

This means that the three functions $e^{-\lambda/2}\lambda^{-n}Q(\lambda)$, $e^{\lambda/2}\lambda^{-n}P(\lambda)$, $e^{-\lambda/2}\lambda^{-n}R(\lambda)$ all satisfy (3.2) with $R(\lambda)$ defined by

$$R(\lambda) = F(\lambda)P(\lambda) - Q(\lambda)\,. \tag{3.3}$$

Olver [Ol74] provides the tools for a rigorous Liouville-Green analysis, including error bounds, of the solutions of (3.2) for large n, and he discusses this example in detail (pp. 260, 401). Define $h(\lambda)$ by

$$h(\lambda) = \frac{1}{4} + \frac{\nu^2}{\lambda^2} \tag{3.4}$$

so that $h(\lambda)$ has zeros at the turning points $\lambda_+, \lambda_- = \pm 2i\nu$. Then, except near the turning points, first order approximations to the three functions satisfying (3.2) are given by appropriate linear combinations of

$$h(\lambda)^{-1/4}\exp\left(\pm\Phi(\lambda)\;\right), \tag{3.5}$$

where

$$\Phi(\lambda) = \int_{\lambda_+}^{\lambda} dt\, h(t)^{1/2}\;. \tag{3.6}$$

The locus $\operatorname{Re}\Phi(\lambda) = 0$ is independent of which sheet $\Phi(\lambda)$ is evaluated on, and it consists of three arcs joining λ_+ to λ_-, intersecting only at these two points (see Fig. 1).

From now on, to correspond to our previous treatment, we will use the variable $z = 1/\lambda$ so that (3.5) becomes, apart from a constant factor,

$$y(z)^{-1/2}\exp\left(\pm\nu\phi(z)\right), \tag{3.7}$$

where

$$\phi(z) = \int_{z_+}^{z} dt\, t^{-2} y(t)\,, \tag{3.8}$$

$z_+, z_- = \pm i\,(2\nu)^{-1}$ and $y(z) = (z^2 + (2\nu)^{-2})^{1/2}$.

With the notation of (1.3) and (2.12), $f(z) = \exp(1/z)$, and first order approximations to $r(z), p(z), q(z))$ are

$$\begin{aligned} &r(z): \quad \chi_1(z) = e^{i\pi/2}\, y_1(z)^{-1/2} \exp\left(-\nu\phi_1(z) + (2z)^{-1}\right) \\ &p(z): \quad \chi_2(z) = y_2(z)^{-1/2} \exp\left(\nu\phi_2(z) - (2z)^{-1}\right) \\ &q(z): \quad \chi_3(z) = y_3(z)^{-1/2} \exp\left(\nu\phi_3(z) + (2z)^{-1}\right) \end{aligned} \tag{3.9}$$

In each of the expressions of (3.9) for $\chi_j(z),\ j = 1,2,3$, the function $y_j(z)$ is taken to be single-valued outside the arc S_j shown in Fig. 2, which shows the same arcs as Fig.1 but in the z-plane, and also $y_j(z) \sim z,\ z \to \infty$. The path of integration in $\phi_j(z)$ must not cross S_j. We take $y_j(z)^{1/2}$ to mean the same thing on the positive real axis for all j.

For $z \in \Lambda_1$ of Fig. 2 the functions $y_j(z), \chi_j(z)$ are independent of j, and $\mathrm{Re}\,\phi_j(z) > 0$, so that, for n large, $\chi_1(z)$ is much smaller than $\chi_2(z), \chi_3(z)$, which satisfy the relation

$$f(z)\chi_2(z) - \chi_3(z) = 0, \quad z \in \Lambda_1. \tag{3.10}$$

In Λ_2, Λ_3 it is found that

$$\chi_1(z) + \chi_3(z) = 0, \quad z \in \Lambda_2; \qquad \chi_1(z) - f(z)\chi_2(z) = 0, \quad z \in \Lambda_3 \tag{3.11}$$

These relations follow because, for example,

$$\phi_1(z)^+ = \phi_1(z)^-; \quad \phi_3(z)^+ = \phi_3(z)^-; \quad \phi_2(z)^+ = -\phi_2(z)^-, \quad z \in S_2 \tag{3.12}$$

and

$$\left(y_1(z)^{1/2}\right)^- = \left(y_1(z)^{1/2}\right)^+; \quad e^{i\pi/2}\left(y_2(z)^{1/2}\right)^- = \left(y_2(z)^{1/2}\right)^+, \quad z \in S_2. \tag{3.13}$$

In Λ_2, Λ_3 we find that $\chi_2(z), \chi_3(z)$ respectively are much smaller than the other two χ_j for large n.

From relations such as (3.12), (3.13) it also follows that

$$\chi_2(z)^+ \chi_2(z)^- = \left(y_2(z)^+ f(z)\right)^{-1}; \quad \chi_3(z)^+ \chi_3(z)^- = \left(y_2(z)^+\right)^{-1} f(z). \tag{3.14}$$

Now let us consider the zero order approximation which for $p(z)$ we might regard as

$$\chi_2(z)_0 = \exp\left(n\phi_2(z) - (2z)^{-1}\right) \quad . \tag{3.15}$$

Previously in Section 2 we had the equivalent of

$$\psi_2(z) = -n^{-1}\frac{d\log(\chi_2(z)_0)}{dz} = -z^{-2}y_2(z) - (2nz^2)^{-1} \tag{3.16}$$

in this case. Now, instead of (2.4) or (A.2) we have

$$\psi_2(z)^+ + \psi_2(z)^- = -(nz^2)^{-1},\ \ z \in S_2; \qquad \psi_3(z)^+ + \psi_3(z)^- = (nz^2)^{-1},\ \ z \in S_3. \tag{3.17}$$

Again the PA appears to be doing its best. The closed curve $S_2 \cup S_3$ forms a boundary between Λ_1, where the rational approximation is good, and the essential singularity. In the z-plane the set $\Lambda_2 \cup \Lambda_3$, where the rational approximation is poor, shrinks to the origin as $n \to \infty$. The poles on S_2 approach the origin in the sector where $f(z)$ is large, and the zeros on S_3 where $f(z)$ is small. The determination of the location of the 'branch points', the zeros of $y(z)$, is discussed below.

We show next how a heuristic treatment of (1.8) can derive (2.4), (3.17) and a formula for the MPA case that will also be a consequence of our general conjecture.

<u>Heuristic Derivation of Zero Order MPA Asymptotics from the Szego Formula</u>

A heuristic saddle point method approximation to the integral in (1.8) proved to be helpful in the initial analysis of the asymptotics of PAs for functions with branch points [Nu77, Nu80, Nu84a]. Later the approach was extended to obtain (3.17) and similar equations for other entire functions. It appears to apply equally well to at least a class of MPAs, as we shall explain below.

The assumption of the method is that, for a given choice of contour Γ, there will be a set of points $z_k^0 \in \Gamma, k = 1, n$, unique apart from permutation, for which the modulus of the dominant factor in the integrand of (1.8) will be maximum. Distort the contour Γ within the constraints allowed until this maximum is smallest. Then the approximate value of the integral is obtained by expanding the integrand about the resulting point $\{z_1^0, \ldots, z_n^0\}$ as in the saddle point method.

