Central limit theorems and large deviations for the characteristic polynomial of a random unitary matrix and the Riemann zeta function

Notes for talk at Oberwolfach DMV seminar, 15-21 Oct 2000
"The Riemann zeta function and random matrix theory"

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Keating and Snaith [8] found that the local statistics of the Riemann zeta function on the critical line are modelled well by the characteristic polynomial of an $N \times N$ unitary matrix,

$$\begin{aligned} Z(\theta) &= \operatorname{Det}\left(I - Ue^{-\mathrm{i}\theta}\right) \\ &= \prod_{n=1}^{N} \left(1 - e^{\mathrm{i}(\theta_n - \theta)}\right), \end{aligned}$$

when the matrix U (with eigenvalues $e^{\mathrm{i}\theta_1}, \ldots, e^{\mathrm{i}\theta_N}$) is chosen with Haar measure, and the mean density of Riemann zeros at height T is equated with the mean density of eigenangles:

$$N = \ln \frac{T}{2\pi}.$$

For this reason the random variable $Z(\theta)$ has been analysed in depth, and some of those results are the subject of this talk.

In figure 1 the log of the probability density of $\mathfrak{Re} \ln Z(\theta)$ for $N = 42$ is plotted, against the log of the value distribution of $\ln |\zeta(1/2 + \mathrm{i}t)|$ around the 10^{20}th zero. Note that we plot the log of the probability densities so that the tails of the distributions are made visible. This will be discussed in the second part of this talk.

Part 1: Central limit theorems

All the central limit theorems (CLTs) we will prove are theorems of weak convergence.

Definition. *A sequence of random variables, $\{X_N\}$, taking values in some topological space T is said to converge weakly to X (written $X_N \Longrightarrow X$) as $N \to \infty$ if, for all bounded continuous functions $f : T \longrightarrow \mathbb{R}$,*

$$\lim_{N\to\infty} \mathbb{E} f(X_N) = \mathbb{E} f(X).$$

For our purposes, we can take $T = \mathbb{R}^d$. Proving weak convergence using the above definition is usually difficult, so throughout we use:

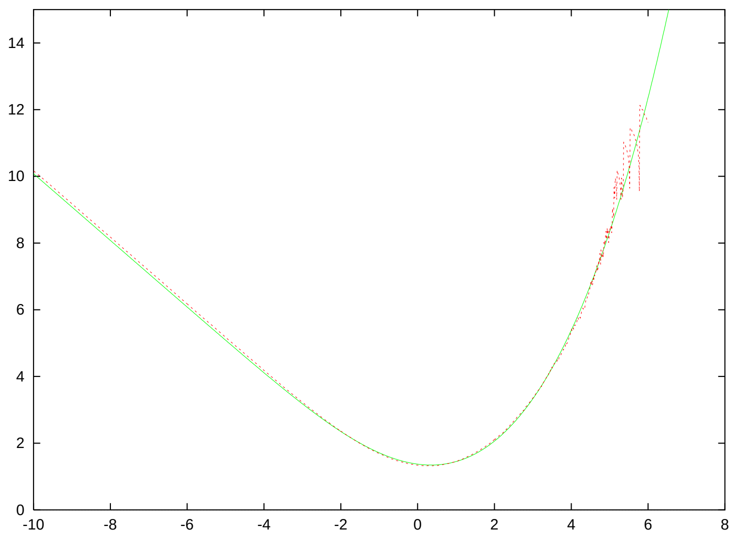

Figure 1: Graph of the negative log of probability density of $\mathfrak{Re} \ln Z(\theta)$ for $N = 42$ (green: data from N.C. Snaith), and for $\ln|\zeta(1/2 + it)|$ around the 10^{20}th zero (red: data from A.M. Odlyzko).

Theorem 1. *If for all finite $\lambda \in \mathbb{R}^d$,*

$$\lim_{N\to\infty} \mathbb{E}e^{\lambda \cdot X_N} = \mathbb{E}e^{\lambda \cdot X} < \infty$$

then $X_N \Longrightarrow X$ as $N \to \infty$.

See [4] for details on weak convergence.

