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Accuracy and Stability of Computing High-order Derivatives of Analytic Functions by Cauchy Integrals

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Abstract High-order derivatives of analytic functions are expressible as Cauchy integrals over circular contours, which can very effectively be approximated, e.g., by trapezoidal sums. Whereas analytically each radius r up to the radius of convergence is equal, numerical stability strongly depends on r. We give a comprehensive study of this effect; in particular, we show that there is a unique radius that minimizes the loss of accuracy caused by round-off errors. For large classes of functions, though not for all, this radius actually gives about full accuracy; a remarkable fact that we explain by the theory of Hardy spaces, by the Wiman–Valiron and Levin–Pfluger theory of entire functions, and by the saddle-point method of asymptotic analysis. Many examples and nontrivial applications are discussed in detail.

Keywords Numerical differentiation · Accuracy · Stability · Analytic functions · Cauchy integral · Optimal radius · Hardy spaces · Entire functions of perfectly and completely regular growth

Mathematics Subject Classification (2000) 65E05 · 65D25 · 65G56 · 30D15

1 Introduction

Real variable formulas for the numerical calculation of high-order derivatives suffer severely from the ill-conditioning of real differentiation. Balancing approximation

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errors with round-off errors yields an inevitable minimum amount of error that blows up as the order of differentiation increases (see, e.g., Miel and Mooney 1985, Theorem 2). It is therefore quite tricky, using these formulas with hardware arithmetic, to obtain any significant digits for derivatives of orders of, say, a hundred or higher. For functions which extend analytically to the complex plane, numerical quadrature applied to Cauchy integrals has on various occasions been suggested as a remedy (see Gautschi 1997, p. 152/187). To be specific, let us consider an analytic function f with the Taylor series[1]

$$f(z) = \sum_{k=0}^{\infty} a_k z^k \quad \bigl(|z| < R\bigr) \tag{1.1}$$

having radius of convergence $R > 0$ (with $R = \infty$ for entire functions). Cauchy's integral formula applied to circular contours yields ($n = 0, 1, 2, \ldots, 0 < r < R$)

$$\begin{aligned} a_n &= \frac{f^{(n)}(0)}{n!} \\ &= \frac{1}{2\pi \mathrm{i}} \int_{|z|=r} \frac{f(z)}{z^{n+1}}\, \mathrm{d}z \\ &= \frac{1}{2\pi r^n} \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}n\theta} f\bigl(r\mathrm{e}^{\mathrm{i}\theta}\bigr)\, \mathrm{d}\theta. \end{aligned} \tag{1.2}$$

Since trapezoidal sums[2] are known to converge geometrically for periodic analytic functions (Davis 1959), the latter integral is amenable to the very simple and yet effective approximation[3]

$$a_n(r, m) = \frac{1}{mr^n} \sum_{j=0}^{m-1} \mathrm{e}^{-2\pi \mathrm{i} jn/m} f\bigl(r\mathrm{e}^{2\pi \mathrm{i} j/m}\bigr). \tag{1.3}$$

This procedure for approximating a_n was suggested by Lyness (1967). Later, Lyness and Sande (1971) observed that the correspondence

$$\bigl(r^n a_n(r, m)\bigr)_{n=0}^{m-1} \leftrightarrow \bigl(f\bigl(r\mathrm{e}^{2\pi \mathrm{i} j/m}\bigr)\bigr)_{j=0}^{m-1}$$

induced by (1.3) is, in fact, the discrete Fourier transform; accordingly, they published an algorithm for calculating a set of normalized Taylor coefficients $r^n a_n$ based on the fast Fourier transform (FFT).

Whereas all radii $0 < r < R$ are, by Cauchy's theorem, analytically equal, they are not so numerically. On the one hand, the geometric convergence rate of the trape-

[1]Without loss of generality, the point of development is $z = 0$, which we choose for ease of notation throughout this paper. Though such series are often named after Maclaurin, we keep the name *Taylor series* to stress that we really do not use anything specific to $z = 0$.

[2]Recall that, for periodic functions, the trapezoidal sum and the rectangular rule are the same.

[3]For other quadrature rules see the remarks in Sect. 2.3.

zoidal sums improves for smaller r. On the other hand, for $r \to 0$ there is an increasing amount of cancellation in the Cauchy integral which leads to a blow-up of relative errors (Lyness 1967, p. 130). Moreover, there is generally also a problem of numerical stability for $r \to R$ (see Sect. 3 of this paper). So, once again there arises the question of a proper balance between approximation errors and round-off errors: what choice of r is best and what is the minimum error thus obtained?

There is not much available about this problem in the literature. Lyness and Sande (1971) circumnavigate it altogether by just considering the *absolute* errors of the normalized Taylor coefficients $r^n a_n$ instead of relative errors, leaving the choice of r to the user as an application-specific scale factor. On p. 670 they write:

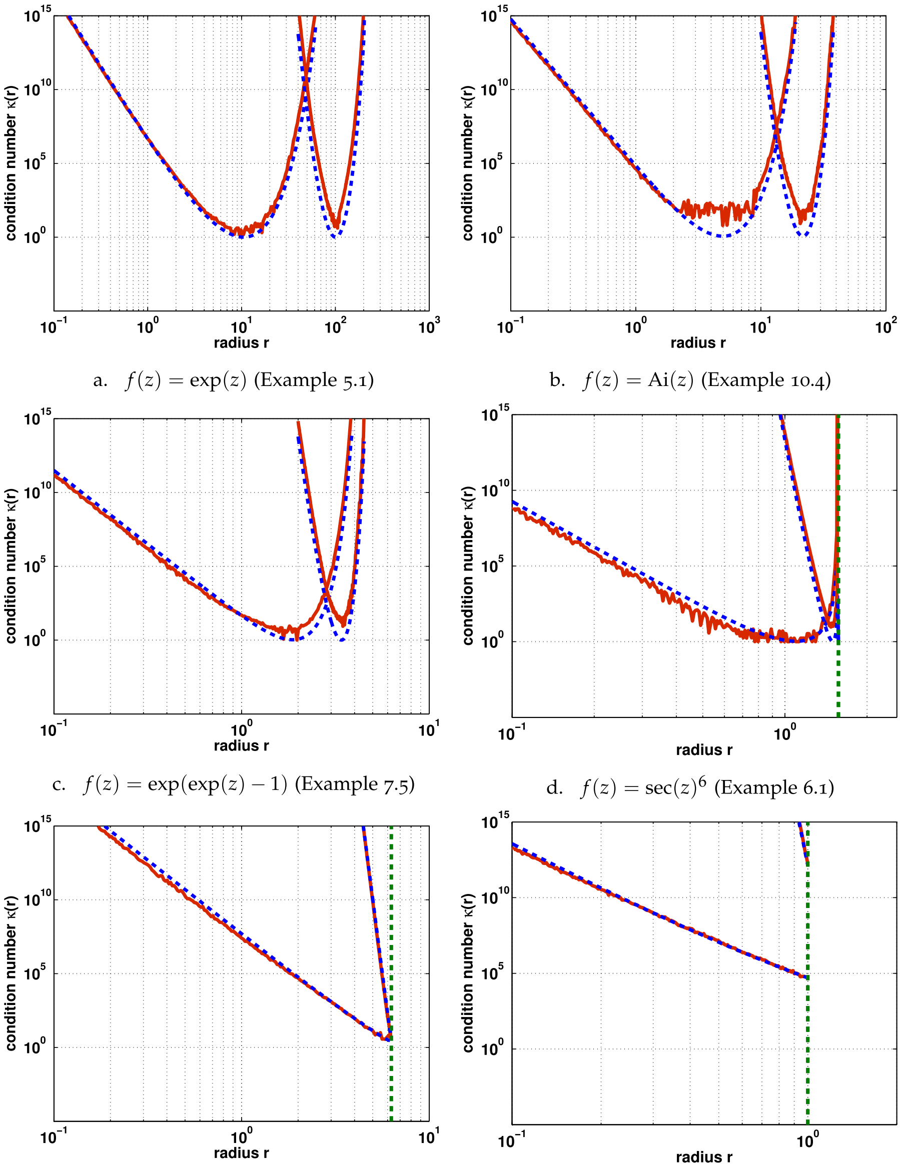
> It is natural to ask why this choice of output [i.e., $r^n a_n$] was made, rather than perhaps a set of Taylor coefficients a_n or a set of derivatives $f^{(n)}(0)$. The most immediate reason is that the algorithm naturally provides a set of normalized Taylor coefficients to a uniform absolute accuracy. If, for example, one is interested in a set of derivatives, the specification of the accuracy requirements becomes very much more complicated. However, if one looks ahead to the use to which the Taylor coefficients are to be put, one finds in many cases that uniform accuracy in normalized Taylor coefficients corresponds to the sort of accuracy requirement which is most convenient.

Fornberg (1981a, 1981b) addresses the choice of a suitable radius r by suggesting a simple search procedure that tries to make $(r^n a_n)_{n=0}^{m-1}$ approximately proportional to the geometric sequence 0.75^n. If accomplished, this results, for $m = 32$, in a loss of at most about $m|\log_{10}(0.75)| \doteq 4.0$ digits;[4] see Sect. 3.1 below. Further, he applies Richardson extrapolation to the last three radii of the search process to enhance the convergence rate of the trapezoidal sums. However, the success of both devices is limited to functions whose Taylor coefficients approximately follow a geometric progression. In fact, Fornberg (1981a, p. 542) identifies some problems:

> Some warning about cases in which full accuracy may not be reached. Such cases are
>
> (1) very low-order polynomials (for example, $f(z) = 1 + z$);
> (2) functions whose Taylor coefficients contain very large isolated terms (for example, $f(z) = 10^6 + 1/(1 - z)$);
> (3) certain entire functions (for example, $f(z) = e^z$);
> (4) functions whose radius of convergence is limited by a branch point at which the function remains many times [real] differentiable (for example, $f(z) = (1 + z)^{10} \log(1 + z)$ expanded around $z = 0$).

As illustrated by the numerical experiments of Fig. 1, an answer to the question of choosing a proper radius r becomes absolutely mandatory for derivatives of orders of about $n = 100$ and higher: outside a narrow region of radii there is a complete loss of accuracy. However, rather surprisingly, Fig. 1 also shows that about full accuracy

[4] We write "$\doteq$" to indicate that a number has been correctly *rounded* to the digits given, "$\sim$" to denote a rigorous asymptotic equality, and "$\approx$" to informally assert some approximate agreement.



a. $f(z) = \exp(z)$ (Example 5.1)

b. $f(z) = \mathrm{Ai}(z)$ (Example 10.4)

c. $f(z) = \exp(\exp(z) - 1)$ (Example 7.5)

d. $f(z) = \sec(z)^6$ (Example 6.1)

e. $f(z) = z/(e^z - 1)$ (Example 6.2)

f. $f(z) = (1 - z)^{11/2}$ (Example 5.2)

Fig. 1 (Color online) Numerical stability of using Cauchy integrals to compute $f^{(n)}(0)$: plots of the empirical loss of digits (*solid red line*), that is, the ratio of the relative error divided by the machine precision, and its prediction by the condition number $\kappa(n, r)$ (*dashed blue line*) vs. the radius r. The vertical lines (*dashed green*) of the last three plots visualize a *finite* radius of convergence $R < \infty$. In each plot the results for *two* different orders of differentiation are shown: $n = 10$ (the less steep curves starting from the *left*) and $n = 100$ (the steeper curves starting farther to the *right*). The number m of nodes of the trapezoidal sum approximation was chosen large enough not to change the picture. The qualitative shape (convexity in the double logarithmic scale, coercivity and monotonicity properties) of these condition number plots can be completely understood from the general results in Sect. 4

can be obtained for some functions if we choose the optimal radius that minimizes the loss of accuracy. We observe that such an optimal radius strongly depends on n (and f). This strong dependence, together with the complete loss of accuracy far off the optimal radius, prevents us from using, for larger n, just a single radius r to calculate all the leading Taylor coefficients $a_0, \dots, a_n$ in one go; it thus puts the FFT effectively out of business for the problem at hand.

The goal of this paper is a deeper mathematical understanding of all these effects. In particular, we would like to automate the choice of the parameters m and r and to predict the possible loss of accuracy. This turns out to be a surprisingly rich and multifaceted topic, with relations to some classical results of complex analysis such as Hadamard's three circles theorem (Sect. 7) as well as to some more advanced topics such as the theory of Hardy spaces (Sects. 4 and 6), the Wiman–Valiron theory of the maximum term of entire functions (Sect. 8), the Levin–Pfluger theory of the distribution of zeros of entire functions (Sect. 10); and with relations to some advanced tools of asymptotic analysis and analytic combinatorics such as the saddle-point method (Sect. 9) and the concept of H-admissibility (Sect. 11).

Outline of the Paper

To guide the reader through the thicket of this paper, we summarize its most relevant findings:

- from the point of approximation theory and convergence rates as $m \to \infty$, smaller radii are better than larger ones (Sect. 2); there are useful explicit upper bounds of the number of nodes m in terms of the desired relative error ϵ, the order of differentiation n, and the chosen radius r ((2.8) and (2.11));
- with respect to *absolute* errors, the calculation of the normalized Taylor coefficients $r^n a_n$ is numerically stable for *any* radius $r < R$ (Sect. 3.1);
- with respect to *relative* errors, the loss of significant digits is modeled by $\log_{10} \kappa(n,r)$ where $\kappa(n,r)$ denotes the condition number of the Cauchy integral (Sect. 3.2, see also Fig. 1), which is *independent* of the particular quadrature rule chosen for the actual approximation; it can be estimated on the fly (algorithm given in Fig. 3);
- $\log \kappa(n,r)$ is a convex function of $\log r$ (Corollary 4.2) and there exists an (essentially unique) optimal radius $r_*(n) = \arg\min_r \kappa(n,r)$ that minimizes the loss of accuracy caused by round-off errors; these optimal radii form an increasing sequence satisfying $r_*(n) \to R$ as $n \to \infty$ (Theorem 4.6);
- for finite radius of convergence $R < \infty$, the corresponding optimal condition number $\kappa_*(n)$ blows up if f belongs to the Hardy space H^1 (Theorem 4.7); on the other hand, $\kappa_*(n)$ remains essentially bounded if f does *not* belong to the Hardy space H^1 and is amenable to Darboux's method (Sects. 5 and 6), in which case there are useful explicit (asymptotic) formulas for $r_*(n)$ and $\kappa_*(n)$ ((6.3) and (6.4));
- for entire transcendental functions it is more convenient to analyze a certain upper bound $\bar\kappa(n,r)$ of the condition number (7); this yields a *unique* radius $r_\diamond(n) = \arg\min_r \bar\kappa(n,r)$, called the *quasi-optimal* radius, with a corresponding quasi-optimal condition number $\kappa_\diamond(n) = \kappa(n, r_\diamond(n)) \geq \kappa_*(n)$; the quasi-optimal radii also form an increasing sequence with $r_\diamond(n) \to R$ as $n \to \infty$ (Theorem 7.3);

- for entire functions of perfectly regular growth there is a simple asymptotic formula for $r_\diamond(n)$ in terms of the order and type of such a function (Theorem 8.4);
- $r_\diamond(n)$ is the modulus of certain saddle points of $|z^{-n} f(z)|$ in the complex plane (Theorem 9.1); the saddle-point method offers a methodology to obtain asymptotic results for $\kappa_\diamond(n)$ (Sect. 9.2);
- for entire functions of completely regular growth (satisfying certain conditions on the zeros), the circular contour of radius $r_\diamond(n)$ is optimal in the sense that it passes the saddle points approximately in the direction of steepest descent (10); this yields the extremely simple asymptotic condition number bound $\limsup_n \kappa_\diamond(n) \le \Omega$ where Ω is the number of maxima of the Phragmén–Lindelöf indicator function of f (Theorem 10.2); in fact, there is an explicit asymptotic formula for $\kappa_\diamond(n)$ in terms of a finite sum (Theorem 10.1) that turns out to yield $\kappa_\diamond(n) \sim 1$ in many relevant examples;
- for H-admissible entire functions we have $\kappa_\diamond(n) \sim 1$ (Corollary 11.3);
- for entire functions f with nonnegative Taylor coefficients the quasi-optimal radius $r_\diamond(n)$ can be calculated as the solution of the scalar convex optimization problem $r_\diamond(n) = \arg\min_r r^{-n} f(r)$ (Theorem 12.1); we prove $\kappa_\diamond(n) \sim 1$ for a model of a Fredholm determinant with nonnegative Taylor coefficients (12.8).

We shall comprehensively discuss many concrete examples and applications throughout this paper: most notably the functions illustrated in Fig. 1, the functions from the list of the Fornberg quote on p. 3, the functions whose properties are listed in Table 2, the functions $f(z) = (1-z)^\beta$ ($\beta \in \mathbb{R} \setminus \mathbb{N}_0$) (Example 5.2), the generalized hypergeometric functions (Example 8.2), the reciprocal gamma function $f(z) = 1/\Gamma(z)$ (10.4), a generating function from the theory of random matrices (Examples 3.1 and 12.3), and a generating function from the theory of random permutations (Example 12.5).

2 Approximation Theory

2.1 Convergence Rates

In this section we recall some basic facts about the convergence of the trapezoidal sums applied to Cauchy integrals on circular contours. We use the notation

$$D_r = \{z \in C : |z| < r\}, \qquad C_r = \{z \in \mathbb{C} : |z| = r\},$$

for (open) disks and circles of radius r. Let f be an analytic function as in Sect. 1, $\mathcal{P}_m$ be the set of all polynomials of degree $\le m$, and let

$$E_m(f;r) = \inf_{p\in\mathcal{P}_m} \|f-p\|_{L^\infty(\overline{D_r})} \quad (0 < r < R)$$

denote the error of best polynomial approximation of f on the closed disk $\overline{D_r}$. Equivalently, by the maximum modulus principle, we have

$$E_m(f;r) = \inf_{p\in\mathcal{P}_m} \|f-p\|_{L^\infty(C_r)} \quad (0 < r < R).$$

The following theorem certainly belongs to the "folklore" of numerical analysis; pinning it down, however, in the literature in exactly the form that we need turned out to be difficult. For accounts of the general techniques used in the proof, see, for the aliasing relation, Henrici (1986, Sects. 13.2/4) and, for the use of best approximation in estimating quadrature errors, Davis and Rabinowitz (1984, Sect. 4.8).

Theorem 2.1 *Let f be analytic in D_R and $0 < r < R$. Then, with the n-th Taylor coefficient a_n and its approximation $a_n(r,m)$ as in* (1.2) *and* (1.3), *we have the aliasing relation*

$$r^n a_n(r,m) = r^{n'} a_{n'}(r,m) \quad (n \equiv n' \bmod m) \tag{2.1}$$

and the error estimate

$$r^n \big|a_n - a_n(r,m)\big| \le 2E_{m-1}(f;r) \quad (0 \le n < m). \tag{2.2}$$

Proof The key to this theorem is the observation that $a_n(r,m)$, with $0 \le n < m$, is the *exact* Taylor coefficient of the polynomial $p_* \in \mathcal{P}_{m-1}$ that interpolates f in the nodes $r\mathrm{e}^{2\pi \mathrm{i} j/m}$ ($j = 0, \ldots, m-1$). This fact, and also the aliasing relation, easily follows from the discrete orthogonality

$$\frac{1}{m}\sum_{j=0}^{m-1} \mathrm{e}^{-2\pi \mathrm{i} jn/m} \mathrm{e}^{2\pi \mathrm{i} jn'/m} = \begin{cases} 1, & n \equiv n' \bmod m; \\ 0, & \text{otherwise.} \end{cases}$$

Now, by introducing the averaging operators

$$\begin{aligned} I_n(f;r) &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{-\mathrm{i}n\theta} f\big(r\mathrm{e}^{\mathrm{i}\theta}\big)\,\mathrm{d}\theta, \\ Q_n(f;r,m) &= \frac{1}{m}\sum_{j=0}^{m-1} \mathrm{e}^{-2\pi \mathrm{i} jn/m} f\big(r\mathrm{e}^{2\pi \mathrm{i} j/m}\big), \end{aligned} \tag{2.3}$$

we have $r^n a_n = I_n(f;r)$ and $r^n a_n(r,m) = Q_n(f;r,m)$. The observation about the approximation being exact for polynomials implies, for $p \in \mathcal{P}_{m-1}$ and $0 \le n < m$, that $I_n(p;r) = Q_n(p;r,m)$ and hence

$$\begin{aligned} &\big|I_n(f;r) - Q_n(f;r,m)\big| \\ &\quad \le \big|I_n(f;r) - I_n(p;r)\big| + \big|Q_n(p;r,m) - Q_n(f;r,m)\big| \le 2\|f - p\|_{L^\infty(C_r)}. \end{aligned}$$

Taking the infimum over all p finally implies (2.2). □

From the aliasing relation we immediately infer an important basic criterion for the choice of the parameter m, namely the

$$\textit{Sampling Condition:} \quad m > n. \tag{2.4}$$

For otherwise, if $m \le n$, the value $a_n(r,m)$ is just a good approximation of $r^{k-n} a_k$, with $0 \le k < m$ the remainder of dividing n by m. However, in general, $r^{k-n} a_k$ will differ considerably from a_n.

2.2 Estimates of the Number of Nodes

To obtain more quantitative bounds of the approximation error as $m \to \infty$, we have a closer look at the error of best approximation. With R the radius of convergence of the Taylor series (1.1) of f, the asymptotic geometric rate of convergence of this error is given by (Walsh 1965, Sect. 4.7)

$$\limsup_{m\to\infty} E_m(f;r)^{1/m} = \frac{r}{R}. \tag{2.5}$$

Thus, if we introduce the relative error (assuming $a_n \neq 0$)

$$\delta_m(n,r) = \frac{|a_n - a_n(r,m)|}{|a_n|}, \tag{2.6}$$

we get from (2.2) and (2.5) that

$$\limsup_{m\to\infty} \delta_m(n,r)^{1/m} \le \frac{r}{R}. \tag{2.7}$$

2.2.1 Finite Radius of Convergence

If $R < \infty$, we obtain from (2.7) that, for n and r fixed,

$$\frac{1}{m}\log\delta_m(n,r)^{-1} \ge \log(R/r) + o(1) \quad (m \to \infty).$$

Therefore, if m_ϵ denotes the *smallest* value such that $\delta_m(n,r) \le \epsilon$ for $m \ge m_\epsilon$ (which implies $\delta_{m_\epsilon} \sim \epsilon$ as $\epsilon \to 0$), we get the asymptotic bound

$$m_\epsilon \le \frac{\log(\epsilon^{-1})}{\log(R/r)}\big(1 + o(1)\big) \quad (\epsilon \to 0). \tag{2.8}$$

Example 2.2 To illustrate the sharpness of this bound, we consider the function $f(z) = z/(e^z - 1)$ for $n = 100$, taking the radius $r = 6.22$, which is about the optimal one shown in Fig. 1.e. Here $R = 2\pi$ and, for a relative error $\epsilon = 10^{-12}$ (which is, for this particular choice of r, large enough to exclude any finite precision effects of the hardware arithmetic), we get

$$m_\epsilon = 2734 \le \underbrace{\frac{\log(\epsilon^{-1})}{\log(R/r)}}_{\doteq 2733.80} \cdot 1.00007;$$

thus, the bound (2.8) is an excellent prediction. In Example 6.2 we will see that, for general n, the radius $r_n = 2\pi(1 - n^{-1})$ is, in terms of numerical stability, about optimal and yields the estimate $m_\epsilon \approx n\log\epsilon^{-1}$. That is, for ϵ fixed, we get $m_\epsilon = O(n)$ as $n \to \infty$, which is the best we could expect in view of the sampling condition (2.4). Further examples of this kind are provided in Sects. 5 and 6.

