Some properties of Hermite–Padé approximants to e^z

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dedicated to Jerry Lange on the occasion of his 70th birthday

ABSTRACT. We investigate questions such as convergence, differential equations, location of zeros of Hermite–Padé approximants to e^z and display some numerical experiments concerning the distribution of zeros. We consider the known results about the more elementary Padé approximants to e^z as a general background for the discussion.

1. Introduction

Padé approximation may be seen as one of the many ways of performing approximation to analytic functions in the complex plane. One of the main features of the Padé approximants comes from the algebraic nature of their definition. Throughout, \mathcal{P}_k will denote the set of polynomials with complex coefficients, of degree at most k.

DEFINITION 1.1. Let f be a function analytic at the origin. The Padé approximant of degree (m,n) is defined as the rational function $P_{m,n}/Q_{m,n}$ such that

$$(Q_{m,n}f - P_{m,n})(z) = O(z^{m+n-1})$$
 as $z \to 0$,

with $P_{m,n} \in \mathcal{P}_m$ and $Q_{m,n} \in \mathcal{P}_n$.

Thus, given the Taylor's coefficients of the function f at the origin, the Padé approximants can be explicitly computed by solving a set of linear equations. There exists a whole theory based on algebraic tools such as determinants which leads to numerous identities, recursion relations and algorithms. In this connection, one can also mention the strong links that exist between Padé approximants, continued fractions and orthogonal polynomials.

The other aspect of the theory is the analytic aspect and the main interest, here, lies in properties such as convergence, asymptotics and distribution of zeros. In this respect, the Padé (or Baker-Gammel-Wills) conjecture plays a prominent role which predicts that, given a meromorphic function f, there exists an infinite subsequence $N \subset \mathbb{N}$ such that the Padé approximants of degree $(n,n), n \in N$ converge locally uniformly to f, away from the poles of f, as n tends to infinity

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(cf. [Sta97] for a recent overview of this conjecture). In general, analyticity is not sufficient in order to ensure convergence of the full sequence of Padé approximants, as the existence of spurious poles shows (cf. [Lub92, Per57, Wal74]).

In this paper, we shall describe a few results and numerical experiments that concern the analytic aspect of a classical generalization of Padé approximants, namely the Hermite–Padé approximants.

DEFINITION 1.2. Let (f_0, \ldots, f_m) be a vector of m+1 functions analytic at the origin. For any multi-index $n=(n_0,\ldots,n_m)\in\mathbb{N}^{m+1}$, the (latin or type I) Hermite–Padé approximants of degree n are defined as the nonzero vector of polynomials

$$(A_0,\ldots,A_m)\in\prod_{j=0}^m\mathcal{P}_{n_j-1}$$

such that

(1.1)
$$\sum_{i=0}^{m} A_i(z) f_i(z) = O(z^{|n|-1}) \quad \text{as} \quad z \to 0,$$

where $|n| = \sum_{i=0}^{m} n_i$.

Let us just recall that there exists another type of Hermite–Padé approximants, the german type or type II, which consists of simultaneous rational approximants. Concerning the algebraic and analytic aspects of Hermite–Padé approximants, we refer to [BGM96, dB85, Coa66, Coa67, Mah68] and [AS92, Nut84, Sta88] respectively.

In the sequel, we shall only consider the approximants in Definition 1.2 when specializing the choice of the vector of functions (f_0, \ldots, f_m) to be the vector of exponentials $(1, e^z, \ldots, e^{mz})$. An important property of such a vector is that it constitutes an example of a perfect system. It means that for any multi-index $n = (n_0, \ldots, n_m)$, any solution A_0, \ldots, A_m of (1.1) satisfies

$$\deg A_j = n_j - 1, \quad j = 0, \dots, m.$$

Hence, the solution to (1.1) is actually unique, up to a constant factor.

In the subsequent sections, we shall start from the known results about Padé approximants and discuss questions such as convergence, differential equations, location and asymptotic distribution of zeros of Hermite–Padé approximants.