Initially [Nu80] this method was applied to diagonal PAs for functions with branch points, with the dominant factor in (1.8) taken to be I, which leads to (2.4), (A.1). Later [Nu84] it was applied to non-diagonal PAs to the exponential and other entire functions. It just as easily applies to the general MPA case where $\omega(z)$ is given by (1.5), and we now outline the method in that case. For the dominant factor we choose $J = I\prod_{k=1}^{n}\omega(z_k)$, so that the equations for $\{z_1^0, \ldots, z_n^0\}$ become

$$\frac{\partial \log J}{\partial z_k} = 0, \quad k = 1, n, \tag{3.18}$$

which leads to

$$2\sum_{j\neq k}(z_k - z_j)^{-1} + (m-n)z_k^{-1} + g(z_k)' = 0, \quad k = 1, n. \tag{3.19}$$

Here we have set

$$f(z)/d(z) = \exp(g(z)). \tag{3.20}$$

We now assume that the points $\{z_1^0, \ldots, z_n^0\}$ are distributed smoothly on the stationary contour S with line density $\rho(z) > 0$ and for large n replace (3.19) by

$$2P\int_S |dt|\rho(t)(z-t)^{-1} + (\eta - 1)z^{-1} + n^{-1}g(z)' = 0, \quad z \in S, \tag{3.21}$$

with $\eta = m/n$. In terms of $\psi_2(z)$ defined by (2.3), equation (3.21) may be written as

$$\psi_2(z)^+ + \psi_2(z)^- = (\eta - 1)z^{-1} + n^{-1}(\log f(z))' - n^{-1}\sum_{j=1}^{n+m+1}(z - \mu_j)^{-1}. \tag{3.22}$$

<u>Application of the Heuristic Method to Example 3.1</u>

Suppose that we did not know about the results of Saff and Varga on $\exp(\lambda)$, and let us try to deduce them from (3.22) and the properties set out in Appendix A. For the case of the diagonal PA to $\exp(\lambda)$, Example 3.1, we have $f(z) = \exp(1/z)$, and (3.22) reduces to (3.17).

In this case there can be only pseudo-branch points, number and location unknown, so we shall try the simplest possibility, two branch points b_1, b_2 first. Let $y_2(z) = [(z-b_1)(z-b_2)]^{1/2}$ with $y_2(z)$ single-valued outside the unknown arc S_2 joining b_1, b_2, and $y_2(z) \sim z, \quad z \to \infty$. To solve (3.17) we apply the techniques of Muskhelishvili [Mu53] to what he would call an inhomogeneous Hilbert problem for arcs. Multiply by $y_2(z)^+ = -y_2(z)^-$ to give

$$[y_2(z)\psi_2(z)]^+ - [y_2(z)\psi_2(z)]^- = -y_2(z)^+(nz^2)^{-1}, \quad z \in S \tag{3.23}$$

which, in view of the behavior of $y_2(z)\psi_2(z)$ at $z = \infty$, leads to

$$y_2(z)\psi_2(z) = -1 - (2n\pi i)^{-1}\int_S dt\, y_2(t)t^{-2}(t-z)^{-1}. \tag{3.24}$$

The integral may be turned into an integral on a closed contour containing S and evaluated by residues to give

$$\psi_2(z) = -\frac{1}{2nz^2} + \frac{\left[-4ny_2(0)z^2 + Y_1 z + 2Y_0\right]}{4ny_2(0)y_2(z)z^2}, \tag{3.25}$$

where

$$y_2(z)^2 = z^2 + Y_1 z + Y_0. \tag{3.26}$$

Condition (A.4) on pseudo-branch points means that the expression in square brackets in (3.25) has to be proportional to $y_2(z)^2$, so that $Y_1 = 0$ and $y_2(0) = -(2n)^{-1}$, or equivalently $b_1, b_2 = \pm i(2n)^{-1}$. This is almost, but not quite, the same as Example 3.1. We attribute the difference to the choice of $h(\lambda)$ in (3.4).

The simplified result for $\psi_2(z)$ is

$$\psi_2(z) = -\frac{1}{2nz^2} - \frac{y_2(z)}{z^2} \tag{3.27}$$

with

$$y_2(z)^2 = z^2 + (2n)^{-2}. \tag{3.28}$$

The fact that $y_2(0) = -(2n)^{-1}$ tells us which of the three possible arcs emanating from b_1 is S_2. It means that the arc S_2 must intersect the positive real axis as we indicated in Fig. 2.

We could repeat the analysis for $q(z)$ and $\psi_3(z)$, starting from the second equation in (3.17). The result would lead to the same branch points but an arc S_3 which in this case is the reflection of S_2 in the origin.

To find the precise location of S_2 we use the fact from (2.3) that, with s as the arc length,

$$\Delta\psi_2(z) \equiv \psi_2(z)^+ - \psi_2(z)^- = 2\pi i\rho(z)ds/dz, \quad z \in S_2, \tag{3.29}$$

so that the equation for S_2 is

$$\frac{dz}{ds} = \frac{i|\Delta\psi_2(z)|}{\Delta\psi_2(z)}. \tag{3.30}$$

4. RIGOROUS ASYMPTOTIC RESULTS

Here we summarize some relevant more general rigorous results on PA and MPA asymptotics.

Results of Stahl and Gonchar/Rakhmanov on Zero Order Asymptotics

Stahl [St89] has devised a method of obtaining zero order asymptotics for close to diagonal PA and MPA polynomials. Define $\mu(p)$, the measure associated with the polynomial $p(z)$ of degree n, as

$$\mu(p) = n^{-1}\sum_j \delta_{t_j} , \tag{4.1}$$

where δ_t is the Dirac measure with support at the point t, and the sum is over all zeros of p (counting multiplicity). Under certain assumptions Stahl shows that, for the polynomial $p(z)$ defined in (1.3), $\mu(p)$ converges weakly to a measure σ as $n \to \infty$ with $m/n \to 1$. This leads to the conclusion that the rational approximants converge in capacity away from $\mathrm{supp}(\sigma)$ (see [St89] for details).

An important case included in Stahl's results is when $F(\lambda)$ is the sum of an algebraic function and a function analytic except for essential singularities on a set of capacity zero. When the algebraic function has branch points, for the PA it is found that $\mathrm{supp}(\sigma)$ is a set S_2 obtained by solving (A.2), and $d\sigma/ds$ is the associated line density $\rho(z)$. Almost all the zeros of $p(z)$ approach the arcs of S_2. When there are no branch points almost all the zeros approach the essential singularities. For a function of the same type, the results for the MPA are similar, but now the set S_2 is obtained from an acceptable solution of (3.22). The MPA results hold only when the set S_2 does not intersect the support of the weak limit of the measure $\mu(d)$, where d is given by (1.6)

Gonchar and Rakhmanov [Go89] have used Stahl's method to extend his results to a class of functions which include the case $F(\lambda) = \exp(n\Pi(\lambda))$, where $\Pi(\lambda)$ is a polynomial with coefficients independent of n. Consider for example the diagonal case. They assume that $\mu(d) \to \alpha$, and that the limit of (3.22)

$$\psi_2(z)^+ + \psi_2(z)^- = \frac{d\Pi(z^{-1})}{dz} - \int d\alpha(t)(z-t)^{-1}, \quad z \in S_2 \tag{4.2}$$

has an acceptable solution $\psi_2(z)$ satisfying the conditions (A.4), (A.5) which leads to a line density $\rho(z)$ positive on S_2. The set S_2 must be bounded and must not intersect $\mathrm{supp}(\alpha)$. If these conditions hold then $\mu(p)$ converges weakly to the measure corresponding to line density ρ.

