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The asymptotic behaviour of Toeplitz determinants $D_n(f)$, as $n \to \infty$, is considered for nonnegative generating functions $f(\theta)$ with a finite number of isolated zeros θ_ν, in the neighborhood of which $f(\theta) \sim | e^{i\theta} - e^{i\theta_\nu} |^{\alpha_\nu}$ where $\alpha_\nu > 0$. Using an argument suggested by Szegö, an upper bound of the form $D_n(f) < C \cdot G^{n+1}(n+1)^\sigma$ is derived, where G is the geometrical mean of f and $\sigma = 1/4 \sum \alpha_\nu^2$. Using some identities in the theory of orthogonal polynomials, and specifically facts about Jacobi polynomials, it is shown that the above bound is actually asymptotically equal D_n, as $n \to \infty$, for some special f's. It is conjectured that this asymptotic equality is generally true for the class of f's considered.

In a paper written more than fifty years ago [9] G. Szegö investigated the asymptotic behavior of the sequence $D_0, D_1, D_2, \cdots$ of determinants (Toeplitz determinants) defined as follows

$$D_n = \det_{0 \leqq p, q \leqq n} (c_{p-q}) , \tag{1}$$

where the entries of the matrix (c_{p-q}) are the Fourier-coefficients of a "generating function"

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-in\theta} f(\theta) d\theta . \tag{2}$$

Here $f(\theta)$ is a real, nonnegative function, periodic modulo 2π, satisfying certain regularity conditions. A refinement of the old results is the following theorem, also due to Szegö [10]:

THEOREM B. *If $f(\theta)$ is a strictly positive and differentiable function, periodic modulo 2π, whose derivative satisfies the condition*

$$| f'(\theta_1) - f'(\theta_2) | < K | \theta_1 - \theta_2 |_\alpha \tag{3}$$

for some constants $K > 0$ and $0 < \alpha < 1$, then

$$D_n \sim C \cdot G^{n+1} \quad (n \longrightarrow \infty) \tag{4}$$

where

$$G = e^{1/2\pi \int_{-\pi}^{\pi} \log f(\theta) d\theta} \tag{5}$$

and

$$C = e^{\sum_{n=1}^{\infty} n|h_n|^2} < \infty \, . \tag{6}$$

The complex numbers h_n are coefficients in a Taylor series

$$\log g(z) = \sum_{n=0}^{\infty} h_n z^n \tag{7}$$

where the function $g(z)$ is determined up to an irrelevant constant factor of unit modulus by the following properties:

(i) *It is analytic on the disk* $|z| < 1$, (ii) *it has no zeros on the disk* $|z| < 1$, *and* (iii) $\lim_{r \to 1-} |g(re^{i\theta})|^2 = f(\theta)$.

When the conditions of the theorem are no longer met, in particular when $f(\theta)$ has zeros, the series (6) for $\log C$ may not converge. However, when the zeros are of a sufficiently mild kind the geometric mean G still exits and is related to the analytic function $g(z)$ by

$$G = |g(0)|^2 \, . \tag{8}$$

In this case the sequence D_n/G^{n+1} $(n = 0, 1, 2, \cdots)$ is nondecreasing (cf. [5], and [8], Appendix A2). The problem then naturally suggests itself to determine its asymptotic behavior as $n \to \infty$.

The writer of these lines has encountered this question some years ago in connection with the mathematical analysis of a problem in quantum mechanics [8]. In the context of that problem the generating function $f(\theta)$ was the following

$$f(\theta) = |e^{i\theta} - e^{i\theta_1}| \cdot |e^{i\theta} - e^{i\theta_2}| \tag{9}$$

where θ_1 and θ_2 are distinct modulo 2π. This function has zeros and it is not immediately evident that Theorem B is relevant. Nevertheless, as Professor Szegö pointed out in a letter to the writer, a deft use of that theorem allows the derivation of an inequality:

$$D_n < C n^{1/2} G^{n+1} \tag{10}$$

where $C = C(\theta_1, \theta_2)$ is an explicitly given function of the zeros θ_1 and θ_2. The argument leading to (10) (cf. [8], §4) may be generalized to generating functions of the form

$$f(\theta) = f_0(\theta) \prod_{\nu} |e^{i\theta} - e^{i\theta_\nu}|^{\alpha_\nu} \, , \tag{11}$$

where the product is finite, the θ_ν are distinct modulo 2π, the α_ν are positive, and $f_0(\theta)$ satisfies the premises of Theorem B. In the following we present this generalization, following closely the argument of the special case treated in [8].

