On the use of the Carathéodory-Fejér method for investigating '1/9' and similar constants

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Abstract. Error norms of best rational approximation of $\exp(-t)$ on $[0,\infty)$ are known to decrease like ρ^n, where n is the degree of the approximant and ρ is the famous number '1/9'= 1/9.28902549192081891875544943595174
Trefethen and Gutknecht have demonstrated this effect on the sequence of singular values of a Hankel matrix, as an example of their use of the Carathéodory-Fejér method.
It is shown here how the rate of decrease of these singular values can be estimated from their symmetric functions. The examples of rational approximation of $\exp(-t^m)$ on $[0,\infty)$, $m = 2,3$ are also explored. The relation with the extremal polynomials method is briefly discussed.

1. Introduction

Best real rational approximants are characterized by equioscillation (equal ripple) properties. Although well known algorithms (as in [7, 74]) are able to produce such approximants, it is highly useful to predict quantitatively the main properties of the result. For polynomial approximation on the standard interval $[-1,1]$, much can be done with Chebyshev polynomial expansions

$$F(x) = \frac{a_0}{2} + \sum_1^\infty a_k T_k(x) = \frac{a_0}{2} + \sum_1^\infty a_k \cos(k\theta) \qquad (x = \cos\theta). \tag{1.1}$$

In particular, the behaviour of the uniform norm of the error of the best approximation by a polynomial of degree n can be predicted for large n from the behaviour of a_n. One would like a similar tool allowing the description of rational approximation errors in terms of the coefficients of (1.1). Several algorithms based on Padé theory [8, 21] have been proposed for constructing useful rational approximations to F, and a suitably modified version was powerful enough for establishing a proof of Meinardus conjecture [4]. However, for most functions continuous on $[-1,1]$, Padé-Chebyshev-like error norms will not decrease with n at the same rate as the actual optimal error norms E_n (see the case of Stieltjes functions, compare [21] with [3]; see

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also [6]). But the long-sought method has finally been found! Table 1 gives a first example of its striking efficiency. The left part of the table shows least uniform error norms of approximation of $\exp(-t)$ on $t \geqslant 0$ by rational functions of degree n. These values come from Table 1 of [7]. Rational approximation of degree n of a function $G(t)$ on $t \geqslant 0$ is the same as rational approximation of degree n of $F(x)$ on $-1 \leqslant x \leqslant 1$ provided

$$F(x) = G(t)\,, \qquad x = \frac{1-t}{1+t} \tag{1.2}$$

So the numbers E_n are also relevant to the approximation of $F(x) = \exp((x-1)/(x+1))$ on $[-1,1]$. On the second part of table 1 are estimates of the same numbers (with signs which will be explained) constructed

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TABLE 1. Remes algorithm results and CF estimates for approximation of $\exp(-t)$. Digits of agreement of the two are in boldtype in the second column.

n	E_n	λ_{n+1}
0	5.000000000000000E-01	**5**.601715174207940E-01
1	6.683104216185045E-02	-**6.68**0573308019967E-02
2	7.358670169580528E-03	**7.35**5581867871742E-03
3	7.993806363356878E-04	-**7.994**517064498902E-04
4	8.652240695288851E-05	**8.652**095258749368E-05
5	9.345713153026646E-06	-**9.3457**40936352446E-06
6	1.008454374899671E-06	**1.00845**3857122026E-06
7	1.087497491375248E-07	-**1.087497**586430036E-07
8	1.172265211633491E-08	**1.172265**194363526E-08
9	1.263292483322314E-09	-**1.26329248**6435714E-09
10	1.361120523345448E-10	**1.36112052**2787731E-10
11	1.466311194937487E-11	-**1.466311195**036850E-11
12	1.579456837051239E-12	**1.5794568370**33622E-12
13	1.701187076340353E-13	-**1.70118707634**3463E-13
14	1.832174378254041E-14	**1.83217437825**3495E-14
15	1.973138996612803E-15	-**1.973138996612**899E-15
16	2.124853710495224E-16	**2.124853710495**207E-16
17	2.288148563247892E-17	-**2.28814856324789**5E-17
18	2.463915737765169E-18	**2.463915737765169**E-18
19	2.653114658063313E-19	-**2.653114658063313**E-19
20	2.856777383549094E-20	**2.856777383549094**E-20

with the coefficients of (1.1) with this $F(x)$. The method of constructing these estimates has been described in [68], and a summary will be given in next section. A first version of table 1 is in Table 5 of [68], and the present one had already be established by L.N. Trefethen [66]

The exponential function was the ideal test: the study of rational approximation to this function on the positive real axis $0 \leqslant t < \infty$ is originally motivated by the numerical solution of differential equations [9, 30]. When it emerged that the uniform error norm E_n decreases exponentially fast with respect to the degree n [9], the determination

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of the precise rate of decrease became a problem interesting on its own right. A history of the approach of this number is given in [5, 7] and [71]. For a moment, it seemed to be $1/9$, and the problem of its determination is known as the '$1/9$' problem [60], but Gutknecht and Trefethen [68], as well as Schönhage [61], showed numerical evidence that it is somewhat smaller, about 1/9.28903. A proof that the number is definitely smaller than $1/9$ is in [53]. Much more numerical evidence is collected in [7], where it is found that E_n very likely[2] behaves according to the asymptotic expansion (from [7, Tables 3-10 and 2]

$$E_n \sim 2\rho^{n+1/2} \exp\left(-\frac{1}{12(n+1/2)} + O(n^{-5})\right),$$

where $\rho = 1/9.28902549192\cdots$ (see table 5 in section 6). Finally, Goncar and Rahmanov ([18, 37, 58]) have suceeded in proving the existence of the limit ρ of $(E_n)^{1/n}$ as $n \to \infty$ by the theory of extremal

[2]The factor 2 is right! It has been shown by A.I. Aptekarev, Sharp constants for rational approximation of analytic functions (in Russian), *Mathematical Sbornik*, Vol **193**(1), 2002, pp. 3-72 = *Sb. Math.* vol. **193**(2002) no. 1-2, 1-72 (in English), MR1906170 (2003g:30070). The $1/12$ is most probably wrong! (2008)

polynomials, which will be described briefly in section 5. From Glover-Karlsson-Trefethen inequalities [14, 33, 67], it follows that $|\lambda_n|^{1/n}$ has the same limit.

I shall try to show here how this rate of decrease can be deduced from Gutknecht and Trefethen's CF constructions. These authors have already shown in [68] the asymptotic matching of real rational approximation and CF approximation for functions analytic in very large regions (for fixed degrees), asymptotic pole matching for meromorphic functions (for unequal degrees, with degree of numerator $\to \infty$ [24]). Braess [6] has established complete asymptotic agreement between real rational approximation and CF approximation for Stieltjes functions, another very interesting test, as rational approximants are very accurately known [3]. CF rational approximation has been adapted to regions which are neither disks nor real intervals by S.W. Ellacott [10].

To give at least one more example of an exponential-like function, here are numerical data for $\exp(-t^2)$ on $0 \leqslant t \leqslant \infty$. Asymptotic matching still seems to hold, but things are less regular, which makes them even more interesting[3].

TABLE 2. Remes algorithm results and CF estimates for approximation of $\exp(-t^2)$. Digits of agreement of the two are in boldtype in the second column.

n	E_n	λ_{n+1}
0	5.000000000000000E-01	6.4950930361073E-01
1	1.688694894223526E-01	-**1.6**652643752795E-01
2	2.284258892248751E-02	**2.29**04765064962E-02
3	6.296734617204572E-03	-**6.29**50348277494E-03
4	6.657190675692884E-04	**6.657**8772442257E-04
5	2.621763610614775E-04	-**2.621**8111332487E-04
6	1.718893455437652E-05	**1.719**5697010430E-05
7	1.308159228579840E-05	-**1.308159**3692197E-05
8	7.148358529429540E-07	-**7.148**8121795910E-07

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2. CF Approximation.

In the CF method, instead of looking for nearly equioscillating approximants in the right set of functions (for instance, the rational n/n functions), one considers an approximant in a broader set of functions, but yielding an exactly equioscillating error function. It is then necessary to modify this approximant in order to return to the required class. Only a sketch of n/n CF approximation on the real interval $[-1,1]$ is given here. As far as possible, the notations of [68] are kept. Let F be a continuous function on $[-1,1]$ and let (1.1) be its Chebyshev polynomial expansion. Using $z = \exp(i\theta)$, one can write

$$F(x) = \frac{a_0}{2} + \frac{f^+(z)}{2} + \frac{f^-(z)}{2},$$

where

$$f^+(z) = \sum_1^\infty a_k z^k \tag{2.1}$$

[3]Recomputed λ_7 and λ_8 have some digits at variance with original publication (added in 2002). I lost even these new computations of 2002 (2010)

(the a_k's need not be real). One considers the approximation of f^+ by meromorphic functions in $|z|>1$ with exactly n poles in that region. Such functions can always be written in the form

$$\tilde{r}(z)=\frac{p(z)}{q(z)}=\frac{\sum_{-\infty}^{n} d_k z^k}{\sum_{0}^{n} e_k z^k}$$

where the n zeros of q must have modulus larger than 1. With respect to the supremum norm on the unit circle, the best approximation $\tilde{r}^*$ to f^+ in this class, the "extended CF approximant" of f^+, is characterized by the property that except in degenerate cases, the error function $f^+(z)-\tilde{r}^*(z)$ describes an exact circle of winding number $2n+1$ centered at the origin, as z describes the unit circle ([1, 14, 23, 28, 41, 42, 43, 65, 67, 68, 69]. A consequence is that the error function can then be written

$$f^+(z)-\tilde{r}^*(z)=b(z)=\frac{b_1(z)}{b_2(z)}=\sigma\frac{\overline{u_1}+\overline{u_2}z+\cdots}{u_1z^{-1}+u_2z^{-2}+\cdots}, \tag{2.2}$$

where the denominator b_2 of b is holomorphic in $|z|>1$ and must have exactly n zeros in $1<|z|<\infty$, which will be precisely the zeros of the denominator q of $\tilde{r}^*$:

$$b_2(z)=u_1z^{-1}+u_2z^{-2}=(e_n+e_{n-1}z^{-1}+\cdots+e_0z^{-n})v(z)=z^{-n}q(z)v(z),$$

where v is still holomorphic (and without zeros in $1<|z|<\infty$. Therefore, multiplying the two sides of (2.2) by $b_2(z)$,

$$f^+(z)b_2(z)-z^{-n}p(z)v(z)=\sigma b_1(z)\,, \qquad \text{or}$$

$$f^+(z)(u_1z^{-1}+u_2z^{-2}+\cdots)=\sigma(\overline{u_1}+\overline{u_2}z+\cdots)+\text{ negative powers of } z,$$

i.e.

$$\boldsymbol{H}U=\sigma\overline{U},$$

where U is the vector $[u_1,u_2,\ldots]^T$, and $\boldsymbol{H}$ is the infinite Hankel matrix

$$\boldsymbol{H}=[a_{k+m-1}],k,m=1,\ldots; \tag{2.3}$$

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σ is a singular value of $\boldsymbol{H}$ (since $\overline{\boldsymbol{H}U}=\sigma U$, i.e., $\overline{\boldsymbol{H}}\boldsymbol{H}U=\sigma^2U$). The fact that the $(n+1)^{\text{th}}$ singular value of $\boldsymbol{H}$ ($\sigma_1\geqslant\sigma_2\geqslant\ldots$) is indeed related to a vector U such that $u_1z^{-1}+u_2z^{-2}+\cdots$ has exactly n zeros in $1<|z|<\infty$ requires a deeper understanding of Hankel matrices theory [1, 14, 41, 42, 43]. However, the authors of [28] succeeded in getting all the fine points with only elementary tools of complex function theory, such as Rouché's theorem. Actually, the picture presented here supposes that σ_{n+1} is non-repeated: $\sigma_n>\sigma_{n+1}>\sigma_{n+2}$ (see [1, 14, 23, 28, 41, 42, 43, 67, 68, 69] for a general treatment).

