ANALYSIS OF RIEMANN ZETA FUNCTION ZEROS USING POCHHAMMER POLYNOMIAL EXPANSIONS

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ABSTRACT. The Riemann Zeta function $\zeta(s)$ can be expressed in terms of the entire function $\xi(s)$ which has an integral representation characteristic of a general class of entire functions symmetric around $s = ½$. Functions in this class can be expanded in terms of a uniformly convergent series of symmetrized Pochhammer polynomials depending on two real continuous affine scaling parameters α and β, which simply reflect different possibilities of grouping terms in an infinite series. One thus obtains polynomial approximations $\Xi_n(t)$, depending on α and β, of degree n in t^2 to the Xi function $\Xi(t) = \xi(½ + it)$ which are valuable for studying its zeros, supposed to be located on the line with t real according to the Riemann Hypothesis.

Although the symmetrized Pochhammer polynomials have real roots only in t and form a sequence with interlacing roots, a sum of n such polynomials may still develop complex roots as n increases, thus making it impossible to make any immediate inference about the reality of the zeros of the limit function $\Xi(t)$. Surprisingly, it turns out that if one chooses $\alpha = \beta$ and tries to let the scaling parameter β grow with n, then one notes that the polynomial $\Xi_n(t,\beta)$ appears to have real roots only in the asymptotic scaling limit $\beta\to\infty$. One may therefore infer the existence of increasing beta-sequences $\beta_n\to\infty$ such that $\Xi_n(t,\beta_n)$ has real roots only for all n, and it is argued that $\beta_n \sim B \log(n)$ is such a sequence. Moreover it can be shown that the approximant $\Xi_n(t, \beta_n)$ converges to $\Xi(t)$ when $n\to\infty$ for B smaller than or equal to a certain critical value B_c at which the convergence rate is $1/\log(n)$. Invoking the Hurwitz theorem of complex analysis, this amounts to confirming the validity of the Riemann Hypothesis.

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I. Introduction

Recently some new insights into possible ways of proving the Riemann Hypothesis have been acquired by studying the properties of the Riemann Zeta function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \text{ , Re(s)>1}$$

in terms of certain polynomial expansions [see e.g. refs. 1-7]. A particularly promising approach uses the Pochhammer polynomials $P_k(s)$ of degree k (related to descending factorials), as defined by

$$P_k(s) = \prod_{j=1}^{k} (1 - \frac{s}{j})$$

with $P_0(s) = 1$, $P_1(s) = 1 - s$, and $P_2(s) = 1 - 3s/2 + s^2/2$, etc. The Pochhammer polynomials have a simple generating function

$$(1-\varepsilon)^s = \sum_{k=0}^{\infty} P_k(s+1)\varepsilon^k$$

with the series being absolutely convergent for $|\varepsilon| < 1$. The usefulness of Pochhammer polynomial expansions is in fact apparent for the more general case of Dirichlet series

$$f(s) = \sum_{n=1}^{\infty} \frac{f_n}{n^s} \text{ , Re(s)>1}$$

where, for example, $f_n = 1$ corresponds to the case of $\zeta(s)$, $f_n = (-1)^n$ corresponds to the case of $(1-2^{1-s})\zeta(s)$, and $f_n = \mu(n)$ (the Möbius function) to the case of the inverse $1/\zeta(s)$. One simply uses the "trick" of introducing two, a priori real, dummy parameters α and β by writing

$$\frac{1}{n^s} = \frac{1}{n^\alpha}(1-(1-\frac{1}{n^\beta}))^{\frac{s-\alpha}{\beta}}$$

and applying the generating function of $P_k(s)$ to obtain

$$f(s) = \sum_{k=0}^{\infty} b_k P_k(\frac{s-\alpha}{\beta}+1)$$

with

$$b_k = \sum_{n=1}^{\infty} \frac{f_n}{n^\alpha}(1-\frac{1}{n^\beta})^k = \sum_{j=0}^{k} P_j(k+1) f(\alpha+\beta j)$$

It should be emphasized that one needs $\beta>0$ to assure convergence of the first expansion in powers of $(1-1/n^\beta)$ and furthermore, to estimate the convergence properties of the general expansion of f(s), one needs information about the growth of the coefficients b_k, as well as on the growth of the $P_k(s)$ factor. The latter one is simple because there is for large k a general uniform estimate (which follows directly from the asymptotics of the gamma function, see also ref. 3) valid in any specific compact subset of the complex plane (circle or rectangular subset of the critical strip):

$$\left|P_k(s)\right| < Ck^{-\mathrm{Re}(s)}$$

The above expansion of the function f(s) is noteworthy in the sense that the coefficients b_k are determined by a discrete set of values of the function itself f(α+βj), depending on the actual choice of α and β, and in some sense the expansion may be seen as an interpolation formula. But in terms of actually using the expansion to prove something about ζ(s) in general, like its behavior for ½<Re(s)<1, and the Riemann Hypothesis in particular, one runs into the problem of quantifying the growth properties of the coefficients b_k to determine the compact subsets of the complex plane where there is convergence of the series.

Nevertheless, it turns out that interesting criteria for the validity of the Riemann Hypothesis may be obtained which for the choice of α = β = 2 are related to the criterion of Riesz [ref. 8], and which for the choice of α =1, β = 2 are related to the criterion of Hardy and Littlewood [ref. 9]. Moreover by studying the expansion of the function 1/ ζ(s) one obtains a new kind of coefficient condition for the Riemann Hypothesis [ref. 2]. So far, however, it has not been possible to demonstrate the validity of these conditions in the chosen context because of difficulties in extending the analysis beyond Re(s)>1.

In the following sections a more general analysis based on the above ideas will be presented whereby new insights into the zeros of ζ(s) on the critical line Re(s) = ½ and in the critical strip 0<Re(s)<1 can be obtained. The result of the analysis is an existence argument for a particular polynomial approximation sequence which confirms the validity of the Riemann Hypothesis.