Let us terminate this introduction by mentionning the well-known application of Padé approximation to number theory, which was initiated by Hermite, in proving the transcendence of e. A few references here, among others, are [Beu81, Pré96, Ass98, dP79].

2. Convergence of Hermite-Padé approximants to e^z

Let us first take a look at the Padé case of type (m, n). We thus consider two polynomials $P_{m,n}$ and $Q_{m,n}$, of respective degree m and n, such that

(2.1)
$$R_{m,n}(z) = Q_{m,n}(z)e^z - P_{m,n}(z) = O(z^{m+n+1}), \ Q_{m,n}(0) = 1.$$

Note that upon dividing the previous equation by e^z and changing z into -z, we get

$$P_{m,n}(-z)e^z - Q_{m,n}(-z) = O(z^{m+n+1}),$$

which implies, by uniqueness, that $Q_{n,m}(z)$ and $P_{m,n}(-z)$ are equal, up to a constant. The following theorem of Padé shows that for a rational function, interpolating the exponential function at zero with an order as high as possible suffices to imply uniform convergence in the complex plane to this exponential function.

THEOREM 2.1. With $P_{m,n}$ and $Q_{m,n}$ satisfying (2.1), we have

$$P_{m,n}/Q_{m,n} \to e^z$$
,

locally uniformly in \mathbb{C} as $m+n\to\infty$. Moreover, if $m/n\to\lambda$, one has separated convergence, namely

$$P_{m,n}(z) \to e^{\lambda z/(1+\lambda)}, \ Q_{m,n}(z) \to e^{-z/(1+\lambda)}.$$

In particular, in the diagonal case $m = n \to \infty$, we have

$$P_{n,n}(z) \to e^{z/2}, \ Q_{n,n}(z) \to e^{-z/2}.$$

The proof relies on the integral expressions of $P_{m,n}$ and $Q_{m,n}$

(2.2)
$$P_{m,n}(z) = \frac{1}{(n+m)!} \int_0^\infty e^{-t} (t+z)^m t^n dt,$$

(2.3)
$$Q_{m,n}(z) = \frac{1}{(n+m)!} \int_0^\infty e^{-t} (t-z)^n t^m dt.$$

Explicit forms are given by

$$P_{m,n}(z) = \sum_{j=0}^{m} \frac{(m+n-j)!m!z^{j}}{(m+n)!j!(m-j)!},$$

$$Q_{m,n}(z) = \sum_{j=0}^{n} \frac{(m+n-j)!n!(-z)^{j}}{(m+n)!j!(n-j)!},$$

(cf. [Per57]). Let us proceed with Hermite–Padé approximants, by considering the vector of exponentials $(1, e^z, \dots, e^{mz})$. This is one of the few cases where integral expressions can be given for the solutions to (1.1). Indeed, it is easily checked that the formulas

(2.4)
$$A_p(z) = \frac{1}{2i\pi} \int_{C_0} \frac{e^{\zeta z} d\zeta}{\prod_{l=0}^m (\zeta + p - l)^{n_l}}, \quad 0 \le p \le m,$$

where C_0 is a circle centered at the origin and of radius less than 1, define polynomials of degree $n_p - 1$ satisfying (1.1). Then, it is natural to ask whether the previous theorem can be generalized to Hermite–Padé approximants. The following result, whose proof can be found in [Wie97], answers this question in the diagonal case, that is when considering m + 1 polynomials A_0, \ldots, A_m such that

(2.5)
$$R(z) = \sum_{p=0}^{m} A_p(z)e^{pz} = O(z^{mn+n-1}),$$

and all the polynomials A_0, \ldots, A_m are of degree less than the same constant integer $n \in \mathbb{N}$.