If the a_k's happen to be real, then $\sigma_{n+1}=|\lambda_{n+1}|$, the absolute value of the $(n+1)^{\text{th}}$ eigenvalue of $\boldsymbol{H}$.

The last step in CF approximation is to project $\widetilde{R}(x)=(a_0+\tilde{r}^*(z)+\tilde{r}^*(z^{-1}))/2$ onto a rational n/n function of $x=(z+z^{-1})/2$. One naturally chooses $Q(x)=q(z)q(z^{-1})$ as the denominator and determines the numerator $P(x)$ such that the Chebyshev expansion of $R_{CF}(x)=P(x)/Q(x)$ and $\widetilde{R}(x)$ agree through the $T_n(x)=(z^n+z^{-n})/2$ term. This operation destroys the exact equioscillation of the error function, but the perturbation is usually very much smaller than σ_{n+1}. This further tratment will not be studied here. The incredible accuracy of CF approximation as quasioptimal real rational approximation is best demonstrated by tables 1 to 3 showing successive values of $\sigma_{n+1}=|\lambda_{n+1}|$ compared to corresponding values of $E_n,n=0,1,\ldots$ It is also striking to discover a Hankel matrices generalized eigenproblem in a step of the Remes algorithm [74]... wether this is another relation between Remes and CF is not clear.

In short, CF allows one to explore rational approximation of a function F by means of quantitative estimates of the eigenvalues of Hankel matrices composed of Chebyshev coefficients of F. For this reason, some properties of the spectra of Hankel matrices are investigated here.

3. An integral form for Hankel matrix invariants.

From now on, we consider only functions with real Chebyshev coefficients in (1.1), so that the eigenvalues $\lambda_1, \lambda_2, \ldots$ of the Hankel matrix (2.3) are the quantities of interest. If F is continuous (a minimal requirement!), $\boldsymbol{H}$ represents a bounded compact operator on the Hilbert sequence space ℓ^2 (these facts are nicely summarized in [41] and [76, § 8], and there is a much more detailed and advanced treatment in [54, 55]), so that its spectrum is a countable set of eigenvalues having the origin as only limit point. Moreover, the meaning of some equalities of the preceding section becomes more rigorous as U is now a square summable sequence: the functions discussed there are

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actually functions in L^2 or H^2.

How can we get information on the behaviour of the eigenvalues of $\boldsymbol{H}$ from the knowledge of F? The simplest identity involves the trace of $\boldsymbol{H}$, which makes immediate reference to values of F:

$$\zeta_1 = \text{ trace}\, \boldsymbol{H} = \sum_1^\infty \lambda_n = \sum_1^\infty a_{2n-1} = \frac{F(1) - F(-1)}{2}.$$

For example, with $F(x) = [(1+x)/2]^{1/2}$, a well-worked example ([12, 32, 49, 72], the value E_n for F equals the value E_{2n} for $|x|$), $\zeta_1 = 1/2$ so that, if the decrease of the λ_n's is fast, λ_1 must be expected to be near $1/2$, which is not surprising, as $E_0 = 1/2$. For more information on the subsequent λ_n's, let us consider the trace of $\boldsymbol{H}^2$, which is still not too hard (it is the sum of the squares of all the elements of the matrix = square of Frobenius norm, or Hilbert-Schmidt norm):

$$\zeta_2 = \text{ trace}\, \boldsymbol{H}^2 = \sum_1^\infty \lambda_n^2 = \sum_1^\infty n\, a_n^2.$$

For $F(x) = [(1+x)/2]^{1/2}$, $a_n = (-1)^{n-1}/[\pi(n^2 - 1/4)]$ and $\zeta_2 = 2/\pi^2$ is easily obtained. Considering only λ_1 and λ_2, this gives $\lambda_1 \approx 0.447$ and $\lambda_2 \approx 0.053$. By numerical[4] means, the following table is obtained; we have added the rational least error norms E_n, completed from [26]:

TABLE 3. Remes algorithm results, CF estimates for approximation of $[(x+1)/2]^{1/2}$ and empirical formula.

n	E_n	λ_{n+1}
0	0.500000	0.448264
1	0.043689	0.040407
2	0.008501	0.008008
3	0.002282	0.002170
4	0.000737	0.000705
5	0.000269	0.000258
	$8\exp(-\pi(2n+3/4)^{1/2})$	$8\exp(-\pi(2n+5/6)^{1/2})$

The link between F and ζ_2 is already more difficult than for ζ_1: ζ_2 requires information on the conjugate function $F_c(x) = \sum_1^\infty a_n \sin n\theta$, as $\zeta_2 = \frac{2}{\pi}\int_0^{2\pi} F(\cos\theta)\, dF_c(\cos\theta)$, by Parseval's relation. In terms of f^+: $\zeta_2 = \frac{1}{2\pi i}\int_{|z|=1} f^+(z^{-1})\, d f^+(z)$.

[4] The π was known [72]; the factor 8 has been established by Herbert Stahl, Best Uniform Rational Approximation of x^a on $[0,1]$, *Bulletin Amer.Math.Soc.* **28** (1993), 116-122, and Poles and Zeros of Best Rational Approximants for $|x|$, *Constr. Approx.*, **10** (1994), 469-522. The $3/4$ and $5/6$ are probably wrong (2008).

Following this line, integral forms for the ζ_p's will be produced, where
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$$\zeta_p = \sum_1^\infty \lambda_n^p. \tag{3.1}$$

Estimates of these values will in turn yield estimates for the λ_n's although ζ_p for large p gives only the largest λ's $(\lambda_1, \lambda_2, \dots)$.

Should there be a way to estimate ζ_p for (non integer) small values of p, then knowledge of the asymptotic behaviour of λ_n, $n \to \infty$, could be reached. The theoretical foundatuions are in [55]; see [73] for this Zeta notation.

In order to manipulate safely thses quantities, a supplementary condition is needed: $\boldsymbol{H}$ will be supposed to be trace-class, i.e., $\sum_1^\infty |\lambda_n| < \infty$. A sufficient condition is the absolute convergence of the double series of all the elements of $\boldsymbol{H}$, turning here into $\sum_1^\infty n|a_n| < \infty$. A necessary condition is that $\boldsymbol{H}$ is Hilbert-Schmidt: $\sum_1^\infty n\,a_n^2 < \infty$. The first condition is much too severe and does not work for instance with $F(x) = (1+x)^{1/2}$, whereas it is known [17, 72] that the E_n's (and consequently the σ_n's, from the Glover-Karlsson-Trefethen inequalities [14, 33, 67]) decreases as fast as $\exp(-\pi(2n)^{1/2})\dots$ The complete characterization has been given by Peller in terms of the function F, actually in terms of f^+:

Theorem 3.1. *The Hankel matrix $\boldsymbol{H} = [a_{k+m-1}]_1^\infty$ is trace-class if and only if $f^+(z) = \sum_1^\infty a_k z^k$ is in the Besov class A_1^1 [54], which means: f^+ is analytic in $|z|<1$, measurable on $|z|=1$, and $\int_{-\pi}^{\pi} h^{-2}\|\Delta^2 f^+(e^{i\theta},h)\|dh < \infty$, where*

$$\|\Delta^2 f^+(e^{i\theta},h)\| = \frac{1}{2\pi i}\int_{-\pi}^{\pi} |f^+(e^{i(\theta+h)}) - 2f^+(e^{i\theta}) + f^+(e^{i(\theta-h)})|d\theta.$$

The condition is satisfied by piecewise analytic continuous functions F with a finite number of power singularities: $F(x) \sim A_k + B_k(x-x_k)^\alpha, \alpha > 0$, although the a_n's decrease no faster than $n^{-\alpha-1}$ ([34, p. 43 and 72], from which the behaviour of $f^+(e^{i\theta})$ near $\theta = \arccos x_k$ may be deduced). For functions like $\exp((x-1)/(x+1))$ the decrease of the a_n's is fast enough to have $\sum n|a_n| < \infty$ (see [77, Example 7.10]).
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When $\boldsymbol{H}$ is trace-class,

$$\det(\boldsymbol{I} - w\boldsymbol{H}) = \prod_1^\infty (1 - w\lambda_j) = \sum_0^\infty \delta_n w^n \tag{3.2}$$

also has a meaning as an entire function of w. The coefficients δ_n's are so far the best source of information on the rate of decrease of the λ_n's, as δ_n is the series made of all the products of n λ's of distinct indexes:

$$\delta_n = (-1)^n \sum_{1 \leqslant i_1 \leqslant \cdots \leqslant i_n} \lambda_{i_1} \cdots \lambda_{i_n}. \tag{3.3}$$

Therefore, if the λ_n's are assumed to decrease like a power ρ^n, the δ_n's will essentially decrease like $\rho^{n^2/2}$, and the detection of such behaviour for the δ_n's will be the subject of section 4.

here is an example of such a behaviour: values of δ_n for $\exp(-t^m)$ (i.e., $F(x) = \exp\left[-\left(\frac{1-x}{1+x}\right)^m\right]$), $m = 1, 2, 3$, are given together with second differences of their exponents. A crude estimate of ρ follows from a mean value of this second difference:

TABLE 4. Samples of δ_n and second differences of exponents.

