

ZEROS AND POLES OF PADÉ APPROXIMATES TO THE SYMMETRIC RIEMANN ZETA FUNCTION

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ABSTRACT. Some of the zeros and poles of Padé approximants approximate zeros and poles of the approximated function. Others, the "spurious" poles and zeros are often arranged in quite remarkable patterns. These patterns display similarity when the ratio of degrees of the numerators to the denominators is kept constant and with scaling according to the total degree appear to converge to a limit curve. We investigate these patterns for the analytic version of the zeta function, $(z-1)\zeta(z)$, and for the symmetric zeta function $\xi(z)$. We develop an algorithm for calculating these approximants along a line of any angle through the Padé table.

1. PADÉ APPROXIMATION

Padé approximation is the extension of polynomial approximation to include rational functions. A degree $[\alpha/\beta]$ approximation, $\frac{P_{\alpha\beta}}{Q_{\alpha\beta}}$, of total degree $\alpha + \beta$, to a function y in x , where the numerator has degree $\leq \alpha$ and the denominator $\leq \beta$ satisfies

$$y - \frac{P_{\alpha\beta}}{Q_{\alpha\beta}} = \mathcal{O}(x^{\alpha+\beta+1}),$$

which is equivalent to

$$(1) \quad yQ_{\alpha\beta} - P_{\alpha\beta} = \mathcal{O}(x^{\alpha+\beta+1}),$$

if $Q_{\alpha\beta}(0) \neq 0$.

The Padé Table for is an array presentation of the various degree representations for a function

$$\begin{array}{cccccc} [0/0] & [1/0] & [2/0] & [3/0] & \dots & \\ [0/1] & [1/1] & [2/1] & [3/1] & \dots & \\ [0/2] & [1/2] & [2/2] & [3/2] & \dots & \\ \vdots & \vdots & \vdots & \vdots & & \end{array}$$

A *diagonal* approximant is one for which the degrees of the numerator and denominator are equal. These lie on a line running at an angle of 45° through the table starting at $[0/0]$. An *anti-diagonal* line is perpendicular to this and contains approximants with the same total degree.

1.1. Algorithms for calculating Padé approximants.

1.1.1. *The Kronecker algorithm.* This uses a modified Euclidean algorithm to calculate approximants along an anti-diagonal line through the table. For degree N approximants, the algorithm starts with the polynomials $r_0 = x^{N+1}$ and $r_1 = [N/0] = y_N = a_0 + a_1x + a_2x^2 + \dots + x^N$, Taylor series of degree N for the function y , and for $k \geq 1$ defines

$$r_{k+1} = r_{k-1} - q_k r_k,$$

where the degree of r_{k+1} is less than the degree of r_k . With the accompanying sequences v_k and u_k defined starting with $v_0 = 0$, $v_1 = 1$ and $u_0 = 1$, $u_1 = 0$ and continuing

$$v_{k+1} = v_{k-1} - q_k v_k$$

$$u_{k+1} = u_{k-1} - q_k u_k$$

the identity

$$r_k = u_k x^{N+1} + y_N v_k$$

is maintained. Provided $v_k(0) \neq 0$,

$$\frac{r_k}{v_k}$$

is a degree N approximant for y . With the particular initialization described here, the polynomials derived are unique. However, we can choose an initialization using any two adjacent entries on an anti-diagonal

$$\frac{P_{\alpha\beta}}{Q_{\alpha\beta}} \text{ and } \frac{P_{\alpha+1,\beta-1}}{Q_{\alpha+1,\beta-1}},$$

namely, $r'_0 = P_{\alpha+1,\beta-1}$, $r'_1 = P_{\alpha\beta}$ and $v'_0 = Q_{\alpha+1,\beta-1}$, $v'_1 = Q_{\alpha\beta}$. Where, for some k , $P_{\alpha\beta} = c_1 r_k$ and $P_{\alpha+1,\beta-1} = c_2 r_{k-1}$, we obtain

$$c_2 r_{k+1} = c_2 r_{k-1} - \left(\frac{c_2 q_k}{c_1} \right) c_1 r_k = P_{\alpha+1,\beta-1} - \left(\frac{c_2 q_k}{c_1} \right) P_{\alpha\beta} = r'_2$$

$$c_2 v_{k+1} = c_2 v_{k-1} - \left(\frac{c_2 q_k}{c_1} \right) c_1 v_k = Q_{\alpha+1,\beta-1} - \left(\frac{c_2 q_k}{c_1} \right) Q_{\alpha\beta} = v'_2$$

giving

$$\frac{r'_2}{v'_2} = \frac{r_{k+1}}{v_{k+1}}.$$

1.1.2. *Solution of linear system and the Frobenius Relations.* Following Frobenius [Fro81], we use the presentation (1) to obtain linear equations for the coefficients of Padé approximants. Let

$$y = a_0 + a_1x + a_2x^2 + \dots$$

with $a_j \in \mathbb{C}$ be the power series representation a function. Let

$$T = t_0 + t_1x + \dots + t_\alpha x^\alpha, \quad U = u_0 + u_1x + \dots + u_\beta x^\beta$$

be polynomials of degrees less than or equal to α and β respectively such that

$$yU - T = V = \mathcal{O}(x^{\alpha+\beta+1}).$$

If $U(0) \neq 0$, then the Padé approximant of order $[\alpha/\beta]$ is given by

$$\frac{T}{U}.$$

Note that T and U are unique up to a constant multiple.

