How well does the Hermite–Padé approximation smooth the Gibbs phenomenon ?

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Abstract

In order to reduce the Gibbs phenomenon exhibited by the partial Fourier sums of a periodic function f, defined on $[-\pi, \pi]$, discontinuous at 0, Driscoll and Fornberg considered so-called singular Fourier-Padé approximants constructed from the Hermite-Padé approximants of the system of functions $(1, g_1(z), g_2(z))$, where $g_1(z) = \log(1-z)$ and $g_2(z)$ is analytic, such that $\mathrm{Re}\,(g_2(e^{it})) = f(t)$. Convincing numerical experiments have been obtained by these authors, but no error estimates have been proven so far. In the present paper we study the special case of Nikishin systems and their Hermite-Padé approximants, both theoretically and numerically. We obtain rates of convergence by using orthogonality properties of the functions involved along with results from logarithmic potential theory. In particular, we address the question of how to choose the degrees of the approximants, by considering diagonal and row sequences, as well as linear Hermite-Padé approximants. Our theoretical findings and numerical experiments confirm that these Hermite-Padé approximants are more efficient than the more elementary Padé approximants, particularly around the discontinuity of the goal function f.

Key words: Hermite-Padé approximants, Gibbs phenomenon, orthogonal polynomials, Nikishin systems, Padé approximants, logarithmic potential theory.

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1 Introduction

To reduce the Gibbs phenomenon exhibited by the truncated Fourier series of a periodic discontinuous function f, many different techniques have been proposed, see [16] and the more recent [4, 5] for a review of some of the recent methods, and [18] for localizing such discontinuities. For a real function f having a logarithmic singularity, the location of which is known, Driscoll and Fornberg [8] suggested the construction of a class of approximants which incorporate the knowledge of that singularity. More precisely, their approach is the following one: let g_2 denote the series on the unit circle such that

$$f(t) = \mathrm{Re}\,(g_2(e^{it})).$$

Then, the goal is to approach g_2 on the unit circle (and more precisely its real part). It is typical that the singularity of the function f, located at 0 say, corresponds to a logarithmic singularity for g_2, then located at 1, and that this function g_2 is analytic in the complex plane, with a branch cut that can be taken as the interval $[1,\infty)$. Defining $g_1(z) = \log(1-z)$, we obtain an explicit function with a singularity at 1 of the same type, and we may consider the problem of determining polynomials p_0, p_1, p_2 such that the residual

$$p_0(z) + p_1(z)g_1(z) + p_2(z)g_2(z)$$

has a zero of highest order at the origin, namely $n_0 + n_1 + n_2 + 2$ where n_j denotes the degree of p_j, $j = 0, 1, 2$. By assumption, the first coefficients of the Fourier expansion of f are known, hence the first coefficients of the Taylor expansion of g_2 at the origin are also known, so that the above problem can be solved.

Driscoll and Fornberg propose the approximation

$$\Pi_{\vec{n}}(z) = -\frac{p_0(z) + p_1(z)g_1(z)}{p_2(z)}, \tag{1.1}$$

of the function g_2. Note that when $p_1(z) = 0$ (or formally $n_1 = -1$) we recover the usual Padé approximant of g_2 of type (n_0, n_2) and if moreover p_2 is constant, then $\Pi_{\vec{n}}(z)$ reduces to the usual Taylor sums. The computation of the Padé approximants, by means of the ϵ-algorithm applied to the sequence of partial Taylor sums of g_2, was already suggested by Wynn [28] as an interesting way to smooth the Gibbs phenomenon for functions with jumps. Brezinski displayed very convincing numerical experiments [6], and, subsequently, an analysis of the convergence of the Padé approximants along the columns of the Padé table for a function g_2 which is the sum of some hypergeometric function and a smooth function was performed by three of the authors in [3]. It is shown there that the consideration of a denominator of degree n_2 in the approximants improves the rate of convergence by a factor $n_0^{-2n_2}$. Note that if g_2 is a Stieltjes function, then the rate of convergence is even geometric for ray sequences where n_0, n_2 both go to infinity with n_0/n_2 tending to some constant. For an application of Padé approximants to filtering in the context of nonlinear partial differential equations such as the incompressible inviscid Boussinesq convection flow see [7].

In their paper, Driscoll and Fornberg gave numerical evidence that considering an additional function g_1 as described above allows one for still better approximations of g_2. Indeed, if the jump location is known it makes sense to incorporate this information into the approximant itself. The approach via Hermite–Padé approximants is motivated by the fact that, provided $p_2(0) \neq 0$, the error of the approximant $\Pi_{\vec{n}}$ has the highest order of vanishing at the origin, among all approximants of the form (1.1). This property entails for instance consistency, namely if g_2 is of the form as on the right-hand side of (1.1), then $\Pi_{\vec{n}}(z) = g_2(z)$.

If both functions g_1 and g_2 are analytic in the unit disk, then one should expect that the above approximants give a small error around the origin, and hopefully on the unit circle $|z| = 1$ (except maybe in a neighborhood of the singularity 1), which is the set of arguments where we are interested in. Of course, the convergence of the approximants $\Pi_{\vec{n}}$ to the goal function g_2 essentially depends on the location of their poles.

The aim of this paper is to study the convergence of sequences of Hermite–Padé approximants for a class of functions known in approximation theory as *Nikishin systems.*

Our analysis is based mainly on orthogonality properties exhibited by the polynomials and functions involved, along with results from the logarithmic potential theory.

In Section 2, we define the model problem we are interested in and recall the definition of the Hermite–Padé approximants we want to study. In Section 3, we derive the rate of convergence achieved by the Hermite–Padé approximants. These estimates include the solution of a vector equilibrium problem with external field. In Section 4, we discuss error estimates for some significant particular cases, namely diagonal and row sequences of approximants and linear Hermite-Padé approximants (approximants without denominator) and compare these estimates with those achieved by the simpler Padé approximants. In the last section, we present numerical experiments. In particular, we describe a numerical procedure to compute the solution of the involved vector equilibrium problem. This illustrate our theoretic results and allows one to verify the agreement of the estimated rates of convergence with the effective errors.

2 Hermite–Padé approximants

Throughout, $\mathcal{P}_n$ will denote the space of complex polynomials of degree at most n. We assume that the function f to be reconstructed has a discontinuity, the location of which is known (say, at 0), but not its amplitude. Let $f \in \mathcal{C}^{n_1}([-\pi,\pi]\setminus\{0\})$ be a periodic function with left and right derivatives of order $0, 1, \ldots, n_1$ at $t = 0$. A typical such function is the saw-tooth function

$$s(t) = \pi + t \quad \text{for } t \in (-\pi, 0], \qquad s(t) = -\pi + t \quad \text{for } t \in (0, \pi], \tag{2.1}$$

with a jump of magnitude 2π at $t = 0$ in $[-\pi, \pi)$, where we notice that $\mathrm{Im}\,(g_1(z)) = \arg(1 - z) = s(t)/2$ for $z = e^{it}$. A basic observation in the work of Eckhoff [9, 10, 11] was that there exist real numbers $d_0, \ldots, d_{n_1}$ such that the function

$$e(t) := f(t) - \left(\sum_{j=0}^{n_1} d_j \sin^j(t)\right) s(t) \in \mathcal{C}^{n_1}([-\pi,\pi])$$

is "smooth" and can be well approximated by a Fourier series of order n_0. In terms of $z = e^{it}$, by writing

$$f(t) = \mathrm{Re}\,(g_2(z)), \qquad \sum_{j=0}^{n_1} d_j \sin^j(t) = -2\,\mathrm{Im}\,(p_1(z)),$$

a reasonable approximation is

$$f(t) \approx \mathrm{Re}\Big(-p_0(z) - p_1(z)\log(1 - z)\Big)$$

with unknown polynomials $p_0 \in \mathcal{P}_{n_0}$, $p_1 \in \mathcal{P}_{n_1}$, such that $p_0(z) + p_1(z)\log(1-z) + g_2(z) = \mathcal{O}(z^{n_0+n_1+2})$ as $z \to 0$. This is a particular case of the Hermite–Padé approximants defined as follows (for more details and properties see for instance [2, Chapter 8, Section 5]).

Definition 2.1. Let $g_1(z)$, $g_2(z)$ be two functions analytic at 0 and define, up to a normalization factor, the polynomials $p_j \in \mathcal{P}_{n_j}$ for $j = 0, 1, 2$ such that

$$p_0(z) + p_1(z)g_1(z) + p_2(z)g_2(z) = \mathcal{O}(z^{n_0+n_1+n_2+2}) \quad \text{as} \quad z \to 0. \tag{2.2}$$

The *Hermite–Padé approximant* of $g_2(z)$ (or in short HP approximant) of order $\vec{n} = (n_0, n_1, n_2)$ is defined as

$$\Pi_{\vec{n}}(z) = -\frac{p_0(z) + p_1(z)g_1(z)}{p_2(z)}. \tag{2.3}$$

Choosing $g_1(z) = \log(1-z)$, the singular Fourier-Padé approximants of $f(t) = \mathrm{Re}\,(g_2(e^{it}))$ introduced by Driscoll and Fornberg [8] are then given by the real part $\mathrm{Re}\,(\Pi_{\vec{n}}(e^{it}))$, and hence we wish to discuss the error of HP approximants on the unit circle. We should notice that (2.3) is an unusual expression for the approximation of functions via Hermite-Padé forms defined by (2.2), for more classical approaches including integral approximants we refer the reader to [2].

For $n_2 = 0$, we recover from (2.3) the approach proposed by Eckhoff, based on approximants with built-in singularity, see [9, 10, 11]. If instead $p_1(z) = 0$ (or formally $n_1 = -1$) then we simply get the Fourier-Padé approximants. A study of these last approximants as a tool to reduce the Gibbs phenomenon has been done in [3]. In particular, their rates of convergence have been estimated for various functions with jumps.

We will restrict ourselves to the above approximants (2.3) for the class of Markov functions

$$g_1(z) = \log(1-z) = z\int_0^1 \frac{dx}{1-xz}, \quad g_2(z) = z\int_0^1 \frac{u(x)\,dx}{1-xz}, \tag{2.4}$$

with

$$u(x) = \int_c^d \frac{d\tau(y)}{x-y}, \quad [c,d] \cap [0,1] = \emptyset. \tag{2.5}$$

In the special case $d\tau(y) = (-y)^\alpha dy$ with $\alpha \in (-1, 0)$, and $(c, d) = (-\infty, 0)$, we obtain for g_2 a scalar multiple of the function $G^{(\alpha,0)}$ whose Padé approximants were considered in [3].

The set of Markov functions $(1, g_1(1/z), g_2(1/z))$ is an example of a Nikishin system. Such systems were originally studied in [20, 21]. It is remarkable that the polynomials and residuals involved in their Hermite–Padé approximants satisfy orthogonality relations with respect to varying weights. As a consequence, their n-th root asymptotics can be given in terms of the solution of a vector equilibrium problem in potential theory. This theory is described in [22, Chapter 5].

3 Potential theory and estimates on the rate of convergence

In this section, we study the rate of convergence of the Hermite–Padé approximants, introduced above, as the total degree $n = n_0 + n_1 + n_2 \to \infty$. Throughout, we assume that $n_0 \geq n_1 \geq n_2$ and consider ray sequences n_0, n_1, n_2 such that

$$\frac{n_0}{n} \to \rho_0, \quad \frac{n_1}{n} \to \rho_1, \quad \frac{n_2}{n} \to \rho_2, \tag{3.1}$$

as n tends to infinity. Note that from the assumption $n_0 \geq n_1 \geq n_2$ follows that

$$\rho_0 \geq \rho_1 \geq \rho_2.$$

The rate of convergence in a nth-root sense can be obtained via a vector equilibrium problem in potential theory with external fields. To state the result, we need the notion of a logarithmic potential in the complex plane,

$$U^{\mu}(z) = \int \log \frac{1}{|z-t|} d\mu(t),$$

associated to a probability measure μ. By probability measure, we mean, as usual, a positive measure of mass 1. An example of such a measure is the Dirac measure δ_0 with a mass 1 at the origin. Note that the potential U^{μ} has a physical interpretation, namely it corresponds to the electric potential of a positive unit charge whose distribution in the plane is described by the measure μ. The usefulness of logarithmic potentials in approximation theory is easily understood from the elementary remark that a polynomial is basically the exponential of a discrete potential, more precisely, for a polynomial p of degree n, we have

$$\frac{1}{n} \log(1/|p(z)|) = U^{\mu_n}(z),$$

where μ_n denotes the discrete measure with masses $1/n$ at the zeros of p. For general facts about logarithmic potential theory, we refer the reader to [19, 23, 24]. The vector equilibrium problem and its numerical resolution is discussed in more details in Section 5.2.

We will also restrict ourselves to the case where the measure τ in the definition (2.5) of $u(x)$ has some kind of regularity. More precisely, we will assume that τ is regular in the sense of [25] (we will write $\tau \in \mathbf{Reg}$ in the sequel), meaning that the corresponding orthonormal polynomials have regular n-th root asymptotic behavior, see [25, Chapter 3] for details. Different criteria for this notion of regularity, as well as their sharpness, are discussed in [25, Chapter 4]. For instance, one of the simplest criteria is the Erdős-Turan condition, which says that the measure τ supported on the interval $[c, d]$ is regular if its Radon–Nikodym derivative with respect to the Lebesgue measure is positive almost everywhere on this interval.