	$\exp(-t)$		$\exp(-t^2)$		$\exp(-t^3)$	
n	δ_n	Δ^2	δ_n	Δ^2	δ_n	Δ^2
0	1.000E 000		1.000E 000		1.000E 000	
5	-1.736E-011	24	-6.676E-009	16	-1.822E-007	16
10	-2.636E-046	24	-1.806E-034	19	-2.920E-030	16
15	2.590E-105	24	-1.237E-078	19	3.885E-069	15
20	1.624E-188	25	6.811E-141	18	2.969E-123	16
25	-6.474E-296	23	-8.510E-222	17	-1.718E-193	17
30	-1.636E-427	25	-3.418E-320	19	-3.555E-280	16
35	2.619E-583		1.177E-437		1.141E-383	
	$10^{-24/25} = 1/9.12$		$10^{-18/25} = 1/5.25$		$10^{-16/25} = 1/4.37$	

Remark that $\sum_0^\infty \delta_n w^n = \exp\left(-\sum_1^\infty \zeta_k w^k/k\right)$, so that the δ_n's can be obtained from the ζ_k's in a finite number of steps:

$$\delta_1 = -\zeta_1, \qquad \delta_2 = \frac{\zeta_1^2 - \zeta_2}{2}, \qquad \delta_3 = \frac{-\zeta_1^3 + 3\zeta_1\zeta_2 - 2\zeta_3}{6}, \ \ldots \tag{3.4}$$

Now that the interest of spectral invariants of the Hankel matrix $\boldsymbol{H}$ seems to have been established, we come to a compact formula for them, which will allow a discussion of their behaviour.

We assume the following integral form:

$$a_k = \int_C z^{k-1}\, d\alpha(z)\ , \qquad\qquad k \geqslant 1, \tag{3.5}$$

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where α is a measure whose support C is in the closed unit disk. There is always at least one way to find (3.5) for any expansion (1.1): from

$$a_k = \frac{2}{\pi}\int_{-1}^{1} F(x)T_k(x)\frac{dx}{\sqrt{1-x^2}} = \frac{1}{\pi i}\int_C z^{k-1}\, F\left(\frac{z+z^{-1}}{2}\right)\, dz, \tag{3.6}$$

where C is the unit circle. Of course, when F is analytic in some region containing the unit circle, the integration contour can be deformed and alternative forms will be available. This happens with Stieltjes functions, where C is a part of the real interval $[-1,1]$ [3,6].

Now, we try to find the traces ζ_n using (3.5):

Theorem 3.2. *Let the Hankel matrix* $\boldsymbol{H} = [a_{k+m-1}]_{k,m=1}^\infty$ *be trace-class, and let* (3.5) *hold with* C *in the closed unit disk. Then,*

$$\zeta_n = \mathit{trace}\, \boldsymbol{H}^n = \int_C \cdots \int_C \frac{d\alpha(z_1)\ldots d\alpha(z_n)}{(1-z_1z_2)(1-z_2z_3)\ldots(1-z_{n-1}z_n)(1-z_nz_1)} \tag{3.7}$$

which must be considered as the limit when $\eta \to 1$, $\eta < 1$, *of*

$$\int_C \cdots \int_C \frac{d\alpha(z_1)\ldots d\alpha(z_n)}{(1-\eta z_1z_2)(1-\eta z_2z_3)\ldots(1-\eta z_{n-1}z_n)(1-\eta z_nz_1)}.$$

This asks first for an integral form for the elements of $\boldsymbol{H}^n$. Let us start the row and column indexes at zero. Then, $\boldsymbol{H}_{m,k} = \int_C z^{m+k}\, d\alpha(z)$. If the whole of C is inside the unit disk, one shows by induction

$$(\boldsymbol{H}^n)_{m,k} = \int_C \cdots \int_C \frac{z_1^m z_n^k\, d\alpha(z_1)\dots d\alpha(z_n)}{(1-z_1z_2)(1-z_2z_3)\dots(1-z_{n-1}z_n)}.$$

and (3.7) follows easily. If at least a part of C touches the unit disk boundary, one must be more careful. One defines $\boldsymbol{H}(\eta) = [\eta^{(m+k)/2} a_{m+k+1}]_{m,k=0}^{\infty}$. Geometric series summations can now be performed in the integrals on $\eta^{1/2}C$, and as $\|\boldsymbol{H}-\boldsymbol{H}(\eta)\| \to 0$ when $\eta \to 1$ ($\|\boldsymbol{H}-\boldsymbol{H}(\eta)\|^2 \leqslant \sum n(1-\eta^{(n-1)/2})^2 a_n^2$), the result follows from from the continuity of the trace with respect to the operator norm (see [76, p. 337]). $\square$

An interesting change of variable is $u = \dfrac{1-z}{1+z}$ $\quad(\leftrightarrow z = \dfrac{1-u}{1+u})$ mapping the unit disk on the right half-plane. Let

$$d\beta(u) = -\frac{\pi i}{2}(1+u)^2\, d\alpha(z)\ , \tag{3.8}$$

Then,

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$(-\pi i)^n \zeta_n = \int_\Gamma \cdots \int_\Gamma (u_1+u_2)^{-1}(u_2+u_3)^{-1}\dots(u_{n-1}+u_n)^{-1}(u_n+u_1)^{-1} d\beta(u_1)\dots d\beta(u_n),$

where $\Gamma = (1-C)/(1+C)$ is a set in the (closed) right half plane.

With $G(t) = \exp(-t)$, $d\beta(u) = \exp(-u^2)du$ (see (4.1) below) produces $\zeta_1 = 1/2$ and $\zeta_2 = 1/\pi$.

For the δ_n's, we have:

Theorem 3.3. *Under the conditions of theorem 3.2, the coefficient δ_n of (3.2) is*

$$\delta_n = \frac{(-1)^n}{n!} \int_C \cdots \int_C S(z_1,\dots,z_n) d\alpha(z_1)\dots d\alpha(z_n) \tag{3.9}$$

with $S(z_1,\dots,z_n) = \prod_{m<j} \left(\dfrac{z_m - z_j}{1-z_m z_j}\right)^2 \prod_1^n (1-z_j^2)^{-1}$ *or, with* $u = (1-z)/(1+z)$, *using (3.8)*

$$\delta_n = (2\pi i)^{-n}(n!)^{-1} \int_C \cdots \int_C \frac{R(u_1,\dots,u_n)}{u_1\cdots u_n} d\beta(u_1)\cdots d\beta(u_n) \tag{3.10}$$

with $R(u_1,\dots,u_n) = \prod_{m<j} \left(\dfrac{u_j-u_m}{u_j+u_m}\right)^2.$

This result was first deduced by A. Hautot [27] by symbolic programmation with low values of n. The proof which follows is by J.Meinguet [44].

We start again from (3.5) and use the fact that $(-1)^n\delta_n$ is the series of all the determinants made with the same combinations $0 \leqslant i_1 < i_2 < \dots < i_n$ of n rows and columns of the matrix $\boldsymbol{H}$. From (3.5), each of these determinants turns into a $n-$uple integral of the determinant of elements $z_m^{i_m+i}$, $1 \leqslant m, j \leqslant n$. As in the proof of the preceding theorem, we may suppose $|z_m| \leqslant \eta^{1/2} < 1$, and take the limit $\eta \to 1$ in fine, as δ_n is an expression involving a finite number of ζ's (from (3.4)). From Binet-Cauchy theorem, $n!$ times the (therefore convergent) series in $i_1 < i_2 < \dots < i_n$ happens to be the determinant of the product

$$\begin{bmatrix} 1 & z_1 & z_1^2 & \dots \\ 1 & z_2 & z_2^2 & \dots \\ \dots & \dots & \dots & \dots \\ 1 & z_n & z_n^2 & \dots \end{bmatrix} \begin{bmatrix} 1 & 1 & \dots & 1 \\ z_1 & z_2 & \dots & z_n \\ z_1^2 & z_2^2 & \dots & z_n^2 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

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i.e., the determinant of the matrix $[(1-z_iz_j)^{-1}]_{i,j=1}^{n}$ giving

$$S(z_1,\dots,z_n) = (-1)^n (n!)^{-1} \det[(1-z_iz_j)^{-1}]_1^n = (-1)^n (n!)^{-1} \prod_{m<j} \left(\frac{z_m - z_j}{1 - z_m z_j}\right)^2 \prod_1^n (1-z_j^2)^{-1}$$

(Cauchy determinant [56] Sect.7 § 1.3) □

It is still not known if a numerical implementation of the forms (3.9) or (3.10) can be achieved in a reasonable way. Tables 1-4 have been constructed from conventional numerical methods applied to a big finite section of $\boldsymbol{H}$ (with a little trick: instead of taking the Chebyshev coefficients of $F(x)$, those of $F((x+\alpha)/(\alpha x+1))$ with a suitable $\alpha \in (-1,1)$ give better approximations of the same eigenvalues, this is to be compared with the use of c_n in [7] p.392).

4. Asymptotic estimates by Nuttall' saddlepoints method.

We proceed now with tentative asymptotic estimates of the multiple integral (3.10). Let us consider the case when the form (3.5) holds with a contour C almost completely inside the unit disk, with $F((z+z^{-1})/2)$ piecewise analytic on C . Then (3.10) holds with

$$d\beta(u) = f(u)du$$

where f is piecewise analytic on Γ almost entirely in the right-half plane. As one can always take $d\alpha(z) = (\pi i)^{-1} F((z+z^{-1})/2)dz$,

$$f(u) = F((1+u^2)/(1-u^2)) = G(-u^2) \tag{4.1}$$

is always a valid choice, from (1.2), (3.6) and (3.8).

The integral (3.10) is then essentially dominated by the configurations $(u_1,\dots,u_n)$ maximizing $|R(u_1,\dots,u_n)f(u_1)\dots f(u_n)|$ on Γ. Moreover, Γ can be deformed in an admissible way (singular points of f must not be crossed) into a new contour Γ_n where this latter maximum is minimized: the expected behaviour of $|\delta_n|$ is therefore essentially

$$|\delta_n| \sim \min_{\Gamma} \max_{u_i \in \Gamma} |R(u_1,\dots,u_n)f(u_1)\dots f(u_n)| \tag{4.2}$$

This leads to a search for saddlepoints, i.e., solutions of the set of nonlinear equations

$$\partial\{R(u_1,\dots,u_n)f(u_1)\dots f(u_n)\}/\partial u_i = 0, \qquad i = 1,\dots,n$$

or
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$$4\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{u_j}{u_i^2 - u_j^2} = -f'(u_i)/f(u_i), \quad i = 1,\dots,n \tag{4.3}$$

Similar derivations have been made by J.Nuttall ([50] § 5.3. [51]) for the asymptotic description of Padé and Hermite-Padé approximants . The discussion of the solutions of (4.3) is by no means simple. For

$$G(t) = \exp(-t^m)$$

i.e.,

$$-f'(u)/f(u) = 2m(-1)^m u^{2m-1},$$

numerical tests have been made for some values of m. For $m = 1$, there seems to be only one solution in the right-half complex plane. For $m > 1$, it seems obvious that several solutions are possible. Figure 1 shows the solutions for $m = 1,2$ and 3 that seem relevant to our problem (with a change of scale which will be explained in section 6).