As a remark, if X has a continuous distribution on $\mathbb{R}^d$ and $X_N \Longrightarrow X$ then for any measurable set $A \subseteq \mathbb{R}^d$,

$$\mathbb{P}\{X_N \in A\} \to \mathbb{P}\{X \in A\} \qquad \text{as } N \to \infty.$$

Central limit theorem for zeta

Theorem 2. (Selberg). *For rectangles $E \subseteq \mathbb{R}^2$,*

$$\lim_{T\to\infty} \frac{1}{T} meas \left\{ T \le t \le 2T \,:\, \frac{\ln \zeta(1/2 + it)}{\sqrt{\frac{1}{2}\ln\ln T}} \in E \right\} = \frac{1}{2\pi} \iint_E e^{-(x^2+y^2)/2}\, \mathrm{d}x\, \mathrm{d}y$$

Although Selberg never published a proof of this (see §2.11 of [10]), a proof following the same philosophy we employ (that is, using moment generating functions) can be found in theorem 2.1 of chapter 4 of [9].

Central limit theorem at one fixed point

Recalling that $N = \ln \frac{T}{2\pi}$ is the conjectured connection between matrix size and height up the critical line, we see that an analogous result holds for $\ln Z(\theta)$:

Theorem 3. (Keating & Snaith [8]). *Let $\sigma^2 = \frac{1}{2}\ln N$, then*

$$\frac{\ln Z(\theta)}{\sigma} \Longrightarrow X + \mathrm{i}Y$$

where X, Y are independent identically distributed (iid) normal random variables with mean zero and variance 1.

Their method of proof was to calculate the joint moment generating function,

$$\mathbb{E}\exp(s\mathfrak{Re}\ln Z(\theta) + t\mathfrak{Im}\ln Z(\theta)),$$

exactly, and then show that

$$\lim_{N\to\infty} \mathbb{E}\exp(\lambda\mathfrak{Re}\ln Z(\theta)/\sigma + \mu\mathfrak{Im}\ln Z(\theta)/\sigma) = e^{\lambda^2/2+\mu^2/2}$$

when $\sigma = \sqrt{\frac{1}{2}\ln N}$.

The one dimensional CLTs for the real and imaginary parts of $\ln Z(\theta)$ treated separately had previously been calculated in [1] using the same approach.

Central limit theorem at many distinct points

An exact calculation of the moment generating function has only proved possible for one fixed point. So in order to generalize theorem 3 to a multidimensional central limit theorem, where $\ln Z(\theta)$ is evaluated at many distinct points, a new approach is called for. This will come in the form of a connection between random unitary matrices and Toeplitz determinants.

Theorem 4. Hughes, Keating & O'Connell [7]). *Let $r_1, \cdots, r_k$ be distinct modulo 2π. Then*

$$(\ln Z(r_1)/\sigma, \dots, \ln Z(r_k)/\sigma) \Longrightarrow (X_1 + \mathrm{i}Y_1, \dots, X_k + \mathrm{i}Y_k).$$

with X_j and Y_j $(j = 1, \dots, k)$ all iid standard normal random variables.

(Diaconis & Evans [5] have given an alternative proof of theorem 4, using representation theory to study the moments of $\ln Z(\theta)/\sigma)$.

The connection between random unitary matrices and Toeplitz determinants mentioned above is called Heine's identity:

$$\mathbb{E}\prod_{n=1}^{N} f(\theta_n) = D_N[f] = \mathrm{Det}\left\{\hat{f}_{j-k}\right\}_{1\le j,k\le N}$$

where $\hat{f}_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(t)e^{-\mathrm{i}nt}\,\mathrm{d}t$ is the n^{th} Fourier coefficient of $f(\cdot)$.

To prove the theorem, we take, for fixed k and fixed and distinct r_j,

$$f(\theta_n) = \exp\left(\sum_{j=1}^{k} s_j\mathfrak{Re}\ln\left(1 - e^{\mathrm{i}(\theta_n - r_j)}\right) + t_j\mathfrak{Im}\ln\left(1 - e^{\mathrm{i}(\theta_n - r_j)}\right)\right)$$

Basor [3] has studied the Toeplitz determinant of such a symbol and, translating her results using Heine's identity, she showed that

$$\mathbb{E}\prod_{j=1}^{k}\exp\left(s_j\mathfrak{Re}\ln Z(r_j)+t_j\mathfrak{Im}\ln Z(r_j)\right)\sim F\prod_{j=1}^{k}N^{s_j^2/4+t_j^2/4}$$

for $s_j>-1$ where

$$F=\prod_{\substack{1\le m,n\le N\\ m\ne n}}\left(1-e^{i(r_m-r_n)}\right)^{-(s_m-\mathrm{i}t_m)(s_n+\mathrm{i}t_n)/4}\times$$

$$\times\prod_{j=1}^{k}\frac{G(1+s_j/2+\mathrm{i}t_j/2)G(1+s_j/2-\mathrm{i}t_j/2)}{G(1+s_j)}$$

where G is the Barnes G–function (see the appendix).