2.2.2 Entire Functions

If f is entire, that is, $R = \infty$, the estimate (2.7) shows that the trapezoidal sums converge even faster than geometrically:

$$\lim_{m\to\infty} \delta_m(n,r)^{1/m} = 0.$$

In fact, if f is a polynomial of degree d, we already know from Theorem 2.1 that the trapezoidal sum is exact for $m > d$, which implies[5] $\delta_m(n,r) = 0$. If f is entire and transcendental, a more detailed resolution of the behavior of δ_m depends on the properties of f at its essential singularity in $z = \infty$. For example, entire functions of finite order $\rho > 0$ and type $\tau > 0$ (for a definition see Sect. 8 below) yield (Batyrev 1951; Giroux 1980)

$$\limsup_{m\to\infty} m^{1/\rho} E_m(f;r)^{1/m} = r(\mathrm{e}\rho\tau)^{1/\rho}. \tag{2.9}$$

We thus get

$$\limsup_{m\to\infty} m^{1/\rho} \delta_m(n,r)^{1/m} \le r(\mathrm{e}\rho\tau)^{1/\rho} \tag{2.10}$$

and therefore, for n and r fixed,

$$\frac{1}{m}\log\delta_m(n,r)^{-1} - \frac{1}{\rho}\log\bigl(m/(\mathrm{e}\rho\tau)\bigr) \ge \log(1/r) + o(1) \quad (m\to\infty).$$

Solving for m_ϵ, as defined in Sect. 2.2.1, yields the asymptotic bound

$$m_\epsilon \le \frac{\rho\log(\epsilon^{-1})}{W(\log(\epsilon^{-1})/(\mathrm{e}\tau r^\rho))}\bigl(1+o(1)\bigr) \quad (\epsilon\to 0). \tag{2.11}$$

Here $W(z)$ denotes the principal branch of the Lambert W-function defined by the equation $z = W(z)\mathrm{e}^{W(z)}$. In Remark 8.5 we will specify this bound, for entire functions of perfectly regular growth, using a particular radius that is about optimal in the sense of numerical stability.

Example 2.3 To illustrate the sharpness of this bound, we consider $f(z) = \mathrm{e}^z$ for $n = 10$ taking the radius $r = 10$, which we read from Fig. 1.a to be close to optimal. Here, the order and type of the exponential functions are $\rho = \tau = 1$ (see Table 2) and we get the results of Table 1 (which were computed using high-precision arithmetic in Mathematica). As we can see, (2.11) turns out to be a very useful upper bound.

2.3 Other Quadrature Rules

To approximate the Cauchy integral (1.2), there are other quite effective quadrature rules available besides the trapezoidal sums; examples are Gauss–Legendre and

[5] Recall that we have assumed $a_n \ne 0$ in the definition of δ_m, which restricts us to $n \le d < m$.

Table 1 Sharpness of the bound (2.11) for $f(z)=\mathrm{e}^z$ ($n=10$, $r=10$)

ϵ	minimal m_ϵ	$\rho\log\epsilon^{-1}/W(\log\epsilon^{-1}/\mathrm{e}\tau r^\rho)$
10^{-12}	32	48.21
10^{-100}	126	140.30
10^{-1000}	694	706.73

Clenshaw–Curtis quadrature. From the point of complexity theory, however, Gensun and Xuehua (2005) have shown (drawing from the pioneering work of Nikolskii in the 1970s) that the trapezoidal sums are, for the problem at hand, *optimal* in the sense of Kolmogorov.[6] Hence, for definiteness and simplicity, we stay with trapezoidal sums in this paper.

It is, however, important to note that the results of this paper apply to other families of quadrature rules as well: first, the estimates (2.8) and (2.11) remain valid if the quadrature error is bounded by the error of polynomial best approximation (as in (2.2), up to some different constant); which is, e.g., the case for Gauss–Legendre and Clenshaw–Curtis quadrature (see Trefethen 2008). Second, the discussion of numerical stability in the next section applies to quadrature rules with *positive* weights in general. In particular, the estimated digit loss (3.7) depends only on the condition number of the Cauchy integral itself, an analytic quantity *independent* of the chosen quadrature rule. Then, starting with Sect. 4, optimizing that condition number is the main objective of this paper.

3 Numerical Stability

As we have seen in Sect. 1 and Fig. 1, there are stability issues with using (1.3) in the realm of finite precision arithmetic. Specifically, small finite precision errors in the evaluation of the function f can be amplified to large errors in the resulting evaluation of the sum (1.3). This error propagation is described by the condition number of the Cauchy integral and depends very much on the chosen radius r and on the underlying error concept.

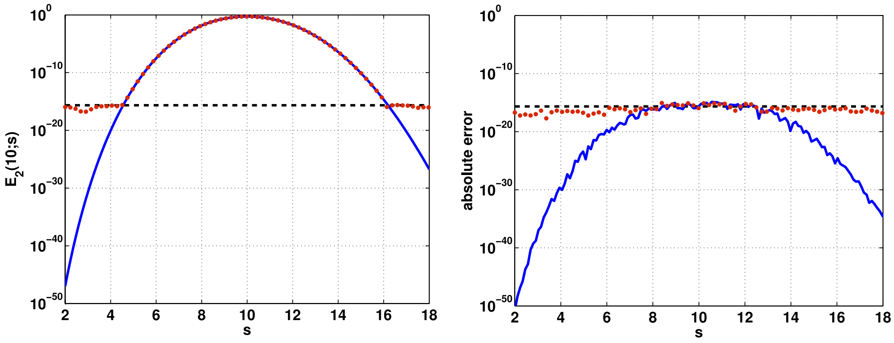
3.1 Absolute Errors

Any perturbation $\hat f$ of the function f within a bound of the *absolute* error,

$$\|f-\hat f\|_{L^\infty(C_r)}\le\epsilon,$$

induces perturbations $\hat a_n(r)$ and $\hat a_n(r,m)$ of the Cauchy integral (1.2) and of its approximation (1.3) by the trapezoidal sum. Note that even though the value of the Cauchy integral does not depend on the specific choice of the radius r (within the

[6] That is, the m-point trapezoidal sum minimizes, among all m-point quadrature formulas, the worst-case quadrature error for the Cauchy integral (1.2) over all analytic functions whose modulus is bounded by some constant in an open disk containing $|z|\le r$.



a. gap probability $E_2(10;s)$ of GUE

b. absolute error

Fig. 2 (Color online) *Left*: the gap probability $E_2(10; s)$ of GUE calculated as the tenth Taylor coefficient of a Fredholm determinant; *right*: the absolute error of the calculation. The *dotted lines* (*red*) show the results for the radius $r = 1$; the *solid lines* (*blue*) show the results for the quasi-optimal radius $r_\diamond$, which depends on s (see Example 12.3 and Fig. 7). The *dashed horizontal lines* show the level of machine precision

range $0 < r < R$), the perturbed value $\hat{a}_n(r)$ generally does depend on it. Because both the integral and the sum are rescaled mean values of f, we get the simple estimates

$$\left|r^n a_n - r^n \hat{a}_n(r)\right| \le \epsilon, \qquad \left|r^n a_n(r,m) - r^n \hat{a}_n(r,m)\right| \le \epsilon. \tag{3.1}$$

Thus, the *normalized* Taylor coefficients $r^n a_n$ are well conditioned with respect to *absolute* errors (with condition number one); a fact that has basically already been observed by Lyness and Sande (1971, p. 670). There are indeed applications where absolute errors of normalized Taylor coefficients are a reasonable concept to consider, which then typically leads to a proper choice of the radius r. We give one such example from our work on the numerical evaluation of distributions in random matrix theory (Bornemann 2009).

Example 3.1 The sequence of hermitian random matrices $X_N \in \mathbb{C}^{N\times N}$ with entries

$$(X_N)_{j,j} = \xi_{j,j}, \quad (X_N)_{j,k} = \frac{\xi_{j,k} + \mathrm{i}\eta_{j,k}}{\sqrt{2}}, \quad (X_N)_{k,j} = \frac{\xi_{j,k} - \mathrm{i}\eta_{j,k}}{\sqrt{2}} \quad (j < k),$$

formed from independent and identically distributed (i.i.d.) families of real standard normal random variables $\xi_{i,j}$ and $\eta_{i,j}$, is called the *Gaussian unitary ensemble* (GUE).[7] The GUE is of considerable interest since, on one hand, various statistical properties of the spectrum $\sigma(X_N)$ enjoy explicit analytic formulas. On the other hand, in the large matrix limit $N \to \infty$, by a kind of "universal" limit law, these properties are often known (or conjectured) to hold for other families of random matrices, too.

[7] In MATLAB, the sequence of commands

```
X = randn(N) + 1i*randn(N); X = (X+X')/2;
```

can be used to sample from the $N \times N$ GUE.

An example of such a property concerns the *bulk scaling* $\hat{X}_N = \pi^{-1}N^{1/2}X_N$, for which the mean spacing of the scaled eigenvalues goes, in the large matrix limit, to one. The basic statistical quantities then considered are the *gap probabilities*[8]

$$E_2(n;s) = \lim_{N\to\infty} \mathbb{P}\big(\#\big(\sigma(\hat{X}_N)\cap[0,s]\big) = n\big),$$

the probability that, in the large matrix limit, exactly n of the scaled eigenvalues are located in the interval $[0,s]$. (For Wigner hermitian matrices with a subexponential decay, Erdős et al. (2010) have, just recently, established the universality of $E_2(0;s)$.) The generating function of the sequence $E_2(0;s)$, $E_2(1;s)$, $E_2(2,s),\ldots$ is given by the Fredholm determinant of Dyson's sine kernel $K(x,y)) = \operatorname{sinc}(\pi(x-y))$ (see, e.g., Mehta 2004, Sect. 6.4), namely,

$$\sum_{k=0}^{\infty} E_2(k;s)z^k = \det\big(I-(1-z)K\big|_{L^2(0,s)}\big).$$

For given values of n and s, the strategy to calculate $E_2(n;s)$ is as follows. First, by using the method of Bornemann (2010) for the numerical evaluation of Fredholm determinants, the function

$$f(z) = \det\big(I-(1-z)K\big|_{L^2(0,s)}\big)$$

can be evaluated for *complex* arguments of z up to an absolute error of about $\epsilon = 10^{-15}$. Second, the Taylor coefficients $E_2(n;s)$ of f are calculated by means of Cauchy integrals. Now, since these Taylor coefficients are *probabilities*, the number 1 is the natural scale for the *absolute* errors, which makes $r = 1$ the proper choice for the radius (Bornemann 2009, Sect. 4.3). By (3.1), we expect an absolute error of about $\epsilon = 10^{-15}$, which is confirmed by numerical experiments; see Fig. 2. However, the figure also illustrates that there is a complete loss of information about the *tails* (that is, those very small probabilities which are about the size of the error level or smaller). By controlling the radius with respect to relative errors using the method exposed in the rest of this paper, we were able to increase the accuracy of the tails considerably. The reader should note, however, that in most applications of random matrix theory the accurate calculation of the tails would be irrelevant. It typically suffices to just identify such small probabilities as being very small; thus, the concept of absolute error is completely appropriate in this example.

There are examples where small *absolute* errors of the normalized Taylor coefficients $r^n a_n$ are not accurate enough. Because of the supergeometric growth of the factorial, examples of such cases are the derivatives $f^{(n)}(0) = n!a_n$, for high orders n. Accuracy will only survive the scaling by $n!$ if the Taylor coefficients themselves already have small *relative* errors.

[8]We denote by $\#S$ the number of elements in a finite set S.

3.2 Relative Errors

We now consider perturbations $\hat{f}$ of the function f whose relative error can be rendered in the form

$$\hat{f}\big(re^{i\theta}\big) = f\big(re^{i\theta}\big)\big(1+\epsilon_r(\theta)\big), \qquad \|\epsilon_r\|_\infty \le \epsilon. \tag{3.2}$$

Such a perturbation induces a perturbation $\hat{a}_n(r)$ of the Cauchy integral (1.2) which satisfies the straightforward bound (Deuflhard and Hohmann 2003, Lemma 9.1)

$$\frac{|a_n - \hat{a}_n(r)|}{|a_n|} \le \kappa(n,r)\cdot\epsilon \tag{3.3}$$

of its relative error (assuming $a_n \ne 0$), where

$$\kappa(n,r) = \frac{\int_0^{2\pi} |f(re^{i\theta})|\,d\theta}{|\int_0^{2\pi} e^{-in\theta} f(re^{i\theta})\,d\theta|} \ge 1 \tag{3.4}$$

is the condition number of the Cauchy integral.[9] Note that this number measures the amount of cancellation within the Cauchy integral: $\kappa(n,r) \gg 1$ indicates a large amount of cancellation, whereas $\kappa(n,r) \approx 1$ if there is virtually no cancellation; see Fig. 4 for an illustration.

Correspondingly, there are perturbations $\hat{a}_n(r,m)$ of the trapezoidal sum approximations (1.3) of the Cauchy integrals. They satisfy the same type of bound, namely

$$\frac{|a_n(r,m) - \hat{a}_n(r,m)|}{|a_n(r,m)|} \le \kappa_m(n,r)\cdot\epsilon, \tag{3.5}$$

of its relative error (assuming $a_n(r,m) \ne 0$), where

$$\kappa_m(n,r) = \frac{\sum_{j=0}^{m-1} |f(re^{2\pi i j/m})|}{|\sum_{j=0}^{m-1} e^{-2\pi i jn/m} f(re^{2\pi i j/m})|} \ge 1 \tag{3.6}$$

is the condition number of the trapezoidal sum (Higham 2002, p. 538).

If m is chosen large enough such that the trapezoidal sum $a_n(r,m)$ is a good approximation of the Cauchy integral a_n, then we typically also have

$$\frac{1}{m}\sum_{j=0}^{m-1}\big|f\big(re^{2\pi i j/m}\big)\big| \approx \frac{1}{2\pi}\int_0^{2\pi}\big|f\big(re^{i\theta}\big)\big|\,d\theta.$$

This is because the integrand $|f(re^{i\theta})|$ is a smooth *periodic* function of θ, and the trapezoidal sum therefore gives excellent approximations of this integral, too.[10]

[9] This condition number is completely *independent* of how the Cauchy integral is actually computed.

[10] By the Euler–Maclaurin summation formula, the approximation error is of *arbitrary* algebraic order (Deuflhard and Hohmann 2003, Theorem 9.16).

```
function [val,err,kappa,m] = D(f,n,r)

fac = exp(gammaln(n+1)-n*log(r));
cauchy = @(t) fac*(exp(-n*t).*f(r*exp(t)));
m = max(n+1,8); tol = 1e-15;
s = cauchy(2i*pi*(1:m)/m); val1 = mean(s); err1 = NaN;
while m < 1e6
    m = 2*m;
    s = reshape([s; cauchy(2i*pi*(1:2:m)/m)],1,m);
    val = mean(s); kappa = mean(abs(s))/abs(val);
    err0 = abs(val-val1)/abs(val); err = (err0/err1)^2*err0;
    if err <= kappa*tol || ~isfinite(kappa); break; end
    val1 = val; err1 = err0;
end
```

Fig. 3 MATLAB implementation of calculating $f^{(n)}(0)$ using the Cauchy integral (1.2) with radius r, approximated by trapezoidal sums. It assumes f to be evaluated up to a relative error `tol`. The number `m` of nodes is determined by a successive doubling procedure until the estimated relative error satisfies a bound corresponding to the level of round-off error given by (3.3). The error estimate (see Lyness 1967, (4.12)) is based on the assumption of a geometric rate of convergence (2.5) which is excellent if $R < \infty$ and an overestimate if $R = \infty$. The initialization of `m` satisfies the sampling condition (2.4). The doubling of nodes is arranged so that already-computed values of f are reused

Moreover, because of positivity, there are no additional stability issues here. That said, for reasonably large m, we have

$$\kappa_m(n,r) \approx \kappa(n,r)$$

as long as the computation of $a_n(r,m)$ is not completely unstable. We use $\kappa(n,r)$ in the theory developed in this paper, but we use $\kappa_m(n,r)$ to monitor stability in our implementation, which is given in Fig. 3. In fact, the examples of Fig. 1 show that $\kappa(n,r)$ gives an excellent prediction of the actual loss of (relative) accuracy in the calculation of the Taylor coefficients; it thus models the dominant effect of the choice of the radius r (in fact, for *any* stable and accurate quadrature rule):

$$\#\text{ lost significant digits} \approx \log_{10}\kappa(n,r). \tag{3.7}$$

4 Optimizing the Condition Number

4.1 General Results on the Condition Number

It is convenient to rewrite the expression (3.4), which defines the condition number, briefly as

$$\kappa(n,r) = \frac{M_1(r)}{|a_n|r^n}, \tag{4.1}$$

using the mean of order 1 of the modulus of f on the circle C_r,

$$M_1(r) = \frac{1}{2\pi}\int_0^{2\pi} \left|f\left(re^{i\theta}\right)\right| d\theta. \tag{4.2}$$

Concerning the properties of M_1, we recall the following classical theorem. For the standard proof, see Dienes (1931, p. 156) or Pólya and Szegö (1964, Sect. III.310).

Theorem 4.1 (Hardy 1915) *Let f be given by a Taylor series with radius of convergence R. The mean value function M_1 satisfies the following, for $0 < r < R$:*

(a) *$M_1(r)$ is continuously differentiable.*
(b) *If $f \not\equiv 0$, $\log M_1(r)$ is a convex function of $\log r$.*
(c) *If $f \not\equiv \text{const}$, $M_1(r)$ is strictly*[11] *increasing.*

Because $\log \kappa(n,r) = \log M_1(r) - \log|a_n| - n\log r$, there are some immediate consequences for the condition number.

Corollary 4.2 *Let $f \not\equiv 0$ be given by a Taylor series with radius of convergence R. Then, for n with $a_n \neq 0$ and for $0 < r < R$:*

(a) *$\kappa(n,r)$ is continuously differentiable with respect to r.*
(b) *$\log\kappa(n,r)$ is a convex function of $\log r$.*

We now study the behavior of $\kappa(n,r)$ as $r \to 0$ and $r \to \infty$. The first direction is simple and gives us the expected numerical instability for small radii.

Theorem 4.3 *Let $f \not\equiv 0$ be given by a Taylor series with radius of convergence R and let a_{n_0} be its first nonzero coefficient. Then, for $n > n_0$,*

$$\kappa(n,r) \to \infty \quad (r \to 0);$$

but $\kappa(n_0,r) \to 1$.

Proof From the expansion

$$M_1(r) = \frac{1}{2\pi}\int_0^{2\pi} \left|f\left(re^{i\theta}\right)\right| d\theta = |a_{n_0}|r^{n_0} + O\left(r^{n_0+1}\right) \quad (r \to 0)$$

we get

$$\kappa(n,r) \sim \frac{|a_{n_0}|}{|a_n|} r^{n_0-n} \quad (r \to 0),$$

which implies both assertions. □

The other direction, $r \to R$, is more involved and depends on further properties of f. Let us begin with entire functions ($R = \infty$).

[11] The fact that the monotonicity is *strict* was added to Hardy's theorem by Taylor (1950).

Theorem 4.4 *Let f be an entire function. If f is transcendental, then, for all $n \in \mathbb{N}$,*

$$\kappa(n,r) \to \infty \quad (r \to \infty).$$

If f is a polynomial of degree d, then this results holds for all $n \neq d$, but $\kappa(d,r) \to 1$.

Proof Let us assume that, for a particular $m \in \mathbb{N}$,

$$\liminf_{r\to\infty} \frac{M_1(r)}{r^m} = \liminf_{r\to\infty} \frac{1}{2\pi r^m} \int_0^{2\pi} \left| f\left(r\mathrm{e}^{\mathrm{i}\theta}\right)\right| \mathrm{d}\theta < \infty.$$

Then, for all $n > m$,

$$0 \le |a_n| \le \liminf_{r\to\infty} \frac{1}{2\pi r^n} \int_0^{2\pi} \left| f\left(r\mathrm{e}^{\mathrm{i}\theta}\right)\right| \mathrm{d}\theta = 0;$$

that is, $a_n = 0$; implying that f is a polynomial of degree $d \le m$. This proves the assertion for transcendental f, and for the cases $n < d$ if f is a polynomial of degree d. The cases $n > d$ follow trivially from $a_n = 0$, which implies $\kappa(n,r) = \infty$. Finally, the case $n = d$ gives, because of $|f(z)| = |a_d||z|^d + O(|z|^{d-1})$ as $z \to \infty$,

$$\kappa(d,r) = \frac{1}{2\pi |a_d| r^d} \int_0^{2\pi} \left| f\left(r\mathrm{e}^{\mathrm{i}\theta}\right)\right| \mathrm{d}\theta = 1 + O\left(r^{-1}\right) \quad (r \to \infty),$$

which completes the proof. □

For finite radius of convergence, $R < \infty$, we recall the definition of the Hardy norm (the last equality follows from the monotonicity of M_1):

$$\|f\|_{H^1(D_R)} = \sup_{0<r<R} M_1(r) = \lim_{r\to R} M_1(r). \tag{4.3}$$

If $\|f\|_{H^1(D_R)} < \infty$ the function f belongs to the Hardy space $H^1(D_R)$. From the *strict* monotonicity and differentiability of $M_1(r)$ we infer that the function

$$\sigma(r) = \log M_1(r)$$

satisfies $\sigma'(r) > 0$ $(0 < r < R)$. Since $\log M_1(r)$ is convex in $\log r$, the function $r\sigma'(r)$ is monotonically increasing. Therefore, the limit

$$\nu = \sup_{0<r<R} r\sigma'(r) = \lim_{r\to R} r\sigma'(r) > 0 \tag{4.4}$$

exists (with $\nu = \infty$ a possibility, however).

