SCIENTIFIC COMPUTATION ON SOME MATHEMATICAL CONJECTURES

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This talk will survey recent results on four mathematical conjectures: the Bernstein Conjecture in polynomial approximation theory, the Pólya Conjecture (related to the Riemann Hypothesis) in function theory, the "1/9" Conjecture in rational approximation theory, and the Ruscheweyh-Varga Conjecture in polynomial function theory. The emphasis here will be on the interaction between high-precision scientific computation and mathematical analysis, and their application to unsolved mathematical conjectures.

1. The Bernstein Conjecture

Scientific computations on an old open conjecture of S. Bernstein in approximation theory, turned out to be both mathematically and computationally interesting, as well as esthetically pleasing. Like other famous unsolved conjectures (such as the Goldbach conjecture in number theory), the Bernstein conjecture is very easy to state.

For notation, given any real continuous function $f(x)$ with domain $[-1,+1]$, let

$$(1.1)\qquad E_n(f) := \inf\left\{ \|f - g\|_{L_\infty[-1,+1]} : g \in \pi_n \right\}$$

denote the error of best uniform approximation of $f(x)$ on $[-1,+1]$ by polynomials in π_n. (Here, π_n denotes the set of all real polynomials of degree at most n ($n=0,1,\cdots$).) For the specific function $|x|$, a well-known result of Jackson (cf. Meinardus [1.7, p.56]) gives that

$$(1.2)\qquad E_n(|x|) \le 6/n \qquad (n=1,2,\cdots),$$

and, because $|x|$ is an even function on $[-1,+1]$, it is easily seen (cf. Rivlin [1.9, p.43]) that

$$(1.3)\qquad E_{2n}(|x|) = E_{2n+1}(|x|) \qquad (n=0,1,\cdots).$$

Thus, it suffices to consider only the manner in which the sequence $\{E_{2n}(|x|)\}_{n=1}^{\infty}$ decreases to zero. From (1.2), there follows

$$(1.4)\qquad 2nE_{2n}(|x|) \le 6 \qquad (n=1,2,\cdots).$$

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In his fundamental paper [1.2] from 1914, Bernstein significantly improved (1.4). Specifically, he showed that there *exists* a constant, which we call β (β for "Bernstein"), such that

$$\lim_{n \to \infty} 2nE_{2n}(|x|) = \beta \quad . \tag{1.5}$$

In addition, Bernstein, using crude calculations based on extremely ingenious methods, deduced in [1.2] the following rigorous upper and lower bounds for β :

$$0.278 < \beta < 0.286 \quad . \tag{1.6}$$

Moreover, Bernstein noted [1.2, p.56] as a "curious coincidence" that the constant

$$\frac{1}{2\sqrt{\pi}} = 0.28209\ 47917 \cdots \tag{1.7}$$

also satisfies the bounds of (1.6) and is very nearly the average of these bounds. This observation has, over the years, become known as the

(1.8) Bernstein Conjecture: $\beta \overset{?}{=} \dfrac{1}{2\sqrt{\pi}}$.

In the 70 years since Bernstein's work [1.2] appeared in 1914, his Conjecture remained unsolved, though there was considerable interest in this Conjecture (cf. Bell and Shah [1.1], Bojanic and Elkins [1.3], and Salvati [1.10]). Recently, we showed in 1985 in [1.11] that Bernstein's Conjecture is *false*. It is important to add that the proof of this depended on numerically implementing some extremely ingenious ideas already devised by Bernstein in 1914!

The high-precision calculations we performed in [1.11] consisted of three basic parts:

i) Determination of $\{2nE_{2n}(|x|)\}_{n=1}^{52}$;

ii) Determination of the upper bounds $\{2\mu_m\}_{m=0}^{100}$ for β;

iii) Determination of the lower bounds $\{l_m\}_{m=1}^{20}$ for β.

The determination in [1.11] of the best approximation errors $E_{2n}(|x|)$ (cf. (1.1)) used an essentially standard mathematical implementation of the (second) Remez algorithm (cf. [1.7, p.105]) on a VAX 11/780, with R. P. Brent's MP package [1.4] to handle the multiple-precision computations. Taking into account guard digits and the possibility of some small rounding errors, we believe that the numbers $\{E_{2n}(|x|)\}_{n=1}^{52}$ we determined are accurate to at least 95 decimal digits. A subset of the numbers $\{2nE_{2n}(|x|)\}_{n=1}^{52}$, truncated to ten decimal digits, is given in Table 1.1 below to show the slow convergence of these numbers. (For a complete listing of the numbers $\{2nE_{2n}(|x|)\}_{n=1}^{52}$ in greater precision, see [1.11].)

n	$2nE_{2n}(\|x\|)$
1	0.25000 00000
10	0.27973 24337
20	0.28005 97447
30	0.28012 06787
40	0.28014 20296
50	0.28015 19162

Table 1.1

The computation of the upper bounds $\{2\mu_m\}_{m=0}^{100}$ for β is based on the following ingenious observation of Bernstein [1.2]. Define the function $F(t)$ on $[0,+\infty)$ by

$$(1.9) \qquad F(t) = t\int_0^1 \frac{x^{t-\frac{1}{2}}\,dx}{x+1} = \frac{1}{2}\int_0^\infty \frac{e^{-u}\,du}{\cosh(u/2t)} .$$