We may find a help in solving our problem of minimizing on admissible curves Γ the maximum of $|R(u_1,\dots,u_n)f(u_1)\dots f(u_n)|$ on Γ by coming to an equivalent problem in electrostatics. To this end, let us consider n particles with a positive unit charge at $u_1,\dots,u_n$ on Γ, and n particles with a negative unit charge at $v_1,\dots,v_n$ on $-\Gamma$. The particles are repelled by the particles of the same family and attracted by the particles of the other family, according to the logarithmic potential . Moreover, they are all submitted to a supplementary field derived from the potential Re $(-f(u)/2)$. The total potential energy of a configuration $\{u_1,\dots,u_n;v_1,\dots,v_n\}$ is therefore

$$W_n = -\sum_{i\neq j}\log|u_i-u_j| - \sum_{i\neq j}\log|v_i-v_j| + \sum_{i,j}\log|u_i-v_j| - \sum_i(\log|f(u_)|+\log|f(v_i)|)/2$$

Remark that, f being even, we may assume that $v_i=-u_i$ will hold at equilibrium. Then we find easily

$$W_n = -\log|R(u_1,\dots,u_n)f(u_1)\dots f(u_n)|$$

so that we may now concentrate on the value of W_n: from (3.10) and (4.2) , a rough asymptotic estimate of $|\delta_n|$ will be given by

$$|\delta_n| = \exp(-W_n+O(n\log n)).$$

provided W_n is found to be much larger than $n\log n$.

For Γ fixed, the particles will take positions on Γ and $-\Gamma$ so as to minimize W_n . The result will be that the forces acting on u_i

$$-\sum_{j\neq i}\overline{(u_j-u_i)^{-1}} + \sum_j\overline{(v_j-u_i)^{-1}} + \frac{1}{2}\overline{f'(u_i)/f(u_i)} \tag{4.4a}$$

and on v_i

$$-\sum_{j\neq i}\overline{(v_j-v_i)^{-1}} + \sum_j\overline{(u_j-v_i)^{-1}} + \frac{1}{2}\overline{f'(v_i)/f(v_i)} \tag{4.4b}$$

will be directed as the normal to Γ and $-\Gamma$.

If we assume that the particles tend to fill a part $\tilde\Gamma_n$ of Γ when n is large, the potential

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function

$$h_n(u) = -\sum_i\log|u-v_i| - \sum_i\log|u-u_i| - \frac{1}{2}\log|f(u)|$$

will take constant values $h_n(\tilde\Gamma_n)$ and $h_n(-\tilde\Gamma_n)$ near $\tilde\Gamma_n$ and $-\tilde\Gamma_n$ (because the force at u is minus the gradient of the potential which is orthogonal to the level lines of the potential; and the gradient of a function of the form Re $H(u)$, H analytic, is $\overline{H'(u)}$. This may be appreciated if we drop the contributions $\log|u-u_i|$ or $\log|u-v_i|$ when u comes to be close to u_i or v_i, typically at a distance to be compared to some (negative) power of n , causing $O(\log n)$ perturbations which are asymptotically inocuous if $h_n(u)$ is much larger than $\log n$ for u near $\pm\tilde\Gamma_n$. With such a rule for estimating the potential function h_n, we find

$$nh_n(\tilde\Gamma_n) \sim \sum_i h_n(u_i) = W_n + \frac{1}{2}\sum_i\log|f(u_i)|.$$

Let us introduce the approximate distribution μ_n o the u_i's on $\tilde\Gamma_n$, so that any sum on the u_i's will be approximated as

$$\sum_i\varphi(u_i) \sim \int_{\tilde\Gamma_n}\varphi(\xi)\,d\mu_n(\xi),$$

then the potential function h_n takes the form (assuming $v_i=-u_i$ at equilibrium)

$$h_n(u) = -\mathrm{Re}\;\Phi_n(u) = \text{constant on } \tilde\Gamma_n \text{ and } -\tilde\Gamma_n$$

with

$$\Phi_n(u) = \int_{\tilde\Gamma_n}\log\frac{u-\xi}{u+\xi}d\mu_n(\xi) + \frac{1}{2}\log f(u). \tag{4.5}$$

So we replaced h_n by a harmonic function taking exactly constant values on $\tilde\Gamma_n$ and $-\tilde\Gamma_n$. This will result in μ_n to be a smooth distribution approximating the actual discrete distribution of $u_1,\dots,u_n$.

At this point, Γ being given, all the unknowns can be estimated asymptotically from the solution of the following boundary problem:

To find a unction Φ_n of the form (4.5) , with

Re $\Phi_n(u) =$ a constant c_n on a part $\tilde\Gamma_n$ of Γ,

Re $\Phi_n(u) < c_n$ on the remaining part $\Gamma\setminus\tilde\Gamma_n$ of Γ (minimality of potential on $\tilde\Gamma_n$),

Increase of imaginary part of Φ_n after a circuit of $\tilde\Gamma_n = 2n\pi$ (principle of argument, or total charge on Γ) .

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Then, $W_n \sim -nc_n - \dfrac{1}{2}\displaystyle\int_{\tilde\Gamma_n} \log|f(\xi)|\,d\mu_n(\xi)$.

Remark that the determination of $\tilde\Gamma_n$ out of Γ is a part of the problem.

Finally, maximizing W_n on admissible curves Γ makes us reach a (therefore unstable) further state of equilibrium where all the forces (4.4) vanish. Remark that, with $v_i = -u_i$, to have (4.4) to vanish is indeed to find a solution of (4.3). The final conditions are then summarized by the following

Rule 4.1. Let us consider the real Hankel matrix (2.3) when (3.5) holds, with

$$d\alpha(z) = -2(ni)^{-1}(1+u)^{-2} f(u)du, \qquad u = (1-z)/(1+z)$$

where f is analytic in a part of the right-half complex plane, whose boundary contains the imaginary axis.

Then we expect the eigenvalues of H to decrease like

$$\exp(2c_n)$$

provided $-c_n/\log n \to \infty$ when $n \to \infty$, where c_n is determined by the following boundary-value problem:

To find a function Φ_n of the form (4.5), with

- Re $\Phi_n(u) =$ a constant on $\tilde\Gamma_n$,
- There exists a curve Γ_n in the right-half plane, containing $\tilde\Gamma_n$, such that Γ_n and the imaginary axis enclose a region where f is holomorphic , and Re $\Phi_n(u) < c_n$ on $\Gamma_n \setminus \tilde\Gamma_n$.
- Increase of imaginary part of Φ_n after a circuit of $\tilde\Gamma_n = 2n\pi$ (equivalent to $\displaystyle\int_{\tilde\Gamma_n} d\mu_n(\xi) = n$).
- The limit values of the derivative Φ_n' at the two sides of $\tilde\Gamma_n$ are opposite:

$$\Phi_{n,+}'(u) \text{ and } \Phi_{n,-}'(u) = \pm\pi i\mu_n'(u), \qquad u\in\tilde\Gamma_n \tag{4.6}$$

  such that Re $\Phi_n(u) > c_n$ when one leaves $\tilde\Gamma_n$ along the normal direction.

The last condition is a consequence of the vanishing of the forces (4.4) and Sokhotskyi-Plemelj formulas([29])

$$\Phi_{n,+}'(u) \text{ and } \Phi_{n,-}'(u) = \fint_{\tilde\Gamma_n} [(u-\xi)^{-1} - (u+\xi)^{-1}]\,d\mu_n(\xi) + \frac{f'(u)}{2f(u)} \pm \pi i\mu_n'(u),$$

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$u\in\tilde\Gamma_n$, giving the limit values of Φ_n' at the two sides of $\tilde\Gamma_n$.

We still have to show that $W_n - W_{n-1} \sim -2c_n$. This comes from an estimate of $W_{n-1} - W_n$ as a mean value of $\log|f(u_n)R(u_1,\dots,u_n)/R(u_1,\dots,u_{n-1})|$ which gives indeed $\log|f(u)| + \displaystyle\int_{\tilde\Gamma_n} \log\left|\frac{u-\xi}{u+\xi}\right|^2 d\mu_n(\xi) = 2c_n$.

5. Relation with the theory of extremal polynomials.

Much of the material of the preceding section is actually found in rational approximation theory. For instance, the electrostatics picture is much used [2] [15]-[20] [51] [59] etc. The function S of (3.9) is almost in [2]. So the connection between CF , Hankel matrices spectral theory, and rational approximation in the complex plane becomes deeper and deeper. Indeed, let us start from $G(t)$ analytic in a region R of the extended complex plane $\overline{\mathbb{C}}$ which we want to approximate on some closed set $K \in \overline{R}$ (the positive real axis in the preceding sections) by a rational function P_n/Q_n of degree n.

As a first step, consider that P_n interpolates Q_nG at $t_1,\ldots,t_{n+1} \in K$. An integral form of the remainder is

$$G(t)-P_n(t)/Q_n(t) = (2\pi i)^{-1}\frac{\omega_n(t)}{Q_n(t)}\int_\Delta \frac{Q_n(\tau)}{\omega_n(\tau)}(\tau-t)^{-1}G(\tau)\,d\tau \tag{5.1}$$

where Δ is a contour in $\overline{R}$ enclosing K and $\omega_n(\tau) = (\tau-t_1)\cdots(\tau-t_{n+1})$. When K is the positive real axis, Δ could be a parabola-like curve. A first bound of the error norm is essentially dominated by

$$\max_{t\in K}|\omega_n(t)/Q_n(t)|\max_{\tau\in\Delta}|Q_n(\tau)G(\tau)/\omega_n(\tau)| \tag{5.2}$$

which we can try to make as small as possible by a suitable choice of the zeros $t_1,\ldots,t_{n+1}$ of ω_n and $p_1,\ldots,p_n$ of Q_n (extended weighted Zolotarev problem [13] [16]).