Theorem 4.5 *Let f be given by a Taylor series with finite radius of convergence $R < \infty$. Then, for $a_n \neq 0$,*

$$\lim_{r\to R} \kappa(n,r) = \frac{\|f\|_{H^1(D_R)}}{|a_n| R^n}.$$

This is finite if and only if f belongs to the Hardy space $H^1(D_R)$. If $n > \nu$ then $\kappa(n,r)$ is strictly decreasing for $0 < r < R$; whereas if $\nu = \infty$ then, for all n, $\kappa(n,r)$ is strictly increasing in the vicinity of $r = R$.

Proof The limit can be directly read from (4.3). If $n > \nu$, we have

$$\frac{\mathrm{d}}{\mathrm{d}r}\log\kappa(n,r) = \sigma'(r) - nr^{-1} \le (\nu - n)r^{-1} < 0 \quad (0 < r < R),$$

which shows that $\kappa(n,r)$ is strictly decreasing. If $\nu = \infty$ then $\sigma'(r) \to \infty$ as $r \to R$, which implies that

$$\frac{\mathrm{d}}{\mathrm{d}r}\log\kappa(n,r) = \sigma'(r) - nr^{-1} \to \infty \quad (r \to R).$$

Hence, $\kappa(n,r)$ must be, for r close to R, strictly increasing. □

4.2 The Optimal Radius

Optimizing the numerical stability of the Cauchy integrals means, by (3.7), to choose a radius r that minimizes the condition number $\kappa(n,r)$. The general results of Sect. 4.1 imply that such a minimum actually exists. Indeed, assuming $n > n_0$ (see Theorem 4.3), $a_n \ne 0$, and that f is not a polynomial,[12] we have the following ingredients allowing the optimization:

- *continuity*: $\kappa(n,r)$ is continuous for $0 < r < R$ (Corollary 4.2) and, if $R < \infty$ and $\|f\|_{H^1(D_R)} < \infty$, can be continuously continued to $r = R$ (Theorem 4.5);
- *convexity*: $\log\kappa(n,r)$ is convex in $\log r$ (Corollary 4.2);
- *coercivity*: $\kappa(n,r) \to \infty$ as $r \to 0$ (Theorem 4.3) and, if $R = \infty$ (Theorem 4.4) or if $R < \infty$ and $\|f\|_{H^1(D_R)} = \infty$ (Theorem 4.5), as $r \to R$.

Hence, by the strict monotonicity of the logarithm, the optimal condition number

$$\kappa_*(n) = \min_{0<r\le R} \kappa(n,r) \tag{4.5}$$

exists and is taken for the optimal radius[13]

$$r_*(n) = \operatorname*{arg\,min}_{0<r\le R} \kappa(n,r). \tag{4.6}$$

Because the functions $r^{-n}M_1(r)$ and $\kappa(n,r)$ only differ by a factor that is independent of r (namely, $|a_n|$), it is convenient to extend the definition of the optimal radius

[12] Polynomials are addressed by Theorem 4.4: first, one detects the degree d from $\lim_{r\to\infty}\kappa(d,r) = 1$; then, the cases $n < d$ are dealt with as for entire transcendental f of order $\rho = 0$ (see Sect. 8).

[13] Since we have no proof of *strict* convexity, we cannot exclude the case that the minimizing radius happens to be not unique (even though we have not encountered a single such example). However, because of convexity, the set of all minimizing radii would form a closed interval. We therefore define $r_*(n)$ as the smallest minimizing radius, which, in view of (2.7) and (2.10), gives the best rates of approximation of the trapezoidal sums.

$r_*(n)$ to the case $a_n = 0$ by setting[14]

$$r_*(n) = \operatorname*{arg\,min}_{0<r\le R} r^{-n} M_1(r). \tag{4.7}$$

Theorem 4.6 *Let the nonpolynomial analytic function f be given by a Taylor series with radius of convergence R. Then, the sequence $r_*(n)$ satisfies the monotonicity*

$$r_*(n) \le r_*(n+1) \quad (n > n_0)$$

and has the limit $\lim_{n\to\infty} r_*(n) = R$. Furthermore, the case $r_*(n) = R$ is characterized by

$$r_*(n) = R \quad \Longrightarrow \quad R < \infty, \quad \|f\|_{H^1(D_R)} < \infty, \quad \textit{and} \quad \nu < \infty,$$

and

$$R < \infty, \quad \|f\|_{H^1(D_R)} < \infty, \quad \textit{and} \quad \nu < n \quad \Longrightarrow \quad r_*(n) = R.$$

Proof Because of the optimality of $r_*(n)$ and since $M_1(r) > 0$, we have, for $0 < r < r_*(n)$,

$$r_*(n)^{-(n+1)} M_1\bigl(r_*(n)\bigr) \le r_*(n)^{-1} r^{-n} M_1(r) < r^{-(n+1)} M_1(r).$$

Hence, the optimal radius $r_*(n+1)$ must satisfy $r_*(n+1) \ge r_*(n)$. This monotonicity implies that $r_0 = \lim_{n\to\infty} r_*(n)$ exists. Let us assume that $r_0 < R$. Then, for each $r_0 < r < R$, by taking the limit $n \to \infty$ in

$$r_*(n)^{-1} M_1\bigl(r_*(n)\bigr)^{1/n} \le r^{-1} M_1(r)^{1/n},$$

and recalling the continuity of M_1, we conclude that $r_0^{-1} \le r^{-1}$. Since this contradicts the choice $r_0 < r$, we must have $r_0 = R$. The characterization of $r_*(n) = R$ follows straightforwardly from Theorem 4.5. □

Bounded analytic functions f that belong to the Hardy space $H^1(D_R)$ are known to possess boundary values (Garnett 1981, Sect. II.3); that is, the radial limits

$$f\bigl(R e^{i\theta}\bigr) = \lim_{r\to R} f\bigl(r e^{i\theta}\bigr)$$

exist for almost all angles θ. These boundary values form an L^1-function,

$$\|f\|_{H^1(D_R)} = \frac{1}{2\pi} \int_0^{2\pi} \bigl|f\bigl(R e^{i\theta}\bigr)\bigr|\, d\theta,$$

whose Fourier coefficients are just the normalized Taylor coefficients of f:

$$a_n R^n = \frac{1}{2\pi} \int_0^{2\pi} e^{-in\theta} f\bigl(R e^{i\theta}\bigr)\, d\theta \quad (n = 0, 1, 2, \ldots).$$

[14] Note that all the *qualitative* results that we stated in Sect. 4.1 for $\kappa(n, r)$ hold *verbatim* for $r^{-n} M_1(r)$, independently of whether $a_n \ne 0$ or not.

As the following theorem shows, this fact is bad news for the optimal condition number of such functions for large n: it grows beyond all bounds, at a rate that is all the faster the more regular the boundary values of f are.

Theorem 4.7 *Let the analytic function f be given by a Taylor series with finite radius of convergence $R < \infty$. If $f \in H^1(D_R)$ then*

$$\kappa_*(n) \to \infty \quad (n \to \infty).$$

For boundary values of f belonging to the class[15] *$C^{k,\alpha}(\mathcal{C}_R)$, the optimal condition number grows at least as fast as $\kappa_*(n) \geq cn^{k+\alpha}$ for some constant $c > 0$.*

Proof Since $a_n R^n$ are the Fourier coefficients of the L^1-function formed by the radial boundary values of f, the Riemann–Lebesgue lemma implies that

$$a_n R^n \to 0 \quad (n \to \infty),$$

with a rate $O(n^{-k-\alpha})$ if these boundary values belong to the class $C^{k,\alpha}$ (see, e.g., Zygmund 1968, Sect. II.4). By Theorem 4.6 we have $r_*(n) \to R$. Hence, for $n \to \infty$,

$$\kappa_*(n) = \kappa\bigl(n, r_*(n)\bigr) = \frac{M_1(r_*(n))}{|a_n| r_*(n)^n} \sim \frac{\|f\|_{H^1(D_R)}}{|a_n| r_*(n)^n} \geq \frac{\|f\|_{H^1(D_R)}}{|a_n| R^n} \to \infty,$$

since $\|f\|_{H^1(D_R)} > 0$ (otherwise, we would have $f = 0$ and $R = \infty$). □

5 Examples of Optimal Radii

Qualitatively, the general results of Sect. 4.1 are nicely illustrated by the examples of Fig. 1. In this section we study a couple of important examples more quantitatively for large n.

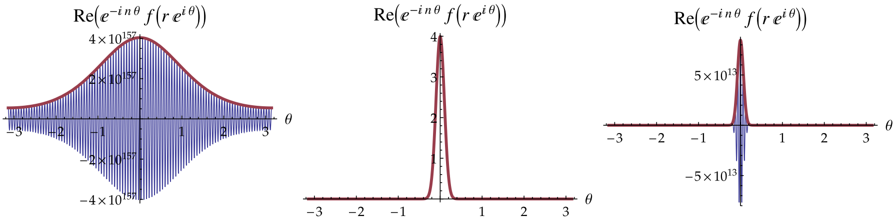
Example 5.1 This example illustrates the excellent behavior of certain entire functions; a general theory will be developed in Sects. 7–12. Here, we consider one of the simplest such functions, namely, the exponential function

$$f(z) = \mathrm{e}^z,$$

which is an entire function ($R = \infty$) with the Taylor coefficients $a_n = 1/n!$. The mean value of the modulus is explicitly given in terms of the modified Bessel function of the first kind of order zero (Watson 1944, Sect. 3.71),

$$M_1(r) = \frac{1}{2\pi} \int_0^{2\pi} \bigl|\exp\bigl(r\mathrm{e}^{\mathrm{i}\theta}\bigr)\bigr| \,\mathrm{d}\theta = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{e}^{r\cos\theta} \,\mathrm{d}\theta = I_0(r) \quad (r \geq 0).$$

[15] $C^{k,\alpha}$ denotes the functions that are k times continuously differentiable with a k-derivative satisfying a Hölder condition of order $0 \leq \alpha \leq 1$.



a. $r = 1$, $\kappa(n,r) = 1.182 \times 10^{158}$ b. $r = 100$, $\kappa(n,r) = 1.002$ c. $r = 200$, $\kappa(n,r) = 1.502 \times 10^{13}$

Fig. 4 (Color online) Real part (oscillatory, *blue line*) and absolute modulus (envelope, *red line*) of the integrand of the Cauchy integral (1.2) for various radii r; $f(z) = \mathrm{e}^z$, $n = 100$. Clearly visible is the huge amount of cancellation if the condition number $\kappa(n,r)$ is large. Note that this is *not* an issue of frequency, which is moderate and perfectly dealt with by the sampling condition (2.4), but rather an issue of amplitude

Hence, the condition number is

$$\kappa(n,r) = r^{-n} n! I_0(r).$$

Figure 4 illustrates the vast cancellations that occur in the Cauchy integral for large condition numbers $\kappa(n,r)$, that is, for far-from-optimal radii r. Using Stirling's formula and the asymptotic expansion of the modified Bessel function (Andrews et al. 1999, (4.12.7)),

$$I_0(r) = \frac{\mathrm{e}^r}{\sqrt{2\pi r}}\left(1 + \frac{1}{8r} + \frac{9}{128r^2} + O\big(r^{-3}\big)\right) \quad (r \to \infty),$$

we get an explicit description of the optimal radius and its condition number: namely, as $n \to \infty$,

$$r_*(n) = n + \frac{1}{2} + \frac{1}{8n} + O\big(n^{-2}\big), \tag{5.1a}$$

$$\kappa_*(n) = 1 + \frac{1}{12n} + \frac{7}{288n^2} + O\big(n^{-3}\big). \tag{5.1b}$$

In fact, even the first term of this expansion for $r_*(n)$ gives uniformly excellent condition numbers:

$$1 < \kappa(n,n) < 1.3 \quad (n \ge 1).$$

Thus, the derivatives of the exponential function can be calculated to full accuracy using Cauchy integrals, for *all* orders n. On the other hand, Fig. 1.a shows that, by choosing a fixed radius r independently of n, it would be impossible to get condition numbers that remain moderately bounded for orders of differentiation between, say, 1 and 100. This explains the failure that Fornberg (1981a, p. 542) has documented using his implementation for the exponential function.

Example 5.2 In preparation for Sect. 6, we consider the family

$$f_\beta(z) = (1 - z)^\beta \quad (\beta \in \mathbb{R} \setminus \mathbb{N}_0)$$

of analytic functions, which are not polynomials for the values of β considered. The radius of convergence of the Taylor series is $R=1$, and the Taylor coefficients are given by

$$a_n = \binom{n-\beta-1}{n} \quad (n=0,1,2,\ldots).$$

By a simple transformation of Euler's integral representation (Andrews et al. 1999, Theorem 2.2.1), the mean value of the modulus can explicitly be expressed in terms of the hypergeometric function ${}_2F_1(a,b;c;z)$:

$$\begin{aligned} M_1(r) &= \frac{1}{2\pi}\int_0^{2\pi} \left|1-re^{i\theta}\right|^\beta \,d\theta = \frac{1}{2\pi}\int_0^{2\pi} \left(\sqrt{1+r^2-2r\cos\theta}\right)^\beta \,d\theta \\ &= (1+r)^\beta {}_2F_1\left(\frac{1}{2}, -\frac{\beta}{2}; 1; \frac{4r}{(1+r)^2}\right) \quad (0\le r<1). \end{aligned} \tag{5.2}$$

The classical results of Gauss (Andrews et al. 1999, Theorems 2.1.3 and 2.2.2) for the hypergeometric function ${}_2F_1(a,b;c;z)$ as $z\to 1$ imply, as $r\to 1$ from below,

$$M_1(r) \sim \begin{cases} \dfrac{2^\beta\Gamma(\frac{\beta+1}{2})}{\sqrt{\pi}\,\Gamma(\frac{\beta}{2}+1)} & (\beta>-1); \\ \frac{1}{\pi}\log(\frac{1}{1-r}) & (\beta=-1); \\ \frac{\Gamma(-\frac{\beta+1}{2})}{2\sqrt{\pi}\,\Gamma(-\frac{\beta}{2})}(1-r)^{\beta+1} & (\beta<-1). \end{cases} \tag{5.3}$$

Therefore, we have to distinguish three cases.

Case I: $\beta>-1$

Here, (5.3) implies that f_β belongs to the Hardy space $H^1(D_1)$ with norm

$$\|f_\beta\|_{H^1(D_1)} = \lim_{r\to 1} M_1(r) = \frac{2^\beta\Gamma(\frac{\beta+1}{2})}{\sqrt{\pi}\,\Gamma(\frac{\beta}{2}+1)} \ge 1.$$

(The estimate from below holds since the last expression of that norm is a convex and coercive function of β, taking its minimum at $\beta=0$.) The constant ν, defined in (4.4), can be computed from

$$\begin{aligned} M_1'(r) = \beta(1+r)^{\beta-3}\biggl((1+r)^2{}_2F_1\left(\frac{1}{2}, -\frac{\beta}{2}; 1; \frac{4r}{(1+r)^2}\right) \\ + (r-1){}_2F_1\left(\frac{3}{2}, 1-\frac{\beta}{2}; 2; \frac{4r}{(1+r)^2}\right)\biggr) \end{aligned}$$

to have the value

$$\nu = \lim_{r\to 1} r\sigma'(r) = \frac{M_1'(1)}{M_1(1)} = \frac{\beta}{2}.$$

Thus, by Theorems 4.5 and 4.6, the condition number $\kappa(n,r)$ is strictly decreasing for $n > \beta/2$ (see Fig. 1.f for an example); hence,

$$r_*(n) = 1 \quad (n > \beta/2), \tag{5.4a}$$

which induces (by Stirling's formula)

$$\kappa_*(n) = \frac{\|f_\beta\|_{H^1(D_1)}}{|\binom{n-\beta-1}{n}|} \geq \frac{1}{|\binom{n-\beta-1}{n}|} \sim \left|\Gamma(-\beta)\right| n^{\beta+1} \to \infty \quad (n \to \infty). \tag{5.4b}$$

Given the $C^{\lfloor\beta\rfloor,\beta-\lfloor\beta\rfloor}$ regularity of the boundary values of f_β, this lower bound on the growth of the optimal condition number is actually just a little sharper than the order n^β bound that can be read from Theorem 4.7.

Thus, for each radius r, there will be a complete loss of significant digits if n is large enough (e.g., there is already a more than 12-digit loss for $\beta = 11/2$ and $n = 100$, see Fig. 1.f); an effect that will be more pronounced for larger β. Now, larger β correspond to higher order real differentiability at the branch point $z = 1$; an observation which helps to explain the failure that Fornberg (1981a, p. 542) has documented of his method for such functions.

Case II: $\beta = -1$

Now, (5.3) shows that f_β does not belong to the Hardy space $H^1(D_1)$ anymore. Thus, by Theorems 4.5 and 4.6, we have $0 < r_*(n) < 1$ with $r_*(n) \to 1$ as $n \to \infty$. Because of $a_n = 1$, and by (5.3) once more, we have the asymptotic expansion

$$\kappa(n,r) = \frac{M_1(r)}{r^n} \sim \frac{1}{\pi r^n} \log\left(\frac{1}{1-r}\right) \quad (r \to 1).$$

It is now a more or less straightforward exercise in asymptotic analysis (de Bruijn 1981, Chap. 2) to get from here to the following expansions of the optimal radius and condition number: as $n \to \infty$,

$$r_*(n) = 1 - \frac{1}{n\log n} + O\left(\frac{\log\log n}{n(\log n)^2}\right), \tag{5.5a}$$

$$\kappa_*(n) = \frac{\log n}{\pi} + O(\log\log n). \tag{5.5b}$$

This logarithmic growth is very moderate; indeed, one has

$$1 < \kappa\left(n, 1 - \frac{1}{n\log n}\right) < 4.8 \quad (3 \leq n \leq 10\,000),$$

which means that less than one digit is lost for a significant range of n.

Remark 5.3 In practice it is not always advisable to use the optimal radius: a small sacrifice in accuracy might considerably speed up the approximation of the Cauchy integral by the trapezoidal sum. In fact, if we recall (2.8), we realize that the near-optimal choice $r_n = 1 - (n \log n)^{-1}$ would need about[16]

$$m_\epsilon \approx n \log n \cdot \log \epsilon^{-1} \tag{5.6}$$

nodes to achieve an approximation of relative error ϵ. We can actually eliminate the factor $\log n$ here if we use the suboptimal radius $\tilde{r}_n = 1 - \alpha n^{-1}$ ($\alpha > 0$) instead. Asymptotically, as $n \to \infty$, the condition number is then

$$\kappa(n, \tilde{r}_n) \sim \frac{1}{\pi \tilde{r}_n^n} \log\left(\frac{1}{1 - \tilde{r}_n}\right) = \frac{1}{\pi(1 - \alpha n^{-1})^n} \log(n/4) \sim \frac{e^\alpha}{\pi} \log n, \tag{5.7}$$

and therefore still of logarithmic growth: compared to r_n we additionally sacrifice just about $\log_{10} e^\alpha \doteq 0.43\,\alpha$ digits, independently of n. However, the corresponding number of nodes now grows like

$$m_\epsilon \approx \frac{n}{\alpha} \log \epsilon^{-1}, \tag{5.8}$$

which is about an $\alpha \log n$ improvement in speed.

To be specific, let us run some numbers for $n = 100$. Since $\kappa(100, r_{100}) \doteq 3.25$, we are about to lose 0.51 digit using r_n; in hardware arithmetic we could therefore strive for a relative error of $\epsilon = 2 \times 10^{-15}$. By (5.6) we have to take about $m_\epsilon \approx 16\,000$ nodes; actually, a computation with $m = 20\,000$ gives us the relative error 2.6×10^{-15}. In contrast, for $\alpha = 4$, we have $\kappa(100, \tilde{r}_{100}) \doteq 101.63$, so we are about to lose 2.0 digits using $\tilde{r}_n$; we could therefore strive for a relative error of $\epsilon = 5 \times 10^{-14}$ here. Because of (5.8) we now have to take just about $m_\epsilon \approx 800$ nodes, and indeed, a computation with $m = 800$ gives us the relative error 4.9×10^{-14}. Thus, sacrificing just a little more than one digit cuts the number of nodes by a factor of 25 (the prediction was $4 \log 100 \doteq 18.4$).

Case III: $\beta < -1$

As for $\beta = -1$, (5.3) shows that these f_β do not belong to the Hardy space $H^1(D_1)$. Thus, by Theorems 4.5 and 4.6, we have $0 < r_*(n) < 1$ with $r_*(n) \to 1$ as $n \to \infty$. Hence, (5.3) implies the asymptotic expansions

$$r_*(n) = 1 + \frac{\beta + 1}{n} + O\big(n^{-2}\big) \quad (n \to \infty) \tag{5.9a}$$

[16]Note that, by (2.8) and (2.11), estimates of the form $m_\epsilon \approx \cdots$ include, among other approximations, a factor of the form $1 + o(1)$ as $\epsilon \to 0$. Therefore, one should not expect too much precision of such estimates, in particular, not if additionally finite precision effects come into play for ϵ close to machine precision. Even then, however, in all the examples of this paper, we observe ratios of the actual values of m_ϵ to their estimates that are smaller than Sect. 1.3; thus, these rough estimates are, in practice, quite useful devices to predict the actual computational effort.

of the optimal radius and

$$\begin{aligned}\kappa_*(n) &\sim \frac{1}{2\sqrt{\pi}\,|\binom{n-\beta-1}{n}|}\,\frac{\Gamma(-\frac{\beta+1}{2})}{\Gamma(-\frac{\beta}{2})}\,\frac{(-\frac{\beta+1}{n})^{\beta+1}}{(1+\frac{\beta+1}{n})^n}\\ &\sim \frac{(2\mathrm{e})^{-\beta-1}(-\beta-1)^{\beta}}{\pi}\Gamma\left(\frac{1-\beta}{2}\right)^2 = c_\beta \end{aligned}\tag{5.9b}$$

of the optimal condition number. Note that there is no explosion in n and that $c_\beta \to 1$ monotonically from above as $\beta \to -\infty$. Quantitatively, we have

$$1 \le c_\beta \le 2 \quad (\beta \le -1.362),$$

that is, we are just about to lose one binary digit of accuracy within this range of values of β (for large n). Finally, to accomplish an approximation of relative error ϵ by using a trapezoidal sum, we would need, in view of (2.8), about the following number of nodes:

$$m_\epsilon \approx \frac{n}{-\beta-1}\cdot \log \epsilon^{-1}. \tag{5.10}$$

Here are some actual numbers: for $\beta = -6$, $n = 100$, $r_n = 1 + (\beta+1)n^{-1}$, and the accuracy requirement $\epsilon = 10^{-15}$, we get

$$\kappa(n, r_n) \doteq 1.0769, \qquad m_\epsilon \approx 700.$$

In fact, a computation in hardware arithmetic secures a relative error of 4×10^{-15} using $m = 900$ nodes.