By noting that Basor's asymptotics are uniform in s_j and t_j close to the origin, writing $s_j=\lambda_j/\sigma$ and $t_j=\mu_j/\sigma$ we obtain

$$\lim_{N\to\infty}\mathbb{E}\exp\left(\sum_{j=1}^{k}\lambda_j\mathfrak{Re}\ln Z(r_j)/\sigma+\mu_j\mathfrak{Im}\ln Z(r_j)/\sigma\right)$$

$$=\exp\left(\sum_{j=1}^{k}\lambda_j^2/2+\mu_j^2/2\right)$$

and so, by theorem 1, this proves theorem 4.

Limiting process

A nice rephrasing of theorem 4 is as follows: As $N\to\infty$, the finite dimensional distributions of $\ln Z(\theta)/\sigma$ weakly converge to those of a centered Gaussian process $\{P(\theta)\,:\,-\pi<\theta\le\pi\}$ with covariance structure

$$\mathbb{E}\{P(\theta)P(\phi)\}=\begin{cases}1 & \theta=\phi\\ 0 & \text{otherwise}\end{cases}$$

Ergodicity

By ergodicity we mean that for almost all matrices, the distribution of $\ln Z(\theta)/\sigma$ over θ is the same as the distribution of $\ln Z(\theta)/\sigma$ over U.

Theorem 5. (Hughes, Keating & O'Connell [7]). *Denote by m the uniform probability measure on $(-\pi,\pi]$ (so that $m(\mathrm{d}\theta)=\mathrm{d}\theta/2\pi$). The sequence of laws $\left\{m\circ(\ln Z(\theta)/\sigma)^{-1}\right\}$ converges weakly in probability to $X+\mathrm{i}Y$, where X,Y are iid standard normal random variables.*

What do we mean by this? For any measurable set $A\subseteq\mathbb{C}$, $(\ln Z(\theta)/\sigma)^{-1}(A)$ is the set of all $\theta\in(-\pi,\pi]$ such that $\ln Z(\theta)/\sigma\in A$. So, for any fixed matrix U,

$$m\circ(\ln Z(\theta)/\sigma)^{-1}(A)=\frac{1}{2\pi}meas\left\{-\pi<\theta\le\pi\,:\,\frac{\ln Z(\theta)}{\sqrt{\frac12\ln N}}\in A\right\}$$

(But remember $m \circ (\ln Z(\theta)/\sigma)^{-1}(A)$ depends on the matrix, not just the matrix size). Weak convergence in probability means that the measure of those matrices which do not converge weakly to $X + \mathrm{i}Y$ is vanishingly small. So, for example, theorem 5 implies that for any $\epsilon > 0$,

$$\lim_{N\to\infty} \mathbb{P}\left\{ \left| m \circ (\ln Z(\theta)/\sigma)^{-1}(A) - \frac{1}{2\pi} \iint_E e^{-(x^2+y^2)/2}\, \mathrm{d}x\, \mathrm{d}y \right| > \epsilon \right\} = 0.$$

Comparing with theorem 2 we see why we have been through all this—the analogy with the zeta function is now much clearer (the original Keating & Snaith CLT is "fix θ and average over all matrices", and the Selberg CLT is "fix the zeta function (there being only one anyway!) and average over t", whereas what we have here is (loosely speaking) "fix a typical matrix and average over θ").