II. Polynomial expansion of the xi function

The application of Pochhammer polynomial expansions is most convenient when instead of the ζ(s) function, one investigates the Riemann xi function given by [see e.g. refs. 10,11]

$$x(s) = \Gamma(s/2+1)(s-1)p^{-s/2}V(s)$$

It is an entire function of s which has the same (non-trivial) zeros as ζ(s) in the critical strip 0<Re(s)<1 and it fulfils the functional equation ξ(s) = ξ(1-s). One has the explicit representation

$$x(s) = \int_1^\infty dx A(x)(x^{-s/2} + x^{(s-1)/2})$$

where A(x) is given in terms of the elliptic theta function

$$y(x) = (J_3(0, \exp(-px)) - 1)/2 = \sum_{n=1}^{\infty} \exp(-n^2 px)$$

by

$$A(x) = 2\frac{d}{dx}(x^{3/2}\psi'(x)) = \sum_{n=1}^{\infty}(2n^4\pi^2 x - 3n^2\pi)x^{1/2}\exp(-n^2\pi x)$$

One notes for this A(x), defined a priori on the interval $[1,\infty]$, that we have $A(x)>0$ and that it is bounded by a power of x times $\exp(-\pi x)$. In fact, our general discussion below of polynomial expansions will apply beyond the special form of A(x) for the Riemann zeta function to the larger class of entire functions with a similar integral representation as for $\xi(s)$, explicitly fulfilling the functional equation, and just requiring A(x) to be a non-negative function for all $x\geq1$ with $A(1)>0$ and decreasing exponentially or faster for large x. For simplicity, we will continue using the notation $\xi(s)$ and refer to it as the Riemann $\xi(s)$ when the specific Riemann representation of A(x) is used.

We recall that the Riemann A(x) fulfills the inversion transformation relation

$$A(x) = x^{-3/2}A(1/x)$$

which means that the combination $A_I(x)$ defined by

$$A_I(x) = x^{3/4}A(x)$$

is invariant under the operation $x \to 1/x$. This property is important for showing that the Riemann $\xi(s)$ has infinitely many zeros on the critical line, but it is not essential for the general discussion of the location of zeros.

Let us introduce the function $\varphi(s)$ by

$$\varphi(s) = \int_1^{\infty} dx A(x) x^{-s/2}$$

so that we have $\xi(s) = \varphi(s) + \varphi(1-s)$, and then expand $\varphi(s)$ in Pochhammer polynomials as done in the previous section:

$$\varphi(s) = \int_1^{\infty} dx A(x) x^{-\alpha/2}(1-(1-x^{-\beta/2}))^{(s-\alpha)/\beta} = \sum_{k=0}^{\infty} b_k P_k\left(\frac{s-\alpha}{\beta}+1\right)$$

where the coefficients $b_k > 0$ are given by

$$b_k = \int_1^{\infty} dx A(x) x^{-\alpha/2}(1-x^{-\beta/2})^k = \sum_{j=0}^{k} P_j(k+1)\varphi(\alpha+\beta j)$$

The expansion is valid for real α and β but we need $\beta > 0$ to assure convergence of the first expansion in terms of powers of $(1-x^{-\beta/2})$. Below we will also assume that α is chosen to be positive. We notice, as observed previously, that $\varphi(s)$ (and $\xi(s)$) can be expressed in terms of its own discrete values $\varphi(\alpha+\beta j)$, but this feature will not be used explicitly for the purpose of the present investigation. The important point of this approach is that we obtain a general expansion

$$x(s)=\sum_{k=0}^{\infty} b_k\,(P_k(\frac{s-a}{b}+1)+P_k(\frac{1-s-a}{b}+1))$$

of the entire function ξ(s) in terms of polynomials in s of degree k depending on arbitrary real parameters α and β, and moreover this expansion is uniformly convergent on any compact subset of the complex plane. To prove this point we just need to note that we have the large k bound for any compact subset of the complex s-plane

$$\left|P_k(\frac{s-a}{b}+1)\right| < C_1 k^{-\mathrm{Re}((s-a)/b+1)}$$

and since $A(x) < C_2\, x^{-m}$ for any m > 0 we have

$$b_k < C_2\int_1^{\infty} dx x^{-m} x^{-a/2}(1-x^{-b/2})^k = \frac{2C_2}{b}\int_0^1 dy y^{2m/b+a/b-1-2/b}(1-y)^k$$

which evaluates to

$$b_k < \frac{2C_2}{b}\frac{\Gamma(2m/b+a/b-2/b)\Gamma(k+1)}{\Gamma(2m/b+a/b-2/b+1+k)}$$

For large k (keeping α and β fixed) we therefore have

$$b_k < \frac{2C_2}{b} k^{-(a/b-2/b+2m/b)}$$

and altogether

$$\left|b_k\,(P_k(\frac{s-a}{b}+1)+P_k(\frac{1-s-a}{b}+1))\right| < \frac{C}{b} k^{|\mathrm{Re}(s-1/2)|/b+3/2b-1-2m/b}$$

Since β is positive and m can be chosen arbitrarily large, one concludes that the series converges uniformly on any compact subset of the complex plane. Clearly the convergence is relatively fast so the polynomial expansion is convenient for the purpose of certain numerical investigations.

In contrast to previous approaches in the literature, we would like here to think of the parameters α and β as having a more dynamical role rather than being subject to some ad hoc fixed choice. In fact, the arbitrary nature of the parameters α and β may be seen simply as a reflection of the multiple ways of regrouping the terms of the infinite Taylor expansion of the function ξ(s). Choosing α and β small produces a faster convergence of the polynomial expansion. However, for the present purpose of studying the zeros of ξ(s), it turns out that interesting features appear when the parameters become large. In particular the limit when α = β is large will be seen a dynamic scaling limit featuring a real root regime of crucial importance for elucidating the Riemann Hypothesis.