Now, the n-th root asymptotic behavior for the error function is described by the following theorem.

Theorem 3.1. *Assume that $[c, d]$ is a compact interval and that the measure $\tau \in \mathbf{Reg}$. Then, the error function $(g_2 - \Pi_{\vec{n}})(s)$ satisfies, locally uniformly for $s = 1/z$, $z \in \mathbb{C} \setminus ([0, 1] \cup [c, d])$,*

$$\lim_{n\to\infty} \frac{1}{n} \log |(g_2 - \Pi_{\vec{n}})(s)| = (\rho_1 + \rho_2)U^{\mu}(z) + \rho_2 U^{\nu}(z) + (\rho_0 - \rho_2)U^{\delta_0}(z) - W - w, \quad (3.2)$$

In (3.2), the probability measures μ and ν, and the constants W and w, solve a specific vector equilibrium problem in potential theory which is precisely stated in Lemma 3.5.

The proof of Theorem 3.1 is based upon orthogonality relations satisfied by quantities related to the Hermite-Padé approximants, that we introduce now. We set

$$A_n(z) = z^{n_1} p_1(1/z), \quad B_n(z) = z^{n_2} p_2(1/z), \quad C_n(z) = A_n(z) + z^{n_1 - n_2} B_n(z) u(z),$$

where p_1 and p_2 satisfy (2.2). Hence we have that, as $z \to \infty$,

$$R_n(z) := z^{n_0}p_0(1/z) + A_n(z)z^{n_0-n_1}g_1(1/z) + B_n(z)z^{n_0-n_2}g_2(1/z) = \mathcal{O}\left(\frac{1}{z^{n_1+n_2+2}}\right), \quad (3.3)$$

with $\deg A_n \leq n_1$, $\deg B_n \leq n_2$. In the next lemma, we show that $\deg B_n = n_2$. Hence, we may (and do) assume throughout that the normalization of (3.3) is chosen so that B_n is a monic polynomial. Let us also mention that $C_n(z)$ cannot have more than n_1+n_2+1 zeros in $(0,1)$. We let the reader check that this fact follows by using an argument similar to the one given in the proof of [22, Theorem 4.4 p.141].

Lemma 3.2. *The expression $C_n(z)$ satisfies the following orthogonality relations,*

$$\int_0^1 x^{n_0-n_1}C_n(x)x^k dx = 0, \quad k = 0, \ldots, n_1+n_2, \quad (3.4)$$

and it has exactly n_1+n_2+1 simple zeros in $(0,1)$. Let H_n denote the monic polynomial of degree n_1+n_2+1 whose roots are these zeros. Then, the relations (3.4) may be rewritten as

$$\int_c^d x^k x^{n_1-n_2}\frac{B_n(x)}{H_n(x)}d\tau(x) = 0, \quad k = 0, 1, \ldots, n_2-1. \quad (3.5)$$

Hence, B_n is of exact degree n_2 with all its zeros, which are simple, in (c,d).

The ratio C_n/H_n admits the following integral representation in $\mathbb{C} \setminus (c,d)$,

$$\frac{C_n(x)}{H_n(x)} = \frac{1}{B_n(x)}\int_c^d t^{n_1-n_2}\frac{B_n^2(t)}{x-t}\frac{d\tau(t)}{H_n(t)}. \quad (3.6)$$

Proof. By applying Cauchy's formula in a neighbourhood of infinity, we obtain in view of (3.3) that

$$\int_{T_\rho} z^k R_n(z)dz = 0, \quad k = 0, \ldots, n_1+n_2,$$

where T_ρ is any circle of radius ρ large enough. Plugging the integral representations for g_1 and g_2 and using Fubini's formula, we get

$$\int_{x=0}^1 \left(\int_{z\in T_\rho} z^k\left(z^{n_0-n_1}\frac{A_n(z)}{z-x} + z^{n_0-n_2}u(x)\frac{B_n(z)}{z-x}\right)dz\right)dx = 0,$$

which leads to (3.4) by applying Cauchy's formula to the inner integral. These relations imply that $C_n(z)$ has at least n_1+n_2+1 simple zeros in $(0,1)$ and so it has exactly n_1+n_2+1 such zeros by the remark before the statement of the lemma.

Next, $C_n(z)/H_n(z)$ is analytic in $\overline{\mathbb{C}} \setminus (c,d)$ and is of order z^{-n_2-1} at infinity. Let Γ be a contour around (c,d). The Cauchy formula applied in the exterior of Γ shows that

$$\int_\Gamma z^k\frac{C_n(z)}{H_n(z)}dz = 0, \quad k = 0, \ldots, n_2-1.$$

If, moreover, Γ does not enclose $(0,1)$, which is always possible, we deduce by using the expression for C_n that

$$\int_\Gamma z^k z^{n_1-n_2}\frac{B_n(z)}{H_n(z)}u(z)dz = 0, \quad k=0,\ldots,n_2-1.$$

Making use of the integral formula (2.5) for u along with Fubini's formula, we obtain (3.5). Finally, to prove (3.6), we make the additional assumption that the above contour Γ does not enclose the given point x in $\mathbb{C}\setminus(c,d)$. By Cauchy's formula applied outside of Γ, we get

$$\begin{aligned}\frac{C_n(x)}{H_n(x)} &= -\frac{1}{2i\pi}\int_\Gamma \frac{C_n(\zeta)}{H_n(\zeta)}\frac{d\zeta}{\zeta-x} = -\frac{1}{2i\pi}\int_\Gamma \zeta^{n_1-n_2}B_n(\zeta)\frac{u(\zeta)}{H_n(\zeta)}\frac{d\zeta}{\zeta-x}\\ &= \int_c^d t^{n_1-n_2}\frac{B_n(t)}{x-t}\frac{d\tau(t)}{H_n(t)} = \frac{1}{B_n(x)}\int_c^d t^{n_1-n_2}\frac{B_n^2(t)}{x-t}\frac{d\tau(t)}{H_n(t)},\end{aligned}$$

where we have used the orthogonality relations (3.5) in the last equality. □

In order to establish the rate of convergence of the Hermite–Padé approximants, we need additional results. We next give an integral representation of the error function $R_n(z)$ defined in (3.3).

Lemma 3.3. *For z a complex number not in $(0,1)$, it holds that*

$$R_n(z) = \frac{1}{H_n(z)}\int_0^1 x^{n_0-n_1}H_n(x)\frac{C_n(x)}{z-x}dx. \tag{3.7}$$

Proof. From the definitions of g_1, g_2, and R_n, the product H_nR_n may be written as

$$\begin{aligned}H_n(z)R_n(z) = H_n(z)z^{n_0}p_0(1/z) &+ \int_0^1 (z^{n_0-n_1}A_n(z)H_n(z) - x^{n_0-n_1}A_n(x)H_n(x))\frac{dx}{z-x}\\ &+ \int_0^1 (z^{n_0-n_2}B_n(z)H_n(z) - x^{n_0-n_2}B_n(x)H_n(x))\frac{u(x)dx}{z-x}\\ &+ \int_0^1 (x^{n_0-n_1}A_n(x) + x^{n_0-n_2}B_n(x)u(x))\frac{H_n(x)dx}{z-x}.\end{aligned}$$

The first three terms in the right-hand side of the previous equation are polynomials, the sum of which vanishes because $H_n(z)R_n(z)$ and the last integral behave like $\mathcal{O}(1/z)$ at infinity. Hence $H_n(z)R_n(z)$ equals that last integral which gives (3.7) in view of the definition of C_n. □

We also need the following classical result about orthonormal polynomials with respect to varying weights.

Lemma 3.4. *Let σ be a probability measure with support in a given interval $[\alpha,\beta]$, and let w_n, $n\geq 0$, be a sequence of continuous positive weights on $[\alpha,\beta]$ such that $w_n^{1/n}(x)$ tends to $w(x)=e^{-2Q(x)}$ uniformly in $[\alpha,\beta]$. Define $\{p_{k,n}\}$, $k,n\geq 0$, to be the sequence of orthonormal polynomials with respect to the varying weights w_n, satisfying*

$$\int p_{j,n}(x)p_{k,n}(x)w_n(x)d\sigma(x) = \delta_{jk}, \quad n\geq 0.$$

*Moreover, assume that the measure $\sigma \in$ **Reg**. Then, as $n \to \infty$, the normalized zero counting measure χ_n of the polynomial $p_{n,n}$ converges in the weak-star sense to the measure σ_w supported on $[\alpha, \beta]$, characterized by the variational equations*

$$\begin{aligned} U^{\sigma_w}(x) + Q(x) &\geq W, \quad x \in [\alpha, \beta], \\ U^{\sigma_w}(x) + Q(x) &= W, \quad x \in \operatorname{supp}(\sigma_w), \end{aligned}$$

where $U^{\sigma_w}(x)$ denotes the logarithmic potential of the measure σ_w and W is some real constant.

Proof. This well-known result follows for instance from the fact that it holds true for any sequence of monic polynomials, asymptotically minimal for the weighted sup norm on $[\alpha, \beta]$ and the fact that the weighted sup norm and the weighted L^2 norm associated to a regular measure are asymptotically equivalent in the n-th root sense, see respectively [24, Theorem 4.2 p.170] and [25, Theorem 3.2.3 p.84] for details. □

In the next lemma, we describe the vector equilibrium problem in potential theory with external fields that we mentioned in Theorem 3.1.

Lemma 3.5. *The problem of finding two probability measures μ and ν, respectively supported in $[0, 1]$ and $[c, d]$, satisfying the the variational conditions*

$$2(\rho_1 + \rho_2)U^{\mu}(x) - \rho_2 U^{\nu}(x) + (\rho_0 - \rho_1)U^{\delta_0}(x) \geq W, \quad x \in [0, 1], \tag{3.8}$$

$$2(\rho_1 + \rho_2)U^{\mu}(x) - \rho_2 U^{\nu}(x) + (\rho_0 - \rho_1)U^{\delta_0}(x) = W, \quad x \in \operatorname{supp}(\mu), \tag{3.9}$$

and

$$2\rho_2 U^{\nu}(x) - (\rho_1 + \rho_2)U^{\mu}(x) + (\rho_1 - \rho_2)U^{\delta_0}(x) \geq w, \quad x \in [c, d], \tag{3.10}$$

$$2\rho_2 U^{\nu}(x) - (\rho_1 + \rho_2)U^{\mu}(x) + (\rho_1 - \rho_2)U^{\delta_0}(x) = w, \quad x \in \operatorname{supp}(\nu), \tag{3.11}$$

where W and w are some real constants, admits a solution, which is unique.

Remarks. The proof of Lemma 3.5 follows from classical arguments in potential theory. We omit the details, but refer the reader also to the discussion in §5.2. Note that the external field given by the potential U^{δ_0} corresponds to the occurrence of the weights $x^{n_0 - n_1}$ and $x^{n_1 - n_2}$ in the orthogonality relations (3.4)–(3.5). Such an additional weight also appears e.g. in [12], where generalized Hermite–Padé approximants of type II of Nikishin systems are investigated.

Finally, we can give the proof of Theorem 3.1.

Proof of Theorem 3.1. Let μ_n and ν_n respectively denote the normalized zero counting measures of the polynomials H_n and B_n, and let $(\overline{\mu}, \overline{\nu})$ be any limit point in the weak topology of the sequence (μ_n, ν_n). By (3.5), we know that $B_n(x)$ is orthogonal with respect to the varying weight $x^{n_1 - n_2}/H_n(x)d\tau$. Since we are assuming that $d\tau$ is regular and since

$$\lim_{n \to \infty} \frac{1}{n} \log |x^{n_1 - n_2}/H_n(x)| = -(\rho_1 - \rho_2)U^{\delta_0}(x) + (\rho_1 + \rho_2)U^{\overline{\mu}}(x),$$

we deduce from Lemma 3.4 that $\overline{\nu}$ and $\overline{\mu}$ satisfy (3.10)–(3.11).