Other representations of $F(t)$ include

$$(1.10) \qquad F(t) = \frac{t}{2t+1}F\left(1,1;t+\frac{3}{2};\frac{1}{2}\right) ,$$

where $F(a,b;c;z)$ denotes the classical hypergeometric function (cf. Henrici [1.6, p.27]), and

$$(1.11) \qquad F(t) = \frac{t}{2}\left\{\Psi\left(\frac{t}{2}+\frac{3}{4}\right) - \Psi\left(\frac{t}{2}+\frac{1}{4}\right)\right\} \qquad (t \geq 0) ,$$

where $\Psi(z)$, the psi (digamma) function, is defined from the gamma function $\Gamma(z)$ by

$$(1.12) \qquad \Psi(z) := \frac{\Gamma'(z)}{\Gamma(z)} .$$

The connection between $F(t)$ of (1.9) and the Bernstein constant β of (1.5) is the following. For each positive integer m, set

$$(1.13) \qquad \mu_m := \inf_{a_0,\cdots,a_m \text{ real}} \left\| \cos(\pi t)\left[F(t) - \left(a_0 + \sum_{k=1}^{m} \frac{a_k}{t^2-[(2k-1)/2]^2}\right)\right]\right\|_{L_\infty[0,+\infty)}$$

and for $m=0$, set

$$(1.13') \qquad \mu_0 := \inf_{a_0 \text{ real}} \left\| \cos(\pi t)\left[F(t) - a_0\right]\right\|_{L_\infty[0,+\infty)} .$$

Note that the poles of the sum in (1.13) are cancelled by zeros of $\cos(\pi t)$. Because of this, standard arguments show that real constants $\{\hat{a}_k(m)\}_{k=0}^{m}$ exist such that

$$(1.14)\qquad \mu_m = \|\cos(\pi t)\left[F(t) - \left(\hat{a}_0(m) + \sum_{k=1}^{m} \frac{\hat{a}_k(m)}{t^2-[(2k-1)/2]^2}\right)\right]\|_{L_\infty[0,+\infty)} .$$

Moreover, it is evident from (1.13) that the numbers $\{\mu_m\}_{m=0}^{\infty}$ are nonincreasing:

$$(1.15)\qquad \mu_0 \geq \mu_1 \geq \cdots \geq \mu_m \geq \cdots .$$

Now, Bernstein [1.2, p.55] proved that β of (1.5) and the constants μ_m of (1.13) are connected through

$$(1.16)\qquad \beta = 2 \lim_{m \to \infty} \mu_m .$$

Clearly, we see from (1.15) and (1.16) that

$$(1.17)\qquad 2\mu_0 \geq 2\mu_1 \geq \cdots \geq 2\mu_m \geq \beta \qquad (m=0,1,\cdots),$$

so that the calculation of the constants $2\mu_m$ provides increasingly sharper upper bounds for β. We mention that the upper bound 0.286 for β of (1.16), determined by Bernstein in 1914, corresponds to an approximation of the upper bound $2\mu_3$.

What is mathematically and computationally interesting is that the solution of the approximation problem in (1.13) has an oscillation character which permits (cf. [1.11]) the use of a modified form of the (second) Remez algorithm. We mention that Bernstein's work [1.2] of 1914 *predates* the 1934 appearance of Remez's algorithm [1.8].

In Table 1.2 below, we give a subset of the numbers $\{2\mu_m\}_{m=0}^{100}$, each truncated to 10 decimal digits. (For details on the application of this modified Remez algorithm, and on the accuracies in the associated calculations, we refer to [1.11].)

m	$2\mu_m$
5	0.28177 99926
20	0.28026 79181
40	0.28019 38951
60	0.28018 03067
80	0.28017 55680
100	0.28017 33791

Table 1.2

We remark that already from the case $m = 5$ of Table 1.2, we have (cf. (1.7))

$$\frac{1}{2\sqrt{\pi}} > 2\mu_5 = 0.28177 \cdots > \beta ,$$

so that the Bernstein Conjecture (1.8) is necessarily *false.*

The final third part of the calculations for the Bernstein Conjecture from [1.11] involved the calculation of lower bounds l_m for β. This is, as Bernstein [1.2] also showed, is related to a complicated nonlinear optimization involving the function $F(t)$ of (1.9). This was by far the most *time-consuming* of all calculations performed in [1.11]; for details of this and for a discussion of the accuracy of these calculations, we refer the reader to [1.11]. These lower bounds $\{l_m\}_{m=1}^{\infty}$ can be shown to satisfy

(1.18) $$l_1 \le l_2 \le \cdots \le l_m \le \beta \text{ , with } \lim_{m \to \infty} l_m = \beta ,$$

so that the calculation of the constants l_m provides increasingly sharper lower bounds for β. We mention that the lower bound 0.278 for β of (1.6), determined by Bernstein in 1914, corresponds to an approximation of the lower bound l_2. Table 1.3 below gives a subset of the numbers $\{l_m\}_{m=1}^{20}$, each truncated to 10 decimal digits.

m	l_m
1	0.27198 23590
5	0.28009 77913
10	0.28016 13794
15	0.28016 71898
20	0.28016 85460

Table 1.3

From (1.17) and (1.18), we have that

(1.19) $$l_{20} \le \beta \le 2\mu_{100} .$$

Thus, from the appropriate entries of Tables 1.2 and 1.3, this implies that

(1.20) $$0.280168 < \beta < 0.280174 .$$

Hence, these upper and lower bound calculations give us that

(1.21) $$\beta = 0.280171 + \delta \quad \text{where } |\delta| < 3 \times 10^{-6} .$$

It turned out that the use of *Richardson extrapolation* (cf. Brezinski [1.5, p.7] with $x_n = 1/n^2$), applied to the high precision calculations $\{2nE_{2n}(|x|)\}_{n=1}^{52}$, produced unexpectedly beautiful results! This use of Richardson extrapolation in [1.11] suggests that

(1.22) $\beta \doteq 0.28016\ 94990\ 23869\ 13303\ 64364\ 91230\ 67200\ 00424\ 82139\ 81236 \cdots$

to 50 decimal places. And, to leave intact the number of unsolved conjectures in this area, it is *conjectured* in [1.11] that $2nE_{2n}(|x|)$ admits the following asymptotic expansion:

$$2nE_{2n}(|x|) = \beta - \frac{K_1}{n^2} + \frac{K_2}{n^4} - \frac{K_3}{n^6} + \cdots \qquad (n \to \infty), \tag{1.23}$$

where the constants K_j (independent of n) are *all positive*. (For numerical estimates of $\{K_j\}_{j=0}^{10}$, see also [1.11].)