Example 5.4 We analyze a further example that Fornberg (1981a, p. 542) has documented to fail his implementation:

$$f(z) = (1+z)^{10}\log(1+z)$$

with radius of convergence $R = 1$. Having norm $\|f\|_{H^1(D_1)} \doteq 180.14$, this function belongs to the Hardy space $H^1(D_1)$. Theorem 4.7 gives $\kappa_*(n) \to \infty$ as $n \to \infty$. More quantitatively, we get, by Theorem 4.5,

$$\kappa(n,r) \ge \kappa(n,1) \doteq \frac{180.14}{|a_n|} \quad (n > \nu \doteq 5.727).$$

The asymptotics (the first equality is valid for $n \ge 11$)

$$a_n = \frac{(-1)^{n-1}}{11\binom{n}{11}} \sim \frac{(-1)^{n-1}10!}{n^{11}} \quad (n\to\infty)$$

implies

$$\kappa(n,r) \ge \kappa(n,1) \doteq 1981.57\binom{n}{11} \sim 5.46\times 10^{-4}\cdot n^{11} \quad (n\to\infty).$$

For instance, $n=50$ gives $\kappa(50,r) \geq \kappa(50,1) \doteq 7.4 \times 10^{13}$, meaning that a loss of more than about 14 digits is unavoidable here.

Example 5.5 The final example of this section is also taken from the list of failures documented by Fornberg (1981a, p. 542):

$$f(z) = 10^6 + \frac{1}{1-z}$$

with radius of convergence $R=1$. This function is a perturbation of the function f_{-1} from Example 5.2. Denoting by $M_1(f_{-1};r)$ the mean value of the modulus of f_{-1} we get, using (5.3),

$$M_1(r) \leq 10^6 + M_1(f_{-1};r) \sim 10^6 + \frac{\log(\frac{1}{1-r})}{\pi} \quad (r \to 1).$$

The suboptimal choice $r_n = 1 - n^{-1}$ (see Remark 5.3) yields

$$\kappa(n, r_n) \leq 10^6 \mathrm{e} + \frac{\mathrm{e}}{\pi} \log n \approx 3 \times 10^6 \quad \bigl(1 \leq n \leq 10^{100\,000}\bigr).$$

Hence, we expect a loss of (at most) about 6.5 digits throughout this huge range of n. The estimate is, in fact, quite sharp: for instance, $n = 100$ yields

$$\kappa(100, r_{100}) \doteq 2.7 \times 10^6.$$

An actual calculation using a trapezoidal sum with $m = 4096$ nodes yields a relative error of 3.13×10^{-10}, which corresponds to a loss of a little more than 6 digits in hardware arithmetic.

6 Functions Amenable to Darboux's Theorem

Example 5.2 contains, in fact, all the information that is needed to address a large class of analytic functions:

$$f(z) = (1-z)^\beta v(z) \quad (\beta \in \mathbb{R} \setminus \mathbb{N}_0),$$

where $v(z)$ is analytic in a neighborhood of $\overline{D_1}$, $v(1) \neq 0$. In particular, the radius of convergence is $R = 1$. By Darboux's theorem (Wilf 2006, Theorem 5.3.1), the Taylor coefficients are asymptotically given by

$$a_n = v(1) \frac{n^{-\beta-1}}{\Gamma(-\beta)} \bigl(1 + O\bigl(n^{-1}\bigr)\bigr) \quad (n \to \infty). \tag{6.1}$$

Hence, the condition number is asymptotically described by

$$\kappa(n,r) \sim \frac{M_1(r)}{|v(1)| r^n} \bigl|\Gamma(-\beta)\bigr| n^{\beta+1} \quad (n \to \infty). \tag{6.2}$$

The mean value of the modulus satisfies, as $r \to 1$ (compare with (5.3))

$$M_1(r) = \frac{1}{2\pi}\int_0^{2\pi} \left|1 - r\mathrm{e}^{\mathrm{i}\theta}\right|^\beta \cdot \left|v\left(r\mathrm{e}^{\mathrm{i}\theta}\right)\right| \mathrm{d}\theta$$

$$\sim \begin{cases} c & (\beta > -1); \\ c\log(\frac{1}{1-r}) & (\beta = -1); \\ c(1-r)^{\beta+1} & (\beta < -1). \end{cases}$$

Here, c denotes some positive constant that depends on v and β. This implies, just as in Example 5.2, that, as $n \to \infty$,

$$r_*(n) \begin{cases} = 1 & (\beta > -1); \\ \sim 1 - \frac{1}{n\log n} & (\beta = -1); \\ \sim 1 + \frac{\beta+1}{n} & (\beta < -1); \end{cases} \qquad \kappa_*(n) \sim \begin{cases} cn^{\beta+1} & (\beta > -1); \\ c\log n & (\beta = -1); \\ c & (\beta < -1). \end{cases} \tag{6.3}$$

For large orders of differentiation, this means that, once more in accordance with Theorem 4.7, the Hardy space case $\beta > -1$ yields polynomial growth of the condition numbers; whereas for $\beta = -1$ we get just logarithmic growth and for $\beta < -1$ there is a uniform bound of the condition number.

To address the last two cases more quantitatively, we can estimate the mean modulus by

$$M_1(r) \le \frac{\|v\|_{H^\infty(D_1)}}{2\pi}\int_0^{2\pi} \left|1 - r\mathrm{e}^{\mathrm{i}\theta}\right|^\beta \mathrm{d}\theta \quad (0 < r < 1)$$

with the help of yet another Hardy space norm, defined by

$$\|f\|_{H^\infty(D_r)} = \operatorname*{ess\,sup}_{0\le\theta\le 2\pi}\left|f\left(r\mathrm{e}^{\mathrm{i}\theta}\right)\right|.$$

Denoting the condition number of the Cauchy integral for the function f_β by $\kappa(f_\beta; n, r)$ (recall that this expression can be evaluated in terms of the hypergeometric function, see (5.2)), we thus obtain a useful estimate of the condition number itself, namely

$$\kappa(n, r) \le \frac{\|v\|_{H^\infty(D_1)}}{|v(1)|}\kappa(f_\beta; n, r) \quad (0 < r < 1). \tag{6.4}$$

Note that there is nothing special about $R = 1$ here. For functions of the form

$$f(z) = (z_0 - z)^\beta v(z) \quad (\beta \in \mathbb{R} \setminus \mathbb{N}_0)$$

with $|z_0| = R$, $v(z)$ analytic in a neighborhood of $\overline{D_R}$, and $v(z_0) \ne 0$ we get accordingly

$$\kappa(n, r) \le \frac{\|v\|_{H^\infty(D_R)}}{|v(z_0)|}\kappa(f_\beta; n, r/R) \quad (0 < r < R). \tag{6.5}$$

If there is more than one singularity on the circle C_R, we would have to use symmetry arguments, or we would have to consider superpositions of these estimates.

Example 6.1 We study the example of Fig. 1.d, that is,

$$f(z) = \sec(z)^6$$

which has radius of convergence $R = \pi/2$. To begin with, we extract the poles at $z = \pm\pi/2$ by the factorization

$$f(z) = g(z)^6 \cdot v(z), \qquad v(\pm\pi/2) = 1,$$

with the rational function

$$g(z) = \frac{\operatorname{res}_{\pi/2}\sec}{z - \pi/2} + \frac{\operatorname{res}_{-\pi/2}\sec}{z + \pi/2} = \frac{4\pi^2}{\pi^2 - 4z^2}.$$

One easily checks that $\|v\|_{H^\infty(D_1)} = 1$, so that, by (6.5) and by a symmetry argument,

$$1 \le \kappa(n, r) \le \kappa(f_{-6}; n, r/R) \quad (R = \pi/2).$$

In view of (6.3) we choose the radius

$$r_n = \frac{\pi}{2}\left(1 - \frac{5}{n}\right)$$

and obtain (see (5.9b) for a definition of c_β)

$$1 \le \kappa(n, r_n) \le \kappa\big(f_{-6}; n, 1 - 5n^{-1}\big) \sim c_{-6} = \frac{9\mathrm{e}^5}{1250} \doteq 1.0686 \quad (n \to \infty).$$

We should thus be able to get about full accuracy for large orders of differentiation. In fact, for $n = 100$, we have

$$\kappa(n, r_n) \doteq 1.0767 \le 1.0769 \doteq \kappa(f_{-6}; n, r_n).$$

Striving for a relative error of $\epsilon = 10^{-15}$ requires, see (5.10), a trapezoidal sum with a number of nodes of about

$$m_\epsilon \approx \frac{n}{5}\log\epsilon^{-1} \approx 700.$$

In fact, an actual computation with $m = 880$ yields a little more than 14 correct digits in hardware arithmetic.

Example 6.2 In this example we address the accurate computation of the Bernoulli numbers B_k given by their exponentially generating function (see Fig. 1.e)

$$f(z) = \frac{z}{\mathrm{e}^z - 1} = \sum_{k=0}^{\infty} \frac{B_k}{k!} z^k,$$

which has radius of convergence $R = 2\pi$. We extract the poles at $z = \pm 2\pi\mathrm{i}$ by the factorization

$$f(z) = g(z) \cdot v(z), \qquad v(\pm 2\pi\mathrm{i}) = 1,$$

with the rational function

$$g(z) = \frac{\mathrm{res}_{2\pi\mathrm{i}}\, f}{z - 2\pi\mathrm{i}} + \frac{\mathrm{res}_{-2\pi\mathrm{i}}\, f}{z + 2\pi\mathrm{i}} = -\frac{8\pi^2}{4\pi^2 + z^2}.$$

One easily checks that $\|v\|_{H^\infty(D_1)} = 2\pi/(1 - \mathrm{e}^{-2\pi}) \doteq 6.2949$, so that, by (6.5) and by a symmetry argument,

$$1 \le \kappa(n, r) \le 6.3\, \kappa(f_{-1}; n, r/R) \quad (R = 2\pi).$$

Because of (5.7) we expect just a moderate loss of accuracy using the choice $r_n = 2\pi(1 - n^{-1})$. In fact, for $n = 100$ we get $\kappa(100, r_{100}) \doteq 7.2355$, meaning a loss of less than one digit. In view of (5.8) we expect to accomplish an approximation error $\epsilon = 10^{-15}$ using a trapezoidal sum with a number of nodes of about

$$m_\epsilon \approx n \log \epsilon^{-1} \approx 3500.$$

In fact, an actual calculation with $m = 4096$ gives more than 15 correct digits in hardware arithmetic.

7 The Quasi-Optimal Radius

For entire transcendental functions, it turns out that an upper bound of the condition number is actually easier to analyze, namely

$$\kappa(n, r) = \frac{M_1(r)}{|a_n| r^n} \le \frac{M(r)}{|a_n| r^n} = \bar{\kappa}(n, r),$$

where

$$M(r) = \max_{0 \le \theta \le 2\pi} \left| f\left(r\mathrm{e}^{\mathrm{i}\theta}\right) \right|$$

denotes the maximum modulus function of f. In fact, we will see in Sects. 9–12 that the radius that is optimal for this upper bound is in many cases already close to optimal for the condition number itself.

For the maximum modulus, the analogue of Hardy's theorem is a classical theorem of complex analysis (the three circles theorem); for the standard proof see Markushevich (1977, Vol. II, p. 221) or Pólya and Szegö (1964, Sects. III.304/305):

Theorem 7.1 (Hadamard 1896; Blumenthal 1907; Faber 1907) *Let f be given by a Taylor series with radius of convergence R. The maximum modulus function M satisfies the following, for $0 < r < R$:*

(a) *$M(r)$ is continuously differentiable, except for a set of isolated r;*

(b) *if* $f(z)$ *is not a monomial*, $\log M(r)$ *is a strictly convex function of* $\log r$;
(c) *if* $f \not\equiv \mathrm{const}$, $M(r)$ *is strictly increasing*.

With the same proofs as in Sect. 4.1 for the condition number, we deduce from this theorem the following results (however, restricting ourselves to entire transcendental functions).

Theorem 7.2 *Let* f *be an entire transcendental function with Taylor coefficients* a_n, *and let* a_{n_0} *be its first nonzero coefficient. Then, for* $n > n_0$, *with* $a_n \neq 0$ *and* $r > 0$:

(a) $\bar{\kappa}(n,r)$ *is continuously differentiable, except for a set of isolated* r;
(b) $\log \bar{\kappa}(n,r)$ *is a strictly convex function of* $\log r$;
(c) $\bar{\kappa}(n,r) \to \infty$, *as* $r \to 0$ *and* $r \to \infty$.

The same reasoning as in Sect. 4.2 shows the existence of the optimal upper bound

$$\bar{\kappa}_\diamond(n) = \min_{r>0} \bar{\kappa}(n,r), \tag{7.1}$$

which is now taken for the radius

$$r_\diamond(n) = \arg\min_{r>0} \bar{\kappa}(n,r). \tag{7.2}$$

Note that $r_\diamond(n)$ is unique because of the *strict* convexity stated in Theorem 7.2. As for $r_*(n)$ it is convenient to extend the definition of $r_\diamond(n)$ to the case of $a_n = 0$ by setting

$$r_\diamond(n) = \arg\min_{r>0} r^{-n} M(r). \tag{7.3}$$

We call $r_\diamond(n)$ the *quasi-optimal* radius and define, accordingly, the quasi-optimal condition number by

$$\kappa_\diamond(n) = \kappa\bigl(n, r_\diamond(n)\bigr) \geq \kappa_*(n). \tag{7.4}$$

Finally, by repeating the proof of Theorem 4.6, we get the following.

Theorem 7.3 *Let* f *be an entire transcendental function. Then, the sequence* $r_\diamond(n)$ *satisfies the monotonicity*

$$r_\diamond(n) \leq r_\diamond(n+1) \quad (n > n_0)$$

and has the limit $\lim_{n\to\infty} r_\diamond(n) = \infty$.

It turns out that the radius $r_\diamond(n)$ is generally much easier to calculate than the optimal radius $r_*(n)$ (see Theorems 8.4 and 9.1). Surprisingly, in all of these cases the radius $r_\diamond(n)$ is also very close to optimal and the condition number $\kappa_\diamond(n)$ is close to one. Before giving a theoretical frame for these effects, we illustrate them with two examples.

Example 7.4 Since its Taylor coefficients are positive, the exponential function $f(z)=\mathrm{e}^z$ has the maximum modulus function $M(r)=\mathrm{e}^r$. A short calculation shows that

$$r_\diamond(n)=n,\quad \bar{\kappa}_\diamond(n)=n!\left(\frac{\mathrm{e}}{n}\right)^n=\sqrt{2\pi n}\big(1+O\big(n^{-1}\big)\big)\quad (n\to\infty);$$

where the asymptotics follows from Stirling's formula. However, the quasi-optimal condition number $\kappa_\diamond(n)$ behaves much better than just being of order $O(n^{1/2})$. In fact, a comparison with (5.1) yields, as $n\to\infty$,

$$r_\diamond(n)\sim r_*(n),\qquad \kappa_\diamond(n)=1+\frac{5}{24n}+\frac{97}{1152n^2}+O\big(n^{-3}\big),$$

which is very close to optimal indeed.

Example 7.5 We consider the example of Fig. 1.c, that is, the entire function

$$f(z)=\mathrm{e}^{\mathrm{e}^z-1}.$$

By the positivity of the Taylor coefficients, the maximum modulus function is also given by $M(r)=\mathrm{e}^{\mathrm{e}^r-1}$. A short calculation yields an explicit formula for the quasi-optimal radius,

$$r_\diamond=W(n),$$

with the Lambert W-function as introduced in Sect. 2.2.2. To find the corresponding condition number bound, we realize that $n!a_n$ is the n-th Bell number whose asymptotics is well studied in the literature. Flajolet and Sedgewick (2009, Prop. VIII.3) prove (using the concept of H-admissibility that we will study in Sect. 11)

$$a_n\sim\frac{\mathrm{e}^{\mathrm{e}^{r_\diamond}-1}}{r_\diamond^n\sqrt{2\pi r_\diamond(r_\diamond+1)\mathrm{e}^{r_\diamond}}}=\frac{\mathrm{e}^{\mathrm{e}^{r_\diamond}-1}}{r_\diamond^n\sqrt{2\pi n(r_\diamond+1)}}\quad (n\to\infty).$$

Hence, asymptotically, we obtain the condition number bound

$$\bar{\kappa}_\diamond(n)=\frac{\mathrm{e}^{\mathrm{e}^{r_\diamond}-1}}{a_n r_\diamond^n}\sim\sqrt{2\pi n(r_\diamond+1)}\sim\sqrt{2\pi n\log n}\quad (n\to\infty),\tag{7.5}$$

where we have used the asymptotic expansion (de Bruijn 1981, (2.4.3))

$$W(t)=\log t-\log\log t+O\left(\frac{\log\log t}{\log t}\right)\quad (t\to\infty).\tag{7.6}$$

Even though (7.5) looks like a possible, though moderate, $O(n^{1/2}(\log n)^{1/2})$ growth of the condition number, things turn out to be much better than this. For instance, $n=100$ yields the excellent quasi-optimal condition number $\kappa_\diamond(100)\doteq 1.013$. In Sect. 11 we will explain the surprising effect that $\kappa_\diamond(n)$ is close to one for any order n, see Corollary 11.3.

8 Entire Functions of Perfectly Regular Growth

8.1 Order and Type of Entire Functions

Since $r_\diamond(n) \to \infty$, an explicit asymptotic description of the optimization (7.3) requires a detailed study of the growth of the maximum modulus function $M(r)$ as $r \to \infty$. A fruitful characterization is by the order and type of f; for the following see Markushevich (1977, Theorems II.9.2–9.5).

The order ρ of an entire function f is given by

$$\rho = \limsup_{r\to\infty} \frac{\log\log M(r)}{\log r} \geq 0. \tag{8.1}$$

Note that polynomials have order $\rho = 0$. If $0 < \rho < \infty$ (which means that f is transcendental), the type τ of f is given by

$$\tau = \limsup_{r\to\infty} \frac{\log M(r)}{r^\rho} \geq 0. \tag{8.2}$$

We say that f is of minimal type if $\tau = 0$, of normal type if $0 < \tau < \infty$, and of maximal type if $\tau = \infty$. Order and type can also be read from the coefficients a_n of the Taylor series; if f is of order ρ, then

$$\rho = \limsup_{n\to\infty} \frac{n \log n}{\log(1/|a_n|)}; \tag{8.3}$$

if f is of order ρ and type τ, then

$$\tau = \frac{1}{\mathrm{e}\rho} \limsup_{n\to\infty} n|a_n|^{\rho/n}. \tag{8.4}$$

However, to arrive at an explicit asymptotic formula for $r_\diamond(n)$ (see Theorem 8.4) we need to consider a somewhat stricter class of entire functions (Valiron 1949, p. 45): an entire transcendental function of order $0 < \rho < \infty$ is said to be of *perfectly regular growth* if the limit

$$\tau = \lim_{r\to\infty} \frac{\log M(r)}{r^\rho} \tag{8.5}$$

exists and is positive and finite; f is then of normal type τ. The following fundamental theorem is extremely helpful for the purpose of identifying such functions; for a proof see Valiron (1949, p. 108).

Theorem 8.1 (Wiman 1916; Valiron 1923) *Let f be an entire transcendental function. If f is the solution of a holonomic*[17] *differential equation of order q, then f is of perfectly regular growth with a rational order $\rho \geq 1/q$.*

[17] Holonomic differential equations are homogeneous linear with polynomial coefficients.

Example 8.2 The generalized hypergeometric functions

$$ {}_pF_q(b_1,\dots,b_p;c_1,\dots,c_q;z)=\sum_{n=0}^{\infty}\frac{(b_1)_n\cdots(b_p)_n}{(c_1)_n\cdots(c_q)_n}\frac{z^n}{n!} \quad (-b_j,-c_k\notin\mathbb{N}_0) \tag{8.6} $$

are known to be (Luke 1969, Sects. 3.3/5.1)

- entire transcendental if and only if $p\le q$;
- satisfying a holonomic differential equation of order $\max(p,q+1)$.

Thus, by Theorem 8.1, if $p\le q$, these functions are entire transcendental of perfectly regular growth with a rational order $\rho\ge 1/(q+1)$. It is an easy exercise in dealing with Stirling's formula[18] to calculate from (8.3) and (8.4) the order and type of these functions:

$$ \rho=\frac{1}{q+1-p},\qquad \tau=q+1-p\quad (p\le q). \tag{8.7} $$

Many transcendental functions can be identified as a generalized hypergeometric function (see Luke 1969, Sect. 6.2); if this relation is of the form

$$ f(z)=\alpha z^{\mu}\cdot {}_pF_q\big(b_1,\dots,b_p;c_1,\dots,c_q;\beta z^{\nu}\big)\quad (\alpha,\beta\ne 0,\ \mu\in\mathbb{N}_0,\ \nu\in\mathbb{N}), $$

then f is also of perfectly regular growth and we easily obtain, using (8.7), that the order and type of f are given by

$$ \rho=\frac{\nu}{q+1-p},\qquad \tau=(q+1-p)|\beta|^{1/(q+1-p)}. $$

With the exception of the Airy functions, all the functions in the first section of Table 2 can be dealt with directly this way. It suffices to demonstrate just one such example in detail:

$$ \cos z={}_0F_1\left(;\frac{1}{2};-\frac{1}{4}z^2\right) $$

has $p=0$, $q=1$, $\nu=2$, and $\beta=-1/4$; therefore $\rho=\tau=1$.

Example 8.3 The Airy functions $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ satisfy a holonomic differential equation of second order,

$$ y''(z)-zy(z)=0. $$

By the theory of linear analytic differential equations (Hartman 1982, p. 70), because the leading coefficient of this equation is 1, the Airy functions are entire transcendental. Thus, Theorem 8.1 tells us that the Airy functions are of perfectly regular growth with a rational order $\rho\ge 1/2$. The precise values of the order and type can be read

[18] Stirling's formula implies, for $-c\notin\mathbb{N}_0$, that $\log|(c)_n|=n\log n-n+O(\log n)$ as $n\to\infty$.