Next we determine the n-th root asymptotics of the ratio $|C_n(x)/H_n(x)|$. For that we use the integral representation (3.6). We have

$$\left|\int_c^d t^{n_1-n_2}\frac{B_n^2(t)}{x-t}\frac{d\tau(t)}{H_n(t)}\right| \le \frac{1}{\min_{t\in[c,d]}|x-t|}\int_c^d |t|^{n_1-n_2}B_n^2(t)\frac{d\tau(t)}{|H_n(t)|},$$

and

$$\left|\int_c^d t^{n_1-n_2}\frac{B_n^2(t)}{x-t}\frac{d\tau(t)}{H_n(t)}\right| \ge \begin{cases} \dfrac{1}{\max_{t\in[c,d]}|x-t|}\int_c^d |t|^{n_1-n_2}B_n^2(t)\dfrac{d\tau(t)}{|H_n(t)|}, & \text{if } x \text{ is real,} \\ \dfrac{|\operatorname{Im} x|}{\max_{t\in[c,d]}|x-t|^2}\int_c^d |t|^{n_1-n_2}B_n^2(t)\dfrac{d\tau(t)}{|H_n(t)|}, & \text{if } \operatorname{Im} x \neq 0. \end{cases}$$

Consequently, since we assume that the interval (c,d) is compact, the previous lower bound does not vanish and the problem of estimating the integral in (3.6) is equivalent to that of estimating

$$\int_c^d |t|^{n_1-n_2}B_n^2(t)\frac{d\tau(t)}{|H_n(t)|},$$

in the n-th root sense. Applying [25, Theorem 3.2.3], the above weighted L^2 norm of B_n behaves in the n-th root sense just as its weighted sup norm

$$\sup_{t\in(c,d)} |t|^{n_1-n_2}\frac{B_n^2(t)}{|H_n(t)|}.$$

In terms of the limit measures $\overline{\mu}$ and $\overline{\nu}$, the logarithm of its n-th root tends, as $n\to\infty$, to $-\overline{w}$ where we set

$$\overline{w} = \inf_{t\in(c,d)}(2\rho_2 U^{\overline{\nu}} + (\rho_1-\rho_2)U^{\delta_0} - (\rho_1+\rho_2)U^{\overline{\mu}}).$$

Note that this uses the fact that the polynomials B_n have been normalized to be monic. Now, with (3.6), we get

$$\lim_{n\to\infty}\frac{1}{n}\log\left|\frac{C_n(z)}{H_n(z)}\right| = \rho_2 U^{\nu}(z) - \overline{w}. \tag{3.12}$$

Next, the relations (3.4) may be interpreted as the orthogonality of $H_n(x)$ with respect to the varying weights $x^{n_0-n_1}C_n(x)/H_n(x)$. Lemma 3.4 and (3.12) thus show that $\overline{\nu}$ and $\overline{\mu}$ satisfy (3.8)–(3.9). Therefore, by uniqueness of the solution to the problem displayed in Lemma 3.5, we must have $\overline{\nu}=\nu$ and $\overline{\mu}=\mu$. This also shows the weak convergence of the entire sequences of measures

$$\nu_n \to \nu, \quad \mu_n \to \mu, \quad \text{as } n\to\infty.$$

Finally, we use the integral representation (3.7) to prove that the function $R_n(z)$, defined by (3.3), satisfies

$$\lim_{n\to\infty}\frac{1}{n}\log|R_n(z)| = (\rho_1+\rho_2)U^{\mu}(z) - W - w, \quad z\in\mathbb{C}\setminus[0,1], \tag{3.13}$$

locally uniformly. By an argument as above, the integral in (3.7) behaves in a n-th root sense as the L^2-norm of H_n with respect to the varying weights $x^{n_0-n_1}C_n(x)/H_n(x)$, which itself behaves like its weighted sup norm

$$\sup_{x\in(0,1)} |x|^{n_0-n_1} \left|\frac{C_n(x)}{H_n(x)}\right| H_n^2(x).$$

The logarithm of the n-th root of the above sup tends, as $n\to\infty$, to

$$\sup_{x\in(0,1)} (-(\rho_0-\rho_1)U^{\delta_0}(x) + \rho_2 U^{\nu}(x) - 2(\rho_1+\rho_2)U^{\mu}(x)) - w = -W - w,$$

where we have used (3.12), the fact that $\overline{w} = w$, and the variational conditions (3.8)–(3.9) in the last equality. Along with the fact that $\mu_n \to \mu$ as $n\to\infty$, we get (3.13). From that, the definition (3.3) of $R_n(z)$, and the fact that $\nu_n \to \nu$ as $n\to\infty$, (3.2) follows. □

4 Comparison of particular sequences of Hermite–Padé approximants with Padé approximants

In this section we compare the rate achieved by the Hermite–Padé approximants, obtained in Theorem 3.1, with that of the simpler Padé approximants. In particular, the latter do not incorporate a singularity corresponding to the one found in the goal function g_2. We perform this comparison for sequences of approximants of some specific degrees (n_0, n_1, n_2), as $n\to\infty$, which we think are of some significance with respect to numerical experiments. Namely, we will consider the case of approximants corresponding to ray sequences with limits $\rho_0 \geq \rho_1 = \rho_2 > 0$ (which we will call here the diagonal case), the case of linear approximants, that is, without denominator ($n_2 = 0$), which was studied by Eckhoff, and finally the "row case" such that the degree of denominator n_2 remains constant as $n = n_0 + n_1 + n_2$ goes to infinity. Here the denomination "row case" refers to the usual Padé table where Padé approximants with denominators of the same degree are put in rows, see [2, Chapter 1]. Of course, in each case, the comparison will be made with Padé approximants of a type $\vec{m} = (m_0, -1, m_2)$, $m_0 \geq m_2$, such that the total degree $m = m_0 + m_2$ equals $n+1$, so that the calculations of the Hermite–Padé and Padé approximants assume the knowledge of the same number of Taylor coefficients of the goal function g_2. Moreover, since the computations of the Hermite–Padé approximants of type (n_0, n_1, n_2) and of the Padé approximants of type $(m_0, -1, m_2)$ require the resolutions of linear systems of dimensions $n_1 + n_2 + 1$ and m_2 respectively, we shall choose $m_2 = n_1 + n_2 + 1$. In this way, the computations of the two kinds of approximants will be of the same order of complexity, in the sense that they are based on the resolution of linear systems of equal dimensions. Note that the previous conditions completely determine the type of the Padé approximant, namely it has to be chosen so that

$$m_0 = n_0, \quad m_2 = n_1 + n_2 + 1.$$

To perform our comparison, we first recall the rate of approximation achieved by the Padé approximants. Assume that the rational fraction $\Theta_{\vec{m}} = -\widetilde{P}_0/\widetilde{P}_2$ is the (unique)

Padé approximant of type $(m_0, -1, m_2)$, $m = m_0 + m_2$, of the function g_2 at the origin, that is, the following property holds true,

$$\widetilde{P}_0(z) + \widetilde{P}_2(z) g_2(z) = \mathcal{O}(z^{m_0+m_2+1}) \quad \text{as } z \to 0,$$

or equivalently,

$$\widetilde{R}_m(z) = z^{m_0} \widetilde{P}_0(1/z) + \widetilde{B}_m(z) z^{m_0-m_2} g_2(1/z) = \mathcal{O}\left(\frac{1}{z^{m_2+1}}\right) \quad \text{as } z \to \infty, \tag{4.1}$$

where $\widetilde{B}_m(z) = z^{m_2} \widetilde{P}_2(1/z)$. Throughout, the normalization is chosen so that $\widetilde{B}_m$ is a monic polynomial. As in the proof of Lemma 3.2, by using the Cauchy formula and the assumption that $m_0 \geq m_2$, we can show the orthogonality relations,

$$\int_0^1 x^{m_0-m_2} \widetilde{B}_m(x) x^k u(x) dx = 0, \quad k = 0, \ldots, m_2 - 1, \tag{4.2}$$

from which follows in particular that all the zeros of $\widetilde{B}_m$ lie in $(0, 1)$ and are simple. Moreover, the function $\widetilde{R}_m(z)$ has the following integral representation,

$$\widetilde{R}_m(z) = \frac{1}{\widetilde{B}_m(z)} \int_0^1 x^{m_0-m_2} \widetilde{B}_m^2(x) \frac{u(x)}{z - x} dx. \tag{4.3}$$

Next, consider a ray sequence $m_0, m_2 \to \infty$ such that

$$\frac{m_0}{m} \to \sigma_0, \quad \frac{m_2}{m} \to \sigma_2,$$

as $m = m_0 + m_2$ tends to infinity. Note that the assumption $m_0 \geq m_2$ implies that $\sigma_0 \geq \sigma_2$. Then, as in the previous section, the rate of convergence in a m-th root sense of the corresponding Padé approximants can be given in terms of an extremal probability measure $\widetilde{\mu}$, supported on $[0, 1]$, solution of an equilibrium problem in potential theory. Here, the measure is characterized by the following variational conditions:

$$2\sigma_2 U^{\widetilde{\mu}}(x) + (\sigma_0 - \sigma_2) U^{\delta_0}(x) \geq \widetilde{W}, \quad x \in [0, 1], \tag{4.4}$$

$$2\sigma_2 U^{\widetilde{\mu}}(x) + (\sigma_0 - \sigma_2) U^{\delta_0}(x) = \widetilde{W}, \quad x \in \operatorname{supp}(\widetilde{\mu}). \tag{4.5}$$

Then, it can be proved, in the same way as in the previous section, that

$$\lim_{m\to\infty} \frac{1}{m} \log |\widetilde{R}_m(z)| = \sigma_2 U^{\widetilde{\mu}}(z) - \widetilde{W}, \quad z \in \mathbb{C} \setminus [0, 1], \tag{4.6}$$

and that the error function $(g_2 - \Theta_{\vec{m}})(s)$, $s = 1/z$, satisfies for $z \in \mathbb{C} \setminus [0, 1]$,

$$\lim_{m\to\infty} \frac{1}{m} \log |(g_2 - \Theta_{\vec{m}})(s)| = 2\sigma_2 U^{\widetilde{\mu}}(z) + (\sigma_0 - \sigma_2) U^{\delta_0}(z) - \widetilde{W}. \tag{4.7}$$

4.1 Diagonal Hermite–Padé approximants

Here, as explained at the beginning of the section, we study a sequence of approximants of type $\vec{n} = (n_0, n_1, n_2)$ such that the ratios in (3.1) satisfy $\rho_0 \geq 2\rho_1 = 2\rho_2 > 0$. We compare these approximants to Padé approximants of type $\vec{m} = (n_0, -1, n_1 + n_2 + 1)$ and show that the two kinds of approximants behave differently near the point 1, which is the point of special interest regarding the Gibbs phenomenon. For our conclusion to hold, the type of the Padé approximants is not important, and we could have chosen different types, as long as the limits $\sigma_0 \geq \sigma_2$ remain positive. Note that, with our choice of degrees, we have $\sigma_0 = \rho_0 > 0$ and $\sigma_2 = \rho_1 + \rho_2 = 2\rho_1 > 0$.

Proposition 4.1. *Assume that the hypotheses of Theorem 3.1 are satisfied and that the degrees of the Hermite–Padé and Padé approximants $\Pi_{\vec{n}}$ and $\Theta_{\vec{m}}$ are chosen as above. Then,*

$$\lim_{\substack{z\to 1\\ |z|=1, z\neq 1}} \lim_{n\to\infty} |(g_2 - \Pi_{\vec{n}})(z)|^{1/n} < 1, \qquad \lim_{\substack{z\to 1\\ |z|=1, z\neq 1}} \lim_{m\to\infty} |(g_2 - \Theta_{\vec{m}})(z)|^{1/m} = 1. \tag{4.8}$$

Consequently, there exists a neighborhood of 1 in $\mathbb{C} \setminus (0, 1)$ in which the Hermite–Padé approximants achieve a rate of convergence which is better than the rate of the Padé approximants.

Proof. According to Theorem 3.1, the rate of convergence of the Hermite–Padé approximants is given by (3.2) where the right-hand side can be decomposed as

$$(2\rho_1 U^\nu(x) - 2\rho_1 U^\mu(x) - w) - (W - 4\rho_1 U^\mu(x) + \rho_1 U^\nu(x) - (\rho_0 - \rho_1)U^{\delta_0}(x)). \tag{4.9}$$

The variational conditions on $[c, d]$ imply that the measure ν is the balayage of μ on $[c, d]$, and also that

$$w = 2\rho_1 \int g_{\overline{\mathbb{C}}\setminus[c,d]}(\zeta, \infty) d\mu(\zeta)$$

and

$$2\rho_1 U^\nu(z) - 2\rho_1 U^\mu(z) - w = -2\rho_1 \int g_{\overline{\mathbb{C}}\setminus[c,d]}(\zeta, z) d\mu(\zeta), \quad z \in \mathbb{C} \setminus [c, d], \tag{4.10}$$

where $g_{\overline{\mathbb{C}}\setminus[c,d]}(\zeta, x)$ denotes the Green function of the unbounded domain $\overline{\mathbb{C}} \setminus [c, d]$, see [24, Chapter II, Sections 4 and 5] for details. Since the Green function is positive in the complement of $[c, d]$, we deduce from (4.10) that the first term in (4.9) is negative outside $[c, d]$, and in particular in a neighborhood of 1. Next, the measure μ must also satisfy variational conditions on $[0, 1]$, namely

$$4\rho_1 U^\mu(x) - \rho_1 U^\nu(x) + (\rho_0 - \rho_1)U^{\delta_0}(x) \geq W, \quad x \in [0, 1], \tag{4.11}$$

$$4\rho_1 U^\mu(x) - \rho_1 U^\nu(x) + (\rho_0 - \rho_1)U^{\delta_0}(x) = W, \quad x \in \operatorname{supp}(\mu). \tag{4.12}$$

Let us prove that the point 1 belongs to $\operatorname{supp}(\mu)$. Assume this is not the case and that $a = \max(\operatorname{supp}(\mu)) < 1$. Then, denoting by $F(x)$ the expression in the left-hand sides of (4.11)–(4.12), we get, for $x \in (a, 1]$,

$$F'(x) = -4\rho_1 \int_0^1 \frac{d\mu(t)}{x - t} + \rho_1 \int_c^d \frac{d\nu(t)}{x - t} - (\rho_0 - \rho_1)\frac{1}{x}.$$

If $[c,d]$ lies on the right of $[0,1]$, then all terms are negative, while, if $[c,d]$ lies on the left of $[0,1]$, then the second term becomes positive but the sum of the first two terms remains negative. In both cases, we conclude that the derivative is negative on $(a,1]$, which contradicts the facts that $F(a) = W$ and $F(1) \geq W$. Hence, $1 \in \operatorname{supp}(\mu)$ and $F(1) = W$ which implies that the second term in (4.9) vanishes at 1. Consequently, we obtain that the rate of convergence of the Hermite–Padé approximants remains geometric in a neighborhood of 1.