Finally, because the Bernstein constant β is intimately associated with the function $F(t)$ of (1.10), it is not implausible that β, as well as the constants K_j in (1.23), *may* admit a closed-form expression in terms of classical hypergeometric functions and/or known mathematical constants!

References

1.1 R. A. Bell, S. M. Shah (1969): Oscillating polynomials and approximations to $|x|$. Publ. of the Ramanujan Inst. 1: 167-177.

1.2 S. Bernstein (1914): Sur la meilleure approximation de $|x|$ par des polynomes de degrés donnés. Acta Math. 37: 1-57.

1.3 R. Bojanic, J. M. Elkins (1975): Bernstein's constant and best approximation on $[0,+\infty)$. Publ. de l'Inst. Math., Nouvelle série 18 (32):19-30.

1.4 R. P. Brent (1978): A FORTRAN multiple-precision arithmetic package. Assoc. Comput. Mach. Trans. Math. Software 4 :57-70.

1.5 C. Brezinski (1978): Algorithmes d'Accélération de la Convergence. Paris: Editions Technip.

1.6 P. Henrici (1974): Applied and Computational Complex Analysis, vol. 1. New York: John Wiley and Sons.

1.7 G. Meinardus (1967): Approximation of Functions: Theory and Numerical Methods. New York: Springer-Verlag.

1.8 E. Ya. Remez (1934): Sur le calcul effectiv des polynômes d'approximation de Tchebichef. C. R. Acad. Sci. Paris, 199: 337-340.

1.9 T. J. Rivlin (1969): An Introduction to the Approximation of Functions. Waltham, Mass.: Blaisdell Publishing Co.

1.10 D. A. Salvati (1980): Numerical Computation of Polynomials of Best Uniform Approximation to the Function $|x|$. Master's Thesis, Ohio State University, Columbus, Ohio, 39 pp.

1.11 R. S. Varga and A. J. Carpenter (1975): On the Bernstein Conjecture in approximation theory. Constr. Approx. 1: 333-348. (This will also appear as a Russian translation in Math. Sbornik (1986).)

2. The Pólya Conjecture

This section is devoted to an old conjecture from 1927 of G. Pólya (related to the famous Riemann Hypothesis). To begin, let Riemann's ξ-function (cf. Titchmarsh [2.9, p.16]) be defined by

$$(2.1)\qquad \xi(iz) := \frac{1}{2}\left(z^2 - \frac{1}{4}\right)\pi^{-\frac{z}{2}-\frac{1}{4}}\Gamma\left(\frac{z}{2}+\frac{1}{4}\right)\varsigma\left(z+\frac{1}{2}\right),$$

where ς denotes the Riemann ς-function. It is known that ξ is an entire function of order one which admits (cf. Pólya [2.8], p.11]) the integral representation

$$(2.2)\qquad \frac{1}{8}\xi\left(\frac{x}{2}\right) = \int_0^\infty \Phi(t)\cos(xt)\,dt\ ,$$

where

$$(2.3)\qquad \Phi(t) := \sum_{n=1}^{\infty}\left(2\pi^2 n^4 e^{9t} - 3\pi n^2 e^{5t}\right)\exp\left(-\pi n^2 e^{4t}\right)\ .$$

Now, expanding $\cos(xt)$ and integrating termwise in (2.2) show that ξ can be written in Taylor series form as

$$(2.4)\qquad \frac{1}{8}\xi\left(\frac{x}{2}\right) = \sum_{m=0}^{\infty}\frac{(-1)^m\,\hat{b}_m\,x^{2m}}{(2m)!}\ ,$$

where

$$(2.5)\qquad \hat{b}_m := \int_0^\infty t^{2m}\,\Phi(t)\,dt \qquad (m=0,1,\cdots)\ .$$

On setting $z = -x^2$ in (2.4), the function $F(z)$ is then defined by

$$(2.6)\qquad F(z) := \sum_{m=0}^{\infty}\frac{\hat{b}_m\,z^m}{(2m)!}\ ,$$

so that F is an entire function of order 1/2 which is real for real z. From (2.4) and (2.6), it follows that

$$(2.7)\qquad \frac{1}{8}\xi\left(\frac{x}{2}\right) = F(-x^2)\ .$$

Concerning the Riemann ζ-function, it is known that $\{-2m\}_{m=1}^{\infty}$ are the real zeros of ζ, and the Riemann Hypothesis asserts that all remaining zeros of the function $\zeta(z)$ lie on the line Re $z=1/2$. It is known (cf. Titchmarsh [2.9]) that all the nonreal zeros of $\zeta(z)$ lie in the strip $0<\text{Re } z<1$, and that infintely many zeros lie on Re $z=1/2$. To add to this, the Riemann Hypothesis has been attacked numerically over the years, and it is now known (cf. van de Lune et al. [2.10]) that the first 200,000,000 nonreal zeros of $\zeta(z)$ closest to the real axis *do* lie exactly on Re $z=1/2$!