The contour Δ can also be deformed provided it is still in $\overline{R}$ and encloses K, in order to minimize (5.2) . However, the integral in (5.1) constructed with the best rational approximant is often still very much smaller than the best possible bound (5.2). This is explained by the fact that P_n/Q_n can satisfy up to $2n+1$ interpolation conditions, so that the integral in (5.1) vanishes at n further points $t_{n+2},\ldots,t_{2n+1}$. Introducing $\Omega_n(t) = (t-t_1)\cdots(t-t_{2n+1})$, the new conditions become

$$\int_\Delta \frac{Q_n(\tau)}{\Omega_n(\tau)}\Pi(\tau)G(\tau)\,d\tau = 0, \text{ any polynomial } \Pi \text{ of degree } < n \tag{5.3}$$

and the remainder can now be written

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$$G(t)-P_n(t)/Q_n(t) = (2\pi i)^{-1}\frac{\Omega_n(t)}{Q_n^2(t)}\int_\Delta \frac{Q_n^2(\tau)}{\Omega_n(\tau)}(\tau-t)^{-1}G(\tau)\,d\tau \tag{5.4}$$

Now, we consider again (5.2) with Ω_n and Q_n^2 instead of ω_n and Q_n, and let $2\lambda_n$ and Q_n be smooth approximations of the distributions of $\{t_1,\ldots,t_{2n+1}\}$ and $\{p_1,\ldots,p_n\}$. Then, with

$$\Psi_n(t) = \int_{\tilde{\Delta}_n}\log(t-\eta)d\nu_n(\eta) - \int_K \log(t-\eta)d\lambda_n(\eta) + \frac{1}{2}\log G(t) \tag{5.5}$$

where $\tilde{\Delta}_n$ is the actual support of $d\nu_n$ (with $\int_{\tilde{\Delta}_n} d\nu_n(\eta) = \int_K d\lambda_n(\eta) = n$), the : best bound of the remainder (5.4) can be estimated as

$$\log E_n \sim 2\left[\max_{t\in K}\text{ Re }\left(-\Psi_n(t)+\frac{1}{2}\log(G(t)\right)+\max_{\tau\in\tilde{\Delta}_n}\text{Re }\Psi_n(\tau)\right]$$

and this kind of problem is again related to a boundary problem

Rule 5.1.

Find Ψ_n *of the form (5.5) , with*

(1) Re $\left(\Psi_n - \frac{1}{2}\log G(t)\right) =$ a constant a_n on K,
(2) Re $\Psi_n(t) =$ a constant b_n on $\tilde{\Delta}_n$,
(3) There exists a curve Δ_n in $\overline{R}$, enclosing K and containing $\tilde{\Delta}_n$, such that Re $\Psi_n < b_n$ on $\Delta_n \setminus \tilde{\Delta}_n$,
(4) $\int_{\tilde{\Delta}_n} d\nu_n(\eta) = \int_K d\lambda_n(\eta) = n$,
(5) The limit values of the derivative Ψ_n' at the two sides of $\tilde{\Delta}_n$ are opposite:
$\Psi_{n,+}'(t)$ and $\Psi_{n,-}'(t) = \pm\pi i\nu_n'(t), \qquad t\in\tilde{\Delta}_n$
such that Re $\Psi_n(t) > b_n$ when one leaves $\tilde{\Delta}_n$ along the normal direction.

Then, we expect

$$G(t)-P_n(t)/Q_n(t)\sim\exp(2b_n-2\Psi_n(t)+\log G(t)), t\notin K, t\notin\tilde{\Delta}_n,$$

$$E_n\sim\exp(2(b_n-a_n)).$$

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The conditions of validity of the rule are by no means simple!! They have been worked a.o. by Goncar, Lopez, Rahmanov, Stahl [15]-[20] [35] [37] [62][63] [64]. It sems important that G must be analytic in the whole complex plane excepting a set of vanishing capacity, so that Δ_n may be deformed almost at will (as before, $\tilde{\Delta}_n$ (the place where Q_n 'lives' [45]) is an unknown of the problem and is related to the boundary of so-called extremal regions [62]) . The most difficult part is to show that (5.3) is asymptotically compatible with rule 5.1, that is that if (5.3) holds, the distribution of the zeros of Q_n and Ω_n behave indeed asymptotically as given by rule 5.1. This has been established by Stahl for functions with branch points [63] .

Relation (5.3) may be considered as defining Q_n to be (formally) orthogonal to polynomials of degree less than n with respect to a "weight" $G(\tau)/\Omega_n(\tau)$. Should Δ be allowed to shrink to a real set where $G(\tau)/\Omega_n(\tau)>0$, then (5.3) is equivalent to saying that Q_n is the monic polynomial of degree n minimizing $\int_\Delta (Q_n(\tau))^2 G(\tau)/\Omega_n(\tau)\,d\tau$, whence the name extremal polynomial given to Q_n: denominators of best rational approximations behave like extremal polynomials. The real set case has received recently extremely dramatic and impressive accelerations of knowledge [36]-[39] [45] [47] [57] [70]: see the big recent surveys by two active workers in this field, P.Hevai ([47] including added note on p.144, the subject has been declared by P.Hevai [48] as one of the hottest in approximation theory) and D.Lubinsky [39].

For the complex set case, Q_n could rightly be called extremal if it would minimize a true norm $\int_\Delta |Q_n(\tau)|^2|G(\tau)/\Omega_n(\tau)|\,|d\tau|$, (Szegő's complex orthogonality, see [75]), and this does not seem to be the same as (5.3) and (5.4). However, near $\tilde{\Delta}_n$ but not on $\tilde{\Delta}_n$, one has $Q_n(G/\Omega_n)^{1/2}\sim\exp(\Psi_n)$ which has a discontinuous derivative when one crosses $\tilde{\Delta}_n$, whereas the true $Q_n(G/\Omega_n)^{1/2}$ is of course regular. A better description of this function on $\tilde{\Delta}_n$ is $Q_n(G/\Omega_n)^{1/2}\sim\exp(\Psi_n)+\exp(2b_n-\Psi_n)$ (see [50] 3.2.7 for such a situation) which takes into account the actual distribution of zeros of Q_n on $\tilde{\Delta}_n$. This suggests that the phase of $(Q_n)^2G/\Omega_n$ has only slow variation on $\tilde{\Delta}_n$ and that Q_n still behaves like an extremal polynomial .

Finally, here is the compatibility of rules 4.1 and 5.1 :

Remark 5.2. *When $K=[0,\infty]$, $f(u)=G(-u^2)$ with $f(\overline{u})=\overline{f(u)}$, let us*

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take $\tilde{\Gamma}_n$ symmetrically with respect to the real axis in the right half complex plane and satisfying the conditions of rule 4.1 . Then

$$\tilde{\Delta}_n=-(\tilde{\Gamma}_n)^2, \Psi_n(t)=\Psi_n(-u^2)=\Phi_n(u)$$

satisfy rule 5.1 with $a_n=0$ and $b_n=c_n$.

Indeed, as $\Gamma=\tilde{\Gamma}_n$ and $d\mu_n$ are symmetric with respect to the real axis, (4.5) may be uritten $\Phi_n(u)=\int_{\tilde{\Gamma}_n}\log\frac{u\overline{\xi}}{u+\xi}d\mu_n(\xi)+\frac{1}{2}\log(f(u))$, so that $\Phi_n(u)-\log(f(u))/2=-2i\int_{\tilde{\Gamma}_n}\text{Arctan}\,[(u/i+\text{Im}\,\xi)/\text{Re}\,\xi]d\mu_n(\xi)=-2in\kappa_n(u)$ is pure imaginazy when u is on the imaginary axis, that is when $t\in K$. Remark that $\kappa_n(i\infty)-\kappa_n(-i\infty)=n$, and that $i\kappa_n'(u)>O$ on the imaginary axis. The derivative $\Phi_n'(u)-f'(u)/(2f(u))$ is given in the right half plane (avoiding $\tilde{\Gamma}_n$ where the jump of derivative values is $2\pi i\mu' n(u)$) by the Cauchy integral $(2\pi i)^{-1}\int_{-i\infty}^{i\infty}(\xi-u)^{-1}2i\pi\kappa_n'(\xi)d\xi-(2\pi i)^{-1}\int_{\tilde{\Gamma}_n}(\xi-u)^{-1}2i\pi d\mu_n(\xi)$. Multiplying by two and subtracting the known form $\int_{\tilde{\Gamma}_n}[(u-\xi)^{-1}-(u+\xi)^{-1}]\mu_n'(\xi)d\xi$, we get $2\int_{-i\infty}^{i\infty}(\xi-u)^{-1}d\kappa_n(\xi)+\int_{\tilde{\Gamma}_n}\log(\xi^2-u^2)d\mu_n(\xi)$. After integrating in u , one recovers a new form

$$\Phi_n(u)-(\log f(u))/2=-2\int_{-i\infty}^{i\infty}\log(\xi-u)d\kappa_n(\xi)+\int_{\tilde{\Gamma}_n}\log(\xi^2-u^2)d\mu_n(\xi).$$