Let us adopt the following notation: If $f(\theta)$ is the generating function, we write $D_n(f)$, $G(f)$, $g(z; f)$ and $h_n(f)$ for the associated quantities that occur in Theorem B, and in case the series converges,

$$H(f) = \sum_{n=1}^{\infty} n|h_n(f)|^2 . \tag{12}$$

For $R > 1$, let

$$f_R(\theta) = f_0(\theta) \prod_\nu |Re^{i\theta} - e^{i\theta_\nu}|^{\alpha_\nu} \tag{13}$$

where the θ_ν, the α_ν and $f_0(\theta)$ are the same as in (11). Then

$$f_R(\theta) > f(\theta) ; \tag{14}$$

in particular, f_R has no zeros. Moreover, it satisfies the other conditions of Theorem B as well. It is a fact that the Toeplitz determinants depend monotonically on the generating function (cf. [5], p. 38), so that (14) implies

$$D_n(f_R) > D_n(f) . \tag{15}$$

On the other hand, the ratio D_n/G^{n+1} is nondecreasing with increasing n (cf. [5], *ibid.*); therefore

$$D_n(f_R) \leqq G(f_R)^{n+1} \lim_{m\to\infty} \frac{D_m(f_R)}{G(f_R)^{m+1}} = G(f_R)^{n+1} e^{H(f_R)} \tag{16}$$

by Theorem B. The geometric mean is

$$G(f_R) = G(f_0)R^\alpha = G(f)R^\alpha \tag{17}$$

where

$$\alpha = \sum_\nu \alpha_\nu . \tag{18}$$

We now compute $H(f_R)$ as prescribed by the theorem.

One verifies directly that

$$g(z; f_R) = g(z; f_0) \prod_\nu (z - Re^{i\theta_\nu})^{\alpha_\nu/2} , \tag{19}$$

since the properties of g identify this function uniquely up to the irrelevant phase factor (which makes it also unecessary to specify the banch of the multi-valued factors). Expanding its logarithm in powers of z, it follows that for $n \geqq 1$

$$h_n(f_R) = h_n(f_0) - Re \sum_\nu \frac{\alpha_\nu}{2n} R^{-n} e^{in\theta_\nu} . \tag{20}$$

A direct computation yields

$$H(f_R) = H(f_0) - Re \sum_\nu \alpha_\nu \log g\left(\frac{e^{i\theta_\nu}}{R}; f_0\right) \tag{21}$$
$$- \frac{1}{8} \sum_\nu \sum_\mu \alpha_\nu \alpha_\mu \log\left(1 - \frac{2}{R^2} \cos(\theta_\nu - \theta_\mu) + \frac{1}{R^4}\right).$$

Let

$$k_0 = \operatorname*{Inf}_{|z|<1} |g(z; f_0)| . \tag{22}$$

Since $g(z; f_0)$ is analytic without zeros on the open unit disk and its squared absolute value has the radial limit $|g(e^{i\theta}; f_0)|^2 = f_0(\theta)$, continuous and bounded away from zero, we have $k_0 > 0$. Thus

$$\exp\left\{-Re \sum_\nu \alpha \log g\left(\frac{e^{i\theta_\nu}}{R}; f_0\right)\right\} \leqq k_0^{-\alpha} \tag{23}$$

where α is defined by (18). It follows then from (15), (16) and (21) that

$$D_n(f) < k_0^{-\alpha} e^{H(f_0)} [G(f) R^\alpha]^{n+1} \tag{24}$$
$$\cdot \prod_\nu \prod_\mu \left[1 - \frac{2}{R^2} \cos(\theta_\nu - \theta_\mu) + \frac{1}{R^4}\right]^{-\alpha_\nu \alpha_\mu / 8} .$$