In a different direction, as a consequence of (2.1) and (2.7), one obtains the well-known result (cf. [2.4, p.16]) that the Riemann Hypothesis is *equivalent* to the statement that all zeros of $F(z)$ of (2.6) are real and negative. Now, it is known (cf. Boas [2.1, p.24]) that a *necessary condition* that $F(z)$ satisfy the weaker hypothesis that all its zeros be real is that its Taylor coefficients satisfy

$$(2.8) \qquad m\left(\frac{\hat{b}_m}{(2m)!}\right)^2 > (m+1)\frac{\hat{b}_{m-1}}{(2m-2)!}\frac{\hat{b}_{m+1}}{(2m+2)!} \qquad (m=1,2,\cdots),$$

or equivalently that

$$(2.9) \qquad D_m := \left(\hat{b}_m\right)^2 - \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1} > 0 \qquad (m=1,2,\cdots).$$

In 1927, Pólya [2.8], while studying some fragmentary unpublished notes of J. L. W. V. Jensen dealing with the Riemann Hypothesis, raised the question of directly establishing the inequalities (2.9), *without* proving the Riemann Hypothesis. The interest in the inequalities in (2.9) is very natural: the truth of the Riemann Hypothesis obviously implies that all the inequalities of (2.9) are valid, so that if one of the inequalities (2.9) *were* to fail for some $m\geq 1$, then the Riemann Hypothesis would necessarily be *false*! For historical reasons, we call the inequalities of (2.8) and (2.9) the *Pólya-Turán inequalities*.

The history concerning Pólya's problem of 1927 is interesting. For nearly 40 years, this problem was apparently untouched in the literature. Then in 1966, Grosswald [2.4, 2.5] generalized a formula of Hayman [2.6] on *admissible functions*, and, as an application of this generalization, Grosswald proved that

$$(2.10) \qquad D_m = \frac{\left(\hat{b}_m\right)^2}{m}\left\{1+O\left(\frac{1}{\log m}\right)\right\}, \qquad (m\to\infty).$$

As the moments $\{\hat{b}_m\}_{m=0}^{\infty}$ are well-known to be all positive (cf. Thm. A of [2.3]), then Grosswald's result (2.10) proves that (2.9) *is* valid for all m sufficiently large, say $m\geq m_0$, but the exact value of m_0 was not determined in Grosswald's analysis. To our knowledge, this gap in Grosswald's solution of Pólya's problem was not filled subsequently in the literature.

Intrigued by Pólya's problem, in part because of its interesting numerical overtones in the determination of the moments $\{\hat{b}_m\}_{m=0}^{\infty}$, we embarked on a dual program of high-precision computations of the moments $\{\hat{b}_m\}_{m=0}^{109}$ and the numbers $\{D_m\}_{m=1}^{108}$, as well as an attempt of a mathematically rigorous analysis of the Pólya problem. Our mathematical result (cf. Csordas, Norfolk, and Varga [2.3]) is that the *Pólya Conjecture is true*:

Theorem. The Pólya-Turán inequalities (2.9) are valid for all $m = 1, 2, \cdots$.

Our proof of this Theorem, using a technique which is different from Grosswald's approach, has two main steps which we now sketch. Setting

$$(2.11)\qquad K(t) := \int_t^{\infty} \Phi(\sqrt{u}\,)du \qquad (t \geq 0),$$

where Φ is defined in (2.3), our first main step was to establish that $\log K(t)$ is strictly concave on $(0, +\infty)$. Next, on setting

$$(2.12)\qquad \lambda_x := \frac{1}{2\Gamma(x+1)} \int_0^{\infty} u^x K(u)du \qquad (x > -1),$$

the second main step of our analysis was to establish that $\log \lambda_x$ is also strictly concave on $(0, +\infty)$, from which it follows that

$$(2.13)\qquad \lambda_{m-1/2}^2 > \lambda_{m-3/2}\lambda_{m+1/2} \qquad (m = 1, 2, \cdots).$$

Now, integration by parts and the change of variable $u = t^2$ in (2.12) yield

$$(2.14)\qquad \lambda_x = \frac{1}{\Gamma(x+2)} \int_0^{\infty} t^{2x+3}\Phi(t)dt \qquad (x > -1).$$

Thus, on choosing $x = m - 1/2$, the above reduces from (2.5) to

$$(2.15)\qquad \lambda_{m-1/2} = \hat{b}_{m+1}/\Gamma(m + \tfrac{3}{2}) \qquad (m = 1, 2, \cdots).$$

Substituting (2.15) in (2.12) then gives

$$(2.16)\qquad (\hat{b}_{m+1})^2 > \left(\frac{2m+1}{2m+3}\right) \hat{b}_m \hat{b}_{m+2} \qquad (m = 1, 2, \cdots).$$

which directly establishes (2.9) for all $m = 2, 3, \cdots$. (The remaining case $m = 1$ of (2.9) was established numerically by computing the moments $\hat{b}_0, \hat{b}_1$, and $\hat{b}_2$, each to a precision of 50 significant digits.) We mention that high-precision estimates of $\{\hat{b}_m\}_{m=0}^{20}$ and $\{D_m\}_{m=1}^{19}$, can be found in [2.3].