Gonchar and Rakhmanov do not prove that there is always an acceptable solution of (4.2), and indeed we know from examples that there are cases in which for several reasons the conditions cannot be met, but there are also cases to which the theory does apply. One of these is the PA to $F(\lambda) = \exp(n\lambda)$ which can, by writing $\lambda' = n\lambda$, be transformed into Example 3.1. Apart from this case it does not appear that the results of Stahl and Gonchar/Rakhmanov include information about the detailed structure of the polynomial zeros for the MPA to entire functions which are independent of n.

Gonchar and Rakhmanov also provided a rigorous proof of the derivation of the value of the "1/9" constant made by Magnus [Ma88] using heuristic arguments similar to those above.

The method of proof invented by Stahl and used by Gonchar/Rakhmanov is by contradiction. They suppose that $\mu(p)$ does not converge to the measure σ associated with an acceptable set S_2, in which case there must be another measure σ' such that a subsequence of $\mu(p)$ does converge weakly to σ'. They then show using a steepest descent argument that the corresponding polynomials cannot satisfy the defining orthogonality relation (1.4) in the limit $n \to \infty$.

First Order Asymptotics

Rigorous results on first order PA asymptotics are less extensive than those for zero order, and first order results for MPA s are even more limited. However, what is known does suggest, as the examples above imply, that, for many functions, stronger results exist than just the weak convergence of the polynomial measure $\mu(p)$.

Nuttall and Singh [Nu77] considered the case of diagonal PAs to a function with $2l$ actual branch points $\{b_j\}$ such that the set S that follows from the Properties in Appendix A has no pseudo-branch points. The function $\psi(z)$ has the form

$$\psi(z) = -\prod_{j=1}^{l-1}(z-a_j) \Big/ X(z)^{1/2} \qquad (4.3)$$

where

$$X(z) = \prod_{j=1}^{2l}(z-b_j)\,, \qquad (4.4)$$

and the coefficients $\{a_j\}$ are determined from (A.5). The set S consists of l non-intersecting arcs.

Nuttall and Singh studied functions $f(z)$ of the form

$$f(z) = \int_S dt\left[X(t)^+\right]^{-1/2} \sigma(t)(t-z)^{-1} \qquad (4.5)$$

with appropriate restrictions on σ. They effectively showed that the first order approximation $\chi_2(z)$ to $p(z)$ is given by solving (A.10), where $g = l-1$, and described techniques for obtaining the solution, including the determination of the approximate zeros $\{c_j\}$ that do not approach S.

Nuttall and Singh [Nu77] used an extension of the Bernstein-Szego integral equation method which relates the exact polynomial $p(z)$ on S to polynomials orthogonal with respect to a weight in which $\sigma(t)$ of (4.5) is approximated by the reciprocal of a polynomial.

Later Nuttall [Nu90] derived a singular integral equation that applies to diagonal PAs to functions of the form (2.1). The equation is for the remainder function $r(z)$ of (2.12) and involves what we expect to be the first order approximation $\chi_1(z)$ of $r(z)$. If $\sigma(t)$ has the necessary analyticity, the path of integration in the equation can be distorted so that analysis of the solution is straightforward.

In the thesis of Nuttall's student N. H. Li [Li91] this approach was extended and improved to provide the framework that it is hoped will lead to the rigorous derivation of first order asymptotics for diagonal PAs to a class that includes algebraic functions. For a function $f(z)$ with no singularities other than branch points, assume that we have found the unique (see the references in [St97]) set S that has the Properties listed in Appendix A. Take the limit (for the purposes of this outline assume all limits and integrals exist) of (2.12) as $z \to S$ from either side to give

$$r(z)^{+} = f(z)^{+} p(z) - q(z), \quad z \to S$$
$$r(z)^{-} = f(z)^{-} p(z) - q(z), \quad z \to S \,. \tag{4.6}$$

Subtract to eliminate $q(z)$ so that

$$r(z)^{+} - r(z)^{-} = (f(z)^{+} - f(z)^{-})p(z), \quad z \to S \,. \tag{4.7}$$

Now we use the functions $\chi_1(z), \chi_2(z)$ that we expect to give the first order approximations to $r(z), p(z)$. These functions are determined from (2.20), (2.21) for the particular $f(z)$ in question, and they satisfy (2.22). If we define

$$U(z) = r(z) / \chi_1(z); \quad V(z) = p(z) / \chi_2(z) \tag{4.8}$$

then (4.7), (2.22) lead to

$$U(z)^{+} = V(z)^{-} - U(z)^{-} W(z); \quad U(z)^{-} = V(z)^{+} - U(z)^{+} W(z)^{-1}, \quad z \in S \,, \tag{4.9}$$

where $W(z) = \chi_1(z)^{-} / \chi_1(z)^{+}$.

Equations (4.9) may be decoupled by defining

$$K(z) = U(z) + V(z); \quad J(z) = U(z) - V(z) \tag{4.10}$$

to give

$$K(z)^{+} - K(z)^{-} = -U(z)^{-} W(z) + U(z)^{+} W(z)^{-1}$$
$$J(z)^{+} + J(z)^{-} = -U(z)^{-} W(z) - U(z)^{+} W(z)^{-1} \qquad z \in S \,, \tag{4.11}$$

In the simplest case $f(z)$ has two branch points, S is a line segment, $\chi_1(z)$ has no finite zeros, and we can solve (4.11) to give

$$K(z) = C_0 + (2\pi i)^{-1} \int_S dt \left[-U(t)^{-} W(t) + U(t)^{+} W(t)^{-1} \right] (t - z)^{-1} \tag{4.12}$$

$$J(z)=(2\pi i)^{-1}y(z)\int_S dt\left[-U(t)^{-}W(t)+U(t)^{+}W(t)^{-1}\right](y(t)^{+})^{-1}(t-z)^{-1},$$

where $y(z)$ is defined as in Example 2.1 and C_0 is a constant depending on normalization. A singular integral equation for $U(z)$ results by writing $U(z)=(K(z)+J(z))/2$ to give

$$U(z)=C_0/2+(4\pi i)^{-1}\int_S dt\left[1-y(z)(y(t)^{+})^{-1}\right]W(t)^{-1}U(t)^{+}(t-z)^{-1}$$
$$-(4\pi i)^{-1}\int_S dt\left[1-y(z)(y(t)^{-})^{-1}\right]W(t)\ U(t)^{-}(t-z)^{-1} \qquad (4.13)$$

and taking the limits as $z\to S^{+},S^{-}$.

Li [Li91] shows how, if $f(z)$ is suitably analytic, the contours in (4.13) can be distorted away from S in such a way that $W(t)^{-1},W(t)$ are small for large n. The new integral equation involves an operator that is small in a certain B-space, and asymptotic results follow. Li also deals with the case when the underlying Riemann surface has genus 1 so that $\chi_1(z)$ may have a special zero c as in Example 2.2, and with the case when there is a pseudo-branch point as in Example 2.3. The extension to more general functions with branch points should be straightforward.