From the first $\alpha + \beta + 1$ coefficients $v_{\alpha+\beta} = 0, \dots, v_1 = 0, v_0 = 0$, we obtain an undetermined system of $\alpha + \beta + 1$ equations in the $\alpha + \beta + 2$ coefficients of T and U . For the β coefficients from $v_{\alpha+1}$ to $v_{\alpha+\beta}$ give the β equations

$$\begin{aligned} 0 &= a_{\alpha+1}u_0 + a_\alpha u_1 + \dots + a_{\alpha-\beta+1}u_\beta \\ 0 &= a_{\alpha+2}u_0 + a_{\alpha+1}u_1 + \dots + a_{\alpha-\beta+2}u_\beta \\ &\vdots \\ 0 &= a_{\alpha+\beta}u_0 + a_{\alpha+\beta-1}u_1 + \dots + a_\alpha u_\beta \end{aligned}$$

involving the $\beta + 1$ coefficients of U . For this system we choose as a solution

$$U_{\alpha\beta} = \begin{vmatrix} a_{\alpha-\beta+1} & a_{\alpha-\beta+2} & \dots & a_\alpha & x^\beta \\ a_{\alpha-\beta+2} & a_{\alpha-\beta+3} & \dots & a_{\alpha+1} & x^{\beta-1} \\ \cdot & \cdot & \dots & \cdot & \cdot \\ a_{\alpha+1} & a_{\alpha+2} & \dots & a_{\alpha+\beta} & 1 \end{vmatrix}$$

which has $U_{\alpha\beta}(0) = c_{\alpha\beta}$ where we define

$$c_{\alpha\beta} = \begin{vmatrix} a_{\alpha-\beta+1} & a_{\alpha-\beta+2} & \dots & a_\alpha \\ a_{\alpha-\beta+2} & a_{\alpha-\beta+3} & \dots & a_{\alpha+1} \\ \vdots & \vdots & \ddots & \vdots \\ a_\alpha & a_{\alpha+1} & \dots & a_{\alpha+\beta-1} \end{vmatrix}.$$

From this the $\alpha + 1$ coefficients $v_0 = 0, \dots, v_\alpha = 0$ we now obtain

$$\begin{aligned} t_0 &= a_0 u_0 \\ t_1 &= a_1 u_0 + a_0 u_1 \\ &\vdots \\ t_\alpha &= a_\alpha u_0 + a_{\alpha-1} u_1 + \dots + a_{\alpha-\beta} u_\beta \end{aligned}$$

which we may write in the form

$$T_{\alpha\beta} = \begin{vmatrix} a_{\alpha-\beta+1} & a_{\alpha-\beta+2} & \dots & a_\alpha & a_{\alpha-\beta} x^\alpha + a_{\alpha-\beta-1} x^{\alpha-1} + \dots \\ a_{\alpha-\beta+2} & a_{\alpha-\beta+3} & \dots & a_{\alpha+1} & a_{\alpha-\beta+1} x^\alpha + a_{\alpha-\beta} x^{\alpha-1} + \dots \\ \cdot & \cdot & \dots & \cdot & \cdot \\ a_{\alpha+1} & a_{\alpha+2} & \dots & a_{\alpha+\beta} & a_\alpha x^\alpha + a_{\alpha-1} x^{\alpha-1} + \dots \end{vmatrix}.$$

For V , we then have

$$V_{\alpha\beta} = \begin{vmatrix} a_{\alpha-\beta+1} & a_{\alpha-\beta+2} & \dots & a_\alpha & a_{\alpha+1} x^{\alpha+\beta+1} + a_{\alpha+2} x^{\alpha+\beta+2} + \dots \\ a_{\alpha-\beta+2} & a_{\alpha-\beta+3} & \dots & a_{\alpha+1} & a_{\alpha+2} x^{\alpha+\beta+1} + a_{\alpha+3} x^{\alpha+\beta+2} + \dots \\ \cdot & \cdot & \dots & \cdot & \cdot \\ a_{\alpha+1} & a_{\alpha+2} & \dots & a_{\alpha+\beta} & a_{\alpha+\beta+1} x^{\alpha+\beta+1} + a_{\alpha+\beta+2} x^{\alpha+\beta+2} + \dots \end{vmatrix}.$$