It is convenient to separate the factors with $\nu = \mu$ from those with $\nu \neq \mu$; and for the latter we use the inequality, valid for $R > 1$ and real α,

$$(R^4 - 2R^2 \cos \alpha + 1)^{1/2} > |1 - e^{i\alpha}| . \tag{25}$$

Thus

$$D_n(f) < C_0 [G(f)]^{n+1} R^{\alpha(n+1) + \alpha^2/2} (R^2 - 1)^{-\sigma} \tag{26}$$
$$\times \prod_{\nu<\mu} \prod |e^{i\theta_\nu} - e^{i\theta_\mu}|^{-\alpha_\nu \alpha_\mu / 4}$$

where

$$\sigma = \frac{1}{4} \sum_\nu \alpha_\nu^2 \tag{27}$$

and

$$C_0 = k_0^{-\alpha} e^{H(f_0)} . \tag{28}$$

But (26) holds for any $R > 1$, so the best inequality is obtained by minimizing the right hand side with respect to R. A somewhat less precise but simpler inequality results when we put $R^2 = 1 + 1/(n+1)$ and note $R^{\alpha(n+1)} < e^{\alpha/2}$ and $R^{\alpha^2/2} < 2^{\alpha^2}$. We have now proved the following

THEOREM. *For a generating function of the form* (11)

$$D_n(f) < C(f)[G(f)]^{n+1}(n+1)^\sigma \quad (n \geqq 0) \tag{29}$$

where the factor independent of n may be taken

$$C(f) = C_0 \cdot e^{\alpha/2} \cdot 2^{\alpha^2} \prod_{\nu<\mu}\prod |e^{i\theta_\nu} - e^{i\theta_\mu}|^{-\alpha_\nu\alpha_\mu/4} \tag{30}$$

and the rest of the symbols are defined above.

The interesting feature of the bound (29) is its growth with n, and the dependence of this growth on the numbers α_ν (cf. Equ. (27) above) which characterize the behaviour of the generating function near its zeros.

The principal purpose of this note is to record a further important suggestion of Professor Szegö, contained in the correspondence with the writer in 1963. Namely, for some special cases in the class given by the formula (11) it is possible to express D_n in finite terms (the meaning of this phrase will become clear below), so that in these cases another means exists for scrutinizing the behaviour of D_n in the limit $n \to \infty$. This happens when

$$f(\theta) = |e^{i\theta} - 1|^\alpha \cdot |e^{i\theta} + 1|^\beta \tag{31}$$

where $\alpha, \beta > 0$ are arbitrary. Since a multiplicative constant in f affects D_n trivially, we have chosen a normalisation in (31) which makes $G(f) = 1$. In the following we present the calculation suggested by Szegö, and its consequences, in detail.

This calculation makes heavy use of the theory of orthogonal polynomials as presented in Szegö's treatise [11], to which the reader is referred for further information. We follow the notation of this book closely. The starting point is the sequence of identities

$$D_n(f) = \prod_{j=0}^{n} (L\varphi_j)^{-2} \quad (n = 0, 1, 2, \cdots) \tag{32}$$

where $\varphi_j(z)$ is the $(j+1)^{st}$ member of a sequence of polynomials, orthonormal on the unit circle $z = e^{i\theta}$ with respect to the measure $f(\theta)d\theta$ (cf. [11], §11.1); and where L in front of a polynomial stands for "leading coefficient of". We also consider two other polynomial systems $p_n(x)$ and $q_n(x)$ $(n = 0, 1, 2, \cdots)$. These are orthonormal on $-1 \leqq x \leqq 1$ with respect to measures $w(x)dx$ and $(1 - x^2)w(x)dx$ respectively, where w is related to f by

$$f(\theta) = |\sin\theta|\, w(\cos\theta)\ . \tag{33}$$

Writing $x = (z + z^{-1})/2$, there are the following identities between these three systems.

$$p_n(x) = \left(\frac{1}{2\pi}\right)^{1/2}\left(1 + \frac{C\varphi_{2n}}{L\varphi_{2n}}\right)^{-(1/2)}(z^{-n}\varphi_{2n}(z) + z^n\varphi_{2n}(z^{-1})) \tag{34}$$

$$= \left(\frac{1}{2\pi}\right)^{1/2}\left(1 - \frac{C\varphi_{2n}}{L\varphi_{2n}}\right)^{-(1/2)}(z^{-n+1}\varphi_{2n-1}(z) + z^{n-1}\varphi_{2n-1}(z^{-1})) \tag{35}$$

$$(z - z^{-1})q_{n-1}(x) = \left(\frac{2}{\pi}\right)^{1/2}\left(1 - \frac{C\varphi_{2n}}{L\varphi_{2n}}\right)^{-(1/2)}(z^{-n}\varphi_{2n}(z) - z^n\varphi_{2n}(z^{-1})) \tag{36}$$

$$= \left(\frac{2}{\pi}\right)^{1/2}\left(1 - \frac{C\varphi_{2n}}{L\varphi_{2n}}\right)^{-(1/2)} \times (z^{-n+1}\varphi_{2n-1}(z) - z^{n-1}\varphi_{2n-1}(z^{-1}))\ . \tag{37}$$

The symbol C in front of a polynomial stands for "constant term of". These formulae are valid whenever they make sense, i.e. for $n \geqq 1$ in (35)-(37) and for $n \geqq 0$ in (34). For proof see [11], §11.5.