Before coming to this point in the next section, it is perhaps useful to examine one particular case of the polynomial expansion which allows for a quite explicit representation of the Riemann ξ -function. If we choose β = 2, then the integrand of the expansion coefficient b_k simplifies sufficiently to evaluate the integral in terms of known functions. At this point we could keep α arbitrary, but for the purpose of simplifying expressions let us also choose $\alpha = 2$. Then we have

$$b_k = \int_1^\infty dx A(x) x^{-1} (1 - x^{-1})^k$$

and since the Riemann A(x) is a sum of powers of x times exponentials, then the integrand can be expressed directly in terms of Whittaker functions $W_{\mu,\nu}(z)$ (see ref. 12):

$$\int_1^\infty dx x^u (1 - x^{-1})^k e^{-\nu x} = k! \nu^{u/2-1} e^{-\nu/2} W_{u/2-k,u/2-1/2}(\nu)$$

The explicit series expansion (with $\alpha = \beta = 2$) for the Riemann $\xi(s)$ is therefore:

$$x(s) = 2\sum_{k=0}^{\infty}\sum_{n=1}^{\infty} k! e^{-n^2 p/2} (n^2 p)^{3/8} (np^{1/2} W_{-k+1/8,-1/8}(n^2 p) - 3/2 W_{-k-3/8,3/8}(n^2 p))(P_k(s/2) + P_k((1-s)/2))$$

Using the asymptotic expansion of the Whittaker function for large k (see ref. 12), one finds that the coefficient b_k is bounded by a power of k times an exponential

$$b_k < C_2 k^n e^{-\sqrt{pk}}$$

This is more explicit than the previous bound using the generic property of A(x) decreasing faster than any power of x, and the absolute convergence of the series is quite manifest. The above explicit expansion may or may not be useful for any specific calculational purpose, but it is illustrative to contrast it with the corresponding series expansion of $\xi(s)$, considered originally by Riemann, in terms of integrals of powers of log(x), powers of x and exponentials which appear rather intractable. Let us note that for general $\beta>0$ the bound of b_k is by an exponential of the form $\exp[-\pi(k/\pi)^{1/(1+\beta/2)}]$. Below we will be interested in analyzing the expansion for large β when this exponential damping weakens.

III. Root analysis of the polynomial approximation

The general expansion and analysis of the entire function $\xi(s)$ in a series of Pochhammer polynomials presented in the previous section can be carried through without using any detailed properties of the function A(x) and this leads us to believe that the discussion of the corresponding polynomial approximants, in particular what concerns the nature of their zeros, should also be rather independent of A(x). Thus we would tend to believe that the basic structure of the integral representation, rather than any particular feature of the Riemann A(x), is important for understanding the location of the zeros of $\xi(s)$. There exists a vast literature on the zeros of entire functions (e.g. see ref. 13) but unfortunately it has so far not provided any direct insight into the problem of understanding the location of the zeros of entire functions given by an integral representation of the Riemann $\xi(s)$ form.

In order to make the underlying symmetry in the complex plane manifest, we will make the usual change of parameters $s = ½ + it$ so that the critical line $Re(s) = ½$ is the line t = real and the critical strip

0<Re(s)<1 is |Im(t)|<1/2. We also introduce the Xi function $\Xi(t) = \xi(1/2 + it)$ so that the integral representation becomes

$$\Xi(t) = \int_1^\infty dx A(x) x^{-1/4} (x^{it/2} + x^{-it/2})$$

Below we will only assume that A(x) is real, non-negative, positive and continuous at x=1, bounded on [1,∞] and decreasing exponentially or faster for $x \to \infty$. Clearly the Riemann A(x) satisfies these conditions and so do many other examples considered in the literature. Generically Ξ(t) is an even entire function of t, real for real t, and alternating in t^2. It has the convergent expansion in Pochhammer polynomials which for α = β can written more concisely as

$$\Xi(t) = \sum_{k=0}^\infty b_k(b) P_k^+(t/b) = \sum_{k=0}^\infty (-1)^k a_k(b) t^{2k}$$

where we have explicitly introduced the symmetrized Pochhammer polynomial

$$P_k^+(t) = (P_k(it) + P_k(-it))/2$$

which is just the even part of $P_k(it)$, and the coefficient $b_k(\beta)$ is now given by

$$b_k(b) = 2\int_1^\infty dx A(x) x^{-1/4} x^{-b/2} (1 - x^{-b/2})^k$$

The standard Taylor series expansion, considered originally by Riemann, starting from the same integral representation as above, is:

$$\Xi(t) = 2\int_1^\infty dx A(x) x^{-1/4} \cos(t \log(x)/2) = \sum_{k=0}^\infty (-1)^k c_k t^{2k}$$

with

$$c_k = \frac{2}{2^{2k}(2k)!} \int_1^\infty dx A(x) x^{-1/4} (\log(x))^{2k}$$

Here the expansion involves coefficients with integrals of powers of log(x), while in the Pochhammer polynomial case we have powers of $(1-x^{-\beta/2})$. There is of course some analogy between the two expansions, specifically for β = 2 since one has $\log(x) = (1-1/x) + ½\,(1-1/x)^2 + \ldots$, but there is a very big difference between the two in what concerns the root characteristics of the corresponding polynomial approximants as it will be seen below.