5. CONJECTURE ON THE ASYMPTOTICS OF MULTIPOINT PADE APPROXIMANTS TO ENTIRE FUNCTIONS

Now we describe a conjecture about the asymptotics of MPA polynomials for certain entire functions. The conjecture is built on the information presented in the earlier sections.

We restrict attention to two classes of functions

1. $F(\lambda)=\exp(\Pi(\lambda))$
2. $F(\lambda)=\exp(n\Pi(\lambda))$

where $\Pi(\lambda)$ is a polynomial with coefficients independent of λ, although we expect the conjecture to apply to a broader class of functions.

For simplicity we shall consider only the diagonal case. We work in the z-plane ($z=\lambda^{-1}$) so that, for $f(z)=F(z^{-1})$, we are looking for polynomials $p(z),q(z)$ of degree n that are determined by

$$r(\mu_j)=0,\quad j=1,2n+1 \qquad (5.1)$$

where

$$r(z)=f(z)p(z)-q(z), \qquad (5.2)$$

and M is a prescribed set of interpolation points $\{\mu_j, j = 1, 2n+1\}$ depending on n. We assume that no point in M is in a fixed neighborhood of $z = 0$. Here we shall not be concerned with the question of the uniqueness of the polynomials $p(z), q(z)$. See Stahl [St89] and references therein for a discussion of this point.

We set out the conjecture as a set of properties analogous to those for PA in Appendix A. The logical development requires that the properties be presented in a different order.

Property B1

Apart from Dumas zeros and zeros close to the interpolating points of set M, the zeros of $r(z), p(z), q(z)$ approach sets of analytic arcs S_1, S_2, S_3 respectively as $n \to \infty$, with analytic (except at $z = 0$ in the case of $r(z)$) real, limit line densities $\rho_j(z),\ j = 1,2,3$, where $\rho_2(z), \rho_3(z)$ are positive except at the arc ends.

For Class 1, the sets of arcs probably approach zero as $n \to \infty$. For Class 2 they approach limit sets.

For at least some cases the arcs are arranged as a wheel with spokes. The rim consists of alternating arcs of sets S_2, S_3, and arcs of S_1 are spokes which join the origin to the points on the rim where two arcs meet (see Fig. 3).

Property B2

The points on the rim where one arc of each type meet are pseudo-branch points, and the angles between the arcs are $2\pi/3$.

Property B5

The first order approximations to $r(z), p(z), q(z)$ are functions $\chi_j(z)$, analytic in the z-plane cut along S_j, $j = 1,2,3$, respectively. With

$$\eta_1(z) = \chi_1(z); \quad \eta_2(z) = -f(z)\chi_2(z); \quad \eta_3(z) = \chi_3(z) \tag{5.3}$$

functions $\chi_j(z),\ j = 1,2,3$, may be found by solving (Fig. 3 gives the meaning of Λ_j)

$$\eta_k(z) + \eta_l(z) = 0, \quad z \in \Lambda_j, \quad j = 1,2,3, \tag{5.4}$$

where j, k, l are a permutation of $1,2,3$.

The function $\eta_1(z)$ has zeros when $z \in \mathrm{M}$. This implies from (5.4) that $\eta_2(z)$ has zeros for $z \in \mathrm{M} \cap \Lambda_3$, and similarly for $\eta_3(z)$.

We also require

$$\chi_1(z), \chi_2(z), \chi_3(z) = O(z^n), \quad z \to \infty, \tag{5.5}$$

and at a pseudo-branch point b that

$$\chi_j(z) \approx C_j (z-b)^{-1/4}, z \to b, \quad j = 1,2,3 \tag{5.6}$$

for some non-zero constants C_j.

Now suppose that there are $2(g+1)$ pseudo-branch points $\{b_j\}$ (of course in this case there are no real branch points) and define

$$y(z) = \left[\prod_{j=1}^{2(g+1)} (z-b_j) \right]^{1/2} \tag{5.7}$$

with $y(z)$ single valued outside S_2 and $y(z) = O(z^{g+1}), \quad z \to \infty$. Define the piecewise analytic function $\Omega(z)$ as

$$\Omega(z) = \chi_2(z)\chi_3(z), \quad z \in \Lambda_2 \cup \Lambda_3; \quad \Omega(z) = \chi_1(z)\chi_2(z), \quad z \in \Lambda_1. \tag{5.8}$$

Obviously $\Omega(z)$ is analytic for $z \in \Lambda_2 \cup \Lambda_3$. On S_2 we have from B5

$$\eta_2(z)^+ = -\eta_1(z)^+ = -\eta_1(z)^-; \eta_3(z)^+ = \eta_3(z)^- = -\eta_2(z)^-, \quad z \in S_2 \tag{5.9}$$

so that

$$\Omega(z)^+ / \Omega(z)^- = f(z)\chi_2(z)^+ \chi_3(z)^+ / \chi_1(z)^- f(z)\chi_2(z)^- = 1, \quad z \in S_2. \tag{5.10}$$

Similarly

$$\Omega(z)^- / \Omega(z)^+ = -1, \quad z \in S_3. \tag{5.11}$$

Note that the side of S_2, S_3 in Λ_1 is denoted by $-,+$ respectively.

Now define $\Phi(z) = y(z)\Omega(z)$ so that (5.9), (5.10) give

$$\Phi(z)^+ / \Phi(z)^- = 1, \quad z \in S_2 \cup S_3, \tag{5.12}$$

which, since $\Phi(z)$ is bounded, with (5.5) shows that $\Phi(z)$ is a polynomial of degree $2n+g+1$. We know that $\Phi(z)$ is zero at each point of M, so that

$$\Phi(z) = Cd(z)\theta(z) \tag{5.13}$$

for some constant C, $d(z)$ defined by (1.6), and $\theta(z)$ given by

$$\theta(z)=\prod_{j=1}^{g}(z-c_j)\,, \qquad (5.14)$$

with the Dumas zeros $\{c_j\}$ still to be determined.

For $z\in S_2$ we note that from (5.8), (5.9) and (5.13)

$$Cd(z)\theta(z)=\Phi(z)=y(z)^-\chi_1(z)^-\chi_2(z)^- = y(z)^+ f(z)\chi_2(z)^+\chi_2(z)^-\,,\quad z\in S_2 \qquad (5.15)$$

so that, if we choose normalization to make $C=1$, we have the equivalent of Property A6

Property B6

$$\chi_2(z)^+\chi_2(z)^- = d(z)\theta(z)\big/ f(z)y(z)^+\,,\quad z\in S_2\ . \qquad (5.16)$$

Having solved (5.16) for $\chi_2(z)$, the functions $\chi_1(z),\chi_3(z)$ follow immediately from (5.4) and (5.8). Thus for example,

$$\chi_3(z)=d(z)\theta(z)\big/y(z)\chi_2(z)\,,\quad z\in\Lambda_2\cup\Lambda_3\,. \qquad (5.17)$$

In this way we can also obtain two more equations analogous to (5.16), namely

$$\begin{aligned}\chi_3(z)^+\chi_3(z)^- &= f(z)\,d(z)\theta(z)\big/y(z)\ ,\quad z\in S_3\\ \chi_1(z)^+\chi_1(z)^- &= f(z)\,d(z)\theta(z)\big/y(z)\ ,\quad z\in S_1\ .\end{aligned} \qquad (5.18)$$