In the case (31) we are considering one finds from (33)

$$w(x) = 2^{(\alpha+\beta)/2}(1 - x)^{(\alpha-1)/2}(1 + x)^{(\beta-1)/2} \tag{38}$$

and

$$(1 - x^2)w(x) = 2^{(\alpha+\beta)/2}(1 - x)^{(\alpha+1)/2}(1 + x)^{(\beta+1)/2}\ . \tag{39}$$

Thus the p_n and q_{n-1} are, apart from normalization, Jacobi polynomials ([11], Chapter IV.). Equate the coefficients of the leading power of z on both sides of (34)-(37). This yields identities between $C\varphi_{2n}$, $L\varphi_{2n}$, $L\varphi_{2n-1}$ on the one hand, and Lp_n, Lq_{n-1} on the other. But the latter are expressible in terms of Γ-functions whose arguments are simple linear combinations with numerical coefficients of α, β and n ([11], Chapter IV., especially Equs. (4.3.3) and (4.21.6)). Eliminating $C\varphi_{2n}$, one calculates $L\varphi_{2n}$ and $L\varphi_{2n-1}$ explicitly, calculation that is somewhat lengthy though straightforward, and whose details we omit. With an appropriate use of the duplication formula $\pi^{1/2}2^{1-2z}\Gamma(2z) = \Gamma(z)\Gamma(z + 1/2)$, one obtains

$$\begin{aligned}(L\varphi_{2n})^2 &= \Gamma\left(n + \frac{1}{2} + \frac{\alpha}{4} + \frac{\beta}{4}\right)^2\Gamma\left(n + 1 + \frac{\alpha}{4} + \frac{\beta}{4}\right)^2 \\ &\quad \times \Gamma(n+1)^{-1}\Gamma\left(n + 1 + \frac{\alpha}{2} + \frac{\beta}{2}\right)^{-1}\Gamma\left(n + \frac{1}{2} + \frac{\alpha}{2}\right)^{-1} \\ &\quad \times \Gamma\left(n + \frac{1}{2} + \frac{\beta}{2}\right)^{-1}\end{aligned} \tag{40}$$

and

$$(41)\quad \begin{aligned}(L\varphi_{2n-1})^2 &= \Gamma\Big(n+\frac{\alpha}{4}+\frac{\beta}{4}\Big)^2\Gamma\Big(n+\frac{1}{2}+\frac{\alpha}{2}+\frac{\beta}{4}\Big)^2\Gamma(n)^{-1}\\ &\quad\times\Gamma\Big(n+\frac{\alpha}{2}+\frac{\beta}{2}\Big)^{-1}\Gamma\Big(n+\frac{1}{2}+\frac{\alpha}{2}\Big)^{-1}\Big(n+\frac{1}{2}+\frac{\beta}{2}\Big)^{-1}.\end{aligned}$$

Through (32) above this leads to the desired formula for D_n "in finite terms."

One is now faced with the problem of finding the asymptotic formula for D_n as $n \to \infty$. The first minor difficulty is that, due to the differing expressions (40) and (41) there is a corresponding difference in D_n for even and odd n. However, the Stirling formula for Γ shows that

$$(42)\qquad \lim_{n\to\infty} L\varphi_{2n} = \lim_{n\to\infty} L\varphi_{2n-1} = 1\,,$$

so that

$$(43)\qquad D_{2n} \sim D_{2n-1} \quad (\text{as } n \to \infty)\,.$$

Thus, it is sufficient to look at, say, odd n only. It proves convenient to make use of the compact notation offered by a rarely used transcendental function, the G-function of Barnes [1]. This function arises by a natural extension of the ideas leading to the Γ-function and has a similar analytic theory. For our purpose its most essential properties are $G(1) = 1$ and the functional equation

$$(44)\qquad G(z+1) = \Gamma(z)G(z)\,.$$

Thus

$$(45)\qquad \Gamma(z)\Gamma(z+1)\cdots\Gamma(z+n) = \frac{G(z+n+1)}{G(z)}\,,$$

a formula that in view of (32), (40), (41) is obviously relevant in calculating D_{2n+1}. We find