Table 2 Various growth characteristics of some entire transcendental functions; all the functions with normal type are of completely regular growth and, a fortiori, of perfectly regular growth. The column for $r_\diamond(n)$ gives the asymptotics as $n \to \infty$. The angle θ is understood to be restricted to $-\pi \le \theta \le \pi$. For $1/\Gamma(z)$ the limit given is meant to be the interval $(\liminf \kappa_\diamond(n), \limsup \kappa_\diamond(n))$. For the q-series $(-z;q)_\infty$ we assume that $0 < q < 1$

$f(z)$	order ρ	type τ	$r_\diamond(n)$	$\lim \kappa_\diamond(n)$	indicator $h(\theta)$	Ω	ω
e^z	1	1	n	1	$\cos\theta$	1	1
$\cos(z)$	1	1	n	1	$\|\sin\theta\|$	2	1/2
$\sin(z)$	1	1	n	1	$\|\sin\theta\|$	2	1/2
$J_k(z)$	1	1	n	1	$\|\sin\theta\|$	2	1/2
$I_k(z)$	1	1	n	1	$\|\cos\theta\|$	2	1/2
$z^{-k/2} I_k(2\sqrt{z})$	1/2	2	n^2	1	$2\cos(\theta/2)$	1	1
$\mathrm{erf}(z)$	2	1	$\sqrt{n/2}$	1	$(-\cos(2\theta))_+$	2	1/2
e^{-z^2}	2	1	$\sqrt{n/2}$	1	$-\cos(2\theta)$	2	1/2
$\mathrm{Ai}(z)$	3/2	2/3	$n^{2/3}$	$2/\sqrt{3}$	$-\frac{2}{3}\cos(\frac{3}{2}\theta)$	2	$1/\sqrt{3}$
$\mathrm{Bi}(z)$	3/2	2/3	$n^{2/3}$	4/3	$\frac{2}{3}\|\cos(\frac{3}{2}\theta)\|$	3	2/3
$C(z)$	2	$\pi/2$	$\sqrt{n/\pi}$	1	$\frac{\pi}{2}\|\sin(2\theta)\|$	4	1/4
$S(z)$	2	$\pi/2$	$\sqrt{n/\pi}$	1	$\frac{\pi}{2}\|\sin(2\theta)\|$	4	1/4
$(-z;q)_\infty$	0	–	$q^{\frac{1}{2}-n}$	1	–	–	–
$1/\Gamma(z)$	1	∞	$e^{\operatorname{Re} W(\frac{1}{2}-n)}$	$(1,\infty)$	–	–	–
e^{e^z-1}	∞	–	$W(n)$	1	–	–	–

from the asymptotic expansions (Abramowitz and Stegun 1965, (10.4.59–65)) of the Airy functions as $z \to \infty$, which imply

$$M(r) = \frac{c}{\sqrt{\pi} r^{1/4}} e^{\frac{2}{3} r^{3/2}} \bigl(1 + O\bigl(r^{-3/2}\bigr)\bigr) \quad (r \to \infty),$$

with $c = 1/2$ for $\mathrm{Ai}(z)$ and $c = 1$ for $\mathrm{Bi}(z)$. Hence, by (8.1) and (8.2), we get

$$\rho = \frac{3}{2}, \qquad \tau = \frac{2}{3}.$$

8.2 The Asymptotics of the Quasi-Optimal Radius

A short calculation shows that any entire function f with the maximum modulus function

$$\log M(r) = \tau r^\rho \quad (\rho, \tau > 0)$$

would have the quasi-optimal radius

$$r_\diamond(n) = \left(\frac{n}{\tau\rho}\right)^{1/\rho}. \tag{8.8}$$

By the definition (8.5), functions of perfectly regular growth satisfy the asymptotic relation

$$\log M(r) = \tau r^{\rho}\bigl(1 + o(1)\bigr) \quad (r \to \infty), \tag{8.9}$$

which suggests that (8.8) might still hold, at least asymptotically, as $n \to \infty$. The following theorem shows that this is indeed the case; however, the proof is quite involved.[19] Concrete examples of the result can be found in Table 2.

Theorem 8.4 *Let f be an entire transcendental function of perfectly regular growth having order ρ and type τ. Then, the quasi-optimal radius satisfies*

$$r_{\diamond}(n) \sim \left(\frac{n}{\tau\rho}\right)^{1/\rho} \quad (n \to \infty). \tag{8.10}$$

Proof The difficulty of the proof is to deal with the simultaneous limits $r \to \infty$ and $n \to \infty$ whose coupling has yet to be established. To this end we introduce a transformed variable η by

$$r = \left(\frac{n\mathrm{e}^{\eta}}{\tau}\right)^{1/\rho}.$$

We rewrite (8.9) in the form

$$\log\bigl(r^{-n} M(r)\bigr) = n\mathrm{e}^{\eta}\bigl(1 + o(1)\bigr) - \frac{n}{\rho}\eta - \frac{n}{\rho}\log\frac{n}{\tau} = n \cdot f_n(\eta) - \frac{n}{\rho}\log\frac{n}{\tau},$$

defining functions $f_n(\eta)$ that satisfy

$$f_n(\eta) = \mathrm{e}^{\eta}\bigl(1 + o(1)\bigr) - \rho^{-1}\eta;$$

note that the estimate $o(1)$ holds locally uniformly in η as $n \to \infty$. By the properties of the maximum modulus function M stated in Theorem 7.1, we know that these functions f_n are strictly convex in η and coercive, which means that

$$f_n(\eta) \to \infty \quad (\eta \to \pm\infty).$$

The quasi-optimal radius $r_{\diamond}(n)$, which, by definition, minimizes $r^{-n}M(r)$, is now given in the form

$$r_{\diamond}(n) = \left(\frac{n\mathrm{e}^{\eta_n}}{\tau}\right)^{1/\rho},$$

where η_n is the unique minimizer of $f_n(\eta)$. The assertion of the theorem is therefore equivalent to $\lim_{n\to\infty}\eta_n = \log\rho^{-1}$, which remains to be proven.

[19]Under the additional assumption of the nonnegativity of the Taylor coefficients of f, it is possible to give a much shorter proof of this theorem; see Remark 12.2.

To establish the limit of η_n we proceed by constructing a convex enclosure of f_n for large n: for $\epsilon > 0$ small, we define the strictly convex functions

$$f_{\pm\epsilon}(\eta) = \mathrm{e}^{\eta}(1 \pm \epsilon) - \rho^{-1}\eta.$$

The minimizer of f_ϵ is explicitly given by

$$\eta_\epsilon = \arg\min f_\epsilon(\eta) = \log \frac{1}{\rho(1+\epsilon)}.$$

Since $f_{-\epsilon}(\eta) < f_\epsilon(\eta)$ for all η, and because $f_{-\epsilon}$ is convex and coercive, there exist points $\underline{\eta}_\epsilon$ and $\overline{\eta}_\epsilon$ with $\underline{\eta}_\epsilon < \eta_\epsilon < \overline{\eta}_\epsilon$ satisfying

$$f_{-\epsilon}(\underline{\eta}_\epsilon) = f_{-\epsilon}(\overline{\eta}_\epsilon) = f_\epsilon(\eta_\epsilon).$$

It is clear that $\underline{\eta}_\epsilon, \overline{\eta}_\epsilon \to \log \rho^{-1}$ as $\epsilon \to 0$; in particular, $\underline{\eta}_\epsilon$ and $\overline{\eta}_\epsilon$ remain bounded. By the asymptotics of f_n as $n \to \infty$, we have, for $n \geq n_\epsilon$,

$$f_n(\eta_\epsilon) \leq f_\epsilon(\eta_\epsilon) = f_{-\epsilon}(\underline{\eta}_\epsilon) \leq f_n(\underline{\eta}_\epsilon),$$
$$f_n(\eta_\epsilon) \leq f_\epsilon(\eta_\epsilon) = f_{-\epsilon}(\overline{\eta}_\epsilon) \leq f_n(\overline{\eta}_\epsilon).$$

Thus, the strictly convex function f_n is neither strictly increasing nor strictly decreasing between the points $\underline{\eta}_\epsilon$ and $\overline{\eta}_\epsilon$. Hence, its minimizer η_n must lie there,

$$\underline{\eta}_\epsilon < \eta_n < \overline{\eta}_\epsilon.$$

Now, taking the limit $n \to \infty$ yields

$$\underline{\eta}_\epsilon \leq \liminf_{n\to\infty} \eta_n \leq \limsup_{n\to\infty} \eta_n \leq \overline{\eta}_\epsilon.$$

Finally, letting $\epsilon \to 0$ proves that $\lim_{n\to\infty} = \log \rho^{-1}$ as required. □

Remark 8.5 By means of (8.10) and (2.11) we can estimate the number of nodes m_ϵ that a trapezoidal sum would need to achieve the relative approximation error ϵ if we choose the quasi-optimal radius $r = r_\diamond(n)$. To this end we recall the Taylor series

$$W(z) = \sum_{n=1}^{\infty} (-1)^{n-1} n^{n-1} \frac{z^n}{n!} \quad \left(|z| < \mathrm{e}^{-1}\right) \tag{8.11}$$

of the Lambert W-function (see de Bruijn 1981, Sect. 2.3) and obtain

$$m_\epsilon \approx en + \rho \log \epsilon^{-1}. \tag{8.12}$$

Note how close this is already to the lower bound $m > n$ given by the sampling condition (2.4).

8.3 An Upper Bound of the Quasi-Optimal Condition Number

At first sight the precise asymptotic description (8.10) of the quasi-optimal radius $r_\diamond(n)$ does not tell us much about the size of the corresponding condition number $\kappa_\diamond(n)$. In fact, restricting ourselves to subsequences of n which make the limes superior in (8.4) a proper limit, we just get

$$\log\kappa_\diamond(n) \le \log\bar\kappa_\diamond(n) = o(n) \quad (n\to\infty). \tag{8.13}$$

Such a weak estimate could not even exclude a super-polynomial growth of the condition number. However, we can do much better (see the explicit asymptotic bound (8.18) below) by optimizing the upper bound

$$\bar\kappa_\diamond(n) \le \frac{M(r)}{|a_n|r^n} \quad (r>0)$$

from a dual point of view: by choosing the radius r in a way such that the modulus of $a_n r^n$ becomes maximal among all normalized Taylor coefficients, which directly leads us into studying the Wiman–Valiron theory of entire functions. For an account of the basics of this theory, see Pólya and Szegö (1964, Sects. IV.1–76); surveys of some more refined recent results can be found in Hayman (1974) and Gol'dberg et al. (1997, Chap. 1.4).

The fundamental quantities of the Wiman–Valiron theory are the *maximum term* of an entire function f with Taylor coefficients a_n at a given radius r, defined by

$$\mu(r) = \max_n |a_n|r^n, \tag{8.14}$$

and the corresponding maximal index taking this value, called the *central index*,

$$\nu(r) = \max\bigl\{n : |a_n|r^n = \mu(r)\bigr\}. \tag{8.15}$$

The asymptotic properties of these quantities are described in the following theorem; for a proof see Pólya and Szegö (1964, Sect. IV.68).

Theorem 8.6 (Wiman 1914) *If the entire function f is of perfectly regular growth with order ρ and type τ, then*

$$\log M(r) \sim \log\mu(r) \sim \tau r^\rho, \qquad \nu(r) \sim \tau\rho r^\rho \quad (r\to\infty).$$

We restrict ourselves to those entire functions f of perfectly regular growth for which eventually, if n is only large enough, each term $|a_n|r^n$ (with $a_n \ne 0$) can be made the *unique* maximum term for a properly chosen radius. All the functions of Table 2 belong to this class.

Remark 8.7 If $a_n \ne 0$ for n large enough, then this property is known (see Pólya and Szegö 1964, Sect. IV.43) to be equivalent to the fact that $|a_n/a_{n+1}|$ eventually becomes a strictly increasing sequence. This criterion is, for instance, satisfied by the generalized hypergeometric functions (8.6) with $p \le q$: we find

$$\left|\frac{a_n}{a_{n+1}}\right| = (n+1)\left|\frac{(n+c_1)\cdots(n+c_q)}{(n+b_1)\cdots(n+b_p)}\right| \sim n^{q+1-p} + O\big(n^{q-p}\big) \quad (n \to \infty),$$

which is therefore strictly increasing if n is only large enough.

Thus, if $a_n \ne 0$ and n is large enough, then there will be a radius $\bar{r}_n$ with

$$n = \nu(\bar{r}_n), \qquad |a_n|\bar{r}_n^n = \mu(\bar{r}_n).$$

Theorem 8.6 yields the asymptotics (where n runs only through those indices with $a_n \ne 0$)

$$n = \nu(\bar{r}_n) \sim \tau\rho\bar{r}_n^{\rho} \quad (n \to \infty),$$

which implies, in view of Theorem 8.4, the remarkable asymptotic duality

$$\bar{r}_n \sim \left(\frac{n}{\tau\rho}\right)^{1/\rho} \sim r_\diamond(n) \quad (n \to \infty). \tag{8.16}$$

We thus expect the bound (recall that $r_\diamond(n)$ is defined as the minimizer of $\bar{\kappa}(n,r)$)

$$\bar{\kappa}_\diamond(n) = \frac{M(r_\diamond(n))}{|a_n| r_\diamond(n)^n} \le \frac{M(\bar{r}_n)}{|a_n|\bar{r}_n^n} = \frac{M(\bar{r}_n)}{\mu(\bar{r}_n)} \tag{8.17}$$

to be quite sharp for large n. Now, one of the deep results of the Wiman–Valiron theory is the following explicit bound of the ratio $M(r)/\mu(r)$ in general; for a proof see Hayman (1974, Theorem 6).

Theorem 8.8 (Wiman 1914; Valiron 1920) *Let f be an entire function of finite order ρ. Then, for each $\epsilon > 0$, there is an exceptional set E_ϵ of relative logarithmic density smaller than $1/(1+\epsilon)$ such that*

$$M(r) < \rho(1+\epsilon)\mu(r)\sqrt{2\pi \log \mu(r)} \quad (r \notin E_\epsilon).$$

Shchuchinskaya (1982) has characterized those entire functions of finite order for which there are no exceptional radii, that is, for which $E_\epsilon = \emptyset$. However, we did not bother to check her complicated conditions for any concrete functions. Let us simply assume the weaker condition that the sequence $\bar{r}_n$ eventually does not belong to E_ϵ for all $\epsilon > 0$. We would then obtain from Theorems 8.6 and 8.8, and from (8.16) and (8.17), the asymptotic bound (where n runs only through those indices with $a_n \ne 0$)

$$\kappa_\diamond(n) \le \bar{\kappa}_\diamond(n) \le \rho\sqrt{2\pi \log \mu(\bar{r}_n)} \sim \sqrt{2\pi\rho n} \quad (n \to \infty). \tag{8.18}$$

Note that this bound is consistent with the results obtained in Example 7.4 for $f(z) = e^z$, in which particular case the bound of $\bar{\kappa}_\diamond(n)$ is even sharp; quite a success for such a general approach. In preparation for Sect. 10, we rephrase (8.18) by introducing yet another growth characteristic of f, namely the quantity

$$0 \le \omega = \limsup_{n\to\infty: a_n \neq 0} \frac{\bar{\kappa}_\diamond(n)}{\sqrt{2\pi\rho n}} \le 1. \tag{8.19}$$

See Table 2, and also Pólya and Szegö (1964, Sect. IV.50), for some examples of ω.

9 Relation to the Saddle-Point Method

The results of the last section have shown that, for a certain class of entire functions of perfectly regular growth, the quasi-optimal condition number $\kappa_\diamond(n)$ grows at worst like

$$1 \le \kappa_\diamond(n) \le \bar{\kappa}_\diamond(n) = O\big(n^{1/2}\big) \quad (n \to \infty).$$

However, as we have seen in Examples 7.4 and 7.5, there are cases where the quasi-optimal condition number is asymptotically optimal, actually satisfying the best of all possible asymptotic bounds, $\kappa_\diamond(n) \sim 1$. We now develop a methodology which can be used to understand and prove this highly welcome effect for a large class of entire functions; concrete examples will follow in the next sections.

9.1 The Saddle-Point Equation

The key lies in the observation (Hayman 1974, Lemma 6) that the maximum modulus function M of an entire function f satisfies, except for a set of isolated radii (see also Theorem 7.1), the equation

$$r\frac{\mathrm{d}}{\mathrm{d}r}\log M(r)\bigg|_{r=r_0} = z\frac{\mathrm{d}}{\mathrm{d}z}\log f(z)\bigg|_{z=z_0},$$

where $z_0 \in \mathbb{C}$ is one of the points for which $|z_0| = r_0$ and $|f(z_0)| = M(r_0)$. We apply this observation to the quasi-optimal radius $r_n = r_\diamond(n)$ which, by definition, minimizes $r^{-n}M(r)$. If not accidentally one of those isolated exceptions, this radius must fulfill the differential optimality condition

$$r\frac{\mathrm{d}}{\mathrm{d}r}\log M(r)\bigg|_{r=r_n} = n.$$

Thus, there is a complex number z_n with

$$r_n = |z_n|, \qquad M(r_n) = \big|f(z_n)\big|,$$

that satisfies the transcendental equation

$$n = z\frac{\mathrm{d}}{\mathrm{d}z}\log f(z)\bigg|_{z=z_n} = z_n\frac{f'(z_n)}{f(z_n)}.$$

Table 3 For $f(z) = \mathrm{Ai}(z)$, a comparison of the quasi-optimal radius $r_\diamond(n)$ with its asymptotic value (8.10) as taken from Table 2. This asymptotic value is already quite accurate for small n. The value of $r_\diamond(n) = |z_n|$ was actually computed by numerically solving the saddle-point equation $z_n f'(z_n)/f(z_n) = n$ in the complex plane. Note that $\lim_{n\to\infty} \kappa_\diamond(n) = 2/\sqrt{3} \doteq 1.15470$, see (10.15)

n	$r_\diamond(n)$	$\kappa_\diamond(n)$	$n^{2/3}$	$\kappa(n, n^{2/3})$
1	1.21575	1.37413	1.00000	1.56499
10	4.72421	1.19188	4.64159	1.21120
100	21.58047	1.15832	21.54435	1.16003
1000	100.01668	1.15506	100.00000	1.15523

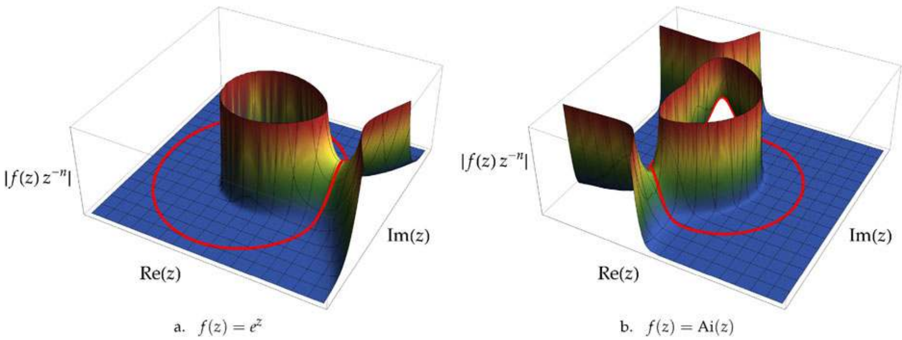


Fig. 5 (Color online) Plots of $|z^{-n} f(z)|$ for $n = 31$; *left*: $f(z) = \mathrm{e}^z$; *right*: $f(z) = \mathrm{Ai}(z)$. The *solid curve* (*red*) is the image of the circle $|z| = r_\diamond(n)$, showing that the maximum modulus along this circle is taken right at some saddle points. Note that the circle leaves these saddle points approximately in the direction of steepest descent. The *left plot* explains nicely the qualitative differences between the plots in Fig. 4: where a circle gets close to being a level line of $|z^{-n} f(z)|$, there must be oscillations of the integrand of the Cauchy integral

This equation can be rewritten in the form

$$F'(z_n) = 0, \qquad F(z) = z^{-n} f(z). \tag{9.1}$$

For functions $F(z)$ that are analytic in a neighborhood of a point z_n (with $F(z_n) \neq 0$) it is well known (see de Bruijn 1981, Sect. 5.2) that $F'(z_n) = 0$ holds if and only if the modulus $|F(z)|$ forms a saddle at $z = z_n$. Since, by construction, $|F(z)|$ has a local maximum at the saddle point z_n in the angular direction, it must thus show a local minimum in the radial direction there; see Fig. 5 for an illustration. On the other hand, by the convexity properties of the maximum modulus function M stated in Theorem 7.1, any saddle point z_n of $|F(z)|$ satisfying $|f(z_n)| = M(|z_n|)$ such that the saddle is oriented this way (local minimum in the radial direction and local maximum in the angular direction) will give us in turn the *unique* quasi-optimal radius $r_\diamond(n) = r_n = |z_n|$. We have thus proven the following theorem.

Theorem 9.1 *Let f be an entire transcendental function and let $z_n \in \mathbb{C}$ be a solution of the saddle-point equation $F'(z_n) = 0$ with $F(z) = z^{-n} f(z)$, that is,*

$$n = z_n \frac{f'(z_n)}{f(z_n)}. \tag{9.2a}$$

If $z_n = r_n \mathrm{e}^{\mathrm{i}\theta_n}$ satisfies $|f(z_n)| = M(|z_n|)$, $\partial_{\theta\theta}|F(r_n \mathrm{e}^{\mathrm{i}\theta_n})| < 0$, and $\partial_{rr}|F(r_n \mathrm{e}^{\mathrm{i}\theta_n})| > 0$, then we get the following representation of the quasi-optimal radius:

$$r_\diamond(n) = |z_n|. \tag{9.2b}$$

On the other hand, if $r_\diamond(n)$ is a point of differentiability of $M(r)$, then there is a solution z_n of the saddle-point equation that satisfies these three conditions.

Theorem 9.1 allows us the actual computation of $r_\diamond(n)$; see Tables 3/4 and Sect. 10.4 for some examples.