We can formally obtain the equation for the zero order approximation to $\chi_2(z)$ by writing

$$\chi_2(z)=\exp\left[n\phi_2(z)+O(1)\right], \qquad (5.19)$$

substituting in (5.16) and taking logarithms to give

$$n(\phi_2(z)^+ + \phi_2(z)^-) = \log(d(z)) - \log(f(z)) + O(1),\quad z\in S_2\,. \qquad (5.20)$$

Differentiating with respect to z, dividing by n, and disregarding terms $O(1)$ leads to (3.22), i.e. the equivalent of Property A3

Property B3

$$\psi_2(z)^+ + \psi_2(z)^- = n^{-1}\left(\log f(z)\right)' - n^{-1}\sum_{j=1}^{2n+1}(z-\mu_j)^{-1}, \quad z \in S_2, \tag{5.21}$$

with $\psi_2(z) = -d\phi_2/dz$, where $\psi_2(z)$ has a representation

$$\psi_2(z) = \int_{S_2} |dt|\rho_2(t)(t-z)^{-1}. \tag{5.22}$$

We can define $\psi_1(z), \phi_1(z), \psi_3(z), \phi_3(z)$ in the same way as above.

We maintain conditions (A.4), (A.5) which are now:

Near a pseudo-branch point b, $\psi_2(z)$ has an expansion $\psi_2(z) = \sum_{k=0}^{\infty} B_k (z-b)^{k/2}$ (5.23)

which in particular means that

$$\Delta\psi_2(b) = 0 \quad \text{at each pseudo-branch point } b. \tag{5.24}$$

where $\Delta\psi(z) = \psi(z)^+ - \psi(z)^-$.

$$\mathrm{Re}\int_b^{b'} dt\Delta\psi_2(t) = 0 \text{ for any two pseudo-branch points } b, b'. \tag{5.25}$$

We conjecture that, given a solution of (5.21), equations (5.24), (5.25) and the positivity of $\rho_2(z), z \in S_2$ are sufficient to determine g, the pseudo-branch points, and the arc locations and line densities, if a solution exists.

It is of interest to show that the above procedure applied to $\psi_3(z)$ will give rise to the same values for the pseudo-branch points. From formulas such as (5.9) it is possible to show that there is a double-valued function, analytic on a closed curve surrounding one branch point, that on one circuit takes on the values

$$\begin{aligned} &\chi_1(z)^+/\chi_1(z)^-, \quad z \in S_1; \quad -\chi_2(z)^-/\chi_2(z)^+, \quad z \in S_2; \\ &\chi_3(z)^+/\chi_3(z)^-, \quad z \in S_3; \quad \chi_1(z)^-/\chi_1(z)^+, \quad z \in S_1. \end{aligned} \tag{5.26}$$

This means that the functions $\Delta\psi_j(z), \quad j = 1,2,3$, are analytic continuations of each other up to a sign, so that (5.24), (5.25) are independent of the subscript.

6. TECHNICAL DETAILS RELATING TO THE CONJECTURE

Starting from the simple equations (5.4) we have shown that the conjecture leads to two boundary value problems. First we must solve (5.21) to describe the zero order behavior and then (5.15) to obtain the first order results. We comment on these two problems.

Zero Order Boundary Value Problem

Assuming a knowledge of the pseudo-branch points $\{b_j\}$, we can easily solve (5.21) to give an expression for $\psi_2(z)$, just as we solved (3.17) to give (3.24). There are several alternative ways of proceeding, but the method that gave (3.24) provides a solution of (5.21) (when all pseudo-branch points are finite) in the form

$$\psi_2(z) = y(z)^{-1}\left[-z^g + \sum_{k=0}^{g-1} C_k z^k + (2\pi i)^{-1}\int_{S_2} dt y(t)^+ \sigma(t)(t-z)^{-1}\right] \tag{6.1}$$

where

$$\sigma(z) = n^{-1}\left(\log f(z)\right)' - n^{-1}\sum_{j=1}^{2n+1}(z-\mu_j)^{-1}, \quad z \in S_2, \tag{6.2}$$

and $y(z)$ is given by (5.7). From (6.1) may be derived an explicit expression for $\Delta\psi_2(z)$ to be inserted into the $2(g+1)$ complex equations (5.24) and the $2g$ real equations (5.25) for the complex quantities $\{b_j\}$ and the C_k of (6.1). A solution is acceptable only if the density $\rho(z)$ defined in (5.22) is positive on the arcs of S_2 (except at the ends, where it is zero). The arcs of S_2 are located by the procedure described at the end of Section 3.

If the conjecture is correct, only for at most one value of g will there be an acceptable solution of (5.24) and (5.25), and that solution will be unique, at least for large n . Except for simple cases the equations will have to be solved numerically. Often there is a parameter in $f(z)$, the function being approximated, and the solution will depend smoothly on the parameter in certain regions of parameter space. For a particular value of the parameter there may be symmetries in the problem which simplify the solution, in which case it is sensible to find the solution there and then travel through the parameter space using a non-linear equation solver or a differential equation.

Such a procedure can fail at a value of the parameter where the required value of g changes. It can also fail because there is no solution of the equations for any value of g. The NLS problem shows that, for functions of Class 2, it may be necessary to change the function $F(\lambda)$ being approximated in order for the conjecture to work. Thus, the MPA polynomials are unchanged if we multiply $F(\lambda)$ by a function $H(\lambda)$, possibly piecewise analytic, such that

$$H(\lambda_j) = 1, \quad j = 1, 2n+1. \tag{6.3}$$

Only for one particular choice of $H(\lambda)$ will the remainder function $r(z)$ be relatively small in Λ_1. How to determine $H(\lambda)$ in general is an interesting open problem.

First Order Boundary Value Problem

After finding the pseudo-branch points $\{b_j\}$ it remains to solve (5.16) for $\chi_2(z)$, the first order approximation to $p(z)$. This done, approximations to $q(z), r(z)$ follow immediately. Included in the solution of (5.16) is the determination of the Dumas zeros $\{c_j\}$.

The techniques needed for the solution of (5.16) have been previously developed to solve equations such as (2.24) that arise in the case of PAs to functions with branch points. Lemma 5.2 of Nuttall and Singh [Nu77a] gives the solution to Equation (5.2) of that article which is very similar to (5.16) in its essentials. Results of much the same form are found in Widom [Wi69] who treats the problems of true orthogonal polynomials (with complex conjugation) and Chebychev polynomials on a set of arcs, where the location of the arcs is predetermined.