For the Padé approximants, according to (4.4)–(4.5), the rate of convergence depends on the measure $\widetilde{\mu}$ satisfying the variational conditions

$$4\rho_1 U^{\widetilde{\mu}}(x) + (\rho_0 - 2\rho_1)U^{\delta_0}(x) \geq \widetilde{W}, \quad x \in [0,1], \tag{4.13}$$

$$4\rho_1 U^{\widetilde{\mu}}(x) + (\rho_0 - 2\rho_1)U^{\delta_0}(x) = \widetilde{W}, \quad x \in \operatorname{supp}(\widetilde{\mu}), \tag{4.14}$$

where $\widetilde{W}$ is some real constant. This extremal problem also appears in the study of the incomplete polynomials of Lorentz, see [24, Chapter IV, Example 1.16] for details. In particular, it is known that

$$\operatorname{supp} \widetilde{\mu} = [\theta^2, 1] \quad \text{with } \theta = \frac{\rho_0 - 2\rho_1}{\rho_0 + 2\rho_1}.$$

Then, according to (4.7), the rate of convergence is given by

$$\lim_{m\to\infty} \frac{1}{m} \log |(g_2 - \Theta_{\vec{m}})(s)| = 4\rho_1 U^{\widetilde{\mu}}(z) + (\rho_0 - 2\rho_1)U^{\delta_0}(z) - \widetilde{W}. \tag{4.15}$$

From (4.14) evaluated at $x = 1$ and from the continuity principle for potentials, we obtain in (4.15) a rate which tends to zero as z tends to 1. This finishes the proof of the proposition. □

4.2 Linear Hermite–Padé approximants ($n_2 = 0$)

Let us now consider linear Hermite–Padé approximants, that is without denominators, of type $\vec{n} = (n_0, n_1, 0)$, with $\rho_0 \geq \rho_1 > 0$, corresponding to the approximants studied by Eckhoff, see [9, 10, 11]. We compare these approximants with Padé approximants of type $\vec{m} = (n_0, -1, n_1 + 1)$.

Proposition 4.2. *Assume that the hypotheses of Theorem 3.1 are satisfied and that the degrees of the linear Hermite–Padé approximants $\Pi_{\vec{n}}$ and of the Padé approximants $\Theta_{\vec{m}}$ are chosen as above. Then, the same conclusions as in Proposition 4.1, in particular (4.8), hold true.*

Proof. By adapting the proofs of Lemmas 3.2, 3.3 and Theorem 3.1, one may check that, in the present case, there is only one measure μ that governs the convergence of the Hermite–Padé approximants, which must satisfies the variational conditions

$$2\rho_1 U^{\mu}(x) + (\rho_0 - \rho_1)U^{\delta_0}(x) \geq W, \quad x \in [0,1], \tag{4.16}$$

$$2\rho_1 U^{\mu}(x) + (\rho_0 - \rho_1)U^{\delta_0}(x) = W, \quad x \in \operatorname{supp}(\mu), \tag{4.17}$$

for some real constant W. This extremal problem is of the same type as the one in (4.13)–(4.14). Here, we have

$$\operatorname{supp}\mu = [\theta^2, 1] \quad \text{with } \theta = \frac{\rho_0 - \rho_1}{\rho_0 + \rho_1}. \tag{4.18}$$

Then, Theorem 3.1 tells us that the rate of convergence of the Hermite–Padé approximants is given by

$$\begin{aligned}\lim_{n\to\infty} \frac{1}{n} \log |(g_2 - \Pi_{\vec{n}})(s)| &= \rho_1 U^\mu(z) + \rho_0 U^{\delta_0}(z) - W - w, \\ &= (2\rho_1 U^\mu(z) + (\rho_0 - \rho_1)U^{\delta_0}(z) - W) - \rho_1(U^\mu(z) - U^{\delta_0}(z) + w),\end{aligned}$$

where $n = n_0 + n_1$, $s = 1/z$ and

$$w = \inf_{x\in[c,d]} (-U^\mu(x) + U^{\delta_0}(x)). \tag{4.19}$$

In view of (4.17) and (4.18), to derive the inequality in (4.8), it is sufficient to show that

$$U^\mu(1) - U^{\delta_0}(1) + w > 0. \tag{4.20}$$

From the value of the constant w in (4.19), we rewrite inequality (4.20) as

$$\inf_{x\in[c,d]} (-U^\mu(x) + U^{\delta_0}(x)) > -U^\mu(1) + U^{\delta_0}(1).$$

The function $-U^\mu(z) + U^{\delta_0}(z)$ is superharmonic in $\overline{\mathbb{C}} \setminus \operatorname{supp}\mu$ (note that it vanishes at infinity). Hence by the minimum principle for superharmonic functions,

$$\inf_{x\in[c,d]} (-U^\mu(x) + U^{\delta_0}(x)) > \inf_{x\in\operatorname{supp}\mu} (-U^\mu(x) + U^{\delta_0}(x)).$$

On $\operatorname{supp}(\mu)$, we have by (4.17) that

$$-U^\mu(x) + U^{\delta_0}(x) = -\frac{W}{2\rho_1} + \frac{\rho_0 + \rho_1}{2\rho_1} U^{\delta_0}(x),$$

so that the minimum of $-U^\mu(x) + U^{\delta_0}(x)$ on $\operatorname{supp}\mu = [\theta^2, 1]$ is attained at 1, whence

$$\inf_{x\in[c,d]} (-U^\mu(x) + U^{\delta_0}(x)) > -U^\mu(1) + U^{\delta_0}(1),$$

which proves our contention.

Next, observe that the convergence of the Padé approximants is governed by the same extremal problem as (4.16)–(4.17). Indeed, if we set $\sigma_0 = \rho_0$ and $\sigma_2 = \rho_1$ in (4.4)–(4.5), we get the variational conditions (4.16)–(4.17). Hence the measure μ also appears in the rate of convergence of the Padé approximants which, according to (4.7), is given by

$$\lim_{m\to\infty} \frac{1}{m} \log |(g_2 - \Theta_{\vec{m}})(s)| = 2\rho_1 U^\mu(z) + (\rho_0 - \rho_1) U^{\delta_0}(z) - W. \tag{4.21}$$

Then, the equality in (4.8) follows from (4.17) and the fact that $1 \in \operatorname{supp}(\mu)$, see (4.18) (note that (4.17) implies that the potential U^μ is continuous when restricted to its support so that, by the principle of continuity for potentials, it is also continuous there considered as a function on $\mathbb{C}$). $\square$

4.3 Hermite–Padé approximants with fixed denominator degree

We now consider sequences of approximants $\Pi_{\vec{n}}$ of type $\vec{n} = (n_0, n_1, n_1)$ such that the degree n_0 tends to infinity while n_1 remains constant. Hence, here we have $\rho_0 = 1$, $\rho_1 = \rho_2 = 0$. We estimate the error function corresponding to $\Pi_{\vec{n}}$ and compare these Hermite–Padé approximants with Padé approximants of type $\vec{m} = (n_0, -1, 2n_1 + 1)$ in the vicinity of 1.

In the sequel we shall use the following notations. We denote by $P_n^{(\beta)}(x)$, $n \geq 0$, the orthonormal polynomial of degree n on $[0, 1]$, satisfying the orthogonality relations

$$\int_0^1 P_n^{(\beta)}(x) P_m^{(\beta)}(x) x^\beta dx = \delta_{n,m},$$

with respect to the Jacobi type weight x^β. We also set $\alpha_n^{(\beta)} > 0$ for its leading coefficient, $\gamma_n^{(\beta)}$ for its smallest zero, and $p_n^{(\beta)}(x) = P_n^{(\beta)}(x)/\alpha_n^{(\beta)}$ for the corresponding monic polynomial.

Then, the following proposition holds true.

Proposition 4.3. *Assume that the degrees of the Hermite-Padé and Padé approximants are chosen as above, that the measure $d\tau(y)$ in the definition (2.5) of the function $u(x)$ is regular and that its support lies on the negative real axis, that is $[c, d] \subset (-\infty, 0)$. Let $s = 1/z$ on the unit circle, with $|z - 1| \leq 1/2$. Then, for n_0 sufficiently large so that*

$$C \leq (n_0 - 2n_1 - 2)(1 - \mathrm{Re}\,(z)), \tag{4.22}$$

we have

$$|(g_2 - \Pi_{\vec{n}})(s)| \leq \frac{\widetilde{C} |z - 1|^{2n_1}}{\left| P_{2n_1+1}^{(n_0 - 2n_1 - 1)}(z) \right|^2}, \tag{4.23}$$

and

$$\frac{|(g_2 - \Pi_{\vec{n}})(s)|}{|(g_2 - \Theta_{\vec{m}})(s)|} \leq \widehat{C} |z - 1|^{2n_1 - 1}, \tag{4.24}$$

where C, $\widetilde{C}$ and $\widehat{C}$ are some constants that depend only on n_1.

Remarks. It can be checked that $P_{2n_1+1}^{(n_0-2n_1-1)}(1) = \sqrt{n_0 + 2n_1 + 2}$. Hence, for z fixed near 1, the upper bound in (4.23) is of order $\mathcal{O}(n_0^{-1})$ as n_0 tends to infinity. Inequality (4.24) shows that, for z sufficiently close to 1, the Hermite–Padé approximants do somewhat better than the Padé ones.

For the proof, we need two lemmas. The first one is a classical result from Markov, see [27, Theorem 6.12.2 p.116].

Lemma 4.4. *Denote by x_k and $\widetilde{x}_k$ the zeros in increasing order of the orthogonal polynomials of degree n with respect to the measures $d\mu$ and $w(x)d\mu$ where $w(x)$ is a positive continuous weight, increasing on the support of $d\mu$. Then,*

$$x_k < \widetilde{x}_k, \quad k = 1, \ldots, n.$$

The second lemma gives a lower bound for the smallest zero of the Jacobi type polynomial $P_n^{(\beta)}(x)$.

Lemma 4.5. *There exists a constant C_n depending only on n such that for any β larger than 1, say, it holds that*

$$\gamma_n^{(\beta)} \geq 1 - \frac{C_n}{\beta}. \tag{4.25}$$

Proof. For the smallest zero $\widehat{\gamma}_n^{(0,\beta)}$ of the usual Jacobi polynomial $\widehat{P}_n^{(0,\beta)}(x)$ on $[-1,1]$, it is known that

$$\lim_{\beta\to\infty} \beta(1-\widehat{\gamma}_n^{(0,\beta)}) = 2\xi_n,$$

where ξ_n denotes the largest zero of the Laguerre polynomial $L_n^{(0)}(x)$, see [27, Formula 6.71.11 p.144]. Hence, (4.25) follows from the fact that $\beta(1-\widehat{\gamma}_n^{(\beta)})$ is a positive continuous function of β on $[1,\infty)$ and the fact that $\gamma_n^{(0,\beta)} = (\widehat{\gamma}_n^{(0,\beta)}+1)/2$. $\square$

We are now in a position to prove Proposition 4.3.