9.2 The Saddle-Point Method

Taking the quasi-optimal radius $r_\diamond = r_\diamond(n)$, we write the Cauchy integral (1.2) in the form

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} F\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right) \mathrm{d}\theta$$

with $F(z) = z^{-n} f(z)$. If $|f(z)|$, and thus $|F(z)|$, is small for those z on the circle that are not close to the saddle points z_n of Theorem 9.1, the integral localizes to the vicinity of these saddle points, and we can estimate

$$a_n \approx \frac{1}{2\pi} \sum_{\substack{\theta_n : z_n = r_\diamond \mathrm{e}^{\mathrm{i}\theta_n} \\ \text{saddle point}}} \int_{\theta \approx \theta_n} F\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right) \mathrm{d}\theta.$$

It is actually possible to estimate each of the integrals

$$\frac{1}{2\pi} \int_{\theta \approx \theta_n} F\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right) \mathrm{d}\theta = \frac{1}{2\pi} \int_{\theta \approx \theta_n} \mathrm{e}^{\log F(r_\diamond \mathrm{e}^{\mathrm{i}\theta})} \mathrm{d}\theta$$

by the Laplace method (see de Bruijn 1981, Sect. 5.7). To this end we expand the function $\log f(r\mathrm{e}^{\mathrm{i}\theta})$ with respect to the angular variable θ; for $\theta \to \theta_*$ we calculate that

$$\log f\left(r\mathrm{e}^{\mathrm{i}\theta}\right) = \log f(z_*) + \mathrm{i}a(z_*)(\theta - \theta_*) - \frac{1}{2} b(z_*)(\theta - \theta_*)^2 + O(\theta - \theta_*)^3 \tag{9.3a}$$

with $z_* = r\mathrm{e}^{\mathrm{i}\theta_*}$ and the coefficients

$$a(z) = z\frac{f'(z)}{f(z)}, \qquad b(z) = za'(z). \tag{9.3b}$$

By specifying as the expansion point z_* a saddle point $z_n = r_\diamond \mathrm{e}^{\mathrm{i}\theta_n}$ as in Theorem 9.1, we thus have $a(z_n) = n$ and therefore

$$\log F\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right) = \log F(z_n) - \frac{1}{2} b(z_n)(\theta - \theta_n)^2 + O(\theta - \theta_n)^3;$$

hence, by taking real parts,

$$\log\left|F\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right)\right| = \log|F(z_n)| - \frac{1}{2} \operatorname{Re} b(z_n)(\theta - \theta_n)^2 + O(\theta - \theta_n)^3.$$

In particular, if $|F(z)|$ takes, when moving along the circle, a *strict* local maximum at the saddle point z_n, we infer that necessarily

$$\operatorname{Re} b(z_n) > 0. \tag{9.4}$$

Thus, the Laplace method is applicable and gives, by "trading tails,"

$$\begin{aligned} \frac{1}{2\pi} \int_{\theta \approx \theta_n} \mathrm{e}^{\log F(r_\diamond \mathrm{e}^{\mathrm{i}\theta})}\, \mathrm{d}\theta &\approx \frac{1}{2\pi} \int_{\theta \approx \theta_n} \mathrm{e}^{\log F(z_n) - \frac{1}{2} b(z_n)(\theta - \theta_n)^2}\, \mathrm{d}\theta \\ &\approx \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{\log F(z_n) - \frac{1}{2} b(z_n)\theta^2}\, \mathrm{d}\theta = \frac{F(z_n)}{\sqrt{2\pi b(z_n)}}. \end{aligned} \tag{9.5}$$

Summarizing our results so far, we get the following estimate of the Taylor coefficient a_n:

$$a_n \approx \frac{1}{\sqrt{2\pi}} \sum_{\substack{\theta: z = r_\diamond \mathrm{e}^{\mathrm{i}\theta} \\ \text{saddle point}}} \frac{F(z)}{\sqrt{b(z)}}. \tag{9.6}$$

Correspondingly, we estimate the mean modulus by

$$\begin{aligned} \frac{1}{2\pi} \int_0^{2\pi} \left|F\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right)\right| \mathrm{d}\theta &\approx \frac{1}{2\pi} \sum_{\substack{\theta_n: z_n = r_\diamond \mathrm{e}^{\mathrm{i}\theta_n} \\ \text{saddle point}}} \int_{\theta \approx \theta_n} \left|F\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right)\right| \mathrm{d}\theta \\ &= \frac{1}{2\pi} \sum_{\substack{\theta_n: z_n = r_\diamond \mathrm{e}^{i\theta_n} \\ \text{saddle point}}} \int_{\theta \approx \theta_n} \mathrm{e}^{\operatorname{Re} \log F(r_\diamond \mathrm{e}^{\mathrm{i}\theta})}\, \mathrm{d}\theta \\ &\approx \frac{1}{\sqrt{2\pi}} \sum_{\substack{\theta: z = r_\diamond \mathrm{e}^{\mathrm{i}\theta} \\ \text{saddle point}}} \frac{|F(z)|}{\sqrt{\operatorname{Re} b(z)}} \end{aligned} \tag{9.7}$$

and, therefore, the quasi-optimal condition number by

$$\kappa_\diamond(n) = \kappa(n, r_\diamond) = \frac{\int_0^{2\pi} |F(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|\, \mathrm{d}\theta}{|\int_0^{2\pi} F(r_\diamond \mathrm{e}^{\mathrm{i}\theta})\, \mathrm{d}\theta|} \approx \frac{\sum_{\substack{\theta: z = r_\diamond \mathrm{e}^{\mathrm{i}\theta} \\ \text{saddle point}}} \frac{|F(z)|}{\sqrt{\operatorname{Re} b(z)}}}{|\sum_{\substack{\theta: z = r_\diamond \mathrm{e}^{\mathrm{i}\theta} \\ \text{saddle point}}} \frac{F(z)}{\sqrt{b(z)}}|}. \tag{9.8}$$

As we will see in the following sections, for some interesting classes of entire functions our reasoning can eventually be sharpened by replacing the somewhat vague "$\approx$" signs of approximation with rigorous asymptotic equality as $n \to \infty$. Moreover, the estimate (9.8) is actually quite precise even for small n, as is typical for such asymptotic estimates of integrals; see Sect. 10.4 for an example.

9.3 Steepest Descent

In general, there is not much to further conclude about the approximate values of $\kappa_\diamond(n)$ from the estimate (9.8). Thus, to obtain a result like $\kappa_\diamond(n) \approx 1$ we need some additional structure: a look at the examples of Fig. 5 tells us that there the circle of radius $r_\diamond$ passes through the saddle points of $|F(z)|$ approximately in the direction of steepest descent. In the following sections we will explain why this is the case for some larger classes of entire functions.

From general facts about the method of steepest descent in asymptotic analysis[20] we learn (see de Bruijn 1981, p. 84) that the circular contour through the saddle point z_n is approximately of steepest descent if and only if $b(z_n)$ is approximately real, that is, if and only if

$$\operatorname{Im} b(z_n) \approx 0. \tag{9.9}$$

Note that this implies that the integrand in (9.5) has approximately constant phase. In fact, geometrically it is straightforward to see that the circle is the contour of steepest descent if and only if the off-diagonal elements of the Hessian of $G(r,\theta) = \log|F(re^{i\theta})|$ vanish; at a saddle point $z_n = r_\diamond e^{i\theta_n}$ as in Theorem 9.1, we actually obtain

$$\operatorname{hess} G(r_\diamond, \theta_n) = \begin{pmatrix} \operatorname{Re} b(z_n) r_\diamond^{-2} & -\operatorname{Im} b(z_n) r_\diamond^{-1} \\ -\operatorname{Im} b(z_n) r_\diamond^{-1} & -\operatorname{Re} b(z_n) \end{pmatrix}. \tag{9.10}$$

Now, assume additionally that the circle of radius $r_\diamond = r_\diamond(n)$ passes through *just one* saddle point z_n (this amounts to the case $\Omega = 1$ in Sect. 10.3). Then, we infer from the condition number estimate (9.8) and the steepest descent condition (9.9) that

$$\kappa_\diamond(n) \approx \frac{\frac{|F(z_n)|}{\sqrt{\operatorname{Re} b(z_n)}}}{\left|\frac{F(z_n)}{\sqrt{b(z_n)}}\right|} = \sqrt[4]{1 + \left(\frac{\operatorname{Im} b(z_n)}{\operatorname{Re} b(z_n)}\right)^2} \approx 1.$$

This line of reasoning thus explains why the best of all possible results, $\kappa_\diamond(n) \approx 1$, actually may come into place even though the radius $r_\diamond = r_\diamond(n)$ itself was first introduced by optimizing just the upper bound $\bar\kappa(n,r)$ of the condition number.

[20] For a detailed exposition see de Bruijn (1981, Chap. 5), Miller (2006, Chap. 4), and Flajolet and Sedgewick (2009, Chap. VIII). Gil et al. (2007, Sect. 5.5) explain how steepest descent contours are used as an analytic tool for obtaining numerically stable integral representations of certain special functions, a topic that is certainly closely related to the theme of this paper.

10 Entire Functions of Completely Regular Growth

10.1 The Indicator Function

The reasoning of Sect. 9.3 relies on the remarkable fact (observed in Fig. 5) that for certain functions the circle passing through the relevant saddle points is approximately tangential to the contour of steepest descent. This could be understood if $F(z) = z^{-n} f(z)$ happens to grow predominantly in a radial direction. A first hint that this is exactly the right picture is the existence of the Phragmén–Lindelöf indicator function

$$h(\theta) = \limsup_{r\to\infty} r^{-\rho} \log\bigl|f\bigl(re^{i\theta}\bigr)\bigr| \tag{10.1}$$

for entire functions of finite order ρ and normal type τ. We recall some of its properties; see Markushevich (1977, Sect. II.45) or Levin (1980, Sect. I.15/16) for proofs:

- $h(\theta)$ is 2π-periodic;
- $h(\theta)$ is continuous and has a derivative except possibly on a countable set;
- if $0 < \rho \le 1/2$, then $0 \le h(\theta) \le \tau$; if $\rho > 1/2$, then $-\tau \le h(\theta) \le \tau$;
- $\tau = \max_\theta h(\theta)$.

As it was convenient in Sect. 8 to consider the functions of perfectly regular growth, for which the limes superior in the definition (8.2) of the type τ becomes the proper limit (8.5), we do the same with the limes superior in the definition of the indicator function here.

An entire function of finite order ρ and normal type τ is said to be of *completely regular growth* (Levin 1980, Chap. III) if

$$h(\theta) = \lim_{r\to\infty: r\notin E} \frac{\log|f(re^{i\theta})|}{r^\rho}, \tag{10.2}$$

uniformly in θ. Here, the exceptional set E is required to have relative linear density zero; it will obviously be related to the zeros of f. In fact, if there are no zeros of f in an open sector containing the ray of direction θ, then (10.2) holds in a closed subsector without the need of an exceptional set. An important result of Levin (1980, p. 142) states that if (10.2) holds just pointwise for θ in a set that is dense in $[-\pi, \pi]$, then f is already of completely regular growth. This criterion can be used to check that all of the functions in the first section of Table 2 are of completely regular growth with the indicator functions given there: one just has to look at the known asymptotic expansions of $f(z)$ as $z \to \infty$ within certain sectors of the complex plane, as they are found, e.g., in Abramowitz and Stegun (1965). It is also known that the statement of Theorem 8.1 extends to completely regular functions, see Müller (1997, p. 747).

As developed mainly by Pfluger and Levin in the 1930s, there is a deep relation between the angular density of zeros of a function f of completely regular growth and the properties of its indicator function $h(\theta)$. The following characterization of a density of zero will be of importance to us (Levin 1980, p. 155):

$$\lim_{r\to\infty} \frac{\#\text{ zeros } |z| \le r \text{ of } f \text{ in an open sector containing the ray at } \theta_0}{r^\rho} = 0$$
$$\iff \quad h(\theta) \text{ is } \rho\text{-trigonometric in the vicinity of } \theta_0, \tag{10.3}$$

where a function of θ is called ρ-trigonometric if it is of the form $\alpha\sin(\rho\theta+\beta)$ for some real α and β.

10.2 Circles Are Contours of Asymptotic Steepest Descent

We now look at a direction θ_* in which there is predominantly growth of f, that is, $h(\theta_*)=\tau$. If there are at most finitely many zeros of f in an open sector containing the ray at θ_* (which is the case for all of the functions in the first section of Table 2), then f will also be of perfectly regular growth and the indicator will be, by (10.3), ρ-trigonometric in the vicinity of θ_*. In particular, we get

$$h(\theta_*)=\tau, \qquad h'(\theta_*)=0, \qquad h''(\theta_*)=-\tau\rho^2. \tag{10.4}$$

By the reasoning of Sect. 9 there will be a sequence $z_n=r_\diamond e^{i\theta_n}$ (writing $r_\diamond=r_\diamond(n)$ for brevity) satisfying the saddle-point equation (9.2a) with $\theta_n\to\theta_*$ as $n\to\infty$. To show that the circle passing through z_n is asymptotically a contour of steepest descent there, we look at the Hessian of $\log|F(z_n)|$. From (10.2) we first get

$$\begin{aligned}\log\bigl|F(z_n)\bigr| &= \log\bigl|f\bigl(r_\diamond e^{i\theta_n}\bigr)\bigr| - n\log r_\diamond \\ &\sim r_\diamond^\rho h(\theta_n) - n\log r_\diamond \quad (n\to\infty).\end{aligned} \tag{10.5}$$

Next, by Theorem 8.4 and (10.4), the Hessian of the right-hand side, $G(r,\theta)=r^\rho h(\theta)-n\log r$, becomes asymptotically diagonal:

$$\operatorname{hess} G(r_\diamond,\theta_n)\sim n\rho\begin{pmatrix} r_\diamond^{-2} & 0 \\ 0 & -1\end{pmatrix} \quad (n\to\infty);$$

note that this form of the Hessian is actually consistent with (9.10) and (9.4). Since the off-diagonal terms are zero, the θ-direction is, asymptotically, the direction of steepest descent.

10.3 Condition Number Bounds

We follow the strategy of Sect. 9.2 and apply the Laplace method to the contour integral with radius $r_\diamond=r_\diamond(n)$. However, instead of using the Taylor expansion (9.3) to simplify $\log F(re^{i\theta})$, we now proceed by first recalling from Sect. 9.3 that contours of steepest descent yield integrands of an asymptotically constant phase and by next using the indicator function (10.2) to simplify $\log|F(re^{i\theta})|$, asymptotically as $r\to\infty$. Note that the Laplace method rigorously applies if there is a proper decay of $\log|F(re^{i\theta})|$, as $r\to\infty$, for directions θ far off those θ_* that belong to the saddle points. Assuming this to be the case for the given f (it can be checked to be true for all the functions in the first section of Table 2), we get for the Cauchy integral (1.2), because of (10.5), (10.4), and (8.10), as $n\to\infty$:

$$a_n=\frac{1}{2\pi r_\diamond^n}\int_{-\pi}^{\pi} e^{-in\theta} f\bigl(r_\diamond e^{i\theta}\bigr)\,d\theta=\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{\log F(r_\diamond e^{i\theta})}\,d\theta$$

$$
\begin{aligned}
&\sim \frac{1}{2\pi} \sum_{\theta:h(\theta)=\tau} \mathrm{e}^{\mathrm{i}\,\mathrm{Im}\log F(r_\diamond \mathrm{e}^{\mathrm{i}\theta})} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{Re}\log F(r_\diamond \mathrm{e}^{\mathrm{i}\theta}) + \frac{1}{2} r_\diamond^\rho (t-\theta)^2 h''(\theta)}\, \mathrm{d}t \\
&= \frac{1}{2\pi} \sum_{\theta:h(\theta)=\tau} \sqrt{\frac{2\pi}{-r_\diamond^\rho h''(\theta)}}\, F\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr) \\
&\sim \frac{1}{\sqrt{2\pi\rho n} \cdot r_\diamond^n} \sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-\mathrm{i}n\theta} f\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr).
\end{aligned}
$$

Likewise, we get, as $n \to \infty$,

$$
\begin{aligned}
\frac{M_1(r_\diamond)}{r_\diamond^n} &= \frac{1}{2\pi r_\diamond^n} \int_{-\pi}^{\pi} \bigl| f\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr)\bigr|\, \mathrm{d}\theta = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{Re}\log F(r_\diamond \mathrm{e}^{\mathrm{i}\theta})}\, \mathrm{d}\theta \\
&\sim \frac{1}{\sqrt{2\pi\rho n} \cdot r_\diamond^n} \sum_{\theta:h(\theta)=\tau} \bigl| f\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr)\bigr|
\end{aligned}
$$

and certainly

$$
\frac{M(r_\diamond)}{r_\diamond^n} \sim r_\diamond^{-n} \max_{\theta:h(\theta)=\tau} \bigl| f\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr)\bigr|.
$$

To summarize, we have proven the following theorem.

Theorem 10.1 *Let f be an entire function of completely regular growth with order ρ, type τ, and Phragmén–Lindelöf indicator function $h(\theta)$. If f has at most finitely many zeros in some sectorial neighborhoods of those rays of direction θ for which $h(\theta) = \tau$ and if $|f|$ decays properly, for large radius r, in the angular direction off these rays, then we have*

$$
\frac{\bar{\kappa}_\diamond(n)}{\sqrt{2\pi\rho n}} \sim \frac{\max_{\theta:h(\theta)=\tau} |f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|}{|\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-\mathrm{i}n\theta} f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|} \qquad (n \to \infty : a_n \neq 0) \tag{10.6}
$$

and

$$
\kappa_\diamond(n) \sim \frac{\sum_{\theta:h(\theta)=\tau} |f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|}{|\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-\mathrm{i}n\theta} f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|} \qquad (n \to \infty : a_n \neq 0). \tag{10.7}
$$

That is, the quasi-optimal condition number $\kappa_\diamond(n)$ of the Cauchy integral is asymptotically equal to the condition number of the finite sum $\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-\mathrm{i}n\theta} f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})$.

Let us introduce the number of global maxima of the indicator function,

$$
\Omega = \#\bigl\{\theta : -\pi < \theta \leq \pi, h(\theta) = \tau\bigr\}. \tag{10.8}
$$

Now, by Theorem 10.1, $\Omega = 1$ clearly implies that $\lim_{n\to\infty} \kappa_\diamond(n) = 1$ and that the quantity defined in (8.19) satisfies $\omega = 1$; this observation is precisely matched by two examples in Table 2. On the other hand, if $\Omega > 1$ then it seems, at first glance, that the condition number of the finite sum $\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-in\theta} f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})$ could suffer from severe cancellation. However, as the next theorem shows, there will be generally no such cancellation for the class of functions considered in this section. (But see Sect. 10.4 for an example of severe resonant cancellations in a different setting.)

Theorem 10.2 *Let f be an entire function of completely regular growth which satisfies the assumptions of Theorem 10.1 as well as those that led to (8.19), that is, to $\omega \le 1$. Then, this bound can be supplemented by*

$$0 < \Omega^{-1} \le \liminf_{n\to\infty:a_n\ne 0} \frac{\bar\kappa_\diamond(n)}{\sqrt{2\pi\rho n}} \le \limsup_{n\to\infty:a_n\ne 0} \frac{\bar\kappa_\diamond(n)}{\sqrt{2\pi\rho n}} = \omega \le 1, \tag{10.9}$$

and the quasi-optimal condition number $\kappa_\diamond(n)$ is asymptotically bounded as follows:

$$1 \le \liminf_{n\to\infty:a_n\ne 0} \kappa_\diamond(n) \le \limsup_{n\to\infty:a_n\ne 0} \kappa_\diamond(n) \le \Omega\cdot\omega. \tag{10.10}$$

In particular, we have

$$\omega = \Omega^{-1} \quad\Longrightarrow\quad \lim_{n\to\infty:a_n\ne 0} \kappa_\diamond(n) = \lim_{n\to\infty:a_n\ne 0} \frac{\bar\kappa_\diamond(n)}{\sqrt{2\pi\rho n}} = 1.$$

Proof The obvious estimate

$$\left|\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-\mathrm{i}n\theta} f\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right)\right| \le \sum_{\theta:h(\theta)=\tau} \left|f\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right)\right| \le \Omega\cdot \max_{\theta:h(\theta)=\tau}\left|f\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right)\right| \tag{10.11}$$

yields, by Theorem 10.1 and (8.19), the asymptotic bounds asserted in (10.9). Moreover, (8.19) and (10.6) imply

$$\limsup_{n\to\infty:a_n\ne 0} \frac{\max_{\theta:h(\theta)=\tau} |f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|}{|\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-in\theta} f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|} = \omega \le 1.$$

Hence, by using (10.11) once more to estimate the numerator in (10.7), we get

$$\limsup_{n\to\infty:a_n\ne 0} \kappa_\diamond(n) \le \Omega \limsup_{n\to\infty:\mathrm{a}_n\ne 0} \frac{\max_{\theta:h(\theta)=\tau} |f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|}{|\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-in\theta} f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|} \le \Omega\cdot\omega,$$

which proves the asserted asymptotic bound (10.10). □

Example 10.3 If, by the symmetries of the function f in the complex plane, there is just one *single* phase $\phi_n \in \mathbb{R}$ that allows us the representation

$$\mathrm{e}^{\mathrm{i}\phi_n}\cdot \mathrm{e}^{-in\theta} f\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\right) = \max_{\theta_*:h(\theta_*)=\tau}\left|f\left(r_\diamond \mathrm{e}^{\mathrm{i}\theta_*}\right)\right| \tag{10.12}$$

for *all* θ with $h(\theta)=\tau$, then we get by Theorem 10.1 that already the best of all possible bounds holds, namely,

$$\lim_{n\to\infty:a_n\ne 0} \kappa_\diamond(n) = 1, \qquad \lim_{n\to\infty:a_n\ne 0} \frac{\bar\kappa_\diamond(n)}{\sqrt{2\pi\rho n}} = \Omega^{-1}. \tag{10.13}$$

We then have, by definition, $\omega = \Omega^{-1}$. Note that the symmetry relation (10.12) applies to all of the functions of the first section of Table 2, except for the Airy functions $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$, which will be dealt with in the next two examples.