Equation (5.16) can be turned into an inhomogeneous Hilbert problem on a set of arcs [Mu53] by taking logarithms. However the function $\chi_2(z)$ may have zeros at the zeros of $d(z), \vartheta(z)$, and it will have a pole at infinity, which should all be removed from $\chi_2(z)$ before taking logarithms to avoid the introduction of singularities outside S_2. Thus, we suppose that $\chi_2(z)$ has finite zeros at $z = \mu_j, \quad j = 1, m_d$ and at $z = c_j, \quad j = 1, m_c$, and for ease of explanation we assume that no zeros of $d(z), \vartheta(z)$ lie on S_2. We define $\xi(z)$ by

$$\chi_2(z) = \xi(z)(z-b_1)^{n-m_d-m_c}\left[\prod_{j=1}^{m_d}(z-\mu_j)\right]\left[\prod_{j=1}^{m_c}(z-c_j)\right] \qquad (6.4)$$

and insert in (5.16) before taking logarithms, with the result that

$$\xi(z)^+\xi(z)^- = \omega(z)\vartheta_2(z)/\vartheta_1(z), \quad z \in S_2. \qquad (6.5)$$

Here

$$\vartheta_1(z) = \left[\prod_{j=1}^{m_c}(z-c_j)\right]; \qquad \vartheta_2(z) = \left[\prod_{j=m_c+1}^{g}(z-c_j)\right] \qquad (6.6)$$

and

$$\omega(z) = d_2(z)(z-b_1)^{-2(n-m_d-m_c)}\big/ d_1(z) f(z) y(z)^+, \quad z \in S_2 \qquad (6.7)$$

with

$$d_1(z) = \left[\prod_{j=1}^{m_d}(z-\mu_j)\right]; \qquad d_2(z) = \left[\prod_{j=m_d+1}^{2n+1}(z-\mu_j)\right] \quad . \qquad (6.8)$$

In order to solve (6.5) as in [Nu77a] we need to define arcs $L_j, \quad j=1, 2g$, joining b_1 to b_j, that do not intersect S_2 except at their ends. Also define differentials of the first kind on the Riemann surface

$$y^2 = X(z) \equiv \prod_{j=1}^{2(g+1)} (z-b_j) \tag{6.9}$$

as

$$dw_k = z^{k-1} y(z)^{-1} dz, \quad k = 1, g, \tag{6.10}$$

and the periods

$$\Omega_{kj} = 2\int_{L_j} dw_k \ . \tag{6.11}$$

The solution of (6.5) may then be written

$$\xi(z) = \exp[y(z)\zeta(z)] \tag{6.12}$$

where

$$\begin{aligned}\zeta(z) = (2\pi i)^{-1} \int_{S_2} dt (y(t)^+)^{-1} (t-z)^{-1} \left\{ \log \omega(t) + \sum_{j=m_c+1}^{g} \log(t-c_j) - \sum_{j=1}^{m_c} \log(t-c_j) \right\} \\ + \sum_{l=1}^{2g} \delta_l \int_{L_l} dt (y(t)^+)^{-1} (t-z)^{-1}\end{aligned} \tag{6.13}$$

The integers $\{\delta_l\}$ and the Dumas zeros $\{c_j\}$ are chosen so that $\zeta(z) = O(z^{-g-1}), \quad z \to \infty$. This requires that

$$\begin{aligned}(2\pi i)^{-1} \int_{S_2} dt (y(t)^+)^{-1} t^k \left\{ \log \omega(t) + \sum_{j=m_c+1}^{g} \log(t-c_j) - \sum_{j=1}^{m_c} \log(t-c_j) \right\} \\ + \sum_{l=1}^{2g} \delta_l \int_{L_l} dt (y(t)^+)^{-1} t^k, \qquad k = 0, \quad g-1.\end{aligned} \tag{6.14}$$

It is explained in [Nu77a] how (6.14) is equivalent to the statement that the divisor $\{c_1 c_2 \cdots c_g\}$ on the Riemann surface is the solution of a certain Jacobi inversion problem. There is always a solution which is unique when $g = 1$. If $g > 1$ the solution may not be unique, and it is shown in [Nu77a] how, in the case of certain diagonal Pade approximants, the non-uniqueness relates to non-uniqueness in the PA polynomials. It is likely that a similar situation arises in the MPA case.

7. PROOF OF THE CONJECTURE IN A PARTICULAR CASE

We now outline a proof of the conjecture of Sec. 5 for a particular case. We expect that it will be possible to generalise the method to other cases. The approach relies heavily on the ideas in the Li thesis [Li91] and many of the details needed to complete the proof should be similar to material in the thesis.

For this example we choose $F(\lambda) = \exp(n\alpha\lambda)$, so that $f(z) = \exp(n\alpha z^{-1})$, and consider diagonal approximants ($\deg(p) = \deg(q) = n$) determined on the set of interpolation points is given by

$$\mathrm{M} = \{ z = n/j,\ j = 0, \pm 1, \ldots, \pm n \}. \tag{7.1}$$

We suppose that α is real, positive and small enough so that it is possible to find pseudo-branch points b_1, b_2, arcs S_1, S_2, S_3, and functions $\chi_1(z), \chi_2(z), \chi_3(z)$ that satisfy the properties of Sec. 5 with $g = 0$ for sufficiently high n, and such that $\mathrm{M} \subset \Lambda_1$. Numerical calculations suggest that such values of α exist. We presume that the numerical errors in the calculation can be analyzed in order to produce a proof of the existence of the above objects for appropriate values of α. The arrangement of the arcs and M is sketched in Fig. 4.

Derivation of the Integral Equation

Define the functions $U_j(z),\ j = 1,2,3$, by

$$U_1(z) = r(z)/\eta_1(z) = r(z)/\chi_1(z)$$

$$U_2(z) = -f(z)p(z)/\eta_2(z) = p(z)/\chi_2(z) \tag{7.2}$$

$$U_3(z) = q(z)/\eta_3(z) = q(z)/\chi_3(z)$$

Note that, due to the assumption about M, the functions $\chi_2(z), \chi_3(z)$ have no zeros, so that $U_j(z)$ is analytic and single-valued outside S_j, $j = 1,2,3$. From the definition of $r(z)$ in (5.2) we have

$$\sum_{j=1}^{3} \eta_j(z) U_j(z) = 0 \tag{7.3}$$

which forms the basis for the subsequent development.

Now for $z \in \Lambda_k$, $k = 1,2,3$, divide (7.3) by $\eta_k(z)$, and take the limit as z approaches the $-$side of S_k, to obtain

$$\begin{aligned} U_1^-(z) - U_3^+(z) &= U_2(z) W_2^-(z), \quad z \in S_1 \\ U_2^-(z) - U_1^+(z) &= U_3(z) W_3^-(z), \quad z \in S_2 \\ U_3^-(z) - U_2^+(z) &= U_1(z) W_1^-(z), \quad z \in S_3, \end{aligned} \tag{7.4}$$

where we have used (5.4), and defined

$$W_j(z) = \eta_j(z) \big/ \eta_{j+1}(z), \quad j = 1,2,3 \tag{7.5}$$

with $\eta_4 = \eta_1$. In (7.4) the $+$ superscripts are superfluous since $U_3(z)$ is analytic across S_1, etc., but they are used in the later discussion.

Next we define three piecewise analytic functions $K(z), J(z), M(z)$ as

$$\begin{aligned} K(z) &= U_3(z) + U_1(z), \quad z \in \Lambda_1 \\ K(z) &= U_1(z) + U_2(z), \quad z \in \Lambda_2 \\ K(z) &= U_2(z) + U_3(z), \quad z \in \Lambda_3 \end{aligned} \tag{7.6}$$

$$\begin{aligned} J(z) &= U_3(z) - U_1(z), \quad z \in \Lambda_1 \\ J(z) &= U_1(z) - U_2(z), \quad z \in \Lambda_2 \\ J(z) &= U_2(z) - U_3(z), \quad z \in \Lambda_3 \end{aligned} \tag{7.7}$$

$$M(z) = y_j^{-1}(z) J(z), \quad z \in \Lambda_j, \quad j = 1,2,3, \tag{7.8}$$

where

$$y_1(z) = y_3(z) = -y_2(z) = y(z) \tag{7.9}$$

with $y(z)$ given by (5.7).