Now let us turn to the proof of theorem 5. Recall that weak convergence is implied by the pointwise convergence of the moment generating function, as $N \to \infty$. For each matrix U denote the moment generating function over θ as

$$\phi_U(\lambda, \mu) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp\left(\lambda \mathfrak{Re} \ln Z(\theta)/\sigma + \mu \mathfrak{Im} \ln Z(\theta)/\sigma\right)\, \mathrm{d}\theta.$$

Theorem 5 will follow from showing that for each λ, μ, for any $\epsilon > 0$,

$$\mathbb{P}\left\{ \left| \phi_U(\lambda,\mu) - e^{(\lambda^2+\mu^2)/2} \right| > \epsilon \right\} \to 0 \quad \text{as } N \to \infty.$$

Proof. The mean of $\phi_U(\lambda, \mu)$ is already known from theorem 3:

$$\mathbb{E}\phi_U(\lambda,\mu) \to e^{(\lambda^2+\mu^2)/2}.$$

To calculate the second moment of $\phi_U(\lambda, \mu)$ we use theorem 4 to show

$$\begin{aligned} &\mathbb{E}\exp\left(\lambda \mathfrak{Re} \ln Z(\theta)/\sigma + \mu \mathfrak{Im} \ln Z(\theta)/\sigma + \lambda \mathfrak{Re} \ln Z(\phi)/\sigma + \mu \mathfrak{Im} \ln Z(\phi)/\sigma\right) \\ &\qquad\qquad \to \begin{cases} e^{\lambda^2+\mu^2} & \theta \neq \phi \\ e^{2\lambda^2+2\mu^2} & \theta = \phi \end{cases} \end{aligned}$$

and so, by the bounded convergence theorem,

$$\mathbb{E}\left\{ \phi_U(\lambda,\mu)^2 \right\} \to e^{\lambda^2+\mu^2}.$$

Therefore, the variance of $\phi_U(\lambda, \mu)$ is

$$\begin{aligned} \operatorname{Var} \phi_U(\lambda,\mu) &= \mathbb{E}\left\{ \phi_U(\lambda,\mu)^2 \right\} - \left(\mathbb{E}\phi_U(\lambda,\mu)\right)^2 \\ &\to 0 \quad \text{as } N \to \infty, \end{aligned}$$

and hence Chebyshev's inequality implies that for any $\epsilon > 0$,

$$\begin{aligned} \mathbb{P}_N(|\phi_U(\lambda,\mu) - e^{(\lambda^2+\mu^2)/2}| > \epsilon) &\le \frac{\operatorname{Var} \phi_U(\lambda,\mu)}{\epsilon^2} \\ &\to 0 \quad \text{as } N \to \infty. \end{aligned}$$

Thus, for each λ, μ, the sequence $\phi_U(\lambda, \mu)$ converges in probability to $e^{(\lambda^2+\mu^2)/2}$. Theorem 5 now follows from the fact that moment generating functions are convergence-determining.

Connections with the zeta function

Do these random matrix results suggest any improvements which might be made to theorem 2? The answer is yes, though we must be careful not to push the analogy too far:

- Theorem 5 suggests that the range over which $\ln \zeta(1/2 + \mathrm{i}t)$ is averaged in theorem 2 (currently $T \leq t \leq 2T$) might be reduced. In [11], it is shown that
$$\frac{\mathfrak{Im} \ln \zeta(1/2 + \mathrm{i}t)}{\sqrt{\frac{1}{2} \ln \ln T}}$$
weakly converges to a Gaussian when averaged over $T \leq t \leq T + H$ with $H = T^\alpha$ for any $\alpha > 0$, if the Riemann hypothesis is assumed.
- Theorem 4 suggests that averaging zeta over k distinct blocks, say from $[T, T+H], [T+H, T+2H], \ldots, [T+(k-1)H, T+kH]$ would produce k iid standard complex normal random variables. The published work, [12], again concerns $\mathfrak{Im} \ln \zeta$, and is consistent with the case $k = 2$, but doesn't imply it.

Part 2: Large deviations

So far we have only looked at central limit theorems, and we have seen that random matrix theory models well the zeta function. But looking at figure 1 we can see that the tails of the distribution of $\ln \zeta(1/2 + it)$ are modelled pretty well by the tails of the distribution of $\ln Z(\theta)$ too.

The formal definition of a large deviation, and complete results for both real and imaginary parts of $\ln Z(\theta)$ can be found in [7]. But in this talk, I will concentrate on the far left deviations of $\mathfrak{Re} \ln Z(\theta)$—the straight-line part of figure 1.

Large left deviations

Theorem 6. (Hughes, Keating & O'Connell [7]). *If*
$$\liminf_{N \to \infty} \frac{x}{\ln N} > \frac{1}{2}$$
then
$$\mathbb{P}\left\{\mathfrak{Re} \ln Z(\theta) \leq -x\right\} \sim e^{-x} \exp\left(3\zeta'(-1) + \tfrac{1}{12} \ln 2 - \tfrac{1}{2} \ln \pi\right) N^{1/4}.$$

Proof.