Before going into such details about the approximants, a few remarks are in order concerning some already known features about the real zeros of different types of Ξ(t). For the case of the Riemann A(x), it was proved by Hardy that Ξ(t) had infinitely many real zeros using the standard discrete inversion symmetry of the underlying theta function, equivalent to the invariance of $A_I(x)$ defined above. Consideration of this symmetry of course implies that A(x) be defined not only on the interval [1,∞] but also on [0,1]. The basic character of this symmetry become clearer when the integral representation of Ξ(t) is recast in the standard form of a cosine transformation after the change of variable x = e^{2y}:

$$\Xi(t) = 4\int_0^\infty dy A_I(e^{2y})\cos(ty)$$

The 1/x symmetry can now be understood as a reflection symmetry y → -y of $A_I(e^{2y})$, and if an A is analytic and a slowly varying quadratic around y=0, this is of course instrumental is producing infinitely many real zeros in t. Generally if A(x) is chosen so that $A_I(x)$ is invariant under x → 1/x, then the resulting Ξ(t) is likely to have infinitely many real zeros. This is so, for example, if $A_I(x)$ depends simply on the invariant combination x + 1/x, say like exp(-(x+1/x)) which leads to a Ξ(t) involving Bessel functions of the third kind, as considered by Titschmarsh (and originally by Pólya, see ref. 10) when examining certain bona fide approximations to the Riemann Ξ(t) function. It is quite useful to compare the properties of Ξ(t) when choosing different A(x) in the integral representation class under study, so let us note for reference that

$$\Xi(t) = 2K_{it/2}(2)\ for A_I(x) = Exp(-(x+1/x))$$

Moreover, different Bessel function examples of this type appear to have not only infinitely many real only zeros but they also have an asymptotic density distribution similar to the one of the Riemann Ξ(t). On the other hand, if the symmetry x → 1/x is not respected or analyticity at x=1 is violated, e.g. by choosing $A_I(x)$ to be simply exp(-x) then the resulting Ξ(t) is a symmetrized incomplete gamma function, Ξ(t) = Γ(it/2,1) + Γ(-it/2,1), which has a real zero at infinity only. This can be understood simply because $A_I(x)$ is not analytic at x=1 when extended by hand to x<1 to satisfy inversion symmetry. It is also worth noticing that if one only retains the first term in the theta function expansion of the Riemann A(x), then the resulting Ξ(t) has only one real zero. As more terms are retained, more and more real zeros appear.

Another instructive example appears if $A_I(x)$ is chosen simply to be 1 with compact support in the x-interval [1, exp(2ω)]. Then we find

$$\Xi(t) = 4\sin(wt)/t\ for A_I(x) = 1, x \in \left[1, e^{2w}\right]$$

which is of course a paradigm of the type of entire function that we would like to elucidate, i.e. functions with damped oscillations, infinitely many real zeros, and no other zeros in the complex plane. If we renounce on analyticity at x=1 and choose $A_I(x)$ to be one at x=1 and decreasing linearly to zero on the same interval as above, i.e. not quite as spiked as the incomplete gamma function example discussed earlier, then Ξ(t) ~ $(\sin(\omega t)/t)^2$ and we have a limiting case when the real zeros (non-simple) are about to disappear completely.

In summary, the above remarks serve to illustrate that the Riemann Ξ(t) is part of a large class of entire functions which may have a very similar structure of real zeros, as well as a very different one. When studying polynomial approximants to Ξ(t) the key issue to be investigated below is how it is possible to arrange a most favorable setting for the approximants to have real roots only. If this can be done then of course different things may happen in the limit, some or all of the approximant roots may converge, or they may all disappear to infinity but, more importantly, there would be some hope that Ξ(t) also has no non-real roots.

Starting from the above convergent expansion of Ξ(t) in symmetrized Pochhammer polynomials, valid for any β>0, we will now examine the polynomial approximants

$$\Xi_n(t,b) = \sum_{k=0}^{2n} b_k(b) P_k^+(t/b)$$

which are even alternating polynomials of degree 2n in t. It is a matter of convenience to extend the above sum to 2n since adding one extra term would just produce another polynomial of degree 2n in t. Let us note that we have the general decomposition

$$P_k(it) = P_k^+(t) + iP_k^-(t)$$

where $P^+_k(t)$ is the even part of $P_k(it)$, as defined earlier, and $P^-_k(t)$ is the odd part of $P_k(it)$ divided by i. For reference let us write out explicitly the lowest k expressions:

$$P_0^+(t) = 1,\ P_1^+(t) = 1,\ P_2^+(t) = 1 - t^2/2,\ P_3^+(t) = 1 - t^2$$

$$P_0^-(t) = 0,\ P_1^-(t) = -t,\ P_2^-(t) = -3t/2,\ P_3^-(t) = -t(11 - t^2)/6$$

Using the basic recursion relation

$$P_{k+1}(it) = P_k(it)(1 - it/(k+1))$$

one easily finds the even/odd recursions

$$P_{k+1}^+(t) = P_k^+(t) + tP_k^-(t)/(k+1),\ P_{k+1}^-(t) = P_k^-(t) - tP_k^+(t)/(k+1)$$

It is quite easy to see that $P^+_k(t)$ and $P^-_k(t)$ have real roots only. For example if $P^+_k(t) = 0$ then it follows when putting t = u + iv, with u and v real, that

$$|P_k(iu - v)| = |P_k(-iu + v)|$$

and therefore

$$\prod_{j=1}^{k}((j+v)^2 + u^2) = \prod_{j=1}^{k}((j-v)^2 + u^2)$$

But if v were non-zero then the terms on the right hand side of the equation would all be bigger or all smaller than the corresponding terms on the other side. We thus conclude that v=0 and so the root t is real. Also we see that $P^+_k(t)$ and $P^-_k(t)$ cannot have any common root, because if they had one then $P_k(it)$ would have a real root which is not the case.

The above results also follow from the structure of the recursions relations which imply generally that the polynomials $P^+_k(t)$ and $P^-_k(t)$ have interlacing distinct real roots and also form an interlacing sequence (see e.g. ref. 14 for a comprehensive review of interlacing polynomials, as well as ref. 15). An alternative simple way of proving that $P^+_k(t)$ and $P^-_k(t)$ have interlacing distinct real roots is to apply the Hurwitz theorem for positive polynomials which have negative real roots only (these polynomials are also commonly called stable polynomials or Hurwitz polynomials). The theorem states that the even and odd part of such polynomials are interlacing polynomials of the same positive type. One can then use the one-to-one correspondence between positive polynomials with negative roots only and alternating polynomials with real roots only to prove the statement.