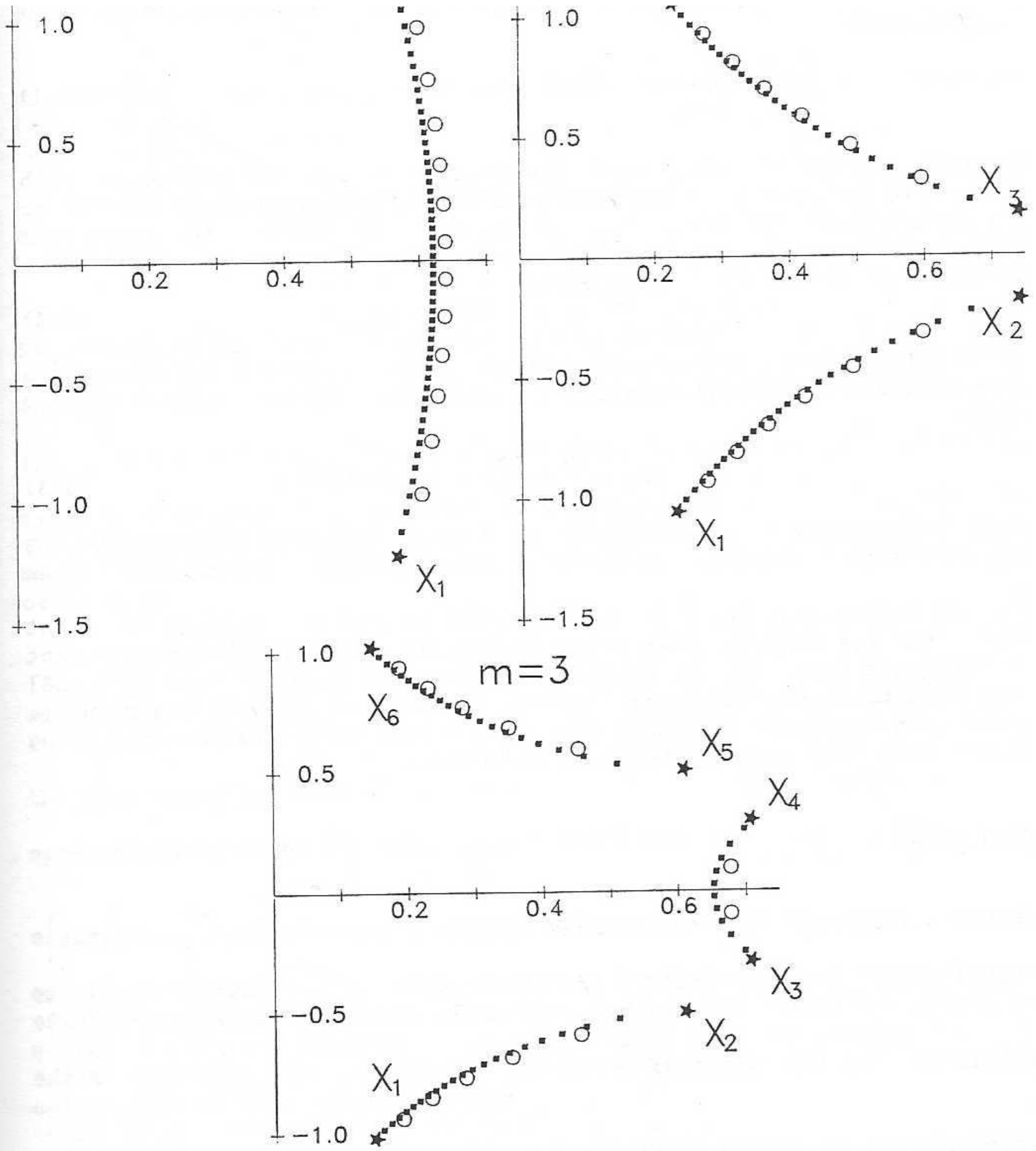

Figure 1 . Positions in the complex plane of remarkable points relevant to rational approximation of exp(−t^m) on t≥0 , for m=1,2,3 . Solid squares : scaled saddlepoints from the integral form of the 50th elementary symmetric function of eigenvalues of Hankel matrix . Hollow circles : scaled square roots of minus the poles of 12th degree approximant . Stars : calculated endpoints of the common locus drawn by the preceding points .

Finally, as κ_n' is even, the first integral is written $-2\int_0^{i\infty}\log(\xi^2-u^2)d\kappa_n(\xi)$ and we have indeed a representation of the required form (5.5) in terms of $t=-u^2$.

So we expect the square roots of minus the zeros of Q_n to be distributed approximately on $\tilde{\Gamma}_n$ with the same distribution μ_n as the saddlepoints in (4.3) . For $G(t) = \exp(-t^m)$, Figure 1 shows saddle-points (squares) and $(-(\text{poles})^{1/2}$ (circles) indeed almost on the same locus. Actually, these values have been divided by $n^{1/(2m)}$ ($n = 50$ for the saddlepoints, $n = 12$ for the rational approximation poles)

6. Solution in terms of (hyper)elliptic integrals.

We come now to a discussion of the solution of (4.3) or an example of rule 4.1, when $G(t) = \exp(-t^m), m = 1, 2, ...,$ i.e., $f(u) = \exp((-1)^{m+1}u^{2m})$ (from 4.1), so that $f'(u)/f(u) = 2m(-1)^{m+1}u^{2m-1}$: (4.3) becomes

$$4\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{u_j}{u_i^2 - u_j^2} = 2m(-1)^m u_i^{2m-1}, \qquad i = 1, \ldots, n \tag{6.1}$$

A simple change of scale will immediately settle the variation with respect to n: in (6.1) , if the u_j's behave like some function $\varphi(n)$ of n, each term of the sum will be of the order of $1/\varphi(n)$, the sum itself will be like $n/\varphi(n)$, and the right-hand side behaves like $(\varphi(n))^{2m-1}$, so that $\varphi(n) = n^{1/(2m)}$. So we expect

$$v_i = n^{-1/(2m)}u_i, \qquad i = 1, \ldots, n \tag{6.2}$$

to be ultimately distributed on a fixed system of arcs $\tilde{\Gamma}$ according to a distribution $d\mu$ of total weight 1, and (4.5) becomes $\Phi_n(u) = n\Phi(v)$, where

$$\Phi(v) = \int_{\tilde{\Gamma}} \log\frac{v-\xi}{v+\xi}\, d\mu(\xi) + (-1)^{m+1}v^{2m}/2 \tag{6.3}$$

Rule 4.1 becomes: *eigenvalues of* $\boldsymbol{H}$ *will decrease like* $\exp(2c_n) = \exp(2nc) = \rho^n$ *(so* $\rho = \exp(2c)$, *where* c *is the constant value of Re* $\Phi(v)$ *on* $\tilde{\Gamma}$.

We assume now that $\tilde{\Gamma}$ is made of a finite number p arcs in the right half plane (it will be shown later that $p \leqslant m$). The proof of such a fact is difficult (see [62] for example). Goncar and Rahmanov [18] [37] [58] were able to do that at least for the case $m = 1$ and they have a complete proof that $(\log E_n)/n \to 2c$ when $n \to \infty$, the actual determination of c being then a mere technicality that will be summarized now.

From (6.3) , $\Phi'(v) + m(-1)^m v^{2m-1} = \displaystyle\int_{\tilde{\Gamma}} 2\xi(v^2-\xi^2)^{-1}\, d\mu(\xi)$ is an even function, analytic in the extended complex plane outside $\pm\tilde{\Gamma}$, and takes values $\pm\pi i\mu'(v) + m(-1)^m v^{2m-1}$ on the two sides of $\tilde{\Gamma}$ (adapting (4.6) to (6.3)). We build now another even analytic function taking opposite values on the two sides of $\tilde{\Gamma}$. Let $X_1, X_2, \ldots, X_{2p-1}, X_{2p}$ be the endpoints of the p arcs of $\tilde{\Gamma}$ (see fig. 1) , and

$$X(v) = v^{4p} + \chi_1 v^{4p-2} + \cdots + \chi_{2p} = (v^2 - X_1^2)\cdots(v^2 - X_{2p}^2). \tag{6.4}$$

We define then $X^{1/2}(v)$ as the square root of X behaving like v^{2p} for
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large v , and continuous outside $\tilde{\Gamma}$. This function takes opposite values $\pm X^{1/2}(v)$ on the two sides of $\tilde{\Gamma}$, so that the function $(\Phi'(v) + m(-1)^m v^{2m-1})/X^{1/2}(v)$ takes the values $\pm m(-1)^m v^{2m-1}/X^{1/2}(v) + \pi i\mu'(v)/X^{1/2}(v)$ on the two sides of $\tilde{\Gamma}$. Applying again Sokhotskyi-Plemelj formulas [29] , we find

$$\begin{aligned}(\Phi'(v) &+ m(-1)^m v^{2m-1})/X^{1/2}(v) \\ &= (\pi i)^{-1}\int_{\tilde{\Gamma}} 2\xi(v^2-\xi^2)^{-1} m(-1)^m \xi^{2m-1} X^{-1/2}(\xi)\, d\xi \\ &= 2m(-1)^m(\pi i)^{-1}\int_{\tilde{\Gamma}} \xi^{2m}(v^2-\xi^2)^{-1} X^{-1/2}(\xi)\, d\xi\end{aligned} \tag{6.5}$$

So everything is known if we find the $2p$ complex numbers $X_1, \ldots, X_{2p}$ (and p)! From (6.3), the left hand side of (6.5) behaves like $\left(2\displaystyle\int_{\tilde{\Gamma}} \xi\, d\mu(\xi)\right) v^{-2p-2}$ for large v, with $\displaystyle\int_{\tilde{\Gamma}} \xi d\mu(\xi) > 0$ (because $\tilde{\Gamma}$ is in the right-half plane and is symmetric with respect to the real axis). So the expansion of the right-hand side of (6.5) in negative powers of v must start with a positive coefficient times v^{-2p-2}, whence the p conditions

$$M_j = \int_{\tilde\Gamma} \xi^{2m+2j} X_+^{-1/2}(\xi)\, d\xi = 0, \qquad j = 0, \ldots, p-1 \tag{6.6}$$

and $(-1)^m i^{-1} M_p > 0$; $p-1$ further real conditions will come from Re $\Phi(v) =$ the same constant c on all the p arcs of $\tilde\Gamma$, we shall assume $\tilde\Gamma$ to be symmetric with respect to the real axis (so that $X_{2p-j+1} = \overline{X_j}$), and $\pi \int_{\tilde\Gamma} d\mu(\xi) = \sum_1^p \mathrm{Im}\,[\Phi(X_{2j}) - \Phi(X_{2j-1})] = \pi$ will be the last condition. Now we transform (6.5) using a technique of [22] (pp.266 and 283) : we multiply (6.5) by the even polynomial $v^2 X(v)$ which is written $v^2 X(v) - \xi^2 X(\xi) + \xi^2 X(\xi)$ inside the integral (6.5) which turns into two integrals, the first involving the polynomial $[v^2 X(v) - \xi^2 X(\xi)]/(v^2 - \xi^2)$. A careful calculation of this integral leaves
$v^2 X^{1/2}(v)\Phi'(v) + m(-1)^m v^{2m+1} X^{1/2}(v) =$
$2m(-1)^m(\pi i)^{-1}\left\{ \sum_{j=0}^{p} \chi_j \sum_{k=p}^{2p-j} M_k v^{4p-2j-2k} + \int_{\tilde\Gamma} \xi^{2m+2} X_+^{1/2}(\xi)(v^2-\xi^2)^{-1}\, d\xi \right\}.$

Differentiating (in v), and integrating by parts (in ξ) the last
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integral, it appears to be $\int_{\tilde\Gamma} (v^2-\xi^2)^{-1} P(\xi) X^{-1/2}(\xi)\xi^{2m}\, d\xi$, wheze $P(\xi)$ is the polynomial $(2m+1)X(\xi) + \xi X'(\xi)/2$. Using the trick $P(\xi) = P(\xi) - P(v) + P(v)$ as before, we get rid of P in the integral and recover the integral of (6.5) . The result is a differential equation for Φ
$\{X^{1/2}(v)[v^2\Phi'(v) + m(-1)^m v^{2m+1}]\}' = vY(v) + vP(v)[\Phi'(v) + m(-1)^m v^{2m-1}]/X^{1/2}(v),$
where Y is the polynomial of degree $2p-2$

$$Y(v) = 2m(-1)^m(\pi i)^{-1} \sum_{j=0}^{p-1} \chi_j \sum_{k=p}^{2p-j-1} (2p-j-2k-2m-1) M_k v^{4p-2j-2k-2}. \tag{6.7}$$