We need to use the exact evaluation [1, 8] of
$$\begin{aligned} M_N(s) &:= \mathbb{E} e^{s \mathfrak{Re} \ln Z(\theta)} \\ &= \frac{G^2\left(1 + \frac{1}{2}s\right) G(N+1) G(N+1+s)}{G(1+s) G^2\left(N+1+\frac{1}{2}s\right)} \end{aligned}$$

where G is the Barnes G–function (see the appendix). If we write $p(t)$ for the probability density of $\mathfrak{Re} \ln Z(\theta)$, which means

$$\mathbb{E}e^{s\mathfrak{Re}\ln Z(\theta)} = \int_{-\infty}^{\infty} e^{st} p(t)\ \mathrm{d}t$$

so that, by Fourier inversion,

$$p(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-\mathrm{i}yt} M_N(\mathrm{i}y)\ \mathrm{d}y.$$

We evaluate

$$\frac{1}{2\pi} \int_C e^{-\mathrm{i}zt} M_N(\mathrm{i}z)\ \ \mathrm{d}z,$$

where C is the rectangle with vertices $-R$, R, $R+\mathrm{i}+\epsilon\mathrm{i}$, $-R+\mathrm{i}+\epsilon\mathrm{i}$, for ϵ a fixed real number subject to $0 < \epsilon < 2$ (see figure 2), and let $R \to \infty$. Note that the contour encloses only a simple pole at $z = \mathrm{i}$.

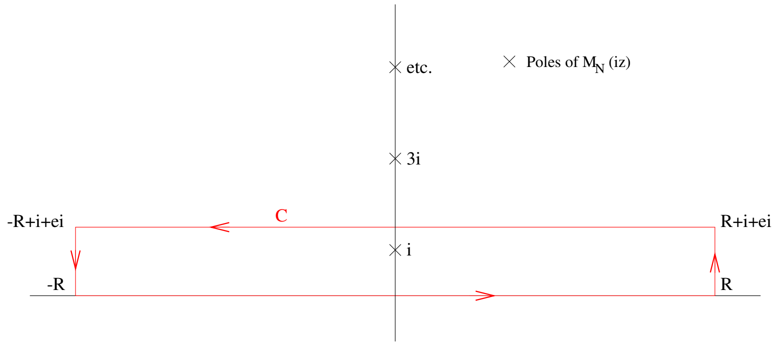

Figure 2: The contour C

The asymptotics for $G(\cdot)$ show that the integral on the sides of the contour vanish as $R \to \infty$, which means

$$p(t) = \mathrm{i}\operatorname*{Res}_{z=\mathrm{i}} \left\{e^{-\mathrm{i}zt} M_N(\mathrm{i}z)\right\} + E,$$

where

$$E = \frac{e^{t+\epsilon t}}{2\pi} \int_{-\infty}^{\infty} e^{-\mathrm{i}yt} M_N(\mathrm{i}y - 1 - \epsilon)\ \ \mathrm{d}y.$$

The pole at $z = \mathrm{i}$ is simple, so

$$\begin{aligned}
\mathrm{i}\operatorname*{Res}_{z=\mathrm{i}} \left\{e^{-\mathrm{i}zt} M_N(\mathrm{i}z)\right\} &= e^t G^2\left(\tfrac{1}{2}\right) \frac{G(N)G(N+1)}{G^2\left(N+\frac{1}{2}\right)} \mathrm{i}\operatorname*{Res}_{z=\mathrm{i}} \left\{\frac{1}{G(1+\mathrm{i}z)}\right\} \\
&= e^t G^2\left(\tfrac{1}{2}\right) \frac{G(N)G(N+1)}{G^2\left(N+\frac{1}{2}\right)} \\
&\sim e^t \exp\left(3\zeta'(-1) + \tfrac{1}{12}\ln 2 - \tfrac{1}{2}\ln\pi\right) N^{1/4},
\end{aligned}$$

and

$$|E| = O\left(e^{t+\epsilon t} N^{1/4+\epsilon/2+\epsilon^2/4} (\ln N)^{-1/2}\right).$$