Then $T_{\alpha\beta}, U_{\alpha\beta}, V_{\alpha\beta}$ represent solutions to the above equation, namely,

$$y U_{\alpha\beta} - T_{\alpha\beta} = V_{\alpha\beta} = \mathcal{O}(x^{\alpha+\beta+1}).$$

From these presentations of T, U, V as determinants we derive the following theorem:

Theorem 1.1. (Frobenius) *The constant coefficient of*

$$(2) \quad U_{\alpha\beta} \text{ is } c_{\alpha\beta},$$

and the coefficient of

$$(3) \quad x^\alpha \quad \text{in} \quad T_{\alpha\beta} \quad \text{is} \quad (-1)^\beta c_{\alpha,\beta+1},$$

$$(4) \quad x^\beta \quad \text{in} \quad U_{\alpha\beta} \quad \text{is} \quad (-1)^\beta c_{\alpha+1,\beta},$$

$$(5) \quad x^{\alpha+\beta+1} \quad \text{in} \quad V_{\alpha\beta} \quad \text{is} \quad c_{\alpha+1,\beta+1}.$$

Further, where in the equations below, each S may be stand for in one case for T , in another for U , or in another for V , we have the following theorem:

Theorem 1.2. (Frobenius)

$$(6) \quad c_{\alpha+1,\beta} S_{\alpha-1,\beta} - c_{\alpha,\beta+1} S_{\alpha,\beta-1} = c_{\alpha\beta} S_{\alpha\beta}$$

$$(7) \quad c_{\alpha,\beta+1} S_{\alpha+1,\beta} - c_{\alpha+1,\beta} S_{\alpha,\beta+1} = c_{\alpha+1,\beta+1} x S_{\alpha,\beta}$$

$$(8) \quad c_{\alpha+1,\beta} S_{\alpha\beta} - c_{\alpha\beta} S_{\alpha+1,\beta} = c_{\alpha+1,\beta+1} x S_{\alpha,\beta-1}$$

$$(9) \quad c_{\alpha,\beta+1} S_{\alpha\beta} - c_{\alpha\beta} S_{\alpha,\beta+1} = c_{\alpha+1,\beta+1} x S_{\alpha-1,\beta}$$

Proof. For the first equation, we start with the representations

$$yU_{\alpha-1,\beta} - T_{\alpha-1,\beta} = V_{\alpha-1,\beta} = c_{\alpha,\beta+1} x^{\alpha+\beta} + \mathcal{O}(x^{\alpha+\beta+1})$$

$$yU_{\alpha,\beta-1} - T_{\alpha,\beta-1} = V_{\alpha,\beta-1} = c_{\alpha+1,\beta} x^{\alpha+\beta} + \mathcal{O}(x^{\alpha+\beta+1})$$

using (5). Where $U = c_{\alpha+1,\beta} U_{\alpha-1,\beta} - c_{\alpha,\beta+1} U_{\alpha,\beta-1}$ and $T = c_{\alpha+1,\beta} T_{\alpha-1,\beta} - c_{\alpha,\beta+1} T_{\alpha,\beta-1}$ we obtain

$$yc_{\alpha+1,\beta} U - c_{\alpha,\beta+1} T = V = \mathcal{O}(x^{\alpha+\beta+1}).$$

Since T and U have degrees α and β we have $T = hT_{\alpha\beta}$, $U = hU_{\alpha\beta}$, $V = hV_{\alpha\beta}$ for some constant h . Equating the coefficients for x^α in the equation for T allows us to calculate $h = c_{\alpha\beta}$.

We obtain (7), (8), and (9) in similar fashion. \square

Corollary 1.1. (Frobenius)

$$(10)$$

$$c_{\alpha\beta} c_{\alpha,\beta+1} S_{\alpha+1,\beta} - (c_{\alpha,\beta+1} + c_{\alpha\beta} c_{\alpha+1,\beta+1} x) S_{\alpha\beta} + c_{\alpha+1,\beta} c_{\alpha+1,\beta+1} x S_{\alpha-1,\beta} = 0$$

$$(11)$$

$$c_{\alpha\beta} c_{\alpha+1,\beta} S_{\alpha,\beta+1} - (c_{\alpha,\beta+1} - c_{\alpha\beta} c_{\alpha+1,\beta+1} x) S_{\alpha\beta} + c_{\alpha,\beta+1} c_{\alpha+1,\beta+1} x S_{\alpha,\beta-1} = 0$$

These are recursion formulas which enable the calculation of the values of the polynomials T and U stepwise along any path starting from the constant entry $[0/0]$. If the polynomials $T_{\alpha\beta}$ and $U_{\alpha\beta}$ are known, then we may calculate the four constants

$$\begin{aligned} c_{\alpha\beta} &= [U_{\alpha\beta}]_0, \\ c_{\alpha+1,\beta} &= (-1)^\beta [U_{\alpha\beta}]_\beta, \\ c_{\alpha,\beta+1} &= (-1)^\beta [T_{\alpha\beta}]_\alpha, \\ c_{\alpha+1,\beta+1} &= \sum_{j=0}^{\beta} a_{\alpha+\beta+1-j} [U_{\alpha\beta}]_j. \end{aligned}$$

Knowing another adjacent set of polynomials T and U for one of the recursion formulas above, we are able to calculate the third set of adjacent polynomials.