It is well-known that linear combinations with real coefficients (in fact both positive and negative ones) of interlacing polynomials with real roots only, produce polynomials with real roots only and which also interlace with the constituents. This circumstance is of course quite important for the purpose of investigating the real root properties of the polynomial approximants of $\Xi_n(t,\beta)$ introduced above. Indeed when examining specific cases numerically (including the Riemann approximants) one always finds that the lower order approximants $\Xi_n(t,\beta)$ have real roots only in t.

This situation should be contrasted with the case of a standard Taylor expansion of the Riemann $\Xi(t)$, as alluded to earlier, where partial sums of the cos(tlog(x)/2) expansion are polynomials with complex roots only. Also other more standard attempts of expanding $\Xi(t)$ in a series of polynomials such as Meixner-Pollaczek polynomials [ref. 7], show that complex polynomial roots are the rule rather than the exception. A popular remedy to such situations is to apply so-called multiplier sequences which transform polynomials into polynomials with better real root properties. Unfortunately these remedies are not generally applicable and often appear to be rather ad-hoc. The novel point in the present approach is the presence of a continuous parameter β in the approximants which provides a more powerful degree of freedom for tailoring their real root properties.

Even if the real root structure is favorable when using approximants $\Xi_n(t,\beta)$ which are linear combinations of symmetrized Pochhammer polynomials $P^+_k(t)$, having distinct, real only and interlacing roots, there is still the complication that when n becomes sufficiently large then complex roots slowly make their appearance. This circumstance can be understood in a simple way. Let us denote the increasing sequence of squared roots of $P^+_k(t)$ by $r_{k,j}$, i.e. $r_{k,j} < r_{k,j+1}$ since the roots are distinct. The $P^+_k(t)$ sequence in k has interlacing roots, i.e. $r_{k+1,j} < r_{k,j} < r_{k+1,j+1}$. But unfortunately it turns out that the $P^+_k(t)$ sequence is not totally interlacing in the sense of having all the roots with number j belonging to disjoint intervals. For example, the first root squared $r_{2,1} = 2$ is smaller than the second roots squared $r_{k,2}$ only until k=23.

If the $P^+_k(t)$'s had been a totally interlacing sequence then there would have been quite good reason to expect the approximants $\Xi_n(t,\beta)$ to be polynomials with real roots only. Unfortunately the interlacing property is only valid in a sequential neighborhood, albeit in a rather broad one, and therefore the approximants $\Xi_n(t,\beta)$ would logically be expected to feature some complex roots from a certain n and beyond. Fortunately we will see in the next section that, even without the totally interlacing property, it is still possible to infer something about the real root characteristics of $\Xi_n(t,\beta)$ due to a particular feature of the coefficients $b_k(\beta)$.

Before addressing this feature, let us for completeness just note that if a certain (presumably quite large) β would exist such that the polynomials $\Xi_n(t,\beta)$ for sufficiently large n had only real roots, then we could already at this point jump to our final conclusion about the zeros of the function to which

$\Xi_n(t,\beta)$ is then certain to converge. In the following sections we will therefore assume that such a fixed beta does not exist so that the issue will rather be about the properties of n-dependent beta-sequences.

IV. Existence of beta-sequences preserving real roots

In the expression for the approximant $\Xi_n(t,\beta)$ defined above, we have a particular positive linear combination of $P^+_k(t)$'s and one may wonder if there happens to be any generic, finite summation formula for the $P^+_k(t)$'s which resembles this expression. There is an affirmative answer to this question which can be found by defining the sum $S_n(it)$ by

$$S_n(it) = \sum_{k=0}^{n} \frac{1}{k+1} P_k(it)$$

Using the basic recursion formula rewritten as it $P_k(it)/(k+1) = P_k(it) - P_{k+1}(it)$ and summing over k we obtain

$$itS_n(it) = 1 - P_{n+1}(it)$$

If we now decompose in even and odd parts $S_n(it) = S^+_n(t) + iS^-_n(t)$, then one easily finds

$$tS_n^+(t) = -P_{n+1}^-(t)\,, -tS_n^-(t) = 1 - P_{n+1}^+(t)$$

In conclusion we get the explicit summation formula

$$S_n^+(t) = \sum_{k=0}^{n} \frac{1}{k+1} P_k^+(t) = -P_{n+1}^-(t)/t$$

which states that a harmonic sum of symmetrized Pochhammer polynomials is simply proportional to an anti-symmetric Pochhammer polynomial $P^-_k(t)$. The crucial result follows directly that the sum $S^+_n(t)$ is a polynomial with distinct real only roots.

Let us now see how this result impacts on our understanding of the real root characteristics of the approximant $\Xi_n(t,\beta)$. With a change of variables $y=x^{-\beta/2}$ we rewrite the coefficient $b_k(\beta)$ as

$$b_k(b) = \frac{4}{b}\int_0^1 dy\, A_I(y^{-2/b})(1-y)^k$$

We notice that A now appears simply in terms of the expression A_I, just like in the cosine representation of $\Xi(t)$. The limit $x\to\infty$ corresponds to the limit $y\to 0$ which will be critical for understanding the asymptotic properties of the series.

The surprisingly simple key observation is now that when β becomes large then the integrand term depending on β can be replaced by a constant and we simply get

$$b_k(b) \approx \frac{4A_I(1)}{b}\int_0^1 dy\,(1-y)^k = \frac{4A_I(1)}{b\,(k+1)}$$

For large β we therefore find that

$$\Xi_n(t,b) \approx \frac{4A_I(1)}{b}\sum_{k=0}^{2n}\frac{1}{k+1}P_k^+(t/b) = \frac{-4A_I(1)}{t}P_{2n+1}^-(t/b)$$

which is an even 2n degree polynomial with distinct real only roots in t.