The differential equation for Φ' turns as $X^{1/2}(v)[v^{1-2m}\Phi'(v)]' = v^{-2m}Y(v)$, so that

$$\Phi'(v) = m(-1)^{m-1} v^{2m-1} + v^{2m-1}\int_\infty^v \xi^{-2m} Y(\xi) X^{-1/2}(\xi) d\xi = v^{2m-1}\int_{X_1}^v \xi^{-2m} Y(\xi) X^{-1/2}(\xi) d\xi \tag{6.8}$$

with the conditions

$$\int_\infty^{X_1} \xi^{-2m} Y(\xi) X^{-1/2}(\xi) d\xi = m(-1)^m,$$

$$\int_{X_j}^{X_{j+1}} \xi^{-2m} Y(\xi) X^{-1/2}(\xi) d\xi = 0, \qquad j = 1, 2, \ldots, 2p-1,$$

as Φ' must vanish at each X_j, this is the only possible way for Φ' to take opposite values on the two sides of each arc of $\tilde\Gamma$. More precisions on $\tilde\Gamma$ can now be given:

Proposition 6.1. *One must have $p \leqslant m$ and Φ' has exactly $m-p$ further zeros in the right half-plane outside $\tilde\Gamma$.*

Indeed, $(\Phi')^2$ is holomorphic in the right half-plane, and has already $2p$ zeros $X_1, \ldots, X_{2p}$ there. For large v , $(\Phi'(v))^2 \sim m^2 v^{4m-2}$. According to the discussion of the remark 5.2, $\Phi'(v) = -2i\kappa'(v) - (-1)^m m v^{2m-1}$ on the imaginary axis, with $-2i\kappa'(v) > 0$, so that the total increase of argument of $(\Phi')^2$ on a big contour enclosing the right half-plane is $4m\pi$: this accounts for the $2p$ known zeros of $(\Phi')^2$ and $m-p$ more (double) zeros. □

If $p < m$, it seems that the remaining critical points of Φ do not allow the existence of a curve Γ (required by rule 4.1) where Re Φ is everywhere $\leqslant c$, but this should be proved. Tests with $m > 1$ and $p = 1$ gave

indeed wrong results. Figure 1 shows $\tilde{\Gamma}$ for $m = 1,2,3$ with $2m$ endpoints (five point stars) calculated as below[5].
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TABLE 5. Results for m=1 , 2 and 3.

$\boldsymbol{m=1}$	
X_1, X_2	$0.564412701731271 \mp 1.230228033100522i$
Y	-3.664045422603946
$2c$	-2.228833648714334
ρ	$1/9.289025491920819$
$\boldsymbol{m=2}$	
X_1, X_4	$0.230299569523605 \mp 1.056043075724618i$
X_2, X_3	$0.740872935366573 \mp 0.181255581301698i$
Y	$-4,089738435714034u^2 + 3.018259576896660$
$2c$	-1.679203056619678
ρ	$1/5.361281630239104$
$\boldsymbol{m=3}$	
X_1, X_6	$0.147466522850900 \mp 1.019380088475020i$
X_2, X_5	$0.610266123777351 \mp 0.504086300206854i$
X_3, X_4	$0.707976575689678 \mp 0.293205472234699i$
Y	$-5.038105707137323u^4 + 3.413952831945491u^2 - 2.465551268021017$
$2c$	-1.472035162993397
ρ	$1/4.358095556608086$

For Φ itself, integration of (6.8) yields

$$\begin{aligned}\Phi(v) &= \frac{(-1)^m v^{2m}}{2} + \frac{1}{2m}\int_\infty^v (v^{2m} - \xi^{2m})\frac{Y(\xi)\,d\xi}{\xi^{2m}X^{1/2}(\xi)} \\ &= \frac{v\Phi'(v)}{2m} - \frac{1}{2m}\int_\infty^v \frac{Y(\xi)\,d\xi}{X^{1/2}(\xi)},\end{aligned}$$

so that

$$c = -(2m)^{-1}\,\mathrm{Re}\int_\infty^{X_1} Y(\xi)X^{-1/2}(\xi)$$

and where the first kind (hyper)elliptic integrals

$$\int_{X_{2j-1}}^{X_{2j}} Y(\xi)X^{-1/2}(\xi)\,d\xi, \qquad j = 1,\ldots,p$$

must he pure imaginary numbers and have a sum πi. Working all these conditions results in table 5 below ($p = m$) . For $m = 1$, elliptic integrals identities yield several equivalent forms. From the conditions above, one finds that $2c = -\pi K'/K$, where K and K' are the complete elliptic integrals of first kind related to modulii k and $(1-k^2)^{1/2}$ such that $K = 2E$, where E is the corresponding elliptic integral of second kind (see [11] [31] [46] for notations; solving equation (6.6) can be interpreted as looking for a zero of the complete elliptic integral of the second kind considered as a function of its modulus [44]). Goncar and Rahmanov presented the equation $\sum_{n=1}^{\infty} n\rho^n/[1-(-1)^n\rho^n] = 1/8$ for $\rho = \exp(2c)$. Equivalence of the two formulations can be established from various identities for Jacobi theta and zeta functions [46] . It

[5]Values for $m = 2$ and $m = 3$ still poorly checked (2010).

is very remarkable that another problem involving theta functions, posed more than 100 years ago by G.H.Halphen [25] , requires the very same number ρ in its solution!

Another equation for ρ is $\sum_{n=0}^{\infty}(2n+1)^2(-\rho)^{n(n+1)/2} = 0$ ([25] pp. 287 and 427) .

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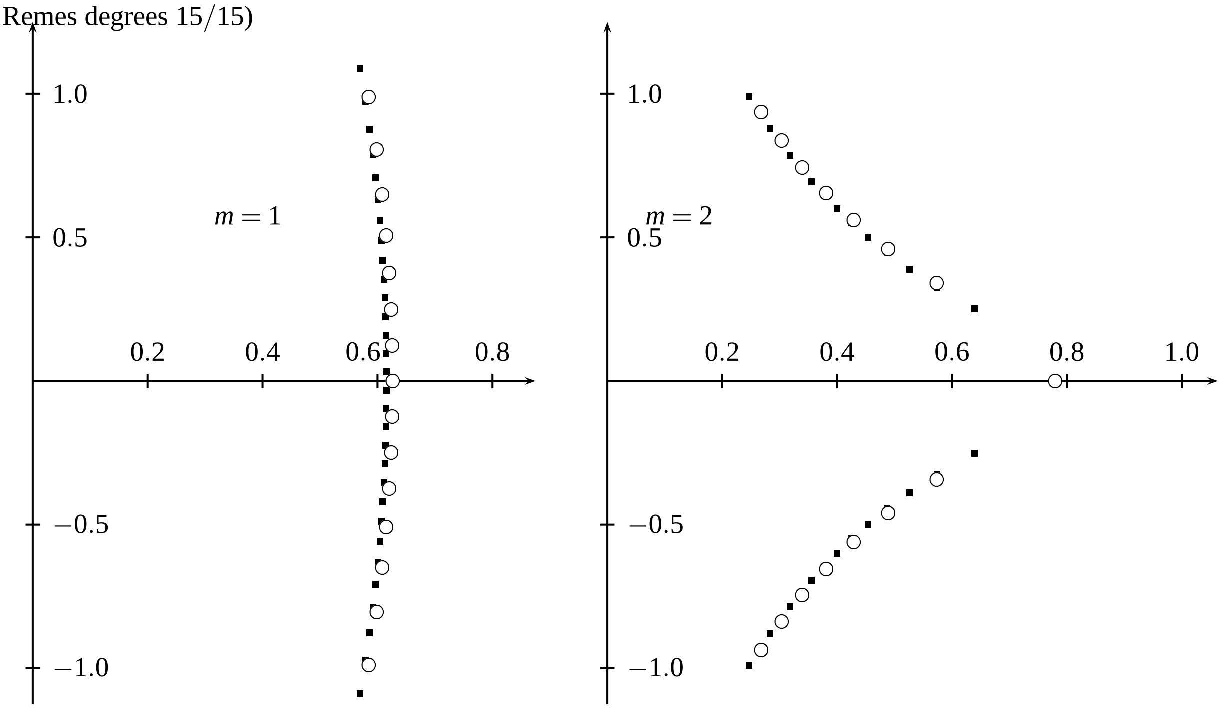
Additions to the retyping (2010).

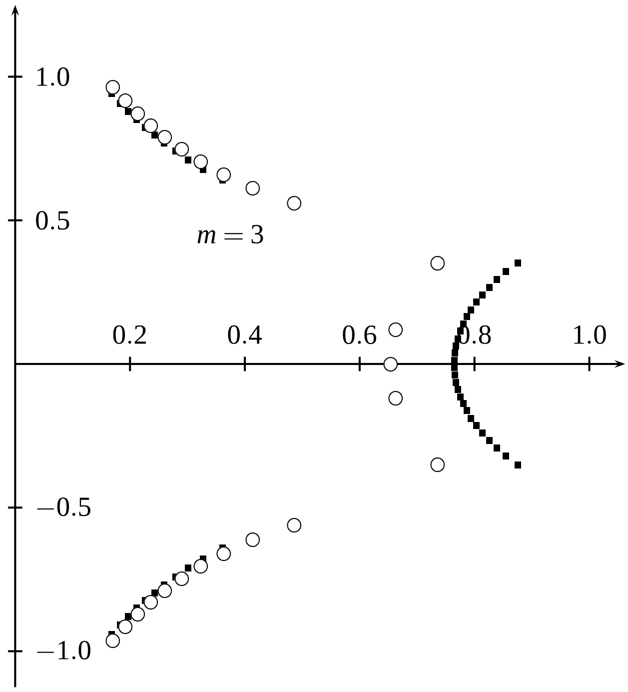
After almost 10 years of retyping (scanning after some time), I fancied to add a big section with enormously more accurate results, as the small laptop of today is as good as the big mainframe of this remote past. However, I only reprogrammed the saddlepoints part, and the Remes part. I do not want to wait 10 more years before finishing my homework, so here is what I have.

Moreover, there were so many computing mistakes to be exposed. I even wonder how some of the conjectures were found to be right (by Herbert in 1993, and by Sasha in 2002).