Proof of Proposition 4.3. First we establish a lower bound for the difference between the function g_2 and its Padé approximants $\Theta_{\vec{m}}$. From (4.1)–(4.3), we know that, for $s = 1/z$,

$$(g_2 - \Theta_{\vec{m}})(s) = \frac{1}{z^{n_0-2n_1-1}\widetilde{B}_m^2(z)} \int_0^1 x^{n_0-2n_1-1}\widetilde{B}_m^2(x)\frac{u(x)}{z-x}dx,$$

where the monic polynomial $\widetilde{B}_m$ of degree $2n_1+1$ is orthogonal with respect to the weight $x^{n_0-2n_1-1}u(x)$ on $[0,1]$. By assumption $|z-1| \leq 1/2$ implies that $\max_{t\in[0,1]}|z-t| = 1$, and thus,

$$|(g_2-\Theta_{\vec{m}})(s)| \geq \frac{|\mathrm{Im}\, z|}{|\widetilde{B}_m^2(z)|}\int_0^1 x^{n_0-2n_1-1}\widetilde{B}_m^2(x)u(x)dx. \tag{4.26}$$

Next, it is easily checked from Lemma 4.5, that if n_0 satisfies (4.22) with $C = C_{2n_1+1}$, then all zeros of $P_{2n_1+1}^{(n_0-2n_1-2)}(x)$ are larger than $\mathrm{Re}\,(z)$. In the sequel, we assume that n_0 is chosen so that the previous inequality is satisfied. On the other hand, in view of the definition (2.5), the function $u(x)$ (resp. $xu(x)$) is decreasing (resp. increasing) on $[0,1]$, hence we know from Lemma 4.4 that the zeros of $\widetilde{B}_m(x)$ lie to the right of those of $P_{2n_1+1}^{(n_0-2n_1-2)}(x)$ and to the left of those of $P_{2n_1+1}^{(n_0-2n_1-1)}(x)$. Consequently

$$|\widetilde{B}_m(z)| \leq |p_{2n_1+1}^{(n_0-2n_1-1)}(z)|. \tag{4.27}$$

Since $\widetilde{B}_m(x)$ is of degree $2n_1+1$, orthogonal with respect to $x^{n_0-2n_1-1}u(x)$, the integral in (4.26) can be written as

$$\min_{p(x)=x^{2n_1+1}+\cdots}\int_0^1 x^{n_0-2n_1-1}p^2(x)u(x)dx \geq u(1)\min_{p(x)=x^{2n_1+1}+\cdots}\int_0^1 x^{n_0-2n_1-1}p^2(x)dx \tag{4.28}$$

$$= u(1)/\left(\alpha_{2n_1+1}^{(n_0-2n_1-1)}\right)^2. \tag{4.29}$$

Hence, together with (4.26) and (4.27), we get

$$|(g_2-\Theta_{\vec{m}})(s)| \geq \frac{|\mathrm{Im}\, z|u(1)}{\left|P_{2n_1+1}^{(n_0-2n_1-1)}(z)\right|^2}. \tag{4.30}$$

Let us now turn to an upper bound for the difference $(g_2 - \Pi_{\vec{n}})(s)$. From (3.3) and (3.7), we have

$$(g_2 - \Pi_{\vec{n}})(s) = \frac{1}{z^{n_0-n_1} B_n(z) H_n(z)} \int_0^1 x^{n_0-n_1} H_n(x) \frac{C_n(x)}{z-x} dx, \tag{4.31}$$

whence

$$|(g_2 - \Pi_{\vec{n}})(s)| \leq \frac{1}{|\mathrm{Im}\,(z) B_n(z) H_n(z)|} \int_0^1 x^{n_0-n_1} H_n^2(x) \left| \frac{C_n(x)}{H_n(x)} \right| dx.$$

Since $H_n(x)$ is a monic orthogonal polynomial of degree $2n_1+1$ with respect to the weight $x^{n_0-n_1}|C_n(x)/H_n(x)|$, we get by an argument similar to (4.28)–(4.29) that

$$\int_0^1 x^{n_0-n_1} H_n^2(x) \left| \frac{C_n(x)}{H_n(x)} \right| dx \leq \frac{\max_{x\in[0,1]} \left| x^{n_1+1} \frac{C_n(x)}{H_n(x)} \right|}{\left(\alpha_{2n_1+1}^{(n_0-2n_1-1)} \right)^2}. \tag{4.32}$$

Furthermore, in view of (3.6), we have, for $x \in [0,1]$,

$$\left| x^{n_1+1} \frac{C_n(x)}{H_n(x)} \right| = \frac{x^{n_1}}{B_n(x)} \int_c^d \frac{B_n^2(t)}{|H_n(t)|} \frac{x d\tau(t)}{x-t}. \tag{4.33}$$

Since $B_n(x)$ is a polynomial of degree n_1 with all its zeros in (c,d), the ratio $x^{n_1}/B_n(x)$ is positive increasing, and the same holds true for the integral as a function of x. Hence, the above expression is increasing on $[0,1]$, from which we deduce together with (4.31) and (4.32) that

$$|(g_2 - \Pi_{\vec{n}})(s)| \leq \frac{|C_n(1)/H_n(1)|}{\alpha_{2n_1+1}^{(n_0-2n_1-1)} |\mathrm{Im}\,(z) B_n(z) P_{2n_1+1}^{(n_0-2n_1-1)}(z)|}. \tag{4.34}$$

In the last inequality, we have also used Lemma 4.4 to ensure that $|H_n(z)| \geq |p_{2n_1+1}^{(n_0-2n_1-1)}(z)|$. Indeed, since (4.33) is increasing on $[0,1]$, the zeros of $H_n(z)$ lie to the right of the zeros of $p_{2n_1+1}^{(n_0-2n_1-1)}(z)$. Moreover, by the assumption (4.22) on n_0, we know that $\mathrm{Re}\,(z)$ is less than all these zeros.

For the numerator in (4.34), we know from (3.6) that

$$\left| \frac{C_n(1)}{H_n(1)} \right| \leq \frac{1}{(1-d) B_n(1)} \int_c^d B_n^2(t) \frac{d\tau(t)}{|H_n(t)|}. \tag{4.35}$$

Let us consider the following measure on $[c,d]$,

$$\frac{d\tau(t)}{(-t)^{2n_1+1}} = \frac{|H_n(t)|}{(-t)^{2n_1+1}} \frac{d\tau(t)}{|H_n(t)|},$$

and denote by $Q_{n_1}^{(2n_1+1)}(x)$ (resp. $q_{n_1}^{(2n_1+1)}(x)$) the associated orthonormal (resp. monic orthogonal) polynomial of degree n_1. Since the monic polynomial $B_n(x)$ is orthogonal with respect to $d\tau(t)/|H_n(t)|$ and the ratio $|H_n(t)|/(-t)^{2n_1+1}$ is increasing on $[c,d]$, it follows that the zeros of $q_{n_1}^{(2n_1+1)}(x)$ lie to the right of the zeros of $B_n(x)$, and consequently

$$|q_{n_1}^{(2n_1+1)}(z)| \leq |B_n(z)|, \quad |q_{n_1}^{(2n_1+1)}(1)| \leq |B_n(1)|.$$

Therefore, from (4.34) and (4.35), we derive that

$$|(g_2 - \Pi_{\vec{n}})(s)| \\ \leq \left((1-d)\alpha_{2n_1+1}^{(n_0-2n_1-1)}|\mathrm{Im}\,(z)Q_{n_1}^{(2n_1+1)}(z)Q_{n_1}^{(2n_1+1)}(1)P_{2n_1+1}^{(n_0-2n_1-1)}(z)|\right)^{-1} \max_{t\in[c,d]} \frac{(-t)^{2n_1+1}}{|H_n(t)|}.$$

We know that the above maximum is attained at $t = c$ and that $|H_n(c)| \geq |p_{2n_1+1}^{(n_0-2n_1-1)}(c)|$. Moreover, since the zeros of $Q_{n_1}^{(2n_1+1)}(x)$ lie in $[c, d]$, we have

$$|Q_{n_1}^{(2n_1+1)}(z)Q_{n_1}^{(2n_1+1)}(1)| \geq \left(Q_{n_1}^{(2n_1+1)}(0)\right)^2,$$

so that, finally, we obtain the upper bound

$$\begin{aligned} |(g_2 - \Pi_{\vec{n}})(s)| &\leq \frac{|c|^{2n_1+1}}{(1-d)|\mathrm{Im}\,z|\left(Q_{n_1}^{(2n_1+1)}(0)\right)^2\left|P_{2n_1+1}^{(n_0-2n_1-1)}(z)\right|^2} \frac{|p_{2n_1+1}^{(n_0-2n_1-1)}(z)|}{|p_{2n_1+1}^{(n_0-2n_1-1)}(c)|} \\ &\leq \frac{|z-1|^{2n_1+1}}{(1-d)|\mathrm{Im}\,z|\left(Q_{n_1}^{(2n_1+1)}(0)\right)^2\left|P_{2n_1+1}^{(n_0-2n_1-1)}(z)\right|^2}, \end{aligned} \tag{4.36}$$

where, in the last inequality, we have used the facts that $|c|^{2n_1+1} \leq |p_{2n_1+1}^{(n_0-2n_1-1)}(c)|$ and that $|p_{2n_1+1}^{(n_0-2n_1-1)}(z)| \leq |z-1|^{2n_1+1}$ since all zeros of $p_{2n_1+1}^{(n_0-2n_1-1)}(x)$ are larger than $\mathrm{Re}\,(z)$. Then, (4.23) follows from (4.36) and the fact that

$$|z-1| \leq \sqrt{2}|\mathrm{Im}\,z|. \tag{4.37}$$

Combining (4.30) together with (4.36), and using again (4.37), we get (4.24). □

5 Numerical experiments

In this section we first compare, in §5.1, the error curves for various Hermite-Padé approximants. Subsequently, in §5.2 we describe the numerical procedure to solve the extremal problem in logarithmic potential theory displayed in Lemma 3.5. Finally, in §5.3 we compare the computed rate of convergence with the nth root behavior predicted by Theorem 3.1.

5.1 Some examples

We start with practical issues for computing our non-linear Hermite-Padé approximant (called singular Fourier-Padé approximant in [8]). Given the first coefficients of a real Fourier series

$$f(t) = \sum_{j=0}^{\infty} a_j \cos(jt) + \sum_{j=1}^{\infty} b_j \sin(jt).$$

supposed to be 2π-periodic, and continuous in $(0, 2\pi)$ except for a jump at $t = 0$, we first construct the associated function

$$g_2(z) = \sum_{j=0}^{\infty} g_{2,j} z^j, \quad g_{2,j} = a_j - ib_j, \quad b_0 = 0,$$

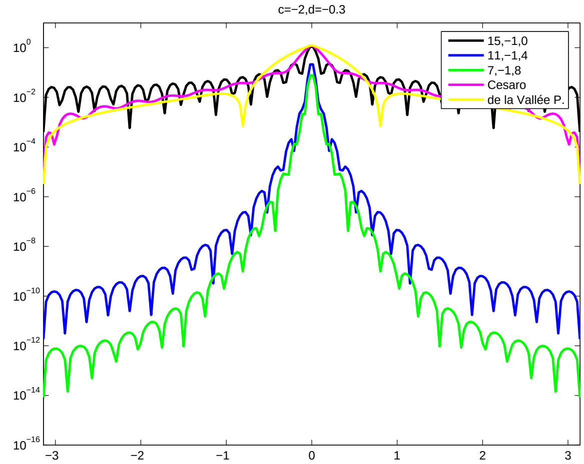

Figure 1: *Error of different approximants for the Lebesgue measure* $d\tau(y) = dy$ *on* $[c, d] = [-2, -.3]$ *using* 16 *Fourier coefficients. One has around the singularity* $t = 0$, *from top to bottom, the partial sum of order* 15, *the Cesaro and de la Vallée–Poussin means, and two nonlinear approximants obtained from Padé approximation of type* $\vec{m} = (11, -1, 4)$ *and* $\vec{m} = (7, -1, 8)$.

such that $f(t) = \mathrm{Re}\,(g_2(e^{it}))$. The function $g_1(z) = i \log(1 - z)$ is such that $\mathrm{Re}\,(g_1(e^{it}))$ has a singularity at $t = 0$ as $f(t)$. Then $f(t) = \mathrm{Re}\,(g_2(e^{it}))$ is approached by $\mathrm{Re}\,(\Pi_{\vec{n}}(e^{it}))$ of order $\vec{n} = (n_0, n_1, n_2)$ defined in (2.3). Equating coefficients in (2.2) it only remains to find polynomials p_1 and p_2 with $\deg p_j \leq n_j$ such that the expansion of $p_1 g_1 + p_2 g_2$ at $z = 0$ does not contains the terms z^j for $j = n_0 + 1, ..., n_0 + n_1 + n_2 + 1$. This leads to a homogeneous linear system of equations with a matrix of the form (T_1, T_2), where T_j is a Toeplitz matrix of size $(n_1 + n_2 + 1) \times (n_j + 1)$, whose elements are the coefficients of g_j.

Though these HP approximants are extremely simple to construct, it is a well-known fact that the underlying matrix of coefficients is quite often very ill conditioned, even for small values of $\vec{n}$. Therefore it is necessary to have accurate data, and to perform the computation of HP approximants in high precision arithmetic, see for instance the discussion in [8, Section 8]. In our case, all Taylor coefficients as well as the HP approximants have been computed with the variable precision artithmetic package vpa of Matlab, handling a precision of 100 digits. However, due to an underlying approximation of the integrals by numerical quadrature, we were only able to evaluate the function f in the interval $[0, 2\pi]$ with double precision. This explains why the error curves below are effected by finite precision arithmetic around the value 10^{-16}.

We now report about our numerical experiments. The error curves $|f(t) - \mathrm{Re}\,(\Pi_{\vec{n}}(e^{it}))|$ drawn in Figure 1 correspond to the theoretical findings and numerical experiments of [3], namely we observe that the partial sum of order 15 has an error of size $\geq 10^{-2}$ (a classical phenomenon for partial Fourier sums of functions with jumps), though there is some phase effect which makes the curve oscillating. The corresponding Cesaro and de la Vallée Poussin means (i.e., linear acceleration schemes) smooth the error curves, but do not lead to an important gain, especially around the singularity. In contrast, the errors given by the Padé approximants ($\vec{m} = (11, -1, 4)$ and $\vec{m} = (7, -1, 8)$), which are nonlinear, are much smaller far from the singularity $t = 0$, but still large close to $t = 0$.