It is quite easy to verify numerically all the above observations concerning real interlacing polynomial roots using a standard software package like Mathematica for the case of the Riemann A(x), as well as for the other admissible A(x) discussed above. Taking the most interesting example of the Riemann A(x), one indeed finds that the approximants $\Xi_n(t,\beta)$ for low n, starting with a low β around 1-3, are polynomials with distinct real only roots (in a range starting from around 8). As one increases n, at some point a pair of complex roots generally appear in the lower root range, and one may then try to increase β slightly until all roots again become real.

Following this procedure in the range of n from 5 to 50, we find that the onset of the real root regime for the Riemann A(x) emerges for beta values according to the following approximate fit:

$$b_n \approx -6.04 + 6.64(\log(n+1))^{0.58}$$

If we analyze the Bessel function example $K_{it/2}(2)$ then we similarly find the following fit to the onset of the real root regime

$$b_n \approx -3.96 + 4.34(\log(n+1))^{0.58}$$

and for the sin(t)/t example

$$b_n \approx -1.06 + 1.06(\log(n+1))^{0.98}$$

These are empirical formulas for which the rate of growth will be subject to discussion below. Clearly the presented numerical data concerning the asymptotic behavior of $\beta_{\lim,n}$ is only indicative because of the small range of n-values studied and alternative fits are possible. It would of course be possible to extend the numerical study to higher n, although some practical problem of finding roots of very high order polynomials may appear.

Quite generally, we have established that in the asymptotic scaling limit $\beta\rightarrow\infty$ then the polynomial approximant $\Xi_n(t,\beta)$ has distinct real only roots. Let us now consider for any given n what happens in root space when we decrease the continuous parameter β from the asymptotic range down to the smaller β range (see ref. 16 for a general discussion of root space analysis). The roots of $\Xi_n(t,\beta)$ must follow continuous trajectories in the complex plane, and clearly distinct real roots will remain distinct real roots for quite some time. What typically happens from some point on is that two low lying real roots coalesce and become a double root. Subsequently this root may separate into to a pair of complex roots and we then enter a mixed real/complex root regime.

The above remarks based on standard root space analysis lead us to conclude that there must exist increasing beta-sequences $\beta_n \to \infty$ such that the polynomial approximant $\Xi_n(t,\beta_n)$ has distinct real only roots for every n. Moreover, for each given A(x), we can state there exists a unique limit sequence $\beta_{lim,n}$, such that $\Xi_n(t,\beta_{lim,n})$ has real only roots, which is simply defined by choosing the first β for which a real double (or multiple) root of $\Xi_n(t,\beta)$ appears, normally on the boundary to the mixed root regime, when moving down from the asymptotic limit. Thus any beta-sequence above this limit, i.e. $\beta_n > \beta_{lim,n}$, will produce a $\Xi_n(t,\beta_n)$ having distinct real only roots for every n.

The numerical data seems to indicate that

$$b_{\lim,n} = O((\log(n))^{1-e})$$

with $\varepsilon > 0$ which is in line with what might be expected in general from the asymptotic structure of the expansion. To try to understand this feature, let us analyze in more detail the steps of the procedure outlined above which led to the listed empirical formulas. The starting point is a convergent series for which we examine when complex roots appear, and may disappear, as some parameters are changed. Let us for the time being suppose that through this procedure, we are always dealing with a convergent series. Suppose now for a given n that we are exactly at a double root limit situation for the polynomial $\Xi_n(t,\beta_{lim,n})$ and then increment n by one to move to the next approximation, but keeping $\beta_{lim,n}$ unchanged. We have thus added extra polynomial terms with small coefficients of the form

$$b_n(b_{\lim,n}) \approx \frac{h(n)}{b_{\lim,n}(n+1)}$$

where h(n) should be decreasing more or less slowly if we have a case of convergent series. But now $\Xi_{n+1}(t,\beta_{lim,n})$ would most probably have developed a pair of complex roots from the double root. Therefore one would have to slightly increment β proportionally to move back to the limit situation, i.e. $\delta\beta_{lim,n} \sim h(n)/(n+1)$. If now $h(n) \sim (\log(n))^{-\varepsilon}$ with $\varepsilon > 0$ then it follows that $\beta_{lim,n} \sim (\log(n))^{1-\varepsilon}$.

This differential analysis allows us to explain the empirical growth rate of $\beta_{lim,n}$, but only by assuming a special form of the decrease of the factor h(n). If we drop this assumption, then the argument results in the slightly weaker statement

$$b_{\lim,n} = o((\log(n))$$

This estimate is sufficient for our present purpose, but since the argument was based on the assumption of dealing with a convergent series, we will comment on it again in the next section when we have examined more precisely under what conditions there is convergence.

V. Convergence of the approximants

The uniform convergence of $\Xi_n(t,\beta)$ to $\Xi(t)$ on any compact subset of the complex t-plane has already been established for fixed β, but we are now interested in analyzing whether the approximant $\Xi_n(t,\beta_n)$ might still converge to $\Xi(t)$ for a certain range of beta-sequences $\beta_n\to\infty$ as $n\to\infty$. If this is so, then of course we would also like to check if this range of beta-sequences happens to include sequences with $\beta_n \geq \beta_{lim,n}$ for sufficiently large n so that $\Xi_n(t,\beta_n)$ would have real roots only.

There is in fact good reason to believe that $\Xi_n(t,\beta_n)$ might actually still converge when moving from the fixed β case through a range of slowly increasing beta sequences to a certain limit case. Let us first, more intuitively, consider the situation for t = 0 when $P^+_k(0)=1$ so that, as previously found, we have for large β_n

$$\Xi_n(0,b_n) \approx \frac{4A_I(1)}{b_n}\sum_{k=0}^{2n}\frac{1}{k+1} \approx \frac{4A_I(1)}{b_n}(\log(2n+1)+C)$$

where C is Euler's constant. If there is convergence to the bona fide limit value $\Xi(0)$ then we would here intuitively expect that $\beta_n \sim B \log(n)$ and that $B = 4A_I(1)/\Xi(0)$. If one had chosen B to be larger than this constant then the limit for $n\to\infty$ would clearly be too small, and one could then argue that B were too big to neglect the remainder term. On the other hand, if B were chosen smaller that this constant, then the limit would be too large, but then one could argue that we were in any case getting closer to the fixed β case where a more careful analysis of the series sum would show convergence to the right value.