To add to our excitement, a review of a 1982 paper by Matiyasevich [2.7] appeared in the Mathematical Reviews (MR 85g:11079), after we had submitted our manuscript [2.3]. Using an approach different from ours or Grosswald's, Matiyasevich also attacked the Pólya problem. Specifically, Matiyasevich first established that the number D_m of (2.9) possesses the interesting triple-integral representation

$$(2.17)\qquad D_m = \frac{1}{2(2m+1)} \int_0^\infty\int_0^\infty u^{2m} v^{2m} \Phi(u)\Phi(v)(u^2-v^2)\int_u^v \frac{\omega(t)}{(t\,\Phi(t))^2} dt\ du\ dv ,$$

where

$$(2.18)\qquad \omega(t) := \big(t\,\Phi(t)\big)'\ \Phi'(t) - t\,\Phi''(t)\Phi(t) \qquad (t \geq 0)$$

As $\Phi(t)$ is well-known to be positive on $[0,+\infty)$ (cf. Wintner [2.11] or Thm. A of [2.3]), it is evident from (2.17) that establishing

$$(2.19)\qquad \omega(t) > 0 \qquad (t > 0)$$

would *directly* gives the positivity of D_m for *all* $m=1,2,\cdots$, and this would affirmatively solve Pólya's problem! By apparently sampling values of $\omega(t)$ and using an interval arithmetic computer package, Matijasevich [2.7] asserts that (2.19) is valid, and that his interval computations "are as powerful as a proof". Of course, a proof that the numbers $\{D_m\}_{m=1}^{\infty}$ are all positive is given in [2.3]. Whether or not Matiyasevich's use of interval arithmetic computations to establish (2.19) will be accepted as a *rigorous* mathematical solution of Pólya's problem, his representation (2.17) will certainly be very useful in further similar investigations associated with the Riemann Hypothesis.

Concerning further possible research in this area, we mention an interesting open problem. In analogy with (2.2) and (2.6), consider the entire function $F_\lambda(z)$ defined by

$$(2.20)\qquad F_\lambda(-x^2) := \int_0^\infty \Phi(t) e^{\lambda t^2} \cos(xt)\, dt ,$$

for any $\lambda \geq 0$. Then, as in (2.4) and (2.5), we can write

$$(2.21)\qquad F_\lambda(z) := \sum_{m=0}^{\infty} \frac{\hat{b}_m(\lambda) z^m}{(2m)!} ,$$

where

$$(2.22)\qquad \hat{b}_m(\lambda) := \int_0^\infty t^{2m} \Phi(t) e^{\lambda t^2} dt \qquad (m=0,1,\cdots) .$$

It is known (cf. de Bruin [2.2]) that $F_\lambda(z)$ has only real zeros for all $\lambda \geq 1/2$.

Moreover, it can be shown that if $F_\lambda(z)$ has only real zeros, then $F_{\lambda'}(z)$ has only real zeros for any $\lambda' \geq \lambda$. Now as the choice $\lambda=0$ in (2.20) gives the function $F(z)$ of (2.6), then the truth of the Riemann Hypothesis would necessarily imply that $F_\lambda(z)$ has only real zeros for each $\lambda \geq 0$, from which it would follow that the numbers

$$(2.23) \qquad D_m(\lambda) := \left(\hat{b}_m(\lambda)\right)^2 - \left(\frac{2m-1}{2m+1}\right) \hat{b}_{m-1}(\lambda)\hat{b}_{m+1}(\lambda) \qquad (m=1,2,\cdots)$$

would satisfy the associated *Pólya-Turán inequalities*:

$$(2.24) \qquad D_m(\lambda) > 0 \qquad (m=1,2,\cdots;\ \text{all } \lambda \geq 0) .$$

We conjecture that, in fact, that (2.24) is valid for *all real* λ, and this is currently being investigated by us.

References

2.1 R. B. Boas (1954): Entire Functions. New York: Academic Press.

2.2 N. G. de Bruijn (1950): The roots of trigonometric integrals. Duke Math. J. 17: 197-226.

2.3 G. Csordas, T. S. Norfolk, and R. S. Varga (1986): The Riemann Hypothesis and the Turán inequalities. Trans. Amer. Math. Soc.: (to appear).

2.4 E. Grosswald (1966): Generalization of a formula of Hayman, and its applications to the study of Riemann's zeta function. Illinois J. Math. 10: 9-23.

2.5 E. Grosswald (1969): Corrections and completion of the paper "Generalization of a formula of Hayman". Illinois J. Math. 13: 276-280.

2.6 W. K. Hayman (1956): A generalization of Stirling's formula. J. Reine Angew. Math. 196: 67-95.

2.7 Yu. V. Matiyasevich (1982): Yet another machine experiment in support of Riemann's Conjecture. Kibernetika 6: 10-22 (MR 85g:11079).

2.8 G. Pólya (1927): Über die algebraisch-funktionentheoretischen Untersuchungen von J. L. W. V. Jensen. Kgl. Danske Vid. Sel. Math. - Fys. Medd. 7: 3-33.

2.9 E. C. Titchmarsh (1951): The Theory of the Riemann Zeta Function. Oxford: The Clarendon Press.

2.10 J. van de Lune, H. J. J. Rielte te, and D. T. Winter (1981): Rigorous high speed separation of zeros of Riemann's zeta function. Stiching Math. Centrum (Amsterdam), No. 113.

2.11 A. Wintner (1935): A note on the Riemann ζ-function. J. London Math. Soc. 10: 82-83.

3. The " 1/9 " Conjecture

The object of this section is to review the more recent results concerning the "1/9" conjecture in approximation theory, and to mention some exciting new developments related to it.

Because rational approximations of e^{-x} occur naturally in the numerical solution of heat-conduction problems (cf. [3.8, Chapter 8]), there has been considerable theoretical interest in the best uniform rational approximations to e^{-x} on $[0,+\infty)$. Specifically, if $\pi_{m,n}$ denotes the set of rational functions $p_m(x)/q_n(x)$, where $p_m(x)$ and $q_n(x)$ are real polynomials of respective degrees m and n, then set

$$(3.1) \qquad \lambda_{m,n} := \min\left\{ \| e^{-x} - r_{m,n}(x) \|_{L_\infty[0,+\infty)} : r_{m,n} \in \pi_{m,n} \right\} \qquad (m \le n),$$

and set

$$(3.2) \qquad \Lambda_1 := \underline{\lim}_{n \to \infty} \lambda_{n,n}^{1/n} ; \quad \Lambda_2 := \overline{\lim}_{n \to \infty} \lambda_{n,n}^{1/n} .$$