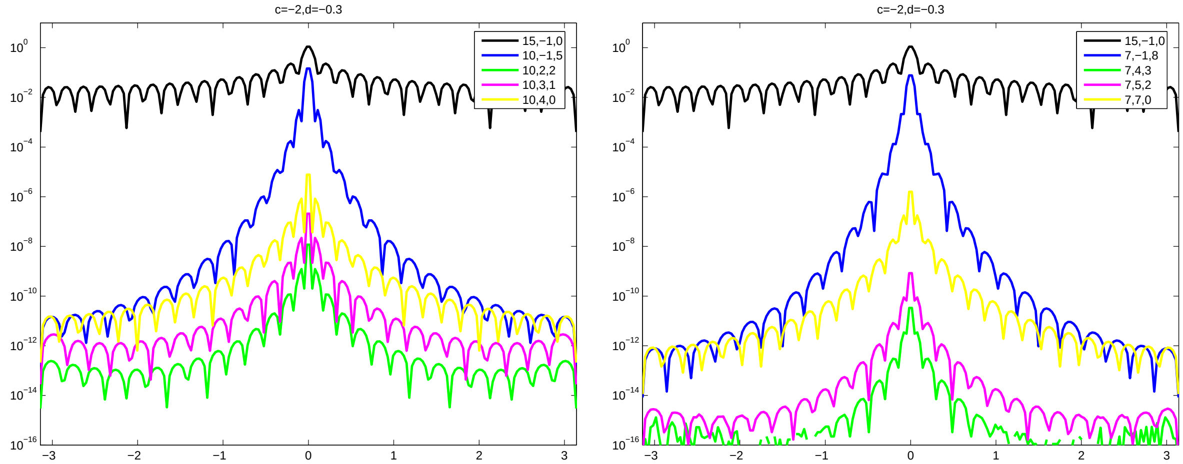

Figure 2: *Error of different approximants for the Lebesgue measure* $d\tau(y) = dy$ *on* $[c, d] = [-2, -.3]$ *using* 16 *Fourier coefficients. In the left-hand plot, one has (beside the same partial sum) four* $\vec{n}$*-HP approximants obtained by solving homogeneous systems with* $n_1 + n_2 + 2 = 6$ *unknowns, namely (around* $t = 0$ *from top to bottom): the Padé approximant* $\vec{n} = (10, -1, 5)$*, the linear HP approximant* $\vec{n} = (10, 4, 0)$, $\vec{n} = (10, 3, 1)$*, and finally the "diagonal" approximant* $\vec{n} = (10, 2, 2)$*. On the right, we obtain (beside the partial sum) homogeneous systems with* $n_1 + n_2 + 2 = 9$ *unknowns, namely (around* $t = 0$ *from top to bottom)* $\vec{n} = (7, -1, 8)$ *(Padé),* $\vec{n} = (7, 7, 0)$ *(linear HP),* $\vec{n} = (7, 5, 2)$*, and* $\vec{n} = (7, 4, 3)$.

In Figure 2 we have drawn the corresponding errors for those Hermite-Padé approximants using the same number of Fourier coefficients as in Figure 1. One observes that, for fixed $n_0 + n_1 + n_2 + 2$ (the number of required Fourier coefficients), it is interesting to choose $n_1 + n_2 + 2$ as large as possible (the size of the underlying system) since, while stepping from the left-hand to the right-hand plot of Figure 2, one gains each time one or two digits. For approximants in the same plot (where each time we solve systems of equal size), one obtains more or less the same precision far from the singularity. More precisely, the linear HP approximants ($n_2 = 0$) are about as good as the Padé approximants ($n_1 = -1$), but the error is the smallest in the diagonal case $n_1 \approx n_2$. Note that the error for $\vec{n} = (7, 4, 3)$ is affected by finite precision arithmetic.

However, close to the singularity, the picture is totally different from Figure 1. By stepping from Padé to linear HP approximants, which are adapted to the singularity, we gain about four digits, in accordance with Proposition 4.2. By going to nearly diagonal approximants we gain another 3 or 4 digits, as predicted by Proposition 4.1. Now, the error is quite small on the whole interval. The numerical results presented in Figure 2 are in accordance with those in [8, Figure 8.1 and Figure 8.3], though, there, the question of how to choose the degrees was not addressed.

In [3], approximants in a row of the Padé table, $n_1 = -1$ and n_2 fixed, $n_0 \to \infty$, were discussed. Rates of convergence of magnitude $\mathcal{O}(n_0^{-2n_2})$ as $n_0 \to \infty$ were established for some particular model problems, and it was shown that the rate does not change if one modifies f by adding a sufficiently differentiable function, a fact which was shown to be

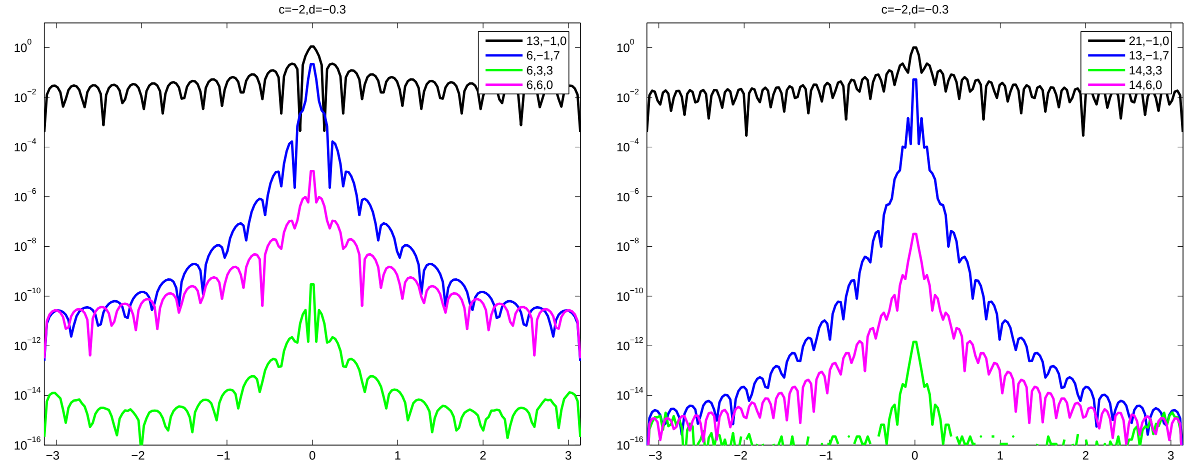

Figure 3: *Error of different approximants for the Lebesgue measure $d\tau(y) = dy$ on $[c, d] = [-2, -.3]$ using 14 Fourier coefficients on the left ($n_0 = 6$), and 22 on the right ($n_0 = 14$). Around the singularity $t = 0$, from top to bottom, one has the partial sum of order $n_0 + 7$, the Padé approximants $\vec{n} = (n_0, -1, 7)$, the linear HP approximants $\vec{n} = (n_0, 6, 0)$ and the diagonal HP approximants $\vec{n} = (n_0, 3, 3)$.*

wrong for diagonal Padé approximants. In relation with Proposition 4.3, we check the decay of the error for increasing n_0 and fixed n_1, n_2. As seen in Figure 3, we gain about two digits for each of the three HP approximants by stepping from $n_0 = 6$ to $n_0 = 14$ for constant n_1, n_2, requiring 8 more Fourier coefficients. This confirms that an increase in n_0 leads to a modest, probably not geometric, improvement, as claimed in Proposition 4.3. However, it is remarkable (and can be read from the proof of Proposition 4.3) that the rate of convergence is strongly influenced by the (not specified) constants occurring in Proposition 4.3. The corresponding constant for diagonal HP approximants is much smaller.

Finally we show in Figure 4 that the rate of convergence for our model problem strongly depends on the choice of the interval $[c, d]$. The error curves drawn in Figure 4 have to be compared with those on the right-hand plot of Figure 3 for $[c, d] = [-2, -0.3]$ with the same degrees. As can be seen on Figure 4, for two intervals close to each other and t far from the singularity, the Padé approximants outperform the other two approximants, but only these latter have an acceptable behavior around the singularity.

5.2 Numerical solution of a vector equilibrium problem in logarithmic potential theory

In this section, we discuss in some more details general vector equilibrium problems, of which the problem appearing in Lemma 3.5 is a particular case. We also explain how we solve it numerically.

To get a feeling of the vector equilibrium problem, we will try in the sequel to display an electrostatic interpretation of the associated variational conditions, such as (3.8)–(3.11) and (4.4)–(4.5) that correspond respectively to the Hermite-Padé and Padé approximants.

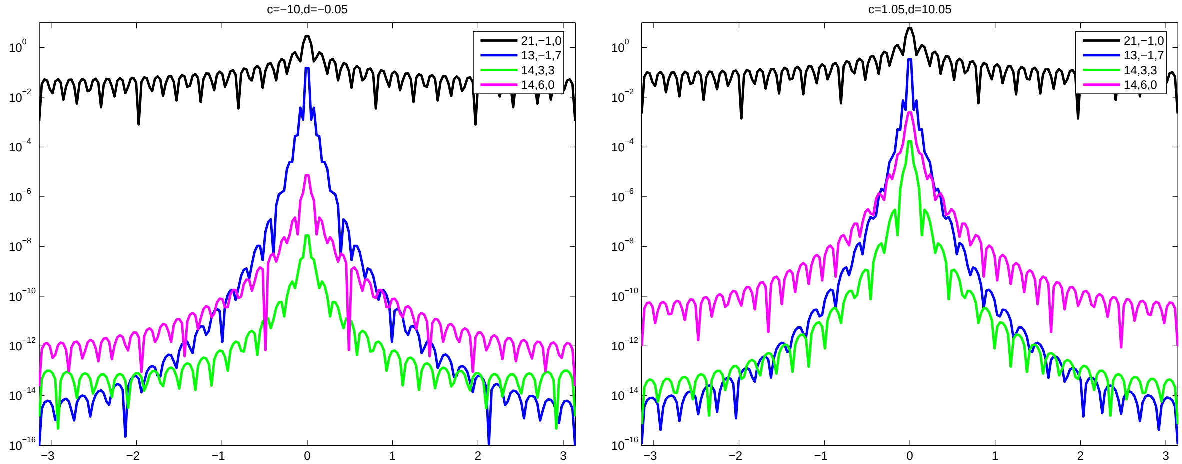

Figure 4: *Error of different approximants for the Lebesgue measure* $d\tau(y) = dy$ *on* $[c, d] = [-10, 0.05]$ *(left), and* $[c, d] = [1.05, 10.05]$ *(right) using* 22 *Fourier coefficients. Around the singularity* $t = 0$*, from top to bottom, one has the partial sum of order* 21*, the Padé approximants* $\vec{n} = (13, -1, 7)$*, the linear HP approximants* $\vec{n} = (14, 6, 0)$ *and the diagonal HP approximants* $\vec{n} = (14, 3, 3)$.

Let $\mathcal{M}(\Sigma)$ be the set of probability measures with support in a given compact set Σ. Let $\Sigma_1, ..., \Sigma_N \subset \mathbb{R}$ be disjoint compact sets (in our case they are real intervals), then we write simply $\mathcal{M}$ for the set of vector measures $\vec{\mu} = (\mu_1, ..., \mu_N)$ with $\mu_j \in \mathcal{M}(\Sigma_j)$. Let $\gamma_1, ..., \gamma_N \geq 0$, and let $A = (a_{j,k}) \in \mathbb{R}^{N\times N}$ be a given symmetric positive semidefinite matrix, the so-called matrix of interactions. Furthermore, let $Q = (Q_1, ..., Q_N)$ be the vector of external fields, where the Q_j are continuous functions on Σ_j. The mutual energy is defined as

$$I(\mu_j, \mu_k) := \int \log \frac{1}{|x-y|}\, d\mu_j(x) d\mu_k(y),$$

and the total energy of the vector measure $\vec{\mu}$ is

$$I_Q(\vec{\mu}) = \sum_{j,k=1}^{N} a_{j,k}\gamma_j\gamma_k I(\mu_j, \mu_k) + 2\sum_{j=1}^{N}\gamma_j \int Q_j \, d\mu_j. \tag{5.1}$$

In the special case $N = 1$, $A = 1$, this corresponds to the physical energy of the positive charge $\gamma_1\mu_1$ on Σ_1 in the external field Q_1. In our case, the external field Q_1 corresponds to the potential U^{δ_0} supported at the origin. For $N = 2$, the special cases

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \text{and} \quad A = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

describe a condenser (Σ_1, Σ_2), with Σ_1 a plate carrying a positive charge, and Σ_2 a plate carrying either a positive or negative charge. The minimum of $I_Q(\vec{\mu})$ for $\vec{\mu} \in \mathcal{M}$ corresponds to the steady state of the condenser formed by the different plates Σ_j in the external fields Q_j. In other words, we are left with a problem of electrostatics, and consequently, one can gain a feeling of the solution by remembering that charges of the same sign are repealing, while charges of different signs are attracting. However, in the case of a Nikishin system of two functions, the interaction matrix is

$$A = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \tag{5.2}$$

which has a more complicated physical meaning since, here, the interaction between charges on a same plate is twice the interaction between charges on different plates.