$$(46)\qquad D_{2n+1} = K\prod_{s=1}^{9} G(a_s+n+1)^{\nu_s}$$

with

$$(47)\qquad K = \prod_{s=1}^{9} G(a_s)^{-\nu_s}\,.$$

The numbers $a_1, \cdots, a_9$ are in order $1/2+\alpha/4+\beta/4$, $1+\alpha/4+\beta/4$, $3/2+\alpha/4+\beta/4$, 1, $1+\alpha/2+\beta/2$, $1/2+\alpha/2$, $3/2+\alpha/2$, $1/2+\beta/2$, $3/2+\beta/2$. The exponents $\nu_1, \cdots, \nu_9$ are in order $-2, -4, -2, 2, 2, 1, 1, 1, 1$. We note the facts

$$\sum_{s=1}^{9} \nu_s = \sum_{s=1}^{9} \nu_s a_s = 0 \,, \tag{48}$$

and

$$\sum_{s=1}^{9} \nu_s a_s^2 = \frac{1}{2}(\alpha^2 + \beta^2) \,. \tag{49}$$

The final step is the application of the analogue of the Stirling formula for the G-function. It reads [1]

$$\begin{aligned} \log G(t + a + 1) &= \frac{1}{12} - \log A - \frac{3t^2}{4} - at + \frac{t + a}{2} \log (2\pi) \\ &\quad + \left(\frac{t^2}{2} + at + \frac{a^2}{2} - \frac{1}{12}\right) \log t + o(1) \quad (\text{as } t \to +\infty) \,. \end{aligned} \tag{50}$$

Here a is any complex number, and A is Glaisher's constant [4]. From (48), (49) we get then

$$D_{2n+1} \sim Kn^{(\alpha^2+\beta^2)/4} \quad (\text{as} \quad n \to \infty) \,. \tag{51}$$

It is remarkable that the contribution of the nine very rapidly growing factors in (46) largely cancel, and the "little left over" yields the asymptotic formula (51). This phenomenon has its origin in the lengthy ratios of Γ-functions that occur in the theory of Jacobi polynomials. Let us record here that the G-functions involved in the definition of $K(\alpha, \beta)$ can be expressed in a variety ways including integral representations [1].

Our interest lies in exponent of n governing the asymptotic increase of D_n. We note that in the cases when the generating function f is of the special form (31) we have

$$\sigma = \frac{1}{4}(\alpha^2 + \beta^2) \tag{52}$$

and therefore the majorization offered by (29) is close enough so that the logarithm of both side divided by $\log n$ tend to the same limit σ. This suggests that the inequality (15) for the best value of R is a very close one, and the sign $>$ may perhaps be replaced by $\sim$ in the limit $n \to \infty$. This leads to the

CONJECTURE. *For a generating function of the form* (11)

$$D_n(f) \sim C(f)[G(f)]^{n+1} n^{\sigma} \quad (n \to \infty) \tag{53}$$

where σ is given by (27) *and $C(f)$ is some positive number depending on f.*

In recent years a number of authors have developed the theory of Toeplitz determinants beyond Szegö's work. See especially the papers by Devinatz [2], the review by Hirschman [6], and the review by Fisher and Hardwig [3], where other references may be found. Noteworthy is the progress in removing the requirement that the generating function f be positive; this is replaced by requirements formulated in terms of the phase of the complex valued $f(\theta)$. In all these generalizations it is necessary to assume, however, that f has no zeros. It is clear from the evidence in the present paper that in the case f has zeros (but $G(f)$ still exists) the asymptotic behaviour of the $D_n(f)$ as $n \to \infty$ is intimately related to the behaviour of $f(\theta)$ near its zeros. The above Conjecture, generalised in an appropriate way for complex valued f, also appears in Fisher and Hartwig [3] and is supported by calculations using ideas of Kac [7], and also by evidence taken from the writer's work [8] and a preliminary unpublished version of the present paper.

It is the authors hope that a rigorous analysis will someday carry the results to the point where the true role of the zeros of the generating function will be understood. When that day comes a capstone will have been put on a beautiful edifice to whose construction many contributed and whose foundations lie in the studies of Gábor Szegö half a century ago.

Notes added after acceptance for publication:

1. The conjecture has now proved by Harold Widom.
2. The author is greatly indebted to Professor Widom for a careful reading of the manuscript and the elimination of a significant error from a previous version.

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