It was first shown in 1969 by Cody, Meinardus, and Varga [3.2], using elementary means, that

$$(3.3) \qquad \overline{\lim}_{n \to \infty} \lambda_{0,n}^{1/n} \le \frac{1}{2.298} .$$

Since it is obvious from (3.1) that

$$(3.4) \qquad \lambda_{0,n} \ge \lambda_{1,n} \ge \cdots \ge \lambda_{n,n} \qquad (n = 0,1,\cdots),$$

then (3.3) gives that

$$(3.5) \qquad 0 \le \Lambda_1 \le \Lambda_2 \le \frac{1}{2.298} .$$

Thus, the error in best uniform rational approximation to e^{-x} on $[0,+\infty)$ by rational functions in $\pi_{n,n}$ enhibits *geometric convergence*, and this phenomenon stimulated much subsequent related research. For further historical remarks and related references, see [3.1] and [3.9].

Now, the paper of Cody, Meinardus, and Varga [3.2] also contained numerical estimates for $\{\lambda_{n,n}\}_{n=0}^{14}$. These numbers, which indicated that the upper bound in (3.3) was certainly crude, led Saff and Varga [3.5] to conjecture that

$$(3.6) \qquad \Lambda_1 \overset{?}{=} \Lambda_2 ,$$

as well as that

$$(3.7) \qquad \Lambda_2 \overset{?}{=} \frac{1}{9} .$$

It was recently shown in 1985 by Opitz and Scherer [3.4] that the conjecture in (3.7) is *false*. More precisely, Optiz and Scherer, using an interesting steepest descent approach and numerical optimizations, established that

$$(3.8) \qquad \Lambda_2 \leq \frac{1}{9.037} \ .$$

In other words, the geometric convergence rate of $\{\lambda_{n,n}\}_{n=0}^{\infty}$ is actually *better* than 1/9! To round out our discussion here, the currently best lower bound for Λ_1 was established in 1982 by Schönhage [3.6], and is

$$(3.9) \qquad \frac{1}{13.928} < \Lambda_1 \ .$$

To describe connections with the Carathéodory-Fejér rational approximation method, let

$$(3.10) \qquad \exp\left[(x-1)/(+1)\right] = \sum_{k=0}^{\infty}{}' c_k T_k(x) \qquad (x \in [-1,+1])$$

denote the Chebyshev expansion of $\exp\left[(x-1)/(+1)\right]$ on $[-1,+1]$, where

$$(3.10') \qquad c_k := \frac{2}{\pi}\int_{-1}^{+1} \exp\left[(x-1)/(+1)\right] T_k(x)dx \Big/ \sqrt{1-x^2} \qquad (k=0,1,\cdots),$$

and where the prime on the summation in (3.10) means that $c_0/2$ is used in place of c_0, defined in (3.10′). On forming the infinite Hankel matrix $H := [c_{i+j-1}]_{i,j=1}^{\infty}$ from the coefficients of (3.10′), set

$$(3.11) \qquad \sigma_n := n\text{-th singular value of } H \ (\text{where } \sigma_1 \geq \sigma_2 \geq \cdots) \ .$$

In 1983, Trefethen and Gutknecht [3.7] conjectured that

$$(3.12) \qquad \lambda_{n,n} \overset{?}{\sim} \sigma_n \qquad (n \to \infty),$$

and, on the basis of numerical estimates of σ_n from [3.7], they further conjectured that

$$(3.13) \qquad \Lambda_2 \overset{?}{=} \frac{1}{9.28903} \ .$$

Subsequently in 1984, Carpenter, Ruttan and Varga [3.1] calculated (by the Remez algorithm) the numbers $\{\lambda_{n,n}\}_{n=0}^{30}$ with very high precision (about 200 decimal digits), and with Richardson extrapolation techniques, they conjectured that

$$(3.14) \qquad \Lambda_2 \overset{?}{=} \frac{1}{9.28902\ 54919\ 2081} \ .$$

Note that this latter conjecture, on rounding, confirms (to the number of digits claimed) the conjecture of Trefethen and Gutknecht in (3.13), which was based on totally different computations and analyses.

In a surprising new development, A. P. Magnus [3.3] has estimated the singular values σ_n of (3.11), and he is convinced that

$$(3.15) \qquad \Lambda_2 \overset{?}{=} e^{-\pi K'/K} ,$$

where K and K' are complete elliptic integrals of the first kind (usual notation), evaluated at the point where $K = 2E$, E being the complete elliptic integral of the second kind. Even more astounding is the fact that the number $e^{-\pi K'/K}$, which can be calculated to arbitrary precision, is given by

$$(3.16) \qquad e^{-\pi K'/K} = \frac{1}{9.28902\ 54919\ 20818\ 91875\ 54494\ 35952 \cdots} ,$$

which agrees with all 15 digits of (3.14), again based on totally different computations and analyses! It is very likely that Magnus' conjecture (3.15) is correct, but there is no complete proof of this as yet.

We conclude this section by stating that it would seem that a sequence of *explicit* and *constructive* rational approximation $\{\hat{r}_{n,n}(x)\}_{n=0}^{\infty}$ of e^{-x} *could* be found (perhaps based on the notions of inner polynomials introduced by Opitz and Scherer [3.4], and on Laguerre polynomials) which would directly settle all these interesting conjectures in this area, without the necessity of indirect use of the Carathéodory-Fejér method. This is currently being investigated by A. Ruttan, R. S. Varga, and others.