THEOREM 2.2. Let A_0, \ldots, A_m be the Hermite-Padé approximants to the exponential function given by (2.4), with $n_l = n$, $0 \le l \le m$, of degree less than n. Let $\{-p - \eta_p, 0 < \eta_p < 1\}_{p=0}^{m-1}$ be the set of the m critical points, that is the m roots of the derivative, of the Pochhammer polynomial

$$(z)_m = z(z+1)\cdots(z+m-1).$$

Then, there exist some explicitly computable nonzero constants $\mu_{p,n}$, $0 \le p < m/2$, such that, as $n \to \infty$,

$$A_p(0) \sim (-1)^{mn} \mu_{p,n}, \ A_{m-p}(0) \sim (-1)^{n-1} \mu_{p,n}, \ 0 \le p < m/2.$$

Consequently, for n large, one can define \widetilde{A}_p as the polynomial obtained upon dividing A_p by its nonzero constant coefficient. Then

$$\widetilde{A}_p(z) \to e^{\eta_p z}, \ \widetilde{A}_{m-p}(z) \to e^{-\eta_p z}, \ 0 \le p < m/2,$$

locally uniformly in \mathbb{C} . If m is even, let $A_{m/2}^{(1)}$ (resp. $A_{m/2}^{(2)}$) be the subsequence of polynomials $A_{m/2}$ corresponding to even (resp. odd) indices n. Then, $A_{m/2}^{(1)}$ is an odd polynomial and $A_{m/2}^{(2)}$ an even polynomial. Moreover, there exists an explicitly computable nonzero constant $\mu_{m/2,n}$ such that, as $n \to \infty$,

$$\frac{dA_{m/2}^{(1)}}{dz}(0) \sim 2\eta_{m/2}\mu_{m/2,n}, \ A_{m/2}^{(2)}(0) \sim 2\mu_{m/2,n}.$$

For n large, let $\widetilde{A}_{m/2}^{(1)}$ and $\widetilde{A}_{m/2}^{(2)}$ be the polynomials obtained upon dividing $A_{m/2}^{(1)}$ and $A_{m/2}^{(2)}$ respectively by the nonzero derivative at zero and nonzero constant coefficient. Then, as $n \to \infty$,

$$(2.6) \quad \widetilde{A}_{m/2}^{(1)}(z) \to \frac{1}{2\eta_{m/2}} (e^{\eta_{m/2}z} - e^{-\eta_{m/2}z}), \ \widetilde{A}_{m/2}^{(2)}(z) \to \frac{1}{2} (e^{\eta_{m/2}z} + e^{-\eta_{m/2}z}),$$

uniformly on compact subsets of \mathbb{C} .

The proof relies on applying the saddle point method to the integral expressions (2.4) of the polynomials A_p . Using in the same way, the integral representation of the remainder term R,

(2.7)
$$R(z) = \frac{1}{2i\pi} \int_{C_{\infty}} \frac{e^{\zeta z} d\zeta}{\prod_{l=0}^{m} (\zeta - l)^{n_{l}}},$$

where C_{∞} is a circle centered at the origin and of radius greater than m, one may also show that in the diagonal case

$$R(z) \sim \frac{z^{mn+n-1}e^{mz/2}}{(mn+n-1)!},$$

uniformly on compact subsets of \mathbb{C} , as $n \to \infty$. The derivation of all the previous asymptotics for the non diagonal case can be obtained similarly.

REMARK 2.3. From Theorem 2.2, one easily recovers the assertions of Theorem 2.1 in the diagonal case. Indeed, the unique critical point of z(z+1) is -1/2 so that $\eta_0 = 1/2$.

EXAMPLE 2.4. When m=2 and

$$A_0(z) + A_1(z)e^z + A_2(z)e^{2z} = O(z^{3n-1}),$$

we consider the critical points of z(z+1)(z+2) which are $-1+1/\sqrt{3}$ and $-1-1/\sqrt{3}$ so that

$$\eta_0 = 1 - 1/\sqrt{3}, \eta_1 = 1/\sqrt{3}.$$

Then, from Theorem 2.2, one gets that

$$A_2(z) \sim (-1)^{n-1} \mu_{0,n} e^{-(1-1/\sqrt{3})z},$$

$$A_1(z) \sim (-1)^n \mu_{0,n} \left(e^{z/\sqrt{3}} + (-1)^{n-1} e^{-z/\sqrt{3}} \right),$$

$$A_0(z) \sim \mu_{0,n} e^{(1-1/\sqrt{3})z},$$

where $\mu_{0,n}$ may be seen to equal $\frac{1}{3\sqrt{2n\pi}} \left(\frac{3\sqrt{3}}{2}\right)^n$.