Example 10.4 The point of departure for discussing the Airy function $\mathrm{Ai}(z)$ is the asymptotic expansion (Abramowitz and Stegun 1965, (10.4.59))

$$\mathrm{Ai}(z) \sim \frac{1}{2\pi} z^{-1/4} \mathrm{e}^{-\frac{2}{3}z^{3/2}} \sum_{k=0}^{\infty} \frac{(-1)^k \Gamma(3k+\frac{1}{2})}{9^k \Gamma(2k+1)} z^{-3k/2} \quad \bigl(z \to \infty : |\arg z| < \pi\bigr). \tag{10.14}$$

This implies, by Levin's criterion given above, that Ai is of completely regular growth. Moreover, we get

$$\bigl|\mathrm{Ai}\bigl(r\mathrm{e}^{\mathrm{i}\theta}\bigr)\bigr| = \frac{1}{2\pi} r^{-1/4} \mathrm{e}^{-\frac{2}{3}r^{3/2}\cos(\frac{3}{2}\theta)} \bigl(1 + O\bigl(r^{-3/2}\bigr)\bigr) \quad \bigl(r \to \infty : |\theta| < \pi\bigr),$$

from which we can directly read the order $\rho = 3/2$, the type $\tau = 2/3$, and the Phragmén–Lindelöf indicator function

$$h(\theta) = -\frac{2}{3}\cos\left(\frac{3}{2}\theta\right) \quad \bigl(|\theta| < \pi\bigr).$$

Note that this indicator $h(\theta)$, continued as a 2π-periodic function, is ρ-trigonometric exactly for $\theta \neq k\pi$ ($k \in \mathbb{Z}$). Thus, by Levin's general theory, there is a positive density of zeros in an arbitrarily small sectorial neighborhood of the ray at $\theta = -\pi$; indeed, $\mathrm{Ai}(z)$ has countably many zeros along the negative real axis and no zeros elsewhere. We have $h(\theta) = \tau$ for $\theta = \pm\frac{2}{3}\pi$; hence $\Omega = 2$. The expansion (10.14) implies for these maximizing angles that

$$\mathrm{Ai}\bigl(r\mathrm{e}^{\pm\frac{2}{3}\pi\mathrm{i}}\bigr) = \frac{\mathrm{e}^{\mp\frac{\pi}{6}\mathrm{i}}}{2\sqrt{\pi}} r^{-1/4} \mathrm{e}^{\frac{2}{3}r^{3/2}} \bigl(1 + O\bigl(r^{-3/2}\bigr)\bigr) \quad (r \to \infty),$$

that is,

$$\arg \mathrm{Ai}\bigl(r\mathrm{e}^{\pm\frac{2}{3}\pi\mathrm{i}}\bigr) = \mp\frac{\pi}{6} + O\bigl(r^{-3/2}\bigr) \quad (r \to \infty).$$

Hence we obtain, because of $h(-\frac{2}{3}\pi) = h(\frac{2}{3}\pi)$: as $n \to \infty$,

$$\begin{aligned}
\left| \sum_{\theta : h(\theta) = \tau} \mathrm{e}^{-\mathrm{i}n\theta} \,\mathrm{Ai}\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr) \right| &\sim \bigl|\mathrm{e}^{\frac{2}{3}\pi n\mathrm{i}} \mathrm{e}^{\frac{\pi}{6}\mathrm{i}} + \mathrm{e}^{-\frac{2}{3}\pi n\mathrm{i}} \mathrm{e}^{-\frac{\pi}{6}\mathrm{i}}\bigr| \cdot \bigl|\mathrm{Ai}\bigl(r_\diamond \mathrm{e}^{\frac{2}{3}\pi\mathrm{i}}\bigr)\bigr| \\
&= 2\left|\cos\left(\frac{\pi}{6} + \frac{2}{3}\pi n\right)\right| \cdot \bigl|\mathrm{Ai}\bigl(r_\diamond \mathrm{e}^{\frac{2}{3}\pi\mathrm{i}}\bigr)\bigr|,
\end{aligned}$$

and

$$\sum_{\theta : h(\theta) = \tau} \bigl|\mathrm{Ai}\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr)\bigr| \sim 2\bigl|\mathrm{Ai}\bigl(r_\diamond \mathrm{e}^{\frac{2}{3}\pi\mathrm{i}}\bigr)\bigr|, \qquad \max_{\theta : h(\theta) = \tau} \bigl|\mathrm{Ai}\bigl(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\bigr)\bigr| \sim \bigl|\mathrm{Ai}\bigl(r_\diamond \mathrm{e}^{\frac{2}{3}\pi\mathrm{i}}\bigr)\bigr|.$$

Now,

$$\left|\cos\left(\frac{\pi}{6}+\frac{2}{3}\pi n\right)\right| = \begin{cases} \sqrt{3}/2, & n \not\equiv 2 \pmod 3, \\ 0, & n \equiv 2 \pmod 3, \end{cases}$$

in accordance with the fact that the Taylor coefficients of $\mathrm{Ai}(z)$ satisfy $a_n \neq 0$ if and only if $n \not\equiv 2 \pmod 3$. Altogether, Theorem 10.1 then gives us

$$\lim_{n\to\infty: a_n\neq 0} \kappa_\diamond(n) = \frac{2}{\sqrt{3}}, \qquad \omega = \lim_{n\to\infty: a_n\neq 0} \frac{\bar{\kappa}(n)}{\sqrt{2\pi\rho n}} = \frac{1}{\sqrt{3}}. \tag{10.15}$$

We observe that the general upper bound given in (10.10) is sharp here. An illustration of the limit result (10.15) by some actual numerical data for various n can be found in Table 3.

Example 10.5 As for $\mathrm{Ai}(z)$ in the last example, the discussion of $\mathrm{Bi}(z)$ begins with its asymptotic expansions (Abramowitz and Stegun 1965, (10.4.63–65)) as $z \to \infty$ in different sectors of the complex plane. Skipping the details, we find that Bi is of completely regular growth with order $\rho = \frac{3}{2}$, type $\tau = \frac{2}{3}$, and Phragmén–Lindelöf indicator

$$h(\theta) = \frac{2}{3}\left|\cos\left(\frac{3}{2}\theta\right)\right| \quad \big(|\theta| < \pi\big).$$

Thus, $h(\theta) = \tau$ for $\theta = \pm\frac{2}{3}\pi$ and also for $\theta = 0$; hence $\Omega = 3$. The asymptotic expansions yield

$$\mathrm{Bi}\big(r\mathrm{e}^{\pm\frac{2}{3}\pi\mathrm{i}}\big) = \frac{\mathrm{e}^{\pm\frac{\pi}{3}\mathrm{i}}}{2\sqrt{\pi}} r^{-1/4}\mathrm{e}^{\frac{2}{3}r^{3/2}}\big(1+O\big(r^{-3/2}\big)\big) \quad (r\to\infty)$$

and

$$\mathrm{Bi}(r) = \frac{1}{\sqrt{\pi}} r^{-1/4}\mathrm{e}^{\frac{2}{3}r^{3/2}}\big(1+O\big(r^{-3/2}\big)\big) \quad (r\to\infty),$$

that is, $\arg\mathrm{Bi}(r) = 0$ and

$$\arg\mathrm{Bi}\big(r\mathrm{e}^{\pm\frac{2}{3}\pi\mathrm{i}}\big) = \pm\frac{\pi}{3} + O\big(r^{-3/2}\big) \quad (r\to\infty).$$

Hence, as $r \to \infty$,

$$\big|\mathrm{Bi}\big(r\mathrm{e}^{\pm\frac{2}{3}\pi\mathrm{i}}\big)\big| \sim \frac{1}{2}\big|\mathrm{Bi}(r)\big|$$

and thus, as $n \to \infty$,

$$\begin{aligned}\left|\sum_{\theta:h(\theta)=\tau} \mathrm{e}^{-\mathrm{i}n\theta}\,\mathrm{Bi}\big(r_\diamond\mathrm{e}^{\mathrm{i}\theta}\big)\right| &\sim \left|\frac{1}{2}\mathrm{e}^{\frac{2}{3}\pi n\mathrm{i}}\mathrm{e}^{-\frac{\pi}{3}\mathrm{i}} + \frac{1}{2}\mathrm{e}^{-\frac{2}{3}\pi n\mathrm{i}}\mathrm{e}^{\frac{\pi}{3}\mathrm{i}} + 1\right| \cdot \big|\mathrm{Bi}(r_\diamond)\big| \\ &= \left|1+\cos\left(\frac{\pi}{3}-\frac{2}{3}\pi n\right)\right| \cdot \big|\mathrm{Bi}(r_\diamond)\big|,\end{aligned}$$

Table 4 For $f(z) = \mathrm{Bi}(z)$, a comparison of the quasi-optimal radius $r_\diamond(n)$ with its asymptotic value (8.10) as taken from Table 2. This asymptotic value is already quite accurate for small n. The value of $r_\diamond(n) = |z_n|$ was actually computed by numerically solving the saddle-point equation $z_n f'(z_n)/f(z_n) = n$ in the complex plane. Note that $\lim_{n\to\infty} \kappa_\diamond(n) = 4/3 \doteq 1.33333$, see (10.16)

n	$r_\diamond(n)$	$\kappa_\diamond(n)$	$n^{2/3}$	$\kappa(n, n^{2/3})$
1	1.36603	1.35408	1.00000	1.57640
10	4.72421	1.37605	4.64159	1.39833
100	21.58047	1.33751	21.54435	1.33948
1000	100.01668	1.33375	100.00000	1.33394

and

$$\sum_{\theta:h(\theta)=\tau} \left|\mathrm{Bi}\left(r_\diamond e^{i\theta}\right)\right| \sim 2\left|\mathrm{Bi}(r_\diamond)\right|, \qquad \max_{\theta:h(\theta)=\tau} \left|\mathrm{Bi}\left(r_\diamond e^{i\theta}\right)\right| \sim \left|\mathrm{Bi}(r_\diamond)\right|.$$

Now,

$$\left|1 + \cos\left(\frac{\pi}{3} - \frac{2}{3}\pi n\right)\right| = \begin{cases} 3/2, & n \not\equiv 2 \pmod 3, \\ 0, & n \equiv 2 \pmod 3, \end{cases}$$

in accordance with the fact that the Taylor coefficients of $\mathrm{Bi}(z)$ satisfy $a_n \neq 0$ if and only if $n \not\equiv 2 \pmod 3$. Altogether, Theorem 10.1 then gives us

$$\lim_{n\to\infty: a_n\neq 0} \kappa_\diamond(n) = \frac{4}{3}, \qquad \omega = \lim_{n\to\infty: a_n\neq 0} \frac{\bar{\kappa}(n)}{\sqrt{2\pi\rho n}} = \frac{2}{3}. \tag{10.16}$$

An illustration of the limit result (10.16) by some actual numerical data for various n can be found in Table 4.

10.4 A Resonant Case: $f(z) = 1/\Gamma(z)$

In the statement of Theorem 10.1 the condition on the zeros of f cannot be disposed of: if f possesses infinitely many zeros in the vicinity of its directions of predominant growth, then it may happen that a *pair* of saddle points recombines in the limit $r \to \infty$ to a *single* maximum of the indicator function $h(\theta)$. That is, even though we have $\Omega = 1$ in the limit, the contributions of the two saddle points may yield resonances in (9.8) as $n \to \infty$; thus $\kappa_\diamond(n)$, as well as $\kappa_*(n)$, may behave quite irregularly.

We demonstrate such a behavior for the entire function $f(z) = 1/\Gamma(z)$, whose zeros are located at $0, -1, -2, -3, \ldots$. This function has order $\rho = 1$, but is of maximal type $\tau = \infty$ (see Levin 1980, p. 27). Therefore, at first glance, the results so far do not seem to be applicable at all. However, using Valiron's concept of a *proximate order* $\rho(r)$ it is possible to extend the definition of functions of completely regular growth and of their indicator functions in such a way that the results cited above still hold true (see Levin 1980, Sect. I.12). By Stirling's formula, and Euler's reflection formula

$$\Gamma(z) \cdot \Gamma(1 - z) = \frac{\pi}{\sin(\pi z)},$$

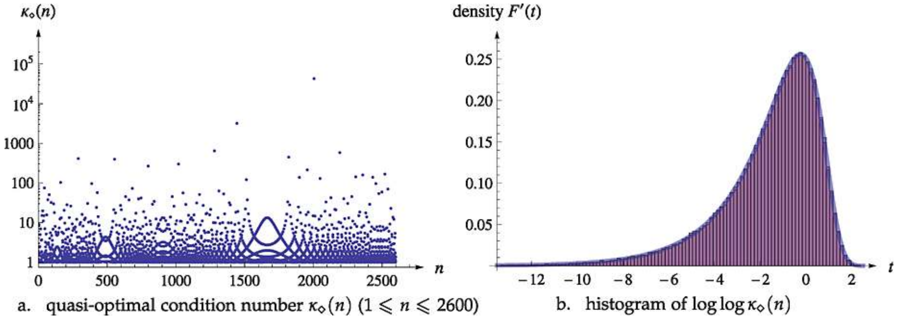


Fig. 6 *Left*: plot of the quasi-optimal condition number $\kappa_\diamond(n)$ $(1 \le n \le 2600)$; $f(z) = 1/\Gamma(z)$. Within the shown range of n, the maximum is taken for $n = 2006$: $\kappa_\diamond(2006) \doteq 47\,067.2$. Note that there is not much to be gained from using the optimal radius $r_*(n)$ instead of $r_\diamond(n)$: $\kappa_*(2006) \doteq 47\,063.9$. *Right*: plot of the density histograms of $t = \log\log\kappa_\diamond(n)$ $(1 \le n \le N)$ for $N = 100\,000$ and $N = 1\,000\,000$ and of the density $F'(t)$ belonging to the distribution $F(t) = \frac{2}{\pi}\arccos(\exp(-e^t))$, printed transparently on top of each other. Since there is such a close agreement, we are led to conjecture the limit law (10.20) and, therefore, $\liminf_{n\to\infty}\kappa_\diamond(n) = 1$ and $\limsup_{n\to\infty}\kappa_\diamond(n) = \infty$

we get the following asymptotic expansion, valid uniformly in θ:

$$\frac{\log|1/\Gamma(re^{i\theta})|}{r\log r} = -\cos\theta + \frac{\cos\theta + \theta\sin\theta}{\log r} + O\big(r^{-1}\big) \quad (r \to \infty : r \notin E), \quad (10.17)$$

where the set E of possible exceptions has relative linear density zero. From this we can read that $1/\Gamma(z)$ is a function of completely regular growth with a proximate order $\rho(r)$ given by $r^{\rho(r)} = r\log r$; the indicator function is then

$$h(\theta) = -\cos\theta.$$

Now, the problem is that this indicator becomes asymptotically maximal at the *single* direction $\theta = \pm\pi$, which is actually the direction of the ray that contains the countably many zeros of $1/\Gamma(z)$. In fact, a closer look at (10.17) reveals that this single maximum is formed, in the limit $r \to \infty$, through a recombination of *two* distinct maxima for finite r. And indeed, Fig. 6.a shows quite an irregular behavior of the quasi-optimal condition number $\kappa_\diamond(n)$ (the picture would be essentially the same for the optimal condition number $\kappa_*(n)$ itself, though much more difficult to compute).

The quasi-optimal radius $r_\diamond(n)$ can straightforwardly be obtained by means of the saddle-point equation (9.2a): that is, $r_\diamond(n) = |z_n|$ where z_n is one of the *two* complex conjugate solutions of

$$n = z\frac{d}{dz}\log\frac{1}{\Gamma(z)} = -z\psi(z);$$

we choose $\operatorname{Im} z_n > 0$ for definiteness. Asymptotically, as $n \to \infty$, this saddle-point equation can actually be solved explicitly in terms of the principal branch of the Lambert W-function: using the asymptotic expansion (Abramowitz and Stegun 1965, (6.3.18)) of the digamma function ψ we obtain

$$-z\psi(z) = -z\log z + \frac{1}{2} + O\big(z^{-1}\big) \quad \big(|\arg z| < \pi\big),$$

and therefore, as $n \to \infty$,

$$z_n \sim \frac{\frac{1}{2}-n}{W(\frac{1}{2}-n)} = \mathrm{e}^{W(\frac{1}{2}-n)} = r_n \mathrm{e}^{\mathrm{i}\theta_n}, \qquad r_\diamond(n) \sim \mathrm{e}^{\mathrm{Re}\, W(\frac{1}{2}-n)} = r_n, \tag{10.18}$$

which we take as the definition of the radius r_n and the angle $\pi/2 < \theta_n < \pi$.

A detailed quantitative analysis of $\kappa_\diamond(n)$ can now be based on the well-known fact (see Hayman 1956, p. 91) that the saddle-point analysis of Sect. 9.2 is applicable to $f(z) = 1/\Gamma(z)$: in fact, the approximations (9.6) and (9.7) are asymptotic equalities as $n \to \infty$. We find that they can be recast in the form

$$a_n \sim \sqrt{\frac{2}{\pi n}} \frac{|1/\Gamma(r_n \mathrm{e}^{\mathrm{i}\theta_n})|}{r_n^n} \cos\phi_n, \tag{10.19a}$$

$$\bar{\kappa}_\diamond(n) \sim \sqrt{\frac{\pi n}{2}} |\sec\phi_n|, \tag{10.19b}$$

$$\kappa_\diamond(n) \sim |\sec\phi_n| \tag{10.19c}$$

with the collective phase approximation[21]

$$\phi_n = \left(n - \frac{1}{2}\right)\left(\frac{\sin^2\theta_n}{\theta_n} - \theta_n + \frac{\theta_n}{12(n-\frac{1}{2})^2}\right) - \frac{1}{2}\operatorname{arccot}\big(\cot\theta_n - \theta_n \csc^2\theta_n\big).$$

The asymptotics (10.19c) not only explains the very *possibility* of resonances, it actually gives excellent *numerical* predictions even for rather small values of n such as those illustrated in Table 5.

Based on Table 5 and Fig. 6.a it is certainly quite reasonable to *conjecture* that $\liminf_{n\to\infty} \kappa_\diamond(n) = 1$. On the other hand, by just looking at the rather randomly distributed positions n of the resonances and the corresponding extreme values of $\kappa_\diamond(n)$ we cannot really establish any serious conjecture about the probable value of $\limsup_{n\to\infty} \kappa_\diamond(n)$. Instead, we look at the *statistics* of the values of $\kappa_\diamond(n)$ for $1 \le n \le N$. The very close agreement of the two histograms shown in Fig. 6.b suggests that there should be a limit law of the form

$$\lim_{N\to\infty} N^{-1} \cdot \#\big\{1 \le n \le N : \log\log\kappa_\diamond(n) \le t\big\} = F(t). \tag{10.20a}$$

If the phases ϕ_n were equidistributed modulo π (and the empirical data of the first one million instances strongly point in that direction), we would immediately find from (10.19c) that the distribution would be

$$F(t) = \frac{2}{\pi}\arccos\big(\mathrm{e}^{-\mathrm{e}^t}\big). \tag{10.20b}$$

[21] Hayman (1956, p. 92) basically states the same results with the much simpler phase approximation

$$\phi_n = \left(n - \frac{1}{2}\right)\big(\theta_n^{-1}\sin^2\theta_n - \theta_n\big),$$

which is, however, numerically far less accurate for small values of n and would not allow such a precise prediction of $\kappa_\diamond(n)$ as in Table 5.

Table 5 The precision of the asymptotics (10.19c) near some resonances

n	$\kappa_\diamond(n)$	$\lvert\sec(\phi_n)\rvert$	n	$\kappa_\diamond(n)$	$\lvert\sec(\phi_n)\rvert$
2002	1.018	1.018	10931	1.006	1.006
2003	1.034	1.033	10932	1.124	1.124
2004	1.301	1.300	10933	1.498	1.497
2005	2.354	2.352	10934	2.798	2.797
2006	47067.162	42811.637	10935	138149.749	143720.416
2007	2.355	2.353	10936	2.798	2.797
2008	1.301	1.300	10937	1.498	1.497
2009	1.034	1.033	10938	1.124	1.124
2010	1.018	1.017	10939	1.006	1.006

In fact, we observe that the thus given density $F'(t)$ is very well approximated by the histograms in Fig. 6.b, and we therefore conjecture that the limit law (10.20) is correct. Now, since $F'(t) > 0$ for all $t \in \mathbb{R}$, this conjecture would also imply that

$$\liminf_{n\to\infty} \kappa_\diamond(n) = 1, \qquad \limsup_{n\to\infty} \kappa_\diamond(n) = \infty.$$

Actually, things are not as bad as such a spread of the condition number might suggest: from $\frac{2}{\pi}\arccos(1/100) \doteq 0.9936$ we infer that just about 0.64% of all n (in the sense of natural density) have $\kappa_\diamond(n) \geq 100$; that is, up to at least 99.36% of all the Taylor coefficients a_n can be computed with a loss of less than two digits. We find that the asymptotic median of $\kappa_\diamond(n)$ would be as small as $\sqrt{2}$.

Remark 10.6 In the same vein, a worst-case analysis based on Fig. 6.a tells us that there will only be a loss of at most *three* digits in computing the first one thousand of the Taylor coefficients of

$$\frac{1}{\Gamma(z)} = \sum_{n=0}^{\infty} a_n z^n$$

by means of a Cauchy integral with radius $r_\diamond(n)$. Note that the only competitor of this approach, namely using the recursion formula (see Luke 1969, Sect. 2.10)

$$a_0 = 0, \qquad a_1 = 1, \qquad a_2 = \gamma,$$
$$a_n = n a_1 a_n - a_2 a_{n-1} + \sum_{k=2}^{n-1} (-1)^k \zeta(k) a_{n-k} \quad (n > 2),$$

shows much worse behavior and suffers from severe numerical instability almost right from the beginning: in hardware arithmetic all the digits are lost for $n \geq 27$.

11 *H*-Admissible Entire Functions

The function $f(z) = \mathrm{e}^{\mathrm{e}^z - 1}$ of Example 7.5 is not covered by our results so far: it has order $\rho = \infty$. Nevertheless, the general idea of using the saddle-point method (see Sect. 9) can certainly also be applied to functions that grow even stronger than f. Hayman (1956) has axiomatized an important class of functions (with predominant growth in the direction of the real axis), for which the saddle-point method is applicable along *circular* contours and which enjoys nice closure properties. Expositions of this method can be found in Wong (1989, Sect. II.79), Odlyzko (1995, Sect. 12.2), Wilf (2006, Sect. 5.4), and Flajolet and Sedgewick (2009, Sect. VIII.5).

Hayman's method is based on the Taylor expansion (9.3) with the expansion point $z_* = r$, that is, on the Taylor expansion

$$\log f\bigl(r\mathrm{e}^{\mathrm{i}\theta}\bigr) = \log f(r) + \mathrm{i}a(r)\theta - \frac{1}{2}b(r)\theta^2 + O\bigl(\theta^3\bigr) \quad (\theta \to 0), \tag{11.1a}$$

where the coefficients are given by

$$a(r) = r\frac{f'(r)}{f(r)} = r\frac{\mathrm{d}}{\mathrm{d}r}\log f(r), \qquad b(r) = ra'(r). \tag{11.1b}$$

Now, an entire function $f(z)$ that is positive on (r_0, ∞) for some $r_0 > 0$ is said to be *H-admissible*, if it satisfies the following three conditions:

- $b(r) \to \infty$ as $r \to \infty$;
- for some function $\theta_0(r)$ defined over (r_0, ∞) and satisfying $0 < \theta_0(r) < \pi$, one has, uniformly in $|\theta| \le \theta_0(r)$,
$$f\bigl(r\mathrm{e}^{\mathrm{i}\theta}\bigr) \sim f(r)\mathrm{e}^{\mathrm{i}\theta a(r) - \theta^2 b(r)/2} \quad (r \to \infty);$$
- uniformly in $\theta_0(r) \le |\theta| \le \pi$
$$f\bigl(r\mathrm{e}^{\mathrm{i}\theta}\bigr) = \frac{o(f(r))}{\sqrt{b(r)}}.$$

However, one rarely checks these conditions directly but relies on the following closure properties instead.

Theorem 11.1 (Hayman 1956) *Let f and g be H-admissible entire functions and let p be a polynomial with real coefficients. Then*:

(a) *the product $f(z)g(z)$ and the exponential $\mathrm{e}^{f(z)}$ are admissible*;
(b) *the sum $f(z) + p(z)$ is admissible*;
(c) *if the leading coefficient of p is positive*, *then $f(z)p(z)$ and $p(f(z))$ are admissible*;
(d) *if the Taylor coefficients of $\mathrm{e}^{p(z)}$ are eventually positive*, *then $\mathrm{e}^{p(z)}$ is admissible.*

For instance, with the help of this theorem it is fairly obvious to see that the functions $f(z) = \mathrm{e}^z$ and $f(z) = \mathrm{e}^{\mathrm{e}^z - 1}$ are both H-admissible. On the other hand, the H-admissibility of functions like $f(z) = z^{-k/2}I_k(2\sqrt{z})$ has to be inferred more labor-intensively from the definition.