Algorithm to calculate Padé approximants stepwise along a line through the table starting from $[0/0]$:

Let $0 < q < 1$. We follow a stepwise path through entries in the Padé Table where the ratio of the degrees of the numerators to the total degree is kept very close to q . Initialize $U_{00} = 1$, $T_{00} = a_0$, $U_{01} = a_0 - a_1x$, $T_{01} = a_0^2$, indicating an initial step downwards, with $\alpha\beta = 01$ for the next step. We calculate $c_{01}, c_{11}, c_{02}, c_{12}$ and set the current ratio $r = q$.

Each step starts with updating $r = r + q$.

If $r > 1$:

This signifies a step to the right and we reset $r = r - 1$.

If the previous step was downward, we use known $T_{\alpha,\beta-1}, U_{\alpha,\beta-1}$ and $T_{\alpha,\beta}, U_{\alpha,\beta}$ in formula 8 to find the new $U_{\alpha+1,\beta}$ and $T_{\alpha+1,\beta}$

If the previous step was to the right, we use formula 10 to calculate the new $U_{\alpha+1,\beta}$ and $T_{\alpha+1,\beta}$.

We complete this step by updating α, β to $\alpha + 1, \beta$ and calculating $c_{\alpha+1,\beta}, c_{\alpha+1,\beta+1}$

If $r < 1$:

This signifies a step downwards.

If the previous step was downward, we use formula 11 to find the new $U_{\alpha,\beta+1}$ and $T_{\alpha,\beta+1}$

If the previous step was to the right, we use formula 9 to calculate the new $U_{\alpha,\beta+1}$ and $T_{\alpha,\beta+1}$.

We complete this step by updating α, β to $\alpha, \beta + 1$ and calculating $c_{\alpha,\beta+1}, c_{\alpha+1,\beta+1}$.

□

Since these relations are homogeneous in S and the c -constants, they are not restrictive to the exact formulations T, U . It is sufficient that for adjacent Padé approximants $\frac{P_{\alpha_1\beta_1}}{Q_{\alpha_1\beta_1}}$ and $\frac{P_{\alpha_2\beta_2}}{Q_{\alpha_2\beta_2}}$ be *normalized*, i.e., that $P_{\alpha_1\beta_1} = kT_{\alpha_1\beta_1}$ and $P_{\alpha_2\beta_2} = kT_{\alpha_2\beta_2}$ for some fixed value k .

Corollary 1.2. *If $\frac{P_{\alpha_1\beta_1}}{Q_{\alpha_1\beta_1}}$ and $\frac{P_{\alpha_2\beta_2}}{Q_{\alpha_2\beta_2}}$ are two adjacent entries in the Padé Table, with $P_{\alpha_1\beta_1} = k_1T_{\alpha_1\beta_1}$ and $P_{\alpha_2\beta_2} = k_2T_{\alpha_2\beta_2}$. Then Theorem allows us to find the ratio $\frac{k_1}{k_2}$ and so normalize the representations.*

Proof. Let $P_{\alpha_1\beta_1} = k_1T_{\alpha_1\beta_1}$ and $P_{\alpha_2\beta_2} = k_2T_{\alpha_2\beta_2}$. There are four cases depending upon the adjacency.

- Horizontal adjacency: $\alpha_1, \beta_1 = \alpha, \beta$; $\alpha_2, \beta_2 = \alpha + 1, \beta$.
Using (2) and (4) establishes that

$$c_{\alpha+1,\beta} = \frac{(-1)^\beta}{k_1} [Q_{\alpha\beta}]_\beta = \frac{[Q_{\alpha+1,\beta}]_0}{k_2}.$$

so

$$(12) \quad [Q_{\alpha+1,\beta}]_0 P_{\alpha\beta} \text{ and } (-1)^\beta [Q_{\alpha\beta}]_\beta P_{\alpha,\beta+1}$$

are normalized.

- Vertical adjacency: $\alpha_1, \beta_1 = \alpha, \beta$; $\alpha_2, \beta_2 = \alpha, \beta + 1$.
Using (2) and (3) establishes that

$$c_{\alpha, \beta+1} = \frac{(-1)^\beta}{k_1} [P_{\alpha\beta}]_\alpha = \frac{[Q_{\alpha, \beta+1}]_0}{k_2}.$$

so

$$(13) \quad [Q_{\alpha, \beta+1}]_0 P_{\alpha\beta} \text{ and } (-1)^\beta [P_{\alpha\beta}]_\alpha P_{\alpha, \beta+1}$$

are normalized.