3. Some differential equations

Let us now establish the differential equations satisfied by the Hermite-Padé approximants A_0, \ldots, A_m such that (2.5) holds. For clarity, as before, we shall limit ourselves to the diagonal case, though the general case can be treated in a similar way. First, in connection with the Padé approximants $P_n := P_{n,n}$ and $Q_n := Q_{n,n}$ defined by (2.1), with m = n, we set

$$w_n(z) = e^{-z/2} z^{-n} P_n(z).$$

Then, $w_n(z)$ satisfies Whittaker's equation (cf. [Olv54, p.260])

$$d^2w(z)/dz^2 = \left\lceil \frac{1}{4} + \frac{n(n+1)}{z^2} \right\rceil w(z),$$

or, equivalently, P_n satisfies

(3.1)
$$nP_n(z) = (z+2n)P'_n(z) - zP''_n(z).$$

Also, from the remark after (2.1), we deduce that

(3.2)
$$nQ_n(z) = (z - 2n)Q'_n(z) + zQ''_n(z).$$

Let us now derive the generalization of (3.1) and (3.2) corresponding to the approximants A_0, \ldots, A_m . Consider the contour integral (2.7) in the diagonal case, that is, $n_l = n$, $0 \le l \le m$ and note that for any polynomial G, we have

(3.3)
$$G(D)R(z) = \frac{1}{2\pi i} \int \frac{G(\zeta)e^{\zeta z}d\zeta}{\prod_{l=0}^{m}(\zeta - l)^{n}},$$

where D denotes the differential operator d/dz. Set

(3.4)
$$L(t) = t(t-1)\dots(t-m).$$

Then we can apply partial integration to (3.3) with (n-1)L' instead of G and obtain

$$(n-1)L'(D)R(z) = \frac{1}{2\pi i} \int \frac{ze^{\zeta z}d\zeta}{\prod_{l=0}^{m} (\zeta - l)^{n-1}}.$$

On the other hand, the right hand side of the previous equation equals zL(D)R(z). Hence we get the differential equation

$$zL(D)R(z) - (n-1)L'(D)R(z) = 0.$$

Since the functions $1, e^z, e^{2z}, \dots, e^{mz}$ are linearly independent over the rational functions, the differential equation holds for each of the summands $A_p(z)e^{pz}$ of R(z). Hence

$$zL(D)(A_p e^{pz}) - (n-1)L'(D)(A_p e^{pz}) = 0.$$

Because of the identity $D(e^{pz}u) = e^{pz}(D+p)u$, this implies that

$$zL(D+p)A_p - (n-1)L'(D+p)A_p = 0.$$

We summarize the result in the next theorem.

THEOREM 3.1. Let A_0, \ldots, A_m be the diagonal Hermite-Padé approximants to the exponential function satisfying (2.5), of degree less than n, and let L be the polynomial defined by (3.4). Then, the following differential equations of order m+1 are satisfied:

(3.5)
$$zL(D+p)A_p = (n-1)L'(D+p)A_p, \quad 0 \le p \le m.$$

EXAMPLE 3.2. Let

$$A_0(z) + A_1(z)e^z + A_2(z)e^{2z} + A_3(z)e^{3z} = O(z^{19}),$$

define, up to a constant, the Hermite–Padé approximants of degree 4 of the vector $(1, e^z, e^{2z}, e^{3z})$. Assuming n=5, m=3 in Theorem 3.1, it is straightforward to check that

$$\begin{aligned} 24A_0 &= (88+6z)A_0' - (72+11z)A_0^{(2)} + (16+6z)A_0^{(3)} - zA_0^{(4)}, \\ 8A_1 &= (8+2z)A_1' + (24-z)A_1^{(2)} - (16+2z)A_1^{(3)} + zA_1^{(4)}, \\ 8A_2 &= (-8+2z)A_2' + (24+z)A_2^{(2)} + (16-2z)A_2^{(3)} - zA_2^{(4)}, \\ 24A_3 &= (-88+6z)A_3' - (72-11z)A_3^{(2)} - (16-6z)A_3^{(3)} + zA_3^{(4)}. \end{aligned}$$