Thus $|E| \ll e^t N^{1/4}$ when

$$e^{t\epsilon} N^{\epsilon/2+\epsilon^2/4} (\ln N)^{-1/2} \ll 1.$$

Thus the error term can be made subdominant if

$$\limsup_{N\to\infty} \frac{t}{\ln N} < -\frac{1}{2}$$

by choosing

$$0 < \epsilon < \min\left\{-2 - 4 \limsup_{N\to\infty} \frac{t}{\ln N}\ ,\ 2\right\},$$

Finally,

$$\mathbb{P}\left\{\mathfrak{Re} \ln Z(\theta) < -x\right\} = \int_{-\infty}^{-x} p(t)\ \mathrm{d}t$$

which completes the proof of the theorem.

Conjecture for the zeta function

Here I will argue that something similar to theorem 6 holds for the Riemann zeta function. Obviously,

$$P(T,x) := \frac{1}{T} meas \left\{0 \le t \le T\ :\ \ln\left|\zeta\left(\tfrac{1}{2} + \mathrm{i}t\right)\right| \le -x\right\}$$

is the analogue of $\mathbb{P}\left\{\ln |Z(\theta)| \le -x\right\}$. So we need to know the equivalent of the moment generating function for $\ln |\zeta(1/2 + it)|$. This is given by the Keating-Snaith conjecture:

Conjecture. (Keating & Snaith [8]). *For fixed k,*

$$\frac{1}{T}\int_0^T |\zeta(\tfrac{1}{2} + \mathrm{i}t)|^{2k}\ \mathrm{d}t \sim \frac{G^2(1+k)}{G(1+2k)} a(k) \left(\ln \frac{T}{2\pi}\right)^{k^2}$$

where

$$a(k) = \prod_{\substack{p \\ \text{prime}}} \left(1 - \frac{1}{p}\right)^{k^2} \sum_{m=0}^{\infty} \left(\frac{\Gamma(m+k)}{m!\,\Gamma(k)}\right)^2 p^{-m}$$

Thus it seems plausible that

$$P(T,x) \approx \int_{-\infty}^{-x} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-\mathrm{i}yz} \frac{G^2(1+\frac{1}{2}\mathrm{i}y)}{G(1+\mathrm{i}y)} a(\tfrac{1}{2}\mathrm{i}y) \left(\ln \frac{T}{2\pi}\right)^{-y^2/4} \mathrm{d}y\ \mathrm{d}z.$$

The Keating-Snaith conjecture is the leading order term in an asymptotic expansion, and there is, *a priori*, no reason to expect the Fourier inverse to make sense. But in [6] it is argued that since the $a(k)$ term has no singularities, maybe for x sufficiently large compared to T, $P(T,x)$ is dominated by the pole at $y = \mathrm{i}$, just as in theorem 6. This argument leads to

Conjecture. (Hughes, Keating & O'Connell [6]). *For large T,*

$$\lim_{x\to\infty} e^x P(T,x) \sim \exp\left(3\zeta'(-1) + \tfrac{1}{12}\ln 2 - \tfrac{1}{2}\ln\pi\right) a(-\tfrac{1}{2}) \left(\ln\frac{T}{2\pi}\right)^{1/4}.$$

Appendix: Barnes' G–function

The Barnes G–function is defined [2] for all z by

$$G(z+1) = (2\pi)^{z/2} \exp\left(-\tfrac{1}{2}\left(z^2 + \gamma z^2 + z\right)\right) \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right)^n e^{-z+z^2/2n}$$

where $\gamma = 0.5772\ldots$ is Euler's constant.

The G-function has the following properties:

Recurrence relation: $G(z+1) = \Gamma(z)G(z)$.

Complex conjugation: $G^*(z) = G(z^*)$.

Asymptotic formula valid for $|z| \to \infty$ with $|\arg(z)| < \pi$,

$$\ln G(z+1) \sim z^2\left(\tfrac{1}{2}\ln z - \tfrac{3}{4}\right) + \tfrac{1}{2}z\ln 2\pi - \tfrac{1}{12}\ln z + \zeta'(-1) + O\left(\frac{1}{z}\right)$$

Special values: $G(1) = 1$ and $G(1/2) = e^{3\zeta'(-1)/2}\pi^{-1/4}2^{1/24}$.

Zeros: $G(z+1)$ has zeros at $z = -n$ of order n, where $n = 1, 2, \ldots$.

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