- Diagonal adjacency 1: $\alpha_1, \beta_1 = \alpha, \beta$; $\alpha_2, \beta_2 = \alpha + 1, \beta + 1$.
Using (2) and (5) establishes that

$$\begin{aligned} c_{\alpha+1, \beta+1} &= [V_{\alpha\beta}]_{\alpha+\beta+1} \\ &= \frac{1}{k_1} \sum_{j=0}^{\beta} a_{\alpha+\beta+1-j} [Q_{\alpha\beta}]_j \\ &= \frac{[Q_{\alpha+1, \beta+1}]_0}{k_2}. \end{aligned}$$

so

$$(14) \quad [Q_{\alpha+1, \beta+1}]_0 P_{\alpha\beta} \text{ and } \left(\sum_{j=0}^{\beta} a_{\alpha+\beta+1-j} [Q_{\alpha\beta}]_j \right) P_{\alpha+1, \beta+1}$$

are normalized.

- Diagonal adjacency 2: $\alpha_1, \beta_1 = \alpha\beta$; $\alpha_2, \beta_2 = \alpha + 1, \beta - 1$.
Using (3) and (4) establishes that

$$c_{\alpha+1, \beta} = \frac{(-1)^\beta}{k_1} [Q_{\alpha\beta}]_\beta = \frac{(-1)^{\beta-1}}{k_2} [P_{\alpha+1, \beta-1}]_\alpha$$

so

$$(15) \quad [P_{\alpha+1, \beta-1}]_\alpha P_{\alpha\beta} \text{ and } -[Q_{\alpha\beta}]_\beta P_{\alpha+1, \beta-1}$$

are normalized. □

An alternative is to adapt the recursion formulas to other standard representations of the Padé components. As an example Baker uses the definition

$$\frac{A_{\alpha\beta}}{B_{\alpha\beta}}$$

to denote the $[\alpha/\beta]$ representative with $B_{\alpha\beta}(0) = 1$.

Theorem 1.3. *Using the Baker definition the Frobenius recursion formulas may be rewritten as*

$$(16) \quad - \left(\frac{\sum_0^{\beta-1} a_{\alpha+\beta-j} [B_{\alpha,\beta-1}]_j}{[A_{\alpha-1,\beta}]_{\alpha-1} [B_{\alpha,\beta-1}]_{\beta-1}} \right) S'_{\alpha-1,\beta} + \left(\frac{\sum_0^{\beta} a_{\alpha+\beta-j} [B_{\alpha-1,\beta}]_j}{[A_{\alpha,\beta-1}]_{\alpha-1} [B_{\alpha-1,\beta}]_{\beta}} \right) S'_{\alpha,\beta-1} = S'_{\alpha\beta}$$

$$(17) \quad S'_{\alpha+1,\beta} - S'_{\alpha,\beta+1} = - \frac{[A_{\alpha,\beta+1}]_{\alpha}}{[A_{\alpha,\beta}]_{\alpha}} x S'_{\alpha\beta}$$

$$(18) \quad = \frac{[B_{\alpha+1,\beta}]_{\beta}}{[B_{\alpha,\beta}]_{\beta}} x S'_{\alpha\beta}$$

$$(19) \quad S'_{\alpha\beta} - S'_{\alpha+1,\beta} = \frac{\sum_0^{\beta} a_{\alpha+\beta+1-j} [B_{\alpha\beta}]_j}{\sum_0^{\beta-1} a_{\alpha+\beta-j} [B_{\alpha,\beta-1}]_j} x S'_{\alpha,\beta-1}$$

$$(20) \quad S'_{\alpha\beta} - S'_{\alpha,\beta+1} = \frac{\sum_0^{\beta} a_{\alpha+\beta+1-j} [B_{\alpha\beta}]_j}{\sum_0^{\beta} a_{\alpha+\beta-j} [B_{\alpha-1,\beta}]_j} x S'_{\alpha-1,\beta}$$

$$(21) \quad S'_{\alpha+1,\beta} - \left(1 + \frac{\sum_{j=0}^{\beta} a_{\alpha+\beta+1-j} [B_{\alpha\beta}]_j}{[A_{\alpha\beta}]_{\alpha} [B_{\alpha\beta}]_{\beta}} x \right) S'_{\alpha\beta} + \frac{\sum_{j=0}^{\beta} a_{\alpha+\beta+1-j} [B_{\alpha\beta}]_j}{\sum_{j=0}^{\beta} a_{\alpha+\beta-j} [B_{\alpha-1,\beta}]_j} x S'_{\alpha-1,\beta} = 0$$

$$(22) \quad S'_{\alpha,\beta+1} - \left(1 - \frac{\sum_{j=0}^{\beta} a_{\alpha+\beta+1-j} [B_{\alpha\beta}]_j}{[A_{\alpha\beta}]_{\alpha} [B_{\alpha\beta}]_{\beta}} x \right) S'_{\alpha\beta} + \frac{\sum_{j=0}^{\beta} a_{\alpha+\beta+1-j} [B_{\alpha\beta}]_j}{\sum_{j=0}^{\beta} a_{\alpha+\beta-j} [B_{\alpha,\beta-1}]_j} x S'_{\alpha,\beta-1} = 0$$

where S' holds the position for either A or B .