REMARK 3.3. The differential equation (3.5) relates $A_p^{(m+1)}$ and the m+1 polynomials $A_p, A_p^{(1)}, \ldots, A_p^{(m)}$. By differentiating (3.5) several times, we get a linear relation with polynomial coefficients between any derivative $A_p^{(j)}, j \geq m+1$ and the polynomials $A_p, A_p^{(1)}, \ldots, A_p^{(m)}$. On the other hand, from the analog of formula (3.3) for the polynomial $A_{p,n}$, where, here, the second subscript denote the degree, we deduce that

$$L(D+p)^{j}A_{p,n} = A_{p,n-j}, \qquad 0 \le j \le n-1.$$

These observations allows one to compute, for each $p, 0 \le p \le m$, a recurrence relation involving the polynomials $A_{p,n}, \ldots, A_{p,n-m-1}$. Indeed, from what precedes, there are linear relations between $A_{p,n-j}$ and $A_{p,n}, A_{p,n}^{(1)}, \ldots, A_{p,n}^{(m)}$. Hence, a linear relation between $A_{p,n}, \ldots, A_{p,n-m-1}$ can be established.

4. On the zeros of Hermite-Padé approximants to e^z

In this section, we shall review some known facts about the zeros of Padé approximants to e^z and display some numerical experiments concerning the zeros of Hermite–Padé approximants. The first result in studying the zeros of such approximants may be the article of Szegő [Sze24], which considers the zeros of the partial sums $s_n(z) = \sum_{k=0}^n z^k/k!$ of the Taylor expansion of e^z . Note that $s_n(z)$ is the Padé approximant of e^z of degree (n,0). Szegő showed that the normalized partial

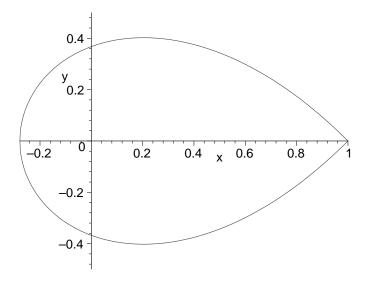


Figure 1

sum $s_n(nz)$ has all its zeros in $|z| \le 1$ for every $n \ge 1$, and that \hat{z} is a limit point of zeros of $\{s_n(nz)\}_{n=1}^{\infty}$ iff

$$|\hat{z}e^{1-\hat{z}}| = 1$$
 and $|\hat{z}| < 1$.

The so-called Szegő curve determined by the previous equations is shown in Figure 1. Concerning general Padé approximants, Saff and Varga have given in a series of papers (cf. [SV75, SV76, SV77, SV78] and the references therein) numerous results concerning the location of their zeros. Mainly using the three-term recurrence relation (or Frobenius relation) and the second-order differential equation satisfied by these approximants, they could prove the existence of a sector, alternatively a parabolic region determined by the type of the approximants, free of zeros. A sharp lower bound as well as an upper bound on the modulus of these zeros could also be established in this way. Moreover, by means of the saddle point method applied to the integral representation (2.2) and (2.3), asymptotic estimates were obtained, from which the asymptotic distribution of the zeros of the normalized Padé approximants and of the error function could be determined. The eye-shaped curve which consists in the limit points of zeros, poles or zeros of the remainders generalizes the Szegő curve. We refer the reader to the original papers for complete statements of the theorems and to [BGM96, pp.268-274] for a nice summary of these results. Let us now proceed with Hermite-Padé approximants of the vector $(1, e^z, \dots, e^{mz})$. To the author's knowledge, such precise results as above are not yet available for the zeros of these approximants. We only state the seemingly weak upper bound (cf. [Wie97]):

PROPOSITION 4.1. For any $m \ge 1$ and $n \ge 2$, all the zeros of the Hermite-Padé approximants $A_p(z)$ satisfying (2.5) lie in