From the definition of H-admissibility we immediately read that the maximum modulus function is given, for r large enough, by

$$M(r) = f(r), \tag{11.2}$$

which, by the strict convexity of $\log M(r)$ with respect to $\log r$,[22] by Theorems 7.3 and 9.1, implies that the quasi-optimal radius $r_\diamond = r_\diamond(n)$ is the *unique* solution of

$$a(r_\diamond) = n \tag{11.3}$$

for n large enough. Hayman's main results are summarized in the following theorem.

Theorem 11.2 (Hayman 1956) *Let f be an entire H-admissible function. Then, for the quasi-optimal radius $r_\diamond = r_\diamond(n)$, we have*[23]

$$a_n \sim r_\diamond^{-n} M_1(r_\diamond) \sim \frac{f(r_\diamond)}{r_\diamond^n \sqrt{2\pi b(r_\diamond)}} \quad (n \to \infty); \tag{11.4}$$

in particular, we get $a_n > 0$ for n large enough. Moreover, we have, uniformly in the integers n,[24]

$$\frac{a_n r^n}{f(r)} = \frac{1}{\sqrt{2\pi b(r)}} \left(\exp\left(-\frac{(n - a(r))^2}{2b(r)} \right) + o(1) \right) \qquad (r \to \infty). \tag{11.5}$$

Finally, the ratio a_n / a_{n+1} forms an eventually increasing sequence since[25]

$$r_\diamond(n) \sim \frac{a_n}{a_{n+1}} \sim \frac{a_{n-1}}{a_n} \quad (n \to \infty). \tag{11.8}$$

---

[22] Note that this strict convexity implies $b(r) = (r \frac{\mathrm{d}}{\mathrm{d}r})^2 \log f(r) > 0$ for all $r > r_0$.

[23] Note that (11.4) can be thought of as being a generalization of Stirling's formula, cf. Examples 5.1 and 7.4: this was the original headline of Hayman's (1956) work.

[24] Because $f(r) = \sum_{k=0}^{\infty} a_k r^k$, the quantities $a_n r^n / f(r)$ form, if $a_n \geq 0$ for all n, a probability distribution in the discrete variable n. The result (11.5) thus tells us that this probability distribution is asymptotically, in the limit of large radius $r \to \infty$, Gaussian with mean $a(r)$ and variance $b(r)$.

[25] Note that the asymptotic representation (11.8) of the quasi-optimal radius holds for the generalized hyperbolic functions (8.6) with $p \leq q$, too: namely, we have by Theorem 8.4, Example 8.2, and Remark 8.7 that

$$r_\diamond(n) \sim n^{q+1-p} \sim \left| \frac{a_n}{a_{n+1}} \right| \sim \left| \frac{a_{n-1}}{a_n} \right| \quad (n \to \infty). \tag{11.6}$$

On the other hand, such a representation is not valid for the function of Example 12.4. However, there the following corollary of (11.6) is nevertheless correct:

$$r_\diamond(n) \sim \sqrt{\left| \frac{a_{n-1}}{a_{n+1}} \right|} \quad (n \to \infty). \tag{11.7}$$

Hence, if we restrict ourselves to those n for which $a_{n-1}, a_{n+1} \neq 0$, we observe that (11.7) does in fact hold for all the functions of Table 2 except the function $1/\Gamma(z)$. Whether this fact is just a contingency or whether it is for some deeper structural reason, we do not yet know.

As for the condition numbers, we straightforwardly get the following corollary; for reasons of a better comparison we have also included the quantities of the Wiman–Valiron theory as introduced in Sect. 8.3 (their asymptotics can directly be read from (11.5)).

Corollary 11.3 *Let f be an entire H-admissible function. Then*

$$\lim_{n\to\infty} \kappa_\diamond(n) = 1, \qquad \lim_{n\to\infty} \frac{\bar{\kappa}_\diamond(n)}{\sqrt{2\pi b(r_\diamond(n))}} = 1.$$

Moreover, we have $\nu(r) \sim a(r)$ as $r \to \infty$ and

$$M\big(r_\diamond(n)\big) \sim \sqrt{2\pi b\big(r_\diamond(n)\big)}\,\mu\big(r_\diamond(n)\big) \quad (n \to \infty).$$

Applications have already been discussed in Examples 7.4 and 7.5.

Remark 11.4 If the entire H-admissible function f is of finite order ρ with normal type τ, it is instructive to compare Corollary 11.3 with Theorem 10.2. From the definition of H-admissibility it then follows that:

- f is of perfectly and completely regular growth;
- there is just one direction of predominant growth, $\Omega = 1$ with $h(0) = \tau$;
- f has at most finitely many zeros in the vicinity of the positive real axis.

Thus, f satisfies the assumptions of Theorem 10.2 and also those that have led to the definition (8.19) of ω. Therefore, by $\Omega = 1$ we get from (10.9) and (10.10) that $\omega = 1$ and

$$\lim_{n\to\infty} \kappa_\diamond(n) = 1, \qquad \lim_{n\to\infty} \frac{\bar{\kappa}_\diamond(n)}{\sqrt{2\pi\rho n}} = 1.$$

(Recall that H-admissible functions have $a_n > 0$ for n large enough.) Further, by Theorem 8.6 we have $\nu(r) \sim \tau\rho r^\rho$. These results are consistent with Corollary 11.3; a comparison gives, by using (8.10), the asymptotic equations

$$a(r) \sim \tau\rho r^\rho, \quad b(r) \sim \tau\rho^2 r^\rho \quad (r \to \infty). \tag{11.9}$$

Formally, as suggested by (11.1b), these equations could have been obtained from differentiating the asymptotic equation $\log f(r) = \log M(r) \sim \tau r^\rho$ (which just states the perfectly regular growth of the function f, see (8.5) for the definition). The differentiability of these asymptotic equations has also been observed by Pólya and Szegö (1964, Sect. IV.70/71) under the weaker assumption that f is a function of perfectly regular growth with $a_n \geq 0$.

12 Entire Functions with Nonnegative Taylor Coefficients

In this final section we consider entire transcendental functions f which have nonnegative Taylor coefficients: $a_n \geq 0$ for all n. Such functions are typically met as generating functions in combinatorial enumeration or in probability theory. The non-negativity of the Taylor coefficients implies at once that

$$M(r) = f(r) \quad (r > 0). \tag{12.1}$$

Thus, by Theorem 7.1, we infer that $\log f(r)$ and hence $\log(r^{-n} f(r))$ are strictly convex functions of $\log r$. Moreover, since

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} r^{-n} f(r) = r^{-n-2} \sum_{k=0}^{\infty} (n+1-k)(n-k) a_k r^k > 0 \quad (r > 0),$$

we conclude that the function $r^{-n} f(r)$ itself is strictly convex, too. The same reasoning that led to (11.3) in the last section proves the following simplification of Theorem 9.1.

Theorem 12.1 *Let f be an entire transcendental function with nonnegative Taylor coefficients*: $a_n \geq 0$ *for all n. Then, the quasi-optimal radius $r_\diamond = r_\diamond(n)$ is given as the unique solution of the convex optimization problem*

$$r_\diamond = \operatorname*{arg\,min}_{r>0} r^{-n} f(r), \tag{12.2}$$

and, *equivalently*, *as the unique solution of the real saddle-point equation*

$$r_\diamond \frac{f'(r_\diamond)}{f(r_\diamond)} = n \quad (r_\diamond > 0). \tag{12.3}$$

Remark 12.2 If f is a function of perfectly regular growth (of order ρ and type τ) with nonnegative Taylor coefficients, Theorem 12.1 yields the assertion of Theorem 8.4 with a proof that is much shorter than the one of the general result given there. First, from the definition of perfectly regular growth in (8.5) and from (12.1) we get

$$\log f(r) \sim \tau r^\rho \quad (r \to \infty);$$

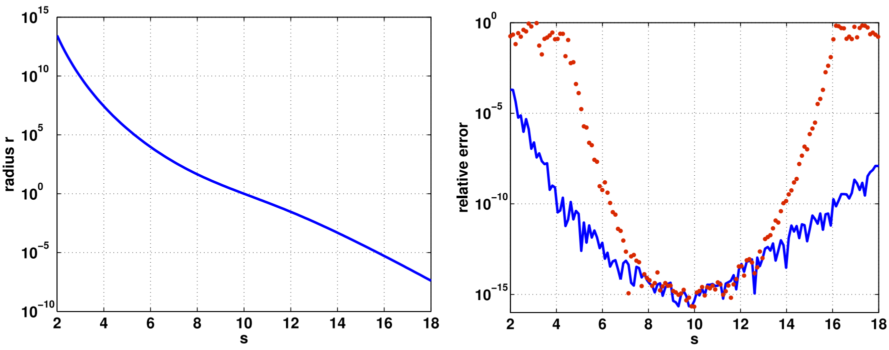
next, since the Taylor coefficients are nonnegative, we may differentiate this asymptotic equation (see Pólya and Szegö 1964, Sect. IV.70) and obtain

$$r \frac{f'(r)}{f(r)} \sim \tau \rho r^\rho \quad (r \to \infty).$$

Therefore, by recalling $r_\diamond(n) \to \infty$ as $n \to \infty$ (see Theorem 4.6), the saddle-point equation (12.3) is asymptotically solved by

$$r_\diamond(n) \sim \left(\frac{n}{\tau\rho}\right)^{1/\rho} \quad (n \to \infty),$$

which is, finally, the assertion of Theorem 8.4.



a. quasi-optimal radius $r = r_\diamond$ as a function of s

b. relative error

Fig. 7 (Color online) *Left*: the quasi-optimal radius $r_\diamond$ as a function of s for calculating the gap probability $E_2(10; s)$ of GUE as the 10-th Taylor coefficient of a Fredholm determinant. *Right*: the relative error of the calculation; the *dotted line* (*red*) shows the errors for the radius $r = 1$, the *solid line* (*blue*) shows the errors for the radius $r_\diamond$ (see also Example 3.1 and Fig. 2). Note that, although $\kappa_\diamond \doteq 1$ throughout the range of s, there is still a noticeable loss of accuracy in the tails: this is because the Fredholm determinant is not computed to small relative but small absolute errors; hence the model assumption (3.2) is violated. Nevertheless, $r_\diamond$ gives a significant improvement over the fixed radius $r = 1$ that belongs to the concept of absolute errors

Example 12.3 We resume the computation of the gap probabilities $E_2(n; s)$ as discussed in Example 3.1, this time striving for small relative errors instead of absolute errors. As we have seen, the generating function is given by the Fredholm determinant

$$f(z) = \sum_{k=0}^{\infty} E_2(k; s) z^k = \det\big(I - (1 - z)K\big|_{L^2(0,s)}\big), \qquad K(x, y) = \operatorname{sinc}\big(\pi(x - y)\big),$$

which is known to be, as a function of z, an entire function of order $\rho = 0$.[26] Figure 7.a shows that, for $n = 10$, the quasi-optimal radius $r_\diamond$ (as computed from (12.2) by means of MATLAB's `fminbnd` command) varies over about 20 orders of magnitude as the parameter s runs through the interval $2 \le s \le 18$. The corresponding condition number satisfies $\kappa_\diamond \doteq 1$, up to machine precision throughout. We will explain this optimal condition number result and the strong variability of the radius by discussing a "mock-up" model in the next example. Note that even though Fig. 7.b shows a significant accuracy improvement in the tails, we do not get the full accuracy that we would have expected from $\kappa_\diamond \doteq 1$. The reason is simply that the numerical evaluation of the Fredholm determinants does not satisfy the model assumption (3.2); see Bornemann (2010, Sect. 4).

[26]Generally, if the kernel $K(x, y)$ satisfies a Hölder condition with exponent α, with respect to either x or y, then $f(z) = \det(I - zK)$ is an entire function of order $\rho \le 2/(1 + 2\alpha)$; see, e.g., Lax (2002, Lemma 24.10).

Example 12.4 Lacking a proof that $\kappa_\diamond \approx 1$ in Example 12.3, we analyze a "mock-up" Fredholm determinant in full detail, namely the q-series

$$f(z) = (-z;q)_\infty = \prod_{k=0}^{\infty}\bigl(1+zq^k\bigr) \quad (0<q<1).$$

By a result of Euler (see Andrews et al. 1999, Corollary 10.2.2) it is known that

$$f(z) = \sum_{k=0}^{\infty} \frac{q^{\binom{k}{2}}}{(q;q)_k} z^k,$$

where

$$(q;q)_k = (1-q)\bigl(1-q^2\bigr)\cdots\bigl(1-q^k\bigr);$$

in particular, f has positive Taylor coefficients. By using (8.3), f is easily seen to be an entire function of order $\rho = 0$. Now, a numerical experiment shows that $\kappa_\diamond(n) \doteq 1$ up to machine precision for $n = 20$ and $q = 1/2$. Hence, we aim at proving that $\kappa_\diamond(n) \to 1$ as $n \to \infty$.

A natural first try would be to check f for H-admissibility; see Corollary 11.3. This approach is doomed to fail, however, since we get the following asymptotics from an application of the Euler–Maclaurin sum formula:

$$a(r) = r\frac{f'(r)}{f(r)} = \sum_{k=0}^{\infty}\frac{rq^k}{1+rq^k} = \frac{\log r}{\log(1/q)} + \frac{1}{2} + O\bigl(r^{-1}\bigr) \quad (r \to \infty); \tag{12.4}$$

but

$$b(r) = ra'(r) = \sum_{k=0}^{\infty}\frac{rq^k}{(1+rq^k)^2} = \frac{1}{\log(1/q)} + O\bigl(r^{-1}\bigr) \quad (r\to\infty),$$

which remains bounded (recall that H-admissibility would require $b(r) \to \infty$). Nevertheless, from (12.3) and (12.4) we get the strong estimate

$$r_\diamond(n) = q^{1/2-n} + O(1) \quad (n \to \infty), \tag{12.5}$$

which not only shows that $r_\diamond(n)$ grows exponentially fast for this slowly growing function $f(z)$, but also that $r_\diamond$ varies very strongly with respect to the parameter q (an effect that we had already observed in Example 12.3).

To study $\kappa_\diamond(n)$ we look more closely at $\log f(re^{i\theta})$ for large values of r. Applying the Euler–Maclaurin sum formula once more and using a uniformity criterion of Levin (1980, p. 142), we get that

$$\operatorname{Re}\log f\bigl(re^{i\theta}\bigr) = \frac{1}{2}\frac{\log(r)^2}{\log(1/q)} + \frac{1}{2}\log r + \frac{1}{12}\log(1/q) + \frac{\pi^2-3\theta^2}{6\log(1/q)} + O\bigl(r^{-1}\bigr), \tag{12.6a}$$

and

$$\operatorname{Im}\log f\bigl(re^{i\theta}\bigr) = \theta\frac{\log r}{\log(1/q)} + \frac{1}{2}\theta + \frac{q}{1-q}\sin(\theta)r^{-1} + O\bigl(r^{-2}\bigr), \tag{12.6b}$$

uniformly in θ as $r \to \infty$ ($r \notin E$) with the possible exception of a set E of relative linear density zero. The first asymptotics, (12.6a), means that f is of completely regular growth with the proximate order $\rho(r)$ (see Levin 1980, Sect. I.12),[27]

$$r^{\rho(r)} = \frac{1}{2}\frac{\log(r)^2}{\log(1/q)}$$

and *constant* indicator function $h(\theta) = 1$. This implies that the growth of f is not localized enough in the angular direction to hope for an application of the Laplace method to estimate the Cauchy integrals. In other words, the second stage of using the saddle-point method (de Bruijn 1981, p. 77) seems to be about to fail. However, this is not the case here, since the *whole* circular contour of radius $r_\diamond = r_\diamond(n)$ is approximately a level line of $\operatorname{Im}\log z^{-n} f(z)$, not just the segment near the saddle point itself. In fact, from (12.6b) we get that

$$\operatorname{Im}\log f\big(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\big) - n\theta = \frac{q^{n+1/2}}{1-q}\sin\theta + O\big(q^{2n}\big) \quad (n \to \infty), \tag{12.7}$$

which is exponentially close to zero. Note that we can arrange for $r_\diamond(n) \notin E$ since E is built from sets of increasingly small neighborhoods of the radii of the zeros of f, which are located at $-q^{-k}$, $k \in \mathbb{N}_0$. That is, (12.7) holds uniformly in θ. Hence, we get

$$\begin{aligned} a_n &= \frac{1}{2\pi r_\diamond^n}\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}n\theta} f\big(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\big)\,\mathrm{d}\theta = \frac{1}{2\pi r_\diamond^n}\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(\operatorname{Im}\log f(r_\diamond \mathrm{e}^{\mathrm{i}\theta}) - n\theta)}\big|f\big(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\big)\big|\,\mathrm{d}\theta \\ &= \frac{1}{2\pi r_\diamond^n}\int_{-\pi}^{\pi}\left(1 + \frac{\mathrm{i}q^{n+1/2}}{1-q}\sin\theta + O\big(q^{2n}\big)\right)\cdot\big|f\big(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\big)\big|\,\mathrm{d}\theta \\ &= \frac{1}{2\pi r_\diamond^n}\int_{-\pi}^{\pi}\big|f\big(r_\diamond \mathrm{e}^{\mathrm{i}\theta}\big)\big|\,\mathrm{d}\theta\cdot\big(1 + O\big(q^{2n}\big)\big), \end{aligned}$$

since the contribution of the odd function $\sin\theta|f(r_\diamond \mathrm{e}^{\mathrm{i}\theta})|$ to the integral is zero. Therefore, we obtain the approximation

$$\kappa_\diamond(n) = 1 + O\big(q^{2n}\big) \quad (n \to \infty), \tag{12.8}$$

whose exponentially small error term helps us to understand the excellent condition numbers observed in Example 12.3.

Example 12.5 We close the paper with a nontrivial example from the theory of random permutations. Let us denote the length of the longest increasing subsequence[28] of a permutation $\sigma \in \mathcal{S}_n$ by $\ell(\sigma)$. The probability distribution of $\ell(\sigma)$ that is induced

[27] Note that, consistent with $\rho = 0$, we have $\rho(r) \to 0$ as $r \to \infty$.

[28] For instance, the longest increasing subsequence of $\sigma = (3, 7, 10, 5, 9, 6, 8, 1, 4, 2) \in \mathcal{S}_{10}$ is given by $(3, 5, 6, 8)$; hence, $\ell(\sigma) = 4$ in this case.

by the uniform distribution on $\mathcal{S}_n$ can be encoded in a family of exponentially generating functions $\phi_\lambda(z)$ via

$$\mathbb{P}\big(\sigma \in \mathcal{S}_n : \ell(\sigma) \le \lambda\big) = \frac{\mathrm{d}^n}{\mathrm{d}z^n}\phi_\lambda^{(n)}(z)\bigg|_{z=0} \qquad (\lambda, n \in \mathbb{N}). \tag{12.9}$$

Now, the seminal work of Gessel (1990) shows that $\phi_\lambda(z)$ can be expressed in terms of a Toeplitz determinant,

$$\phi_\lambda(z) = \det\big(I_{|j-k|}(2\sqrt{z})\big)_{j,k=0}^{\lambda-1}. \tag{12.10}$$

Since the modified Bessel functions $z^{-k/2} I_k(2\sqrt{z})$ ($k \in \mathbb{N}_0$) are entire functions of perfectly regular growth (of order $\rho = 1/2$ and type $\tau = 2$, see Table 2), ϕ_λ must also be an entire function of perfectly regular growth; its order and type are easily inferred to be $\rho = 1/2$ and $\tau = 2\lambda$. Likewise, we obtain that the Phragmén–Lindelöf indicator of $\phi_\lambda(z)$ is given by

$$h(\theta) = 2\lambda\cos(\theta/2) \quad \big(|\theta| \le \pi\big).$$

Hence, we have $\Omega = 1$ and, since there are no zeros of $\phi_\lambda(z)$ in the vicinity of the real axis, $\omega = 1$ and $\lim_{n\to\infty} \kappa_\diamond(n) = 1$ by Theorem 10.2. This explains the very well-behaved quasi-optimal condition numbers shown in Table 6. Theorem 8.4 yields the following asymptotics of the quasi-optimal radius:

$$r_\diamond(n) \sim (n/\lambda)^2 \quad (n \to \infty). \tag{12.11}$$

However, as we can see from Table 6, this asymptotics probably does not hold uniformly in λ and is therefore of limited practical use. Hence, one has to compute the value of the radius $r_\diamond(n)$ itself by numerically solving (12.2). Using these radii and high-precision arithmetic, we were able to reproduce *numerically* the exact rational values of the distributions (12.9) for $n = 15$, 30, 60, 90, and 120 as tabulated by Odlyzko (2000),[29] who has used the *combinatorial* methods exposed in Odlyzko and Rains (2000) for his calculations.

Remark 12.6 The numerical evaluation of $\phi_\lambda(z)$ as given by the Toeplitz determinant (12.10) turns out to suffer from severe numerical instabilities. Instead, we suggest taking one of the famous equivalent expressions in terms of a Fredholm determinant, such as the one given by Borodin and Okounkov (2000, p. 391)

$$\phi_\lambda(z) = \mathrm{e}^z \det\big(I - K\big|_{\ell^2(\lambda,\lambda+1,\ldots)}\big),$$

$$K(j,k) = \sqrt{z}\,\frac{J_j(2\sqrt{z})J_{k+1}(2\sqrt{z}) - J_{j+1}(2\sqrt{z})J_k(2\sqrt{z})}{j-k},$$

or the one given by Baik et al. (2001, p. 629)

$$\phi_\lambda(z) = 2^{-n}\mathrm{e}^z \det(I - K|_{L^2(C_1)}), \qquad K(t,s) = \frac{1 - t^n \mathrm{e}^{\sqrt{z}(t-t^{-1})} s^{-n} \mathrm{e}^{-\sqrt{z}(s-s^{-1})}}{2\pi \mathrm{i}(t-s)};$$

[29] For $n = 30$, 60, and 90, these tables can be found in print in the book of Mehta (2004, pp. 464–467).

Table 6 For $f(z) = \phi_\lambda(z)$, a comparison of the quasi-optimal radius $r_\diamond(n)$ with its asymptotic value (12.11). Note that this asymptotic value is not necessarily useful in practice. The value of $r_\diamond(n) = \arg\min r^{-n} f(r)$ was actually computed by using MATLAB's `fminbnd` command

n	λ	$r_\diamond(n)$	$\kappa_\diamond(n)$	$(n/\lambda)^2$	$\kappa(n, (n/\lambda)^2)$
20	3	55.08575	1.00005	44.44444	1.39833
100	15	108.74559	1.00000	44.44444	$5.17900 \cdot 10^{11}$

see also Basor and Widom (2000) and Böttcher (2002). Both expressions can be evaluated in a numerically stable way; the first using the projection method, the second using the quadrature method exposed in Bornemann (2010, Sects. 5 and 6).

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