From a more mathematical point of view, the extremal problem of minimizing the total energy $I_Q(\vec{\mu})$ over the set of measures $\mathcal{M}$ was first investigated in [13, 14] for matrices A of a special form and without an external field, for the general case see also [12, 15, 22] or the historical remarks in [24, Chapter VIII.8]. It is shown, e.g., in [12, Theorem 4 (1)] that the extremal measure exists and is unique. Note that the components μ_j of this minimizer may not fill the whole plate Σ_j, i.e. $\mathrm{supp}\,(\mu_j) \subsetneq \Sigma_j$. For instance, this may happen if the charges are pushed away by a strong external field. Furthermore, as shown in [12, Theorem 4 (2)], the minimizer is uniquely characterized by the variational conditions, or Euler-Lagrange equations,

$$U_j(\vec{\mu})(z) := \sum_{k=1}^{N} a_{j,k}\gamma_k U^{\mu_k}(z) + Q_j(z) \begin{cases} = W_j & \text{if } z \in \mathrm{supp}\,(\mu_j), \\ \geq W_j & \text{if } z \in \Sigma_j, \end{cases} \tag{5.3}$$

for $j = 1, 2, ..., N$, and for suitable real constants $W_1, ..., W_N$. Physically, this means that the electric potential $U_j(\vec{\mu})$ is constant on the support of the charge $\gamma_j\mu_j$, and larger than this constant elsewhere (otherwise we could decay the energy by distributing differently the charge μ_j).

We now come to the numerical resolution of the vector equilibrium problem. In order to compute our extremal measure, we have to discretize our set $\mathcal{M}$ of measures according to a finite number of free variables. A natural idea would be to restrict ourselves to vectors of discrete measures $\vec{\mu}$. However, in this case, the exponential of the vector potential $U_j(\vec{\mu})$ boils down to a ratio of polynomials taken at some power, and the related max-min problem of [22, Chapter 5.4, Problem C] becomes a coupled extremal problem for polynomials, similar to the one corresponding to Nikishin systems. Hence, this approach would bring us back to the original problem. Thus, here, we have rather considered the subset $\mathcal{M}_0$ of vector measures with piecewise linear weights: we first choose a discretization

$$t_{j,0} < t_{j,1} < .... < t_{j,K}, \quad \Sigma_j = [t_{j,0}, t_{j,K}],$$

and ask μ_j to be a linear function on each subinterval $[t_{j,k}, t_{j,k+1}]$. This gives us $N(K+1)$ parameters $x_{j,k} \geq 0$ in the B-spline representation

$$\frac{d\mu_j}{dx}(x) = \sum_{j=0}^{K} x_{j,k} B_{j,k}(x), \quad B_{j,k}(x) = \begin{cases} \frac{t_{j,k+1}-x}{t_{j,k+1}-t_{j,k}} & \text{if } k < K \text{ and } x \in [t_{j,k}, t_{j,k+1}], \\ \frac{x-t_{j,k-1}}{t_{j,k}-t_{j,k-1}} & \text{if } k > 0 \text{ and } x \in [t_{j,k-1}, t_{j,k}], \\ 0 & \text{otherwise}, \end{cases}$$

with total mass

$$\int d\mu_j = 1 = \sum_{k=0}^{K-1} (x_{j,k} + x_{j,k+1}) \frac{t_{j,k+1} - t_{j,k}}{2}. \tag{5.4}$$

The set of $t_{j,k}$ with $x_{j,k} > 0$ for $j = 0, 1, ..., K$, could then be considered as the discrete support of μ_j, though $t_{j,k} \in \text{supp}\,(\mu_j)$ if $x_{j,k-1} + x_{j,k} + x_{j,k+1} > 0$.

A collocation approach, as used for instance in [17], consists of imposing the equilibrium conditions only pointwise for all $t_{j,k} \in \Sigma_j$, and solving the coupled system of the N linear equations (5.4) together with the equations

$$x_{j,k}[U_j(\vec{\mu})(t_{j,k}) - W_j] = 0, \quad x_{j,k} \geq 0, \quad U_j(\vec{\mu})(t_{j,k}) - W_j \geq 0, \tag{5.5}$$

for the unknowns W_j and $x_{j,k}$ where $j = 1, ..., N$ and $k = 0, 1, ..., K$. Note that the first equations in (5.5) are quadratic in the variables $x_{j,k}$. It is not clear a priori that this system has a simple solution.

In the present paper we prefer to minimize directly the total energy $I_Q(\vec{\mu})$ over $\mathcal{M}_0$, the set of vector measures with piecewise linear densities. It is not difficult to check[1] that I_Q is strictly convex over $\mathcal{M}_0$. Writing the set of $x_{j,k}$ as a (suitably arranged) vector $x \in \mathbb{R}^{N(K+1)}$ and the N equality constrains of (5.4) as $Bx = b$, we are left with the strictly convex quadratic minimization problem with linear constrains

$$\min\{x^T Hx + h^T x : x \geq 0, Bx = b\} \tag{5.6}$$

having a unique minimizer. The matrix H, and the vector h, respectively, contain the entries

$$a_{j,j'}\gamma_j\gamma_{j'} \int \log \frac{1}{|x-y|} B_{j,k}(x) B_{j',k'}(y)\, dx\, dy, \quad \text{and} \quad 2\gamma_j \int Q_j(x) B_{j,k}(x) dx,$$

respectively, for which explicit formulas are available, which have been implemented in our code. Notice that, with the size of each subinterval tending to zero, the sets of piecewise linear densities become dense in the set of all probability measures. Hence, with a sufficiently large K, the minimum of our discrete problem should approach that of our continuous problem. Writing down the Karush-Kuhn-Tucker characterization of our discrete problem, a short calculation shows that there exists constants $W_1, ..., W_N$ such that, for all j, k,

$$x_{j,k} X_{j,k} = 0, \quad x_{j,k} \geq 0, \quad X_{j,k} \geq 0, \quad X_{j,k} = \int [U_j(\vec{\mu})(x) - W_j] B_{j,k}(x) dx.$$

Since

$$\int [U_j(\vec{\mu})(x) - W_j] B_{j,k}(x) dx = [U_j(\vec{\mu})(\xi_{j,k}) - W_j] \int B_{j,k}(x) dx,$$

for some $\xi_{j,k} \in [t_{j,k-1}, t_{j,k+1}]$, we may therefore conclude that the equilibrium conditions (5.3) are true in "local mean", and pointwise at certain $\xi_{j,k}$, as for the collocation methods. However, this does not exclude that the computed vector potential $U_j(\vec{\mu})$ does oscillate, what typically happens at the end points of the supports. There are different methods to

[1] We first notice that all measures in $\mathcal{M}_0$ have finite energy, which allows us to extend the definition of I_Q by linearity to the difference of measures from $\mathcal{M}_0$. By convexity of $\mathcal{M}_0$, we obtain for distinct $\vec{\mu}_1, \vec{\mu}_2 \in \mathcal{M}_0$ and $t \in (0, 1)$ that $tI_Q(\vec{\mu}_1) + (1-t)I_Q(\vec{\mu}_2) - I_Q(t\vec{\mu}_1 + (1-t)\vec{\mu}_2) = t(1-t)I_0(\vec{\mu}_1 - \vec{\mu}_2)$. The strict positivity of the last term follows by considering the Cholesky decomposition $C^T C = \text{diag}\,(\gamma_1, ..., \gamma_N) A \text{diag}\,(\gamma_1, ..., \gamma_N)$ and $\vec{\nu} = C(\vec{\mu}_1 - \vec{\mu}_2) = (\nu_1, ..., \nu_N)$, since then $I_0(\vec{\mu}_1 - \vec{\mu}_2) = \sum_j I(\nu_j, \nu_j)$, where at least one term in the sum is positive by [24, Lemma I.1.8].

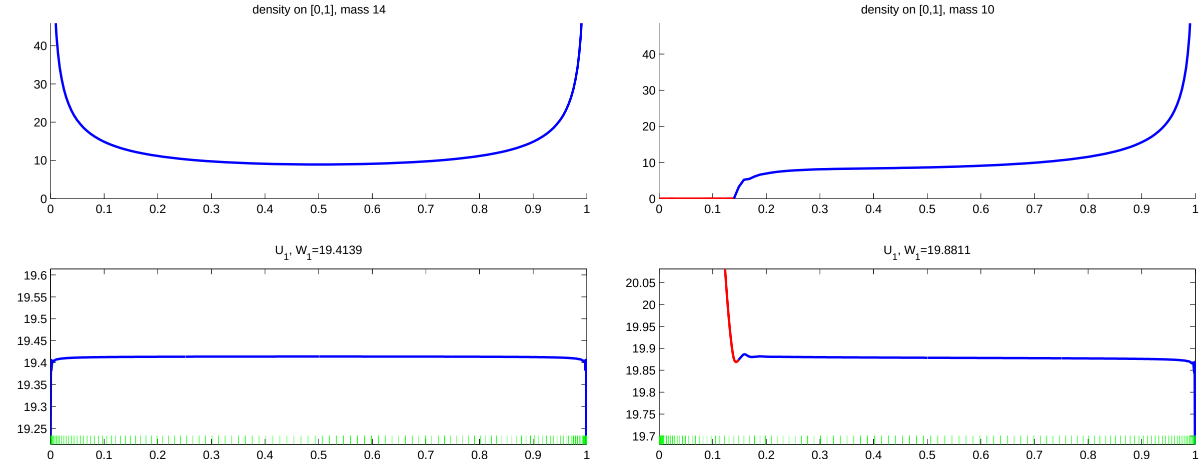

Figure 5: *Extremal measure and vector potential for* $N = 1$, $\Sigma_1 = [0, 1]$, *and* $A = 1$*:* $\gamma_1 = 2n_2 = 14$, *no external field (left),* $\gamma_1 = 2n_2 = 10$, *and the external field* $Q_1 = (n_0 - n_2 + 1)U^{\delta_0} = 6U^{\delta_0}$ *pushes the extremal measure to the right of the interval (right).*

overcome such oscillations: first, one could consider a grid refinement at the endpoints of the sets Σ_j since it is known in the continuous case that at an endpoint a of Σ_j belonging to $\operatorname{supp}(\mu_j)$, the weight typically behaves like $|x - a|^{-1/2}$. Second, it could be interesting to implement an adaptative grid refinement around an endpoint a of $\operatorname{supp}(\mu_j)$ different from an endpoint of Σ_j, so as to match, as well as possible, a with one of the $t_{j,k}$. Since, here, the weight typically behaves like $|x - a|^{1/2}$, we did not implement so far such an adaptative grid refinement. Actually, it is not clear how to measure the deviation of the optimal piecewise linear measure from the optimal one in $\mathcal{M}$, and we will not make any further theoretical analysis in this respect.

Let us now present several numerical experiments, where we draw the weight of the discrete extremal measure $\gamma_j\mu_j$ (top) and the corresponding vector potential $U_j(\vec{\mu})$ (bottom). In each case, one observes, as required by (5.3), that the potential is approximately constant on $\operatorname{supp}(\mu_j)$ and larger than this constant elsewhere in Σ_j (beside some minor oscillations at the endpoints). In our experiments we have chosen $K = 120$, with a grid refinement at the endpoints, obtained by shifting Chebyshev points, see the small vertical ticks in the bottom plot, but with no further adaptative grid refinement. The discrete convex quadratic program (5.6) was solved using the level set algorithm `quadprog` of Matlab with no particular choice of a first iterate, requiring in general no more than a hundred iterations.

Example 5.1. In our first set of experiments, we have chosen $N = 1$ with the interaction matrix $A = 1$ and $\Sigma = [0, 1]$, together with the mass $\gamma_1 = 2n_2$ and the external field $Q_1 = (n_0 - n_2 + 1)U^{\delta_0}$ corresponding (up to normalization with $n = n_0 + n_1 + n_2$) to the case $\vec{n} = (n_0, -1, n_2)$ of (n_0, n_2) Padé approximants for Markov functions with support in $[0, 1]$, compare with (4.4)–(4.5). On the left of Figure 5, the external field $Q_1 = 0$ allows us to recover numerically the equilibrium measure on $[0, 1]$ with weight $\gamma_1/(\pi\sqrt{x(1 - x)})$. The external field in the right-hand plot of Figure 5 represents a positive charge of mass 6 at the origin, which pushes the free positive charge of mass 10 to the right. As mentioned