(4.1)
$$|z| \le 2(n-1/3) \left[\sum_{k=1}^{p} \frac{1}{k} + \sum_{k=1}^{m-p} \frac{1}{k} \right], \ 0 \le p \le m,$$

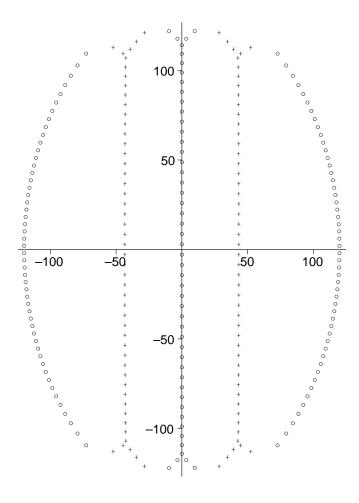


FIGURE 2

where it is understood, in case p = 0 or p = m, that the sum in (4.1) ranging from k = 1 to 0 vanishes.

Finally, we give some numerical results about these zeros. In Figure 2, we have graphed the zeros of the five polynomials A_0 , A_1 , A_2 , A_3 , A_4 , all of degree 50, such that

(4.2)
$$A_0 + A_1 e^z + A_2 e^{2z} + A_3 e^{3z} + A_4 e^{4z} = O(z^{254}).$$

The 50 zeros of the polynomials A_0 to A_4 appear in 5 sequences from the left to the right of the figure. The zeros of A_0 , A_2 , A_4 are denoted by circles "o". Those of A_1 and A_3 are denoted by cross "+".

In the two subsequent figures, Figures 3 and 4, we still represent, in the same way as in Figure 2, the zeros of 5 polynomials such that the expansion (4.2) has maximal vanishing at zero, but now, we consider non diagonal approximation. Indeed, we

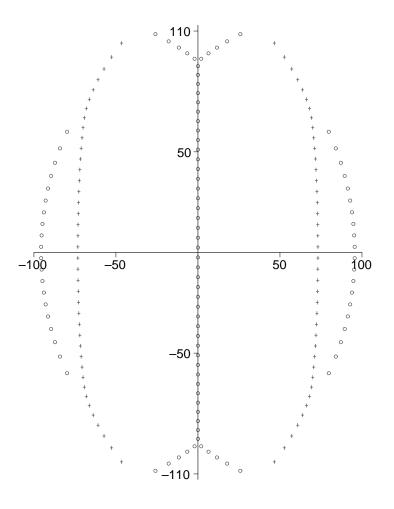


FIGURE 3

choose

$$\deg A_0 = \deg A_4 = 20$$
, $\deg A_1 = \deg A_3 = 40$, $\deg A_2 = 60$,

and

$$\deg A_0 = 12$$
, $\deg A_1 = 24$, $\deg A_2 = 36$, $\deg A_3 = 48$, $\deg A_4 = 60$,

respectively.

We may conjecture that, with a convenient normalization, the zeros of the Hermite–Padé approximants cluster, as the degrees tend to infinity, to fixed curves, analog of the Szegő or eye-shaped curves. As in the Padé case, these curves would be determined by the different ratios of the degrees of the approximants, as they tend to infinity. It seems possible that using the differential equations in Theorem 3.1, one can obtain some information on the location and asymptotic distribution of the zeros of the Hermite–Padé approximants to a vector of exponentials.

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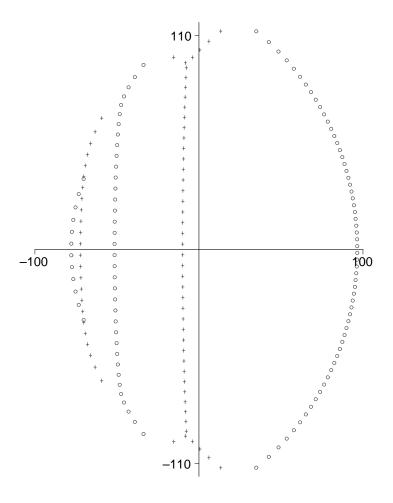


Figure 4

comments and especially for having supplied us with a proof of Theorem 3.1, simpler than that given in a first version of this paper.

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