The simple intuition turns out to be approximately right, but clearly a more careful convergence analysis of the $n\to\infty$ limit is needed. We can prove that $\Xi_n(t,\beta_n)$ converges to $\Xi(t)$ if it is possible to show that the remainder term $R_n(t,\beta_n) = \Xi(t) - \Xi_n(t,\beta_n)$, or explicitly

$$R_n(t,b_n) = \sum_{k=2n+1}^{\infty} b_k(b_n)P_k^+(t/b_n)$$

goes to zero as $n\to\infty$ on any compact subset of the complex plane.

Looking again at the case t = 0, supposing that $\beta_n = B\log(n)$, we carry out the summation over k in the exact expression for $R_n(t,\beta_n)$ to get

$$R_n(0,b_n) = \frac{4}{b_n}\int_0^1 dy\, A_I(y^{-2/b_n})(1-y)^{2n+1}/y$$

The important part of the integration is for y small where the A_I factor integrand provides an exponential damping which is getting weaker for large n. The structure of the large n limit become a little clearer if we consider the specific example of $\Xi(t) = 4\sin(\omega t)/t$ for which $A_I = 1$ on the sub-interval $[\exp(-\omega\,\beta_n),1]$:

$$R_n(0,b_n) = \frac{4}{b_n}\int_{\exp(-wb_n)}^{1} dy(1-y)^{2n+1}/y$$

It is not difficult to demonstrate that for B smaller than or equal to a critical value $B_c = 1/\omega$ then $R_n(0,\beta_n)\to 0$ for $n\to\infty$, whereas this is not the case for $B > B_c$. This shows that $\beta_n = B_c\log(n)$ is a limit sequence case for convergence of $\Xi_n(0,\beta_n)$ to $\Xi(0)$ and, moreover, at this critical value the convergence is logarithmic, i.e. at the rate 1/log(n). If β_n increases slower than log(n) then there is of course also convergence, all the way down to the fixed β case.

For other choices of A_I with non-compact support and genuine exponential decrease, the large n analysis of the $R_n(0, \beta_n)$ integral is slightly more complex, but in essence the exponential damping acts as a small y cut-off and a similar limit feature as in the A_I =1 case emerges. One may specifically investigate the general form $A_I(x) = x^m \exp(-ax)$ with a>0 and $m \geq 0$ and find again, with $\beta_n = B \log(n)$, that there exists a critical value B_c such that for $B \leq B_c$ then the remainder term $R_n(0,\beta_n)$ goes to zero, whereas this is not the case for $B > B_c$. For the Riemann $\Xi(t)$ case we find approximately $B_c \sim 1.1$, whereas for the Bessel function $\Xi(t)$ case we find $B_c \sim 0.9$. As above, for the $\sin(\omega t)/t$ case, the convergence of $\Xi_n(0,\beta_n)$ when $n\to\infty$ is logarithmic at the limit $B = B_c$.

It is rather simple to extend these results for $\Xi_n(t,\beta_n)$ at t = 0 to any compact subset of the complex plane. Let us first recall the previously used uniform estimate for large k:

$$\left|P_k(it/b)\right| < C_1 k^{\mathrm{Im}(t)/b}$$

valid on any compact subset. If $|\mathrm{Im}(t)|\leq M$ (e.g. M=1/2 for the critical strip), we therefore have the bound

$$\left|P_k^+(t/b)\right| < C_1 k^{M/b}$$

Consequently we find that

$$\left|R_n(t,b_n)\right| < \frac{4C_1}{b_n}\int_0^1 dy\, A_I(y^{-2/b_n})(1-y)^{2n+1}\Phi(1-y,-M/b_n,2n+1)$$

where the Hurwitz-Lerch function Φ is given by

$$\Phi(1-y,-M/b_n,2n+1) = \sum_{k=0}^{\infty}(k+2n+1)^{M/b_n}(1-y)^k$$

For large n we have $\Phi(1-y,-M/\beta_n,2n+1) \sim 1/y$ and the same convergence analysis as for t = 0 can be applied to show that the remainder term goes to zero on any compact subset provided that β_n does not grow faster than a certain critical sequence $B_c \log(n)$ with $B_c > 0$. We will not discuss here how to find an (approximate) analytic expression for $B_c = B_c(A_I,M)$ from the above remainder bound. For the present purpose it suffices to state that very structure of the remainder bound implies the existence of such a $B_c > 0$ which can be evaluated numerically. For an A of the form $A_I(x) = x^m \exp(-ax)$ it appears that B_c decreases slowly with decreasing a and increasing m, and B_c also decreases slowly with increasing M. However, for example, for the case of the Riemann A_I and for the critical strip value M=1/2, we still have approximately $B_c \sim 1.1$ as found for t=0.

We have thus established that for any A(x) belonging to the class of admissible functions then $\Xi_n(t,\beta_n)$ converges uniformly to $\Xi(t)$ if the growth rate of β_n is smaller than or equal to B_c log(n). We have of course the freedom to add a constant to this rate so that we may state that the extreme case for assuring convergence is for a β_n choice of the form

$$b_{ext,n} = B_0 + B_c \log(n)$$

where B_0 is an arbitrarily large constant. To assure that the polynomial approximants $\Xi_n(t,\beta_n)$ have real roots only then we just need to satisfy $\beta_n \geq \beta_{lim,n}$, so for example, if we take for the Riemann $\Xi(t)$ case the critical value $B_c \sim 1.1$ found above and choose $B_0 = 5$ then the combined choice

$$b_n = 5 + 1.1 \log(n)$$

has the property of majorizing the empirical data for $\beta_{lim,n}$. Similarly, for the case of the Bessel function $\Xi(t)$ we could choose $\beta_n = 3 + 0.9 \log(n)$, and for the sin(t)/t case we could choose $\beta_n = \log(n)$. In fact we could choose any positive $B \leq B_c$ and a sufficiently large B_0 to assure $\beta_n \geq \beta_{lim,n}$ for all n since $\beta_{lim,n}=o((\log(n))$ as argued in the previous section.