2. PADÉ APPROXIMANTS TO THE SYMMETRIC ZETA FUNCTION

2.1. Zeros of partial sums.

Szegő in his paper of 1924 [Sze24] showed that the zeros of the Taylor series of degree n of the function e^{nz} converge to the section of the curve $|ze^{1-z}| = 1$ lying inside the unit circle.

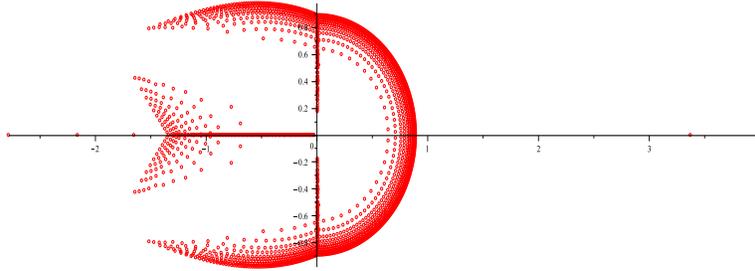


FIGURE 1. Scaled zeros of partial sums for $(z - 1)\zeta(z)$

Since the exponential function has no zeros, these are the so-called “spurious” zeros, and without the scaling, radiate to infinity.

This study was extended to Padé approximants to the exponential function by Saff and Varga in a series of three papers [SV76] [SV77] [SV78], where they showed that where the ratio of the degrees of the numerators and denominators are kept constant, the similarly scaled zeros converge to a curved left-side section of the Szeő curve while the poles converge to a curved right-side section of the reflected Szeő curve.

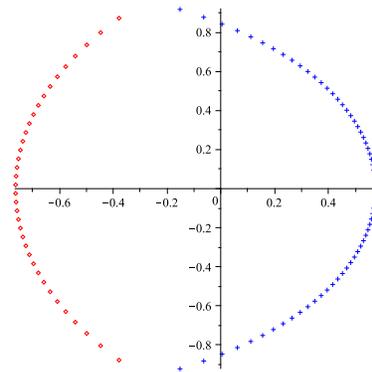


FIGURE 2. Zeros (circles) and poles (crosses) of Padé approximation to e^{100z} , numerator degree 34, denominator degree 64.

Unscaled, these zeros and poles radiate to infinity as well.

Varga and Carpenter [VC00] [VC01] [VC10] extended this again to Taylor series approximations of $\cos(z)$ and $\sin(z)$, which correspond to the real and imaginary parts of the exponential function. In these cases, as the degrees advance, an increasing number of zeros converge to actual zeros of the functions. For the scaled spurious zeros the limit curves are sections of the Szegő curve composed of the positive real component joined with its reflection and rotated by 90° . In this paper we

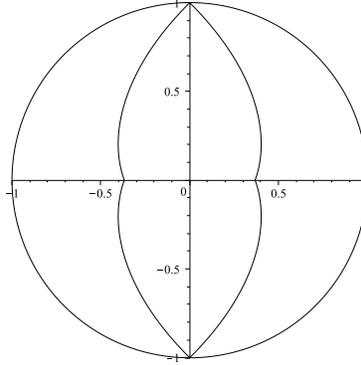


FIGURE 3. Sections of rotated Szegő curves

present computational results on the distributions of zeros for Taylor approximates for the symmetric Riemann zeta function and distributions of zeros and poles of Padé approximates.

3. THE RIEMANN ZETA FUNCTION AND THE SYMMETRIC RIEMANN ZETA FUNCTION

The Riemann zeta function $\zeta(s)$ is defined in the complex plane for $\Re(s) > \frac{1}{2}$ by the formula

$$\zeta(s) = \sum_{n \geq 1} \frac{1}{n^s} = \prod_{p \text{ prime}} \left(1 - \frac{1}{p}\right)^{-1}.$$

The product formula shows that $\zeta(s)$ has no zeros in this region.

It has an analytic continuation to a meromorphic function with a simple pole at $s = 1$ and satisfies the functional equation

$$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s) \zeta(1-s).$$

This also shows that $\zeta(s)$ has simple zeros at the negative even integers on the real line corresponding to the simple poles of the Gamma function, the so-called trivial zeros. All other zeros must be in the critical strip $0 \leq \Re(s) \leq 1$.

Riemann found a symmetric version of this through defining

$$\xi(s) = \frac{1}{2} \pi^{-\frac{s}{2}} s(s-1) \Gamma\left(\frac{s}{2}\right) \zeta(s)$$

which then satisfies

$$\xi(s) = \xi(1-s),$$

In this form, $\xi(s)$ is an analytic function, symmetric about the line $s = \frac{1}{2}$ and with the same zeros as $\zeta(s)$ in the critical strip. The Riemann Hypothesis is equivalent to the statement that all the zeros of $\xi(s)$ are on the line $s = \frac{1}{2}$.