It follows that

$$\begin{aligned} K(z)^+ - K(z)^- &= -U_{j+1}(z) W_{j+1}(z)^-, \\ & \qquad\qquad z \in S_j, \quad j = 1,2,3, \\ M(z)^+ - M(z)^- &= -U_{j+1}(z) W_{j+1}(z)^- \big/ y_{j+1}(z)^- \end{aligned} \tag{7.10}$$

which corresponds to (4.11). As in Sec. 4 the Plemelj formula then leads to

$$\begin{aligned} K(z) &= 2 - (2\pi i)^{-1} \sum_{j=1}^{3} \int_{S_j} dt U_{j+1}(t) W_{j+1}(t)^- (t-z)^{-1} \\ J(z) &= -(2\pi i)^{-1} y_k(z) \sum_{j=1}^{3} \int_{S_j} dt (y_{j+1}(t)^-)^{-1} U_{j+1}(t) W_{j+1}(t)^- (t-z)^{-1}, \quad z \in \Lambda_k . \end{aligned} \tag{7.11}$$

To obtain the constant in the expression for $K(z)$ we have used the conjecture's implication that $U_j(z) \to 1, \quad z \to \infty$, effectively a choice of the overall normalisation of $p(z), q(z), r(z)$.

Subtracting one equation from the other gives

$$U_k(z) = 1-(4\pi i)^{-1}\sum_{j=1}^{3}\int_{S_j} dt(1-y_k(z)/y_{j+1}(t)^-)U_{j+1}(t)W_{j+1}(t)^-(t-z)^{-1}\,, \qquad (7.12)$$

$$z\in\Lambda_k\,,\quad k=1,2,3\,,$$

an integral equation for $U_k(z),\quad k=1,2,3$, analogous to (4.13).

The $-$side of S_j lies in Λ_{j+1}, so that in (7.12) each contour S_j may be distorted into a contour $\Xi_{j+1}\in\Lambda_{j+1}$ joining the two branch points, as shown in Fig. 4, without changing the value of the integrals. Note that $(1-y_k(z)/y_k(t))(t-z)^{-1}$ is analytic in t for $t,z\in\Lambda_k$. The result is that we can rewrite (7.12) as

$$U_k(z) = 1-(4\pi i)^{-1}\sum_{j=1}^{3}\int_{\Xi_j} dt(1-y_k(z)/y_j(t))U_j(t)W_j(t)(t-z)^{-1}\,, \qquad (7.13)$$

$$z\in\Lambda_k\,,\quad k=1,2,3\,.$$

Note that, in the vicinty of $z=0$, $U_2(z)$ is a multiple of $f(z)$ and an analytic function of z. Even though $f(z)$ is not continuous in $S_1\cup\Lambda_2$ at $z=0$, it is bounded, and the distortion of the contour that transforms (7.12) into (7.13) is valid.

If we are able to solve (7.13) to find a solution for $U_j(z),\quad z\in\Xi_j\,,\quad j=1,2,3$, then we can obtain the solution at other values from (7.13) and then (7.11), or by analytic continuation of (7.13).

<u>The Form of the Functions</u> W_j

In order to analyse the integral equation (7.13) we need to use some facts about $W_j(z), z\in\Lambda_j$. The explicit expressions for $\chi_j(z)$ derived in Sec.6 can be analysed to provide the necessary information, but there is a more elegant approach, which we describe now. Equivalent to (5.26) is the statement that there is a double-valued function, say $w(z)$, analytic on a closed curve surrounding one branch point, that on one circuit takes on the values

$$W_1(z),\quad z\in\Lambda_1;\quad -W_2(z)^{-1},\quad z\in\Lambda_2;\quad W_3(z),\quad z\in\Lambda_3;\quad -W_1(z)^{-1},\quad z\in\Lambda_1. \qquad (7.14)$$

On the arcs S_1,S_2,S_3 the properties described in Sec. 5 ensure that $|w(z)|\to 1,\quad n\to\infty$.

Define the two-sheeted Riemann surface **R** as

$$\mathbf{R}\!:\ y^2=(z-b_1)(z-b_2)\,, \qquad (7.15)$$

where the two sheets join at S_1, and $y(z)$ is meromorphic on **R** and such that $y(z)\sim z,\quad z\to\infty^{(1)}$. It follows from (7.14) and Property B5 that $w(z)$ is a single-valued function $z\in\mathbf{R}$, analytic except for simple poles at the points in M on Sheet 2 (i.e. $\mathrm{M}^{(2)}$), and essential singularities at $z = 0^{(1)}, 0^{(2)}$. Near the essential singularities, $w(z)$ has the behavior

$$w(z) = f(z) Anal(z), \quad z = 0^{(1)}; \quad w(z) = f(z)^{-1} Anal(z), \quad z = 0^{(2)}, \tag{7.16}$$

where we take $0^{(1)}$ to be on the $+$ side of S_1 on the Sheet 1. For $z \in \mathrm{M}^{(1)}$, $w(z)$ has simple zeros.

The above information is almost sufficient to determine $w(z)$ as follows. Define $f_1(z), z \in \mathbf{R}$, as

$$f_1(z) = \exp\left[n\alpha z^{-1}\, y(z) / y(0^{(1)})\right], \; z \in \mathbf{R}, \tag{7.17}$$

so that the function $w(z)/f_1(z)$ is meromorphic on $\mathbf{R}$ with zeros, poles at $\mathrm{M}^{(1)}, \mathrm{M}^{(2)}$ respectively, and thus the function is unique apart from a constant factor. We can write $w(z)/f_1(z)$ explicitly in terms of u given by

$$z = \frac{b_1 + b_2}{2} + \frac{(b_1 - b_2)}{4}(u + u^{-1}), \tag{7.18}$$

so that there are the correspondences

$$z = b_1 : u = 1; \quad z = b_2 : u = -1; \quad z \in Sheet\, 1 : |u| > 1; \quad z \in Sheet\, 2 : |u| < 1. \tag{7.19}$$

The explicit form of $w(z)$ is

$$w(z) = C f_1(z) \prod_{j=1}^{2n+1} \left(\frac{u - u_j}{u - u_j^{-1}} \right), \quad z \in \mathbf{R} \tag{7.20}$$

for some constant C, where

$$\mu_j = \frac{b_1 + b_2}{2} + \frac{(b_1 - b_2)}{4}(u_j + u_j^{-1}), \quad |\mu_j| > 1, \quad j = 1, \cdots, 2n+1. \tag{7.21}$$

The formula (7.20) is correct whether or not the condition $\mathrm{M} \subset \Lambda_1$ holds.

To find C we use (5.3), (5.9) to show that

$$W_3(z)^- = \frac{\eta_3(z)^-}{\eta_1(z)^-} = \frac{\chi_2(z)^+}{\chi_2(z)^-}, \quad z \in S_2. \tag{7.22}$$

Using (5.6) and taking the limit as $z \to b$, where b is a branch point, leads to

$$W_3(b) = \pm i, \tag{7.23}$$

the sign depending on whether or not the arcs leave $(+)$ or enter $(-)$ the branch point. It may be checked that the two conditions of (7.23) are consistent with (7.20). It follows for the situation described in Fig. 4 that $C = -i$.