Saddlepoints and Remes poles, these latter scaled by division by $(n+1/2)^{1/m}$ (the $n+1/2$ instead of n is thanks to Sasha too[10]) fit nicely in new computations, at least for $m=1$ and $m=2$ (30 saddlepoints and Remes degrees $15/15$)



But something strange appears at $m=3$ (50 saddlepoints and Remes degree 25) as a part of the saddlepoints do not fit at all with poles close to 0.65:



[10] If the initial function is $\exp(-t^m)$, the circles on the picture are at $\sqrt{-\text{pole}/(n+1/2)^{1/m}}$.

And this part of the picture is not the same as the one of 1987. What happened?

I recently designed a check of the potential function $\Phi(v) = \int_{\tilde{\Gamma}} \log \dfrac{v-\xi}{v+\xi}\, d\mu(\xi) + (-1)^{m+1} v^{2m}/2$ to be estimated from scaled saddlepoints ξ_i as $\dfrac{1}{n}\sum_{i=1}^{n} \log \dfrac{v-\xi_i}{v+\xi_i} + (-1)^{m+1} v^{2m}/2$. On the support, between two saddlepoints, at $(\xi_k + \xi_{k+1})/2$, the real part should be the constant c of Table 5.

It works nicely with $m = 1$ and $m = 2$. With 20 saddlepoints:

```
                  m=1                                                        m=2
 k        ( xi(k)+xi(k+1) )/2              real(potential)        xi(k)+xi(k+1) )/2               real(potential)
 1 0.575870982192689 + 0.970809880769312*I -1.08095236865057 0.264694780530584 + 0.930449835387089*I -0.81373457755362


...
 5 0.602774072210971 + 0.488533855556504*I -1.08130996089973 0.374028282440525 + 0.646698315440168*I -0.80919476548946
...
10 0.610856117644038                       -1.07743194286341 0.609895431609687                        -0.72990104119886
...
15 0.602774072210971 - 0.488533855556504*I -1.08130996089973 0.374028282440525 - 0.646698315440168*I -0.80919476548946
...
19 0.575870982192689 - 0.970809880769312*I -1.08095236865057 0.264694780530584 - 0.930449835387089*I -0.81373457755362
```

And more accurate results with 50 saddlepoints:

```
                  m=1                                                        m=2
 k        ( xi(k)+xi(k+1) )/2              real(potential)        xi(k)+xi(k+1) )/2               real(potential)
 1 0.573030904858412 + 1.08738371602566*I -1.09897713241632 0.249180084946104 + 0.988243761950365*I -0.82742708134669
...
10 0.606111937345503 + 0.59686703666796*I -1.10152351039706 0.348980615322273 + 0.715965857534717*I -0.82834673532988
...
20 0.618869896241061 + 0.19125290653327*I -1.10009480844596 0.511539987008225 + 0.416519452027190*I -0.82319733638440
...
25 0.620285935246128                      -1.09978970700388 0.668254193743779                        -0.78526937857001
...
30 0.618869896241061 - 0.19125290653327*I -1.10009480844596 0.511539987008225 - 0.416519452027190*I -0.82319733638440
...
40 0.606111937345503 - 0.59686703666796*I -1.10152351039706 0.348980615322273 - 0.715965857534717*I -0.82834673532988
...
49 0.573030904858412 - 1.08738371602566*I -1.09897713241632 0.249180084946104 - 0.988243761950365*I -0.82742708134669
```

When $m = 2$, note that there must exist real points where $\Phi(z)$ is ***smaller*** than c.

But here are the values for $m = 3$:

```
 k        ( xi(k)+xi(k+1) )/2              real(potential)
 1 0.175692466657832 + 0.924588613425847*I -0.577103385503801
 2 0.190300092109052 + 0.893175288659714*I -0.577892135454630
...
 8 0.290287680958422 + 0.725677421128352*I -0.575034452596030
 9 0.314361420721404 + 0.694452676098908*I -0.573636858792969
10 0.344352938941608 + 0.659203378565546*I -0.571510408693191
11 0.618327427649441 + 0.496405975881338*I -0.875642071076589
12 0.865296146576558 + 0.336897538281743*I -1.41206581764795
13 0.847189436453089 + 0.307173125697218*I -1.41311939571126
...
24 0.765695473368377 + 0.025222372137298*I -1.41394098023903
25 0.765182627524716                       -1.41393704901930
26 0.765695473368377 - 0.025222372137298*I -1.41394098023903
...
37 0.847189436453089 - 0.307173125697218*I -1.41311939571126
38 0.865296146576558 - 0.336897538281743*I -1.41206581764795
```

```
39 0.618327427649441 - 0.496405975881338*I -0.875642071076589
40 0.344352938941608 - 0.659203378565546*I -0.571510408693191
41 0.314361420721404 - 0.694452676098908*I -0.573636858792969
42 0.290287680958422 - 0.725677421128352*I -0.575034452596030
...
48 0.190300092109052 - 0.893175288659714*I -0.577892135454630
49 0.175692466657832 - 0.924588613425847*I -0.577103385503801
```

The constants on the various arcs of the support are not the same! So even the saddlepoints finder is questionable (the one of 1987 seems to have been better).

So I stick to scaled Remes poles, the estimate of the real part of Φ seems much better there:

```
 k         ( p(k)+p(k+1) )/2              real(potential)
 1 0.181480931530952 + 0.938765803174740*I -0.705438798974375
 2 0.202753295918785 + 0.893245934150062*I -0.709808085969737
 3 0.224779917814115 + 0.850983213885511*I -0.712596238412321
 4 0.248771213330327 + 0.809660029481561*I -0.714557144838279
 5 0.275703592112085 + 0.768189710629888*I -0.715842713907409
 6 0.306750549178130 + 0.725837269404566*I -0.716439757903193
 7 0.343620936572742 + 0.681969860510632*I -0.716285248294386
 8 0.389226084432342 + 0.635894414386978*I -0.715244366498917
 9 0.449984044619928 + 0.586476136463153*I -0.712872529698248
10 0.610579078133332 + 0.455481884173136*I -0.740031270707045
11 0.699475489089291 + 0.235034107772666*I -0.728305446367088
12 0.658504856143687 + 0.059923931212111*I -0.718128281407906
13 0.658504856143687 - 0.059923931212111*I -0.718128281407906
14 0.699475489089291 - 0.235034107772666*I -0.728305446367088
15 0.610579078133332 - 0.455481884173136*I -0.740031270707045
16 0.449984044619928 - 0.586476136463153*I -0.712872529698248
17 0.389226084432342 - 0.635894414386978*I -0.715244366498917
18 0.343620936572742 - 0.681969860510632*I -0.716285248294386
19 0.306750549178130 - 0.725837269404566*I -0.716439757903193
20 0.275703592112085 - 0.768189710629888*I -0.715842713907409
21 0.248771213330327 - 0.809660029481561*I -0.714557144838279
22 0.224779917814115 - 0.850983213885511*I -0.712596238412321
23 0.202753295918785 - 0.893245934150062*I -0.709808085969737
24 0.181480931530952 - 0.938765803174740*I -0.705438798974375
```

Still puzzling is the slow variation of the value of the real part of the discretized potential on the support with the degree n: we have about -0.72 at $n = 25$, whereas $c = -0.736$ in Table 5. At $n = 15$, we have about -0.68.

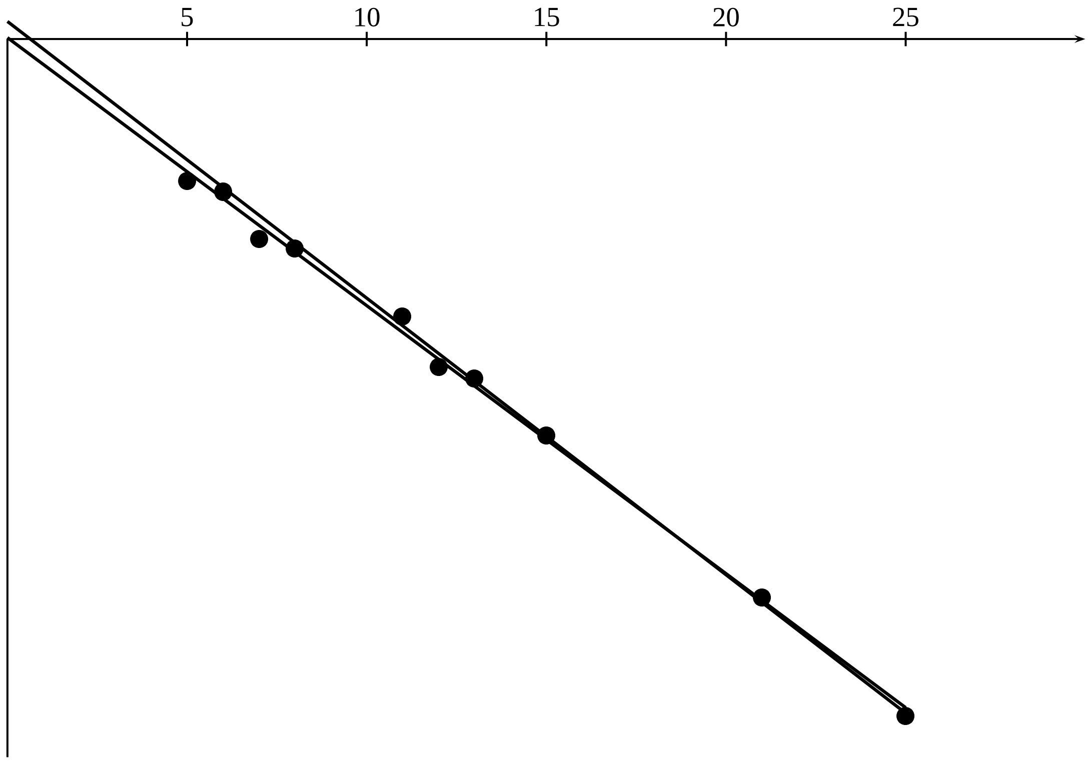
From some error norms:

```
 k           log(Ek) /2
 5 -3.960207867828094697744794222
 6 -4.254405098251466034768636453
 7 -5.571794814451900413481783517
 8 -5.829874088458930779181936372
11 -7.739437560527907153738726031
12 -9.141376215003553322606539777
13 -9.463206549450846865803479738
15 -11.04258558512709576970661894
21 -15.55755153914226454686844673
25 -18.85704041191106161691779962
```

Do we have an average slope of -0.736?

A least squares linear fit yields $0.03815568869506342098626574795 - 0.7463336310333638651274912104n$. Hmm, keeping only degrees > 10, result is now

$0.4894755049694628541652102630 - 0.7704953700100980041302357978n$.



It is clear that whatever I try to do now is clumsier and less accurate than what I did in 1987