4. CALCULATION OF TAYLOR AND PADÉ APPROXIMATES TO THE SYMMETRIC ZETA FUNCTION

First attempts at evaluating Taylor polynomials:

- Calculating exact coefficients of the Taylor series. This was very slow.
- Calculate coefficients using floating point arithmetic. Again too slow.
- Use polynomial interpolation at the even integers. This didn't converge.
- Calculate values for $\xi(s)$ and interpolate to evaluate the coefficients. This worked.

Calculating the Taylor polynomials:

- Values of $\xi(s)$ were calculated to 6144 digit precision at 4096 points equally spaced around a circle of radius $\frac{1}{4}$ centred at the point $s = \frac{1}{2}$.
- Both the Gamma and Zeta functions use the Euler-MacLaurin summation formula to compute numerical values. For this the first 10,000 Bernoulli numbers values were computed once and stored for later use.
- Due to conjugate and even symmetry only 1024 points needed to be evaluated. Translation from $s = \frac{1}{2}$ to the origin gives a series in even powers with real coefficients. This was used as a check in the calculation.
- Most of the CPU time was spent in evaluating the function $\xi(s)$.
- The fastest part of the computation was the polynomial interpolation which used the FFT (Fast Fourier Transform)

Navigating the Padé Table:

- The Taylor polynomial up to some degree were converted to a continued fraction.
- The continued fraction was transformed into a numerator polynomial and a denominator polynomial with the same degree sum.

For Padé approximates $\frac{P_m}{Q_n}$ of fixed total degree $m + n$, we calculate P_m starting from the Taylor polynomial $T_{m+n} = \frac{P_{m+n}}{Q_0}$ and $P_{m+n+1} = z^{m+n+1}$ using the iterations

$$P_{m-1} = P_{m+1} - q_m P_m$$

where q_m is the quotient obtained by dividing the polynomial P_{m+1} by P_m and P_{m+1} is the remainder. For Q_n we start from $Q_{-1} = 0$ and $Q_0 = 1$ and continue, using the iterations

$$Q_{n+1} = Q_{n-1} - q_m Q_n.$$

Defining the associated polynomials U_n starting from $U_{-1} = 1$ and $U_0 = 0$ and continuing inductively

$$U_{n+1} = U_{n-1} - q_m U_n$$

we obtain the Bézout identity

$$P_m = U_n x^{m+n+1} + Q_n T_{m+n}.$$

at each step.

Root finding:

- The roots of the above polynomials were obtained using Madsen's method, which is based on Newton's method.
- The polynomial root finding was the second most time-consuming operation.

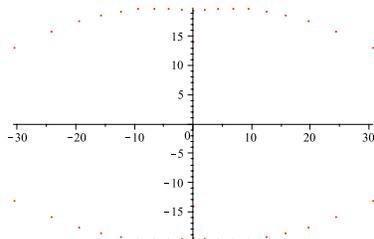


FIGURE 4. Zeros of degree 40 Taylor approximation to $\xi(z)$

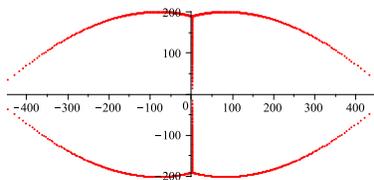


FIGURE 5. Zeros of degree 1024 Taylor approximation to $\xi(z)$

5. PRESENTATION OF RESULTS OF THE COMPUTATIONS

Zeros of Taylor polynomial approximations:

For each degree, zeros of the polynomial approximate the zeros of $\xi(s)$ up to some branch point. Beyond this, the zeros branching off in opposite directions do not correspond to zeros of $\xi(s)$. These are the "spurious" zeros.

Zeros and poles of Padé rational function approximations:

For each degree there are a number of Padé approximates possible, where this is the sum of the degrees of the numerator and denominator. A diagonal approximation has degrees of numerator and denominator equal.

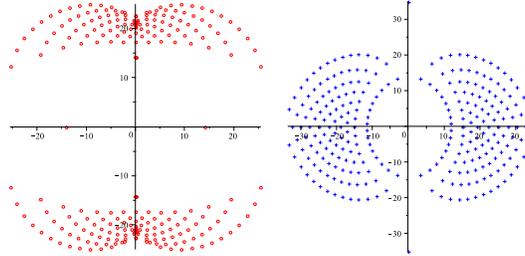


FIGURE 6. Zeros (left) and poles (right) of multiple Padé approximants to $\xi(z)$ of total degree 32 with the ratio of degrees varying