For the above discussion to make sense it is necessary that three arcs of the locus $|w(z)| = 1$ meet at each branch point. On account of (7.14) the function $\log w(z)$ in the vicinity of a branch point b may be written as an imaginary constant plus an expansion in positive odd powers of $(z-b)^{1/2}$. Three arcs of $|w(z)| = 1$ will meet at b if the coefficient of $(z-b)^{1/2}$ in the expansion of $\log w(z)$ vanishes. In this case we will have

$$\mathrm{Re}\left[\log w(z)\right] = Ge^{i\gamma}(z-b)^{3/2} + O(z-b)^{5/2}, \quad z \to b, \tag{7.24}$$

with G, γ real positive, so that, near $z = b$, the locus $|w(z)| = 1$ will be close to the rays

$$\mathrm{Arg}(z-b) = -2\gamma/3 + \pi/3,\ -2\gamma/3 + \pi, -2\gamma/3 + 5\pi/3\ . \tag{7.25}$$

It may be shown that the condition for the vanishing of the coefficient of $(z-b)^{1/2}$ in the expansion of $\log w(z)$ at each branch point is equivalent to the equations (5.24) which we previously used to determine the location of the branch points, at least for large n.

For large n the quantity G in (7.24) will be approximately of the form $G = G_0 n$, where G_0 is real, positive and independent of n. Thus the approximate form of $w(z)$ near to a branch point b is

$$w(z) \approx \pm i \exp(G_0 n (z-b)^{3/2}), \tag{7.26}$$

where G_0 may depend on the branch point.

<u>Analysis of the Integral Equation</u>

The functional analysis of the integral equation (7.13) now proceeds almost exactly as in Li [Li91] Chap. 8. We suppose that the contours $\{\Xi_j\}$ used in (7.13) are analytic arcs which approach each branch point along the bisectors of the angles (each equal to $2\pi/3$) between the arcs $\{S_j\}$ which meet at that branch point.

It follows from the discussion of $\{W_j\}$ that $n^{-1}\,\mathrm{Re}(\log W_j(z)) < 0$ uniformly with n on any closed interval of Ξ_j not containing branch points, so that the behavior of the kernel of the integral equation (7.13) is dominated by parts of Ξ_j near branch points. Chapter 8 of [Li91] showed how to treat a problem with one branch point where the behavior of the kernel near the branch point was effectively the same as in the present case. The extension of the Li approach to two branch points should be trivial.

APPENDIX A. PROPERTIES OF RESULTS ON DIAGONAL PADE APPROXIMANTS TO FUNCTIONS WITH BRANCH POINTS

Here we have collected a number of properties of the results on diagonal PAs which are known and/or conjectured to be of more general applicability. The first four properties relate to zero order asymptotics, and the rest to first order.

As a reminder,

- we assume that $f(z)$ is analytic in the extended complex plane except for a finite number of finite branch points, and is subject to other restrictions,
- $q(z), p(z)$ are polynomials of degree n,
- r(z) is defined by $r(z) = f(z)p(z) - q(z)$, and
- $r(z) = O(z^{-n-1}),\ z \to \infty$

Property A1

All but at most a fixed number (see Property 8) of the zeros of $q(z), p(z)$ approach a set of analytic arcs S as $n \to \infty$, with a smooth real positive limit line density $\rho(z)$. This includes the statement that the polynomial measures (see (4.1)) $\mu(p), \mu(q)$ have the same weak limit.

Property A2

Arcs can end at branch points of the function being approximated (although not necessarily at all branch points), with one arc per branch point. Arcs can also end at points which are not branch points of the function being approximated (pseudo-branch points), with three arcs per pseudo-branch point. These arcs meet at angle $2\pi / 3$.

Property A3

The location of the arcs S, including the location of pseudo-branch points, the limit line density, and the zero order asymptotics of $q(z), p(z)$ can all be determined from the function $\psi(z)$ with a representation

$$\psi(z) = \int_S |dt| \rho(t)(t-z)^{-1} \qquad \text{(A.1)}$$

that satisfies

$$\psi(z)^+ + \psi(z)^- = 0, \quad z \in S. \qquad \text{(A.2)}$$

Three further conditions usually needed to find $\psi(z)$ are

Near a branch point b of $f(z)$ $\psi(z)$ has an expansion $\psi(z) = \sum_{k=-1}^{\infty} A_k (z-b)^{k/2}$ (A.3)

Near a pseudo-branch point a $\psi(z)$ has an expansion $\psi(z)=\sum_{k=0}^{\infty} B_k (z-a)^{k/2}$ (A.4)

$$\mathrm{Re}\int_b^{b'} dz(\psi(z)^+ - \psi(z)^-) = 0 \text{ for any two arc ends } b, b'. \quad \text{(A.5)}$$

<u>Property A4</u>

Away from S the zero order behavior of $p(z)$ (and similarly $q(z)$) is

$$\log(|p(z)|) = n\,\mathrm{Re}\,\phi(z) + O(1),\ n\to\infty \quad \text{(A.6)}$$

where

$$\frac{d\phi(z)}{dz} = -\psi(z). \quad \text{(A.7)}$$

<u>Property A5</u>

The first order approximations to $r(z), p(z), q(z)$ are functions $\chi_1(z), \chi_2(z), \chi_3(z)$, analytic in the z-plane cut along S, with appropriate behavior at the arc ends of S, that may be found by solving the equations

$$\chi_3(z) = f(z\ )\chi_2(z),\quad z\notin S, \quad \text{(A.8)}$$

$$f(z)^{\mp}\chi_2(z)^{\pm} - \chi_3(z)^{\pm} = \chi_1(z)^{\mp},\quad z\in S, \quad \text{(A.9)}$$

with $\chi_1(z) = O(z^{-n-1});\quad \chi_2(z), \chi_3(z) = O(z^n),\quad z\to\infty$.

<u>Property A6</u>

The first order approximation $\chi_2(z)$ to $p(z)$ satisfies

$$\chi_2(z)^+\chi_2(z)^- = \left(y_2(z)^+(f(z)^+ - f(z)^-)\right)^{-1}\prod_{j=1}^{g}(z-c_j),\quad z\in S, \quad \text{(A.10)}$$

where g is the genus of the two-sheeted Riemann surface $y_2(z)^2 = \prod_{j=1}^{2(g+1)}(z-b_j)$, the product running over real and pseudo-branch points at which arcs end.

<u>Property A7</u>

For large n the approximation $\chi_1(z)$ to $r(z)$ is much smaller than $\chi_2(z), \chi_3(z)$ for $z\notin N(S\cup\{c_j\})$, and we have

$$f(z) - \chi_3(z) / \chi_2(z) = small \quad . \tag{A.11}$$

Property A8

The points $\{c_j\}$ are determined by the requirement that (A.10) has a satisfactory solution, and are obtained by solving a Jacobi inversion problem for integrals of the first kind on the Riemann surface. For large n, those points that lie on the second sheet of the Riemann surface are close to zeros of $q(z), p(z)$,and those points on the first sheet are close to zeros of $r(z)$.

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