References

3.1 A. J. Carpenter, A. Ruttan, and R. S. Varga (1984): Extended numerical computations on the "1/9" conjecture in rational approximation theory. Rational Approximation and Interpolation (P. R. Graves-Morris, E. B. Saff, and R. S. Varga, eds.), Lecture Notes in Mathematics 1105, pp.383-411, Heidelberg: Springer-Verlag.

3.2 W. J. Cody, G. Meinardus, and R. S. Varga (1969): Chebyshev rational approximation to e^{-x} in $[0,+\infty)$ and applications to heat-conduction problems. J. Approximation Theory 2: 50-65.

3.3 A. P. Magnus (1985): C F G T determination of Varga's constant "1/9". Personal communication.

3.4 H.-U. Opitz and K. Scherer (1985): On the rational approximation of e^{-x} on $[0,+\infty)$. Constr. Approx. 1: 195-216.

3.5 E. B. Saff and R. S. Varga (1977): Some open questions concerning polynomials and rational functions Padé and Rational Approximation (E. B. Saff and R. S. Varga, eds), pp.483-488. New York: Academic Press, Inc.

3.6 A. Schönhage (1982): Rational approximation to e^{-x} and related L^2- problems. Siam J. Numer. Anal. 19: 1067-1082.

3.7 L. N. Trefethen and M. H. Gutknecht (1983): The Carathéodory-Fejér method for real rational approximation. SIAM J. Numer. Anal. 20: 420-436.

3.8 R. S. Varga (1962): Matrix Iterative Analysis. Englewood Cliffs, NJ: Prentice-Hall, Inc.

3.9 R. S. Varga (1982): Topics in Polynomial and Rational Interpolation and Approximation. Montreal: University of Montreal Press.

4. The Ruscheweyh-Varga Conjecture

There has been a continuing research interest in *global descent methods* for finding zeros of a given polynomial. (For recent contributions on this and for related literature, see Henrici [4.1] and Ruscheweyh [4.3].) To crudely describe such methods, let $p_n(x)$ be a given complex polynomial, and suppose that z_0, our initial starting point of a procedure for finding a zero of $p_n(z)$, is such that $p_n(z_0) \neq 0$. Without loss of generality, assume $z_0=0$, and further normalize $p_n(z)$ so that

$$(4.1) \qquad p_n(z)=1+\sum_{j=1}^{n} a_j z^j, \text{ where } \sum_{j=1}^{n} |a_j| \neq 0 .$$

By a well-known result of Cauchy (cf. Marden [4.2, p.126]), if R (called the *Cauchy radius* of $p_n(z)$) is defined as the unique positive real root of

$$(4.2) \qquad 1 - \sum_{j=1}^{n} |a_j| R^j = 0 ,$$

then each zero $\hat{z}$ of $p_n(z)$ necessarily satisfies $|\hat{z}| \geq R$. On further normalizing R to unity, i.e., on assuming

$$(4.3) \qquad \sum_{j=1}^{n} |a_j| = 1 ,$$

then any polynomial $p_n(z)$ in (4.1) which satisfies (4.3) evidently has no zeros in $|z|<1$. (It may well have zeros on $|z|=1$, as the example $1+z^n$ shows.)

Next, let z_1 be any point on $|z|=1$ for which

$$(4.4) \qquad |p_n(z_1)| = \min_{\theta \text{ real}} \left| p_n(e^{i\theta}) \right| .$$

(In actual numerical applications, $|p_n(z_1)|$ need only be an *approximation* of the minimum of $\left| p_n(e^{i\theta}) \right|$, obtained from sampling $|p_n(z)|$ in a finite number of points on $|z|=1$.) Note that since $p_n(z)$ from (4.1) is not identically constant, then by the minimum principle,

$$(4.5) \qquad |p_n(z_1)| < |p_n(z_0)| \ .$$

In this fashion, one obtains (with appropriate normalizations at each step) a sequence of points $\{z_j\}_{j=0}^{\infty}$ which, because of (4.5), is known to converge to a zero of $p_n(z)$.

Our interest in the problem was in the following question. While (4.5) shows that the point z_1 is in some sense an improvement over z_0 in estimating a zero of $p_n(z)$, it could be that the reduction in $|p_n(z_0)|$, in finding $|p_n(z_1)|$, might be *small.* This led to the question of how *large* $\min_{\theta \text{ real}} |p_n(e^{i\theta})|$ can be for all polynomials $p_n(z)$ satisfying (4.1), and (4.3). Thus, we were led to the problem of investigating the behavior of

$$(4.6) \qquad \Gamma_n := \sup\left\{ \min_{|z|\le 1} |p_n(z)| : p_n(z) = 1 + \sum_{j=1}^{n} a_j z^j \text{ with } \sum_{j=1}^{n} |a_j| = 1 \right\},$$

for each $n \ge 1$.

In Ruscheweyh and Varga [4.4], it was shown that

$$(4.7) \qquad 1 - \frac{1}{n} \le \Gamma_n \le \sqrt{1 - \frac{1}{n}} < 1 - \frac{1}{2n} \qquad (n \ge 1) \ .$$

Analogously, if we set

$$(4.8) \qquad \tilde{\Gamma}_n := \sup\left\{ \min_{|z|\le 1} |p_n(z)| : p_n(z) = 1 + \sum_{j=1}^{n} a_j z^j \right.$$
$$\left. \text{with } p_n(1) = 2 \ , \quad a_j \ge 0 (1 \le j \le n) \right\},$$

then each polynomial considered in (4.8) evidently satisfies the hypotheses for (4.6), so that

$$(4.9) \qquad \tilde{\Gamma}_n \le \Gamma_n \ .$$

It was further shown in [4.4] that

$$(4.10) \qquad 1 - \frac{1}{n} \le \tilde{\Gamma}_n \le \sqrt{1 - \frac{3}{(2n+1)}} = 1 - \frac{3}{4n} + o\left(\frac{1}{n}\right) \qquad (n \to \infty) \ .$$

