# On the Riemann-Siegel formula *

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**Abstract**

In this article we derive a generalization of the Riemann-Siegel asymptotic formula for the Riemann zeta function. By subtracting the singularities closest to the critical point we obtain a significant reduction of the error term at the expense of a few evaluations of the error function. We illustrate the efficiency of this method by comparing it to the classical Riemann-Siegel formula.

**Keywords:** Riemann zeta function, Riemann-Siegel formula, asymptotic expansion, incomplete Gamma function

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# 1 Introduction

The Riemann-Siegel (RS) asymptotic formula is a very efficient method to compute the Riemann zeta function $\zeta\left(\frac{1}{2}+it\right)$ for large $t$ and it has been used extensively in the last seventy years to compute the nontrivial zeros of the zeta function (see Odlyzko (1994)). The RS formula contains the main sum of $N = \left[\sqrt{\frac{t}{2\pi}}\,\right]$ terms and the asymptotic correction terms which allow reduction of the error. The function being approximated is actually $Z(t)$, which is defined as $Z(t) = \zeta\left(\frac{1}{2}+it\right)e^{i\theta(t)}$, where

$$\theta(t) = \mathrm{Im}\left\{\ln\Gamma\left(\tfrac{1}{4}+\tfrac{it}{2}\right)\right\} - \frac{t}{2}\ln(\pi). \tag{1}$$

The function $Z(t)$ is real for real $t$ (this follows from the functional equation for $\zeta$) and $|Z(t)| = |\zeta\left(\frac{1}{2}+it\right)|$.

Below we present the RS formula:

$$Z(t) = 2\sum_{n=1}^{N}\frac{\cos(\theta(t)-t\log(n))}{\sqrt{n}} + (-1)^{N-1}\left(\tfrac{2\pi}{t}\right)^{\frac{1}{4}}\left[\sum_{j=0}^{m-1}\left(\tfrac{2\pi}{t}\right)^{\frac{j}{2}}C_j + O\left(t^{-\frac{m}{2}}\right)\right],$$

where the first three correction terms are

$$\begin{aligned} C_0 &= \Psi(\tau) = \frac{\cos\left(2\pi\left(\tau^2-\tau-\frac{1}{16}\right)\right)}{\cos(2\pi\tau)}, \\ C_1 &= -\tfrac{1}{96\pi^2}\Psi^{(3)}(\tau), \\ C_2 &= \tfrac{1}{18432\pi^4}\Psi^{(6)}(\tau) + \tfrac{1}{64\pi^2}\Psi^{(2)}(\tau), \end{aligned} \tag{2}$$

and $\tau = \sqrt{\frac{t}{2\pi}} - N$. To compute $\theta(t)$ for large $t$ one can use the asymptotic expansion derived from the Stirling series:

$$\theta(t) = \tfrac{t}{2}\ln\left(\tfrac{t}{2\pi}\right) - \tfrac{t}{2} - \tfrac{\pi}{8} + \tfrac{1}{48t} + \tfrac{7}{5760t^3} + \ldots. \tag{3}$$

In the last fifteen years, several new asymptotic expansions for the Riemann zeta function have appeared. In Berry & Keating (1992) the authors use the Cauchy integral formula to derive the asymptotic expansion for $Z(t)$, where the leading term $Z_0(t,K)$ is

$$Z_0(t,K) = \mathrm{Re}\sum_{n\geq 1}\frac{\exp(i[\theta(t)-t\ln(n)])}{\sqrt{n}}\mathrm{Erfc}\left(\frac{\xi(n,t)}{Q(K,t)}\sqrt{\tfrac{t}{2}}\right),$$

where $\xi(n,t) = \ln(n) - \theta'(t)$, $Q^2(K,t) = K^2 - it\theta''(t)$ and $K$ is a free real parameter. Note that the leading term is similar to the main sum of the RS, with the cutoff at $n = N$ being smoothed by the complementary error function, thus the approximation to $Z(t)$ is a smooth function, unlike the RS. Authors show that increasing $K$ gives a better accuracy and that (for suitable $K$) the leading term $Z_0(t,K)$ always gives better accuracy than the RS main sum. As $K$ increases to infinity $Z_0$ also contains at least the first correction term $C_0$. Higher correction terms $Z_j(t,K)$ also provide a significant increase in accuracy.

In Paris (1994) the author uses the Poisson summation formula and the uniform asymptotic expansion for the incomplete Gamma function to derive an asymptotic expansion for $Z(t)$. This expansion also involves the complementary error function, although in a different manner compared to the Berry & Keating (1992) approximation. The free parameters in this approximation can be chosen to decrease the error significantly (though again at the expense of computing error functions), see Paris (1994) for details.

In this article we propose another method of approximating $Z(t)$ for large $t$. The result is a generalization of the RS formula with an additional free parameter $\delta$: in essence we replace $\delta$ highest terms in the main sum by $2\delta$ terms involving the incomplete Gamma function and the function $\Psi(\tau)$ in the correction terms is replaced by a similar function $\Psi(\tau,\delta)$. This approximation is obtained by removing $2\delta$ poles of the integrand around the stationary point and then performing asymptotic expansion. We find that the form of the correction terms is the same as in RS, and when $\delta = 0$ we recover the classical RS formula as a special case. Combined with the asymptotic expansion for the incomplete Gamma function derived in Temme (1979) (see also Dunster et al. (1998)) we obtain a simple and efficient method of reducing the error in the RS formula (see section 3 for the numerical results).