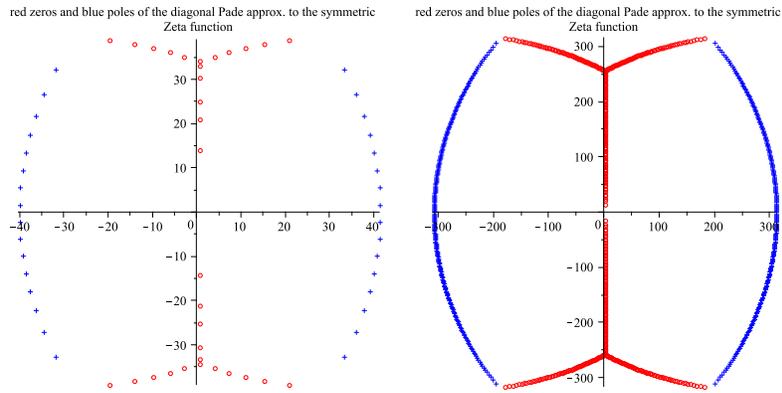


FIGURE 7. Zeros and poles for diagonal Padé approximations of degrees 64 and 1024 to $\xi(z)$

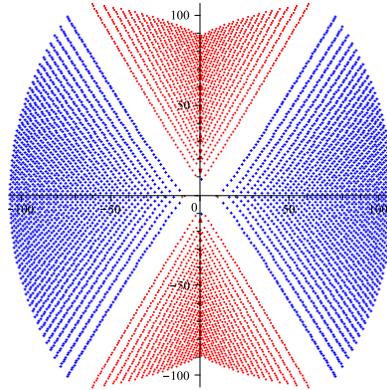


FIGURE 8. Zeros (circles) and poles (crosses) for diagonal Padé approximates to $\xi(s)$ for multiple degrees to 256

6. COMPARISON WITH APPROXIMATIONS TO $\cos(z)$

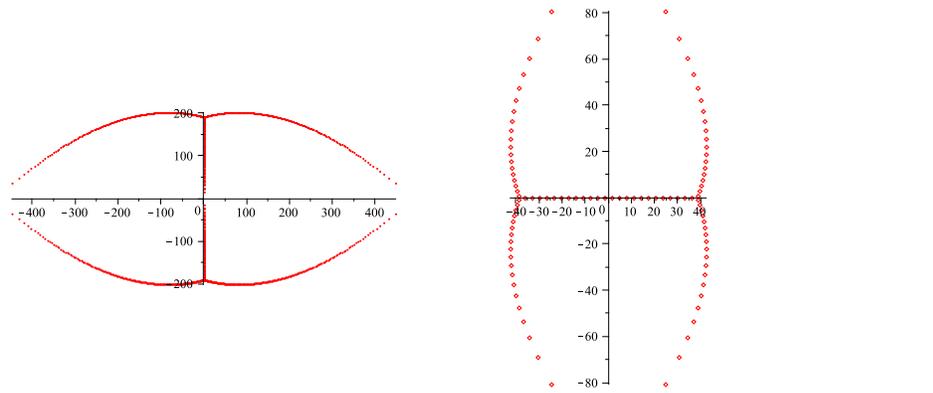


FIGURE 9. Comparison of zeros for Taylor approximations for $\xi(z)$ and $\cos(z)$

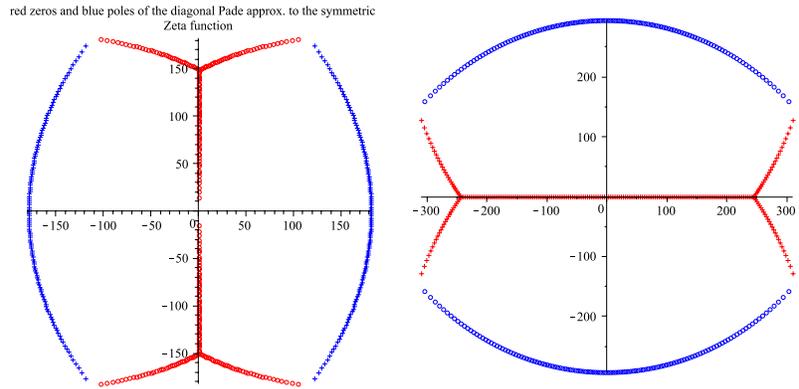


FIGURE 10. Comparison of zeros and poles for diagonal Padé approximations of degree 512 for $\xi(z)$ and $\cos(z)$

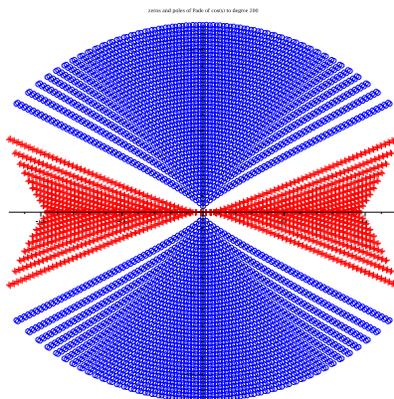


FIGURE 11. Zeros (crosses) and poles (circles) for diagonal Padé approximants to $\cos(z)$ for multiple degrees to 200

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