Next, we conjectured in [4.4] that

$$(4.11) \qquad \Gamma_n \overset{?}{=} \tilde{\Gamma}_n \qquad (n \ge 1) \ ,$$

and that there exists a positive constant γ (independent of n) such that

(4.12) $$\tilde{\Gamma}_n \overset{?}{=} 1 - \frac{\gamma}{n} + o\left(\frac{1}{n}\right) \quad (n \to \infty) \ .$$

Indeed, extended precision calculations given in [4.4] led us to further conjecture in [4.4] that

(4.13) $$\gamma \overset{?}{=} 0.86718\ 9051 \cdots$$

In subsequent research, Ruscheweyh and I [4.5] have focused on the following different, but related, problem. Let $\mathbb{P}_n$ denoting the set of all complex polynomials of degree at most $n\ (n \geq 1)$. Then for each complex number μ, consider the following subset of $\mathbb{P}_n$ of polynomials with *two prescribed values*, defined by

(4.14) $$\mathbb{P}_n(\mu) := \left\{ p_n(z) \in \mathbb{P}_n \ : p_n(0)=1 \text{ and } p_n(1)=\mu \right\} \ .$$

What then can be said about the nonnegative numbers

(4.15) $$S_n(\mu) := \sup\left\{ \min_{|z|\leq 1} |p_n(z)| : p_n \in \mathbb{P}_n(\mu) \right\} \ ,$$

as a function of n and μ?

One of the surprising results of [4.5] is that

(4.16) $$S_n(2) = \tilde{\Gamma}_n = 1 - \frac{1}{2n}\left\{ \text{arccosh}\ (2) \right\}^2 + o\left(\frac{1}{n}\right) \quad (n \to \infty) \ ,$$

so that the quantity γ of (5.12) is *exactly* given by

(4.17) $$\gamma = \left\{ \text{arccosh}\ (2) \right\}^2 / \ 2 = 0.86718\ 90511\ 36318 \cdots \ .$$

Thus, our conjecture of (4.13) (to the number of digits given in (4.13)) is *correct.* The conjecture of (4.11), however, remains open.

We quote from [4.5, Corollary 1] the following result which, for the special case $\mu=2$, gives the result of (4.16).

Theorem. Let $\mu>0$. Then, there holds

(4.18) $$S_n(\mu) = \begin{cases} \mu, \text{ if } 0 < \mu \leq 1 \ ; \\ \sigma, \text{ if } 1 < \mu \leq 2^n \ ; \\ 0, \text{ if } 2^n \leq \mu \ . \end{cases}$$

Here, σ is the uniquely determined solution in (0,1) of the equation

(4.19) $$\mu = \sigma T_{n+1}(\sigma^{-1/(n+1)}) ,$$

where $T_{n+1}(z)$ denotes the Chebyshev polynomial (of the first kind) of degree $n+1$. For n tending to infinity, the solution σ of (4.19) can be expressed as

(4.20) $$\sigma = 1 - \left\{ \operatorname{arccosh}(\mu) \right\}^2 /2n + o\left(\frac{1}{n}\right) \quad (n \to \infty) .$$

In addition, for $\mu \in (1,2^n)$ and for σ defined in (4.19), define the polynomial $Q_{n,\sigma}(z)$ by means of

(4.21) $$Q_{n,\sigma}(w^2) := \frac{-\sigma}{(n+1)} w^{2n+3} \frac{d}{dw} \left\{ w^{-(n+1)} T_{n+1} \left[\sigma^{-1/(n+1)} \left(\frac{1+w^2}{2w} \right) \right] \right\} .$$

Then, $Q_{n,\sigma}(z)$ is an element of $\mathbb{P}_n(\mu)$, and is the unique extremal polynomial for $S_n(\mu)$, i.e.,

(4.22) $$S_n(\mu) = \min_{|z| \leq 1} \left| Q_{n,\sigma}(z) \right| .$$

Moreover, $Q_{n,\sigma}(z)$, when expanded in powers of z, has positive coefficients.

Finally, we can associate to each complex number μ in the complex plane the nonnegative quantity $S_n(\mu)$ of (4.15), thereby generating a three-dimensional surface. This surface, as it turns out, has the interesting shape of a *volcano*. There are different types of volcanoes (active, dormant, extinct), and the present author hopes that this volcano will help convey the *active* interplay between scientific computing and mathematical analysis!

References

4.1 P. Henrici (1983): Methods of descent for polynomial equations. Computational Aspects of Complex Analysis (H. Werner, L. Wuytack, E. Ng, H. J. Bünger, eds.), pp.133-147. Boston: D. Reidel Publishing.

4.2 M. Marden (1966): Geometry of Polynomials. Providence, RI: American Math. Soc. (Mathematical Surveys, No. 3).

4.3 S. Ruscheweyh (1984): On a global descent method for polynomials. Numer. Math. 45: 227-240.

4.4 S. Ruscheweyh and R. S. Varga (1984): On the minimum moduli of normalized polynomials. Rational Approximation and Interpolation (P. R. Graves, E. B. Saff, and R. S. Varga, eds.), Lecture Notes in Mathematics 1105, pp.150-159, Heidelberg: Springer-Verlag.

4.5 S. Ruscheweyh and R. S. Varga (1986): On the minimum moduli of normalized polynomials with two prescribed values. Constr. Approx. (to appear).

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Erratta:

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eq. (3.2). Read " $\Lambda_2 := \overline{\lim_{n\to\infty}} \lambda_{n,n}^{1/n}$ "

eq. (3.3). Read " $\overline{\lim_{n\to\infty}} \lambda_{0,n}^{1/n} \leq \frac{1}{2.298}$ "