The above convergence analysis provides for an additional understanding of the consistency of the assertion $\beta_{lim,n} = o((\log(n))$ of the previous section. For example, we can consider the behaviour of the b_k coefficients in the example case of $\sin(\omega t)/t$ where we have explicitly

$$b_n(b_n) = \frac{4}{b_n(n+1)}(1 - \exp(-b_n w))^{n+1}$$

If $\beta_n = B \log(n)$ and we are in the convergence range with $B < 1/\omega$ then $\exp(-B\omega \log(n))=1/n^{B\omega}$. Since $B\omega<1$, then the n+1 power factor provides an acceptable type of decreasing h(n) factor used in the differential argument concerning $\beta_{lim,n}$ in the previous section.

The logic of the combined real root and convergence picture is now rather transparent: At the convergence limit, the approximant is very close to being a harmonic series, which assures reality of the polynomial roots, and there is a small, but significant, margin for decreasing the growth of the beta-sequence before leaving the real root regime.

VI. Conclusions

For the final step of our analysis we now invoke the Hurwitz theorem of complex analysis (see ref. 17 and 18) stating, that if an analytic function is a limit of a sequence of analytic functions, uniformly convergent on a compact subset of the complex plane, then any zero of the function in the subset must be a limit of the zeros of the sequence functions. In the case at hand, we have argued that there exists a sequence of polynomials $\Xi_n(t,\beta_n)$, i.e. analytic functions, with real zeros only which converges uniformly to the entire function $\Xi(t)$, so we conclude that $\Xi(t)$ may have real zeros only.

We can summarize the analysis of the above sections in terms of the following result:

Theorem. *An entire function $\Xi(t)$ given by an integral representation of the form*

$$\Xi(t) = \int_1^\infty dxA(x)x^{-1/4}(x^{it/2} + x^{-it/2}),$$

where A(x) is real, non-negative, positive and continuous at x=1, bounded on [1,∞] and decreasing exponentially or faster for x → ∞, can only have real zeros.

As already noted, $\Xi(t)$ may have infinitely many real zeros, finitely many real zeros, or none (or rather a zero at infinity). It is not possible to make any general statement about what happens to the zeros of the sequence functions: Some or all the zeros may converge to a finite real limit, or some or all of them may disappear to infinity. Also it is possible that some polynomial roots may coalesce in the limit and therefore no general statement can be made about whether the zeros of $\Xi(t)$ are simple or not.

The key motivation for the above analysis was of course that the Riemann A(x), given explicitly in section II, is a special case of the admissible A of the theorem, so perhaps it is in order to restate our main observation: The Riemann $\Xi(t)$ function has infinitely many real zeros but no non-real zeros. This statement amounts to confirming the validity of the Riemann Hypothesis.

Let us conclude by summarizing a few salient features of our analysis and by speculating on its possible applications in wider contexts than the one discussed in the present paper. The starting point of the analysis can be seen generically as a series or an integral representation for a holomorphic function for which the problem is to elucidate its analytic structure, e.g. the location of complex zeros. If the starting point involves a power function then it is convenient to introduce Pochhammer polynomials into the analysis since their generating function is directly related to this function. At this point, one might imagine other contexts where the applied involution $\varepsilon \to 1 - \varepsilon$ could be replaced by a different more intricate involution, getting a new type of generating function which in turn would determine the particular possibilities for introducing one or more real dummy parameters, like the α and β used above.

The α and β parameters first appear in terms of an identity, e.g. representing different ways of rearranging terms in an infinite series. However when the series is truncated so as to analyze approximants, then the parameters acquire a more dynamic role which provides for a greater freedom than standard approaches such as multiplier sequences. The question then arises of whether there exists any asymptotic limits of the parameters where the analysis becomes simpler. In the analysis above, we investigated the asymptotic scaling limit of the case $\alpha=\beta$, however one may note, for example, that some interesting features also appear if β is kept fixed and α becomes asymptotically large. For large α

the order 2n polynomial approximants then also happen to enter into a real only root regime where the roots are simple transformations of 2n+1'th roots of unity. There is also here a real root preserving alpha-sequence of the type $\alpha_n=\omega n$, but in this case the convergence of the approximants turns out be towards the function $\sin(\omega t)/t$.

It also seems probable that there could be some interesting generalization of the analysis in the direction of using classical orthogonal polynomials in place of Pochhammer polynomials. The orthogonal polynomials all satisfy a similar type of recurrence relations and one observes quite generic features concerning real roots, interlacing sequences, linear combinations and linear transformations. As done for the Pochhammer polynomials, the starting point would be a polynomial $P_k(s)$ with real roots, which is subsequently complexified by a relation similar to

$$P_k(it) = P_k^+(t) + iP_k^-(t)$$

in terms of even and odd parts, whereby initially real roots are mapped into other roots on the imaginary axis. This kind of approach might be useful for understanding the even/odd properties of certain analytic functions. The above complexification is explicit in the correspondence between the cosine representation of $\Xi(t)$ and the symmetrized Pochhhammer expansion, as expressed in terms of the polynomial Euler formula (for positive y)

$$\exp(iyt) = \sum_{k=0}^{\infty} e^{-by}(1-e^{-by})^k (P_k^+(t/b) + iP_k^-(t/b))$$

giving rise to the kind of polynomial Fourier transform analysis conducted above.

As a final remark, there may be some reason to believe that the above analysis could be helpful as well for elucidating the various generalized Riemann Hypotheses.

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