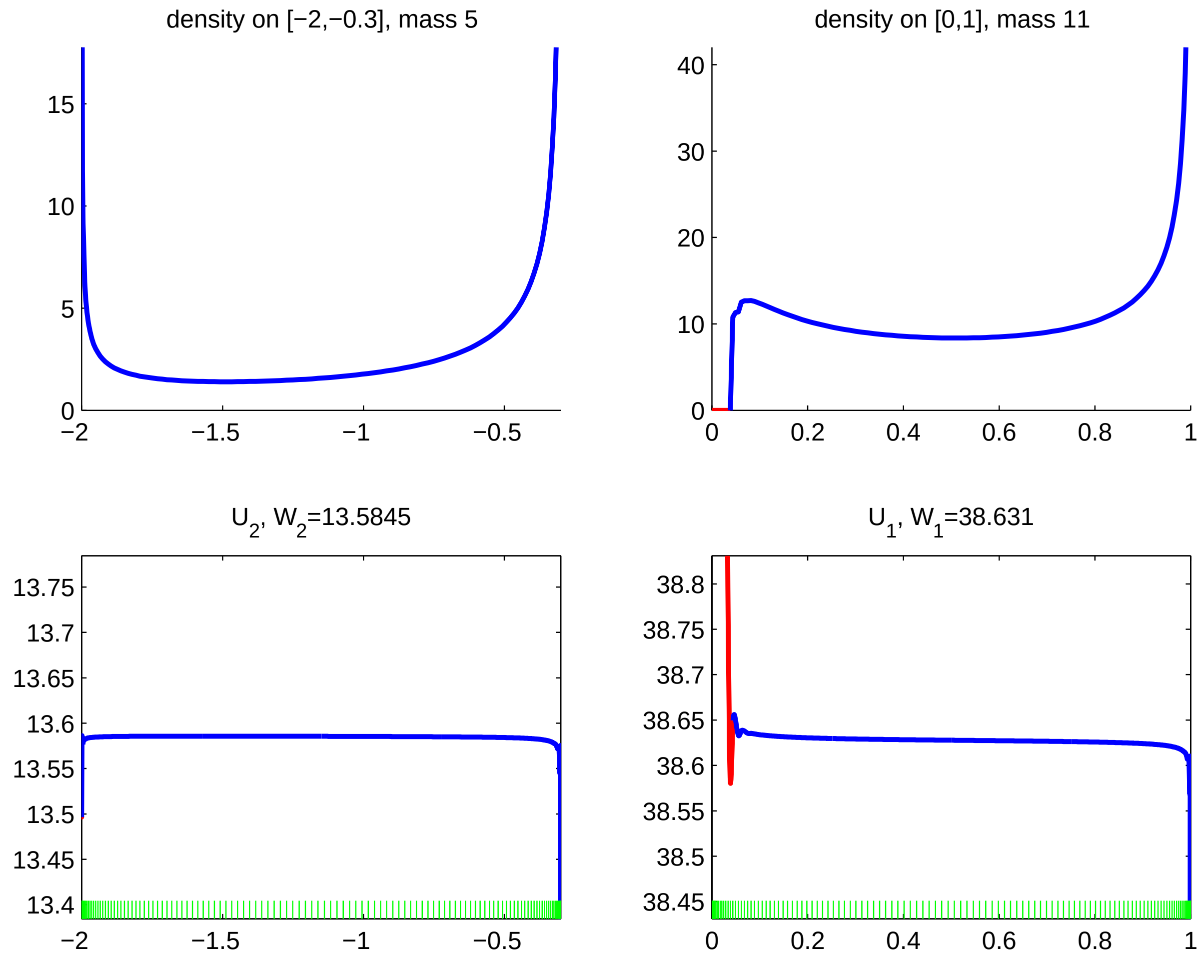

Figure 6: *Extremal measure and vector potential for* $N = 2$ *and the data of Example 5.2,* $[c, d] = [-2, -0.3]$ *and* $\vec{n} = (10, 5, 5)$*, with a trivial external field* $Q_2 = 0$.

before, notice the small oscillation of the vector potential around the left endpoint of $\operatorname{supp}(\mu_1)$, as well as the behavior of the weight around the endpoint.

Example 5.2. We now look at a vector equilibrium problem with $N = 2$ and the Nikishin interaction matrix (5.2), together with $\Sigma_1 = [0, 1]$, $\gamma_1 = n_1 + n_2 + 1$, $Q_1 = (n_0 - n_1 + 1)U^{\delta_0}$, and $\Sigma_2 = [c, d]$ on the left of Σ_1, $\gamma_2 = n_2$, $Q_2 = (n_1 - n_2)U^{\delta_0}$ as required (up to normalization with $n = n_0 + n_1 + n_2$) for the Hermite-Padé approximants of a Nikishin system, compare with (3.8)–(3.11).

In Figure 6, for $\vec{n} = (10, 5, 5)$, we observe that the positive charge $11\mu_1$ on $[0, 1]$ is pushed to the right by the external field Q_1 given by a positive point charge of mass 6 at the origin though it is also attracted weakly by the negative charge $5\mu_2$ on the left. In contrast, the negative charge $5\mu_2$ lives on the whole interval Σ_2 since, here, there is no external field, though it is weakly attracted by the positive mass $11\mu_1$.

In Figure 7, we display a more difficult problem with two plates $\Sigma_1 = [0, 1]$ and $\Sigma_2 = [-2, -0.05]$ closer to each other, and $\vec{n} = (15, 9, 2)$, that is, there is also a nontrivial external field $Q_2 = 7U^{\delta_0}$ corresponding to a negative charge at the origin. Hence $2\mu_2$ is

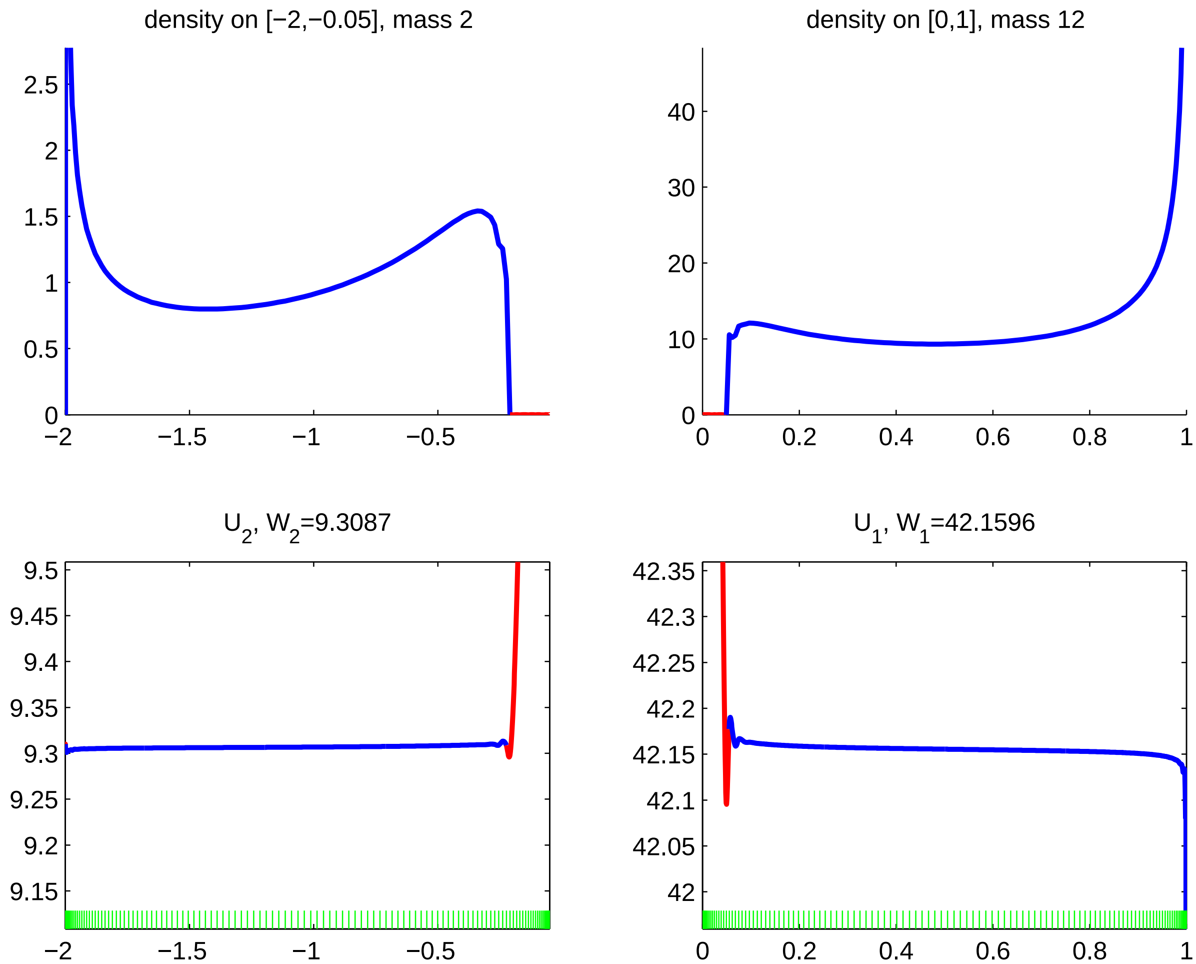

Figure 7: *Extremal measure and vector potential for $N = 2$ and the data of Example 5.2,* $[c, d] = [-2, -0.05]$, $\vec{n} = (15, 9, 2)$, *non-trivial external fields* Q_1 *and* Q_2.

pushed by Q_2 and attracted weakly by $12\mu_1$. Finally we find that $\mathrm{supp}\,(\mu_2) \subsetneq \Sigma_2$. Notice that the vector potential is essentially constant on both supports as required, except for some oscillation at the endpoints.

5.3 Theoretical versus computed rate of convergence

In this last section, we compare the computed error curves

$$|f(t) - \mathrm{Re}\,(\Pi_{\vec{n}}(e^{it})| = |\mathrm{Re}\,((g_2 - \Pi_{\vec{n}})(e^{it}))|, \tag{5.7}$$

with the theoretical rates obtained in Theorem 3.1. Several remarks are in order.

First, the actual error curve is oscillating. This is due to the power of z which factors the error $g_2 - \Pi_{\vec{n}}$. Now, Theorem 3.1 describes the absolute value of $(g_2 - \Pi_{\vec{n}})(e^{it})$, where this factor does not play a role. Hence, it is an upper smooth envelop of our actual error curve which should be compared with the rate predicted by logarithmic potential theory.

Second, it turns out that, at least for sufficiently smooth measures τ on $[c, d]$, the computed and predicted errors not only agree in the weak nth root sense where $n =$

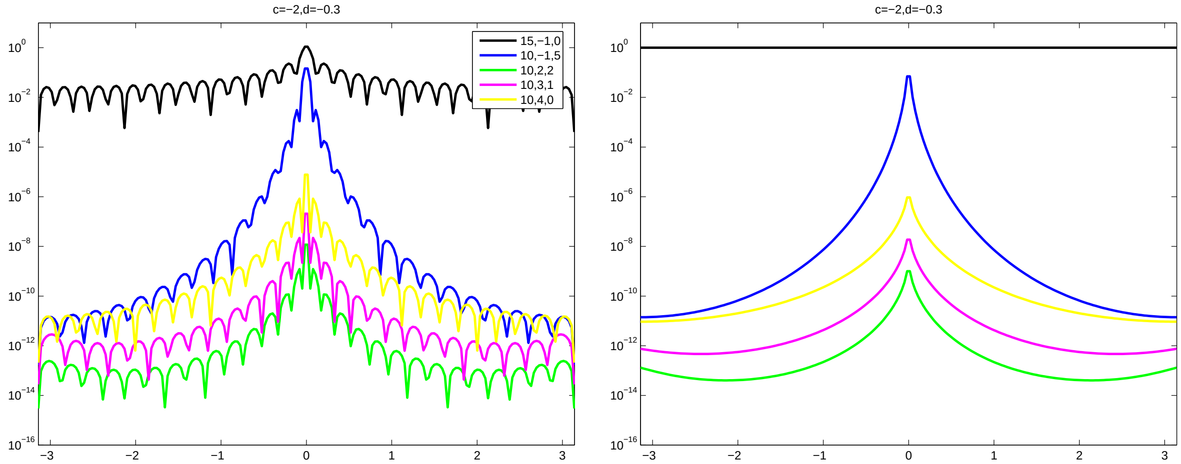

Figure 8: *Error of different approximants for the Lebesgue measure* $d\tau(y) = dy$ *on* $[c, d] = [-2, -.3]$ *using* 16 *Fourier coefficients. In the left-hand plot, one has beside the partial sum, four HP approximants, namely, from top to bottom: the Padé approximant* $\vec{n} = (10, -1, 5)$*, the linear HP approximant* $\vec{n} = (10, 4, 0)$*,* $\vec{n} = (10, 3, 1)$*, and finally the "diagonal" approximant* $\vec{n} = (10, 2, 2)$*. On the right, the corresponding theoretical rate* $\exp(U_1(\vec{\mu})(e^{it}) + U_2(\vec{\mu})(e^{it}) - W_1 - W_2)$*, predicted by logarithmic potential theory, is drawn.*

$n_0 + n_1 + n_2$, but also in the strong sense, meaning that both terms in (3.2) agree even after a multiplication by the total degree n. Hence, we actually depict in the next figure the quantity

$$\exp\Big(\big((n_1 + n_2 + 1)U^{\mu} + n_2 U^{\nu} + (n_0 - n_2 + 1)U^{\delta_0}\big)(e^{it}) - w - W\Big).$$

The argument of the previous exponential corresponds to the quantity $U_1(\vec{\mu}) + U_2(\vec{\mu}) - W_1 - W_2$ of subsection 5.2 where we set as in Example 5.2,

$$\begin{aligned} \Sigma_1 &= [0,1], \quad \gamma_1 = n_1 + n_2 + 1, \quad Q_1 = (n_0 - n_1 + 1)U^{\delta_0}, \\ \Sigma_2 &= [c,d], \quad \gamma_2 = n_2, \quad Q_2 = (n_1 - n_2)U^{\delta_0}. \end{aligned}$$

We present a series of numerical experiments in Figure 8. For other data, the findings are similar, as long as the error (5.7) does not suffer from finite precision arithmetic. We can observe from the curves in Figure 8 that the theoretical convergence rates are very close to the computed errors. The fact that the theoretical asymptotic estimate describes accurately the actual rate, even for small degrees, is less surprising for the Padé approximant of type $\vec{n} = (10, -1, 5)$ because g_2 is a Markov function associated to a smooth density. In this respect, we may refer, for instance, to the findings on strong asymptotics with varying weights obtained in [26]. To our knowledge, there is no similar theory for strong asymptotics of (off-diagonal) Hermite-Padé approximants, for the corresponding second type approximants, though [1] gives results in that direction.

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