# 2 Derivation of the asymptotic formula

We start with the following integral representation for the Riemann zeta function, which Riemann used to prove the functional equation (see Titchmarsh (1986), page 27):

$$\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s) = \Upsilon(s) + \overline{\Upsilon}(1-s), \tag{4}$$

where

$$\Upsilon(s) = e^{-\frac{\pi i s}{2}} 2^{-1-s} \pi^{-\frac{s}{2}-\frac{1}{2}} \Gamma\left(\frac{1-s}{2}\right) \int\limits_{\pi i + e^{\frac{\pi i}{4}}\mathbb{R}} \frac{e^{\frac{iw^2}{4\pi}} w^{s-1}}{\sinh\left(\frac{w}{2}\right)} dw. \tag{5}$$

Note that the integral in equation (5) converges absolutely for all complex $s$. Throughout this article we assume that $s = \frac{1}{2} + it$ and that $t$ is large and positive. To find the stationary point of the integral in (5) we solve $\frac{d}{dw}\left[\frac{iw^2}{4\pi} + it\ln(w)\right] = 0$, thus $w^2 = -2\pi t$ and the stationary points are $\pm i\sqrt{2\pi t}$. We can not move the contour of integration to $w = -i\sqrt{2\pi t}$ because of the branch point at $w = 0$, thus we choose the stationary point $w_0 = i\sqrt{2\pi t}$.

**Remark 1:** Note that equation $w^2 = -2\pi t$ has two real solutions when $t$ is negative, however we do not obtain new asymptotic formulas. We cannot move the contour of integration to $w = \sqrt{-2\pi t}$ because of the branch point at $0$, and if we move the contour of integration to $w = -\sqrt{-2\pi t}$ we would in fact obtain the same asymptotic expansion as by choosing $t$ positive and $w_0 = i\sqrt{2\pi t}$.

In order to obtain the asymptotic representation for the integral in equation (5) we need to move the contour of integration to pass through the stationary point $w_0 = i\sqrt{2\pi t}$, expand function $e^{\frac{iw^2}{4\pi}} w^{s-1}$ in Taylor series around $w_0$ and integrate term by term. However the function $\{\sinh\left(\frac{w}{2}\right)\}^{-1}$ always has poles near the critical point, and this will affect the accuracy of the approximation. Thus we do the following: we fix an integer number $\delta \geq 0$ and subtract $2\delta$ singularities of $\{\sinh\left(\frac{w}{2}\right)\}^{-1}$ around the critical point. Thus we define a function $F_{N,\delta}(w)$ as

$$F_{N,\delta}(w) = \frac{1}{\sinh\left(\frac{w}{2}\right)} - \sum_{n=N+1-\delta}^{N+\delta} \frac{2(-1)^n}{w - 2\pi i n}. \tag{6}$$

Now we move the contour of integration to $w_0$ and we obtain the following decomposition for $\Upsilon(s)$:

$$\begin{aligned}\Upsilon(s) &= \Upsilon_1(s)+\Upsilon_2(s)+\Upsilon_3(s) = \\ &= e^{-\frac{\pi i s}{2}}2^{-1-s}\pi^{-\frac{s}{2}-\frac{1}{2}}\Gamma\left(\frac{1-s}{2}\right)\sum_{n=1}^{N-\delta}2\pi i \text{ Res}_{\,w=2\pi i n}\left[\frac{e^{\frac{iw^2}{4\pi}}w^{s-1}}{\sinh\left(\frac{w}{2}\right)}\right]+ \\ &+ e^{-\frac{\pi i s}{2}}2^{-1-s}\pi^{-\frac{s}{2}-\frac{1}{2}}\Gamma\left(\frac{1-s}{2}\right)\sum_{n=N+1-\delta}^{N+\delta}2(-1)^n\int\limits_{\alpha i+\mathbb{R}}\frac{e^{\frac{iw^2}{4\pi}}w^{s-1}}{w-2\pi i n}dw+ \\ &+ e^{-\frac{\pi i s}{2}}2^{-1-s}\pi^{-\frac{s}{2}-\frac{1}{2}}\Gamma\left(\frac{1-s}{2}\right)\int\limits_{w_0+e^{\frac{\pi i}{4}}\mathbb{R}}e^{\frac{iw^2}{4\pi}}w^{s-1}F_{N,\delta}(w)dw.\end{aligned} \tag{7}$$

First we simplify $\Upsilon_1(s)$ by computing the residues:

$$\Upsilon_1(s)=\pi^{\frac{s-1}{2}}\Gamma\left(\frac{1-s}{2}\right)\sum_{n=1}^{N-\delta}n^{s-1}. \tag{8}$$

Next, we express $\Upsilon_2(s)$ in terms of the incomplete Gamma functions

$$\Upsilon_2(s)=\tfrac{1}{2}\pi^{\frac{s-1}{2}}\Gamma\left(\tfrac{1-s}{2}\right)\sum_{n=N+1-\delta}^{N+\delta}|n|^{s-1}\left[Q\left(\tfrac{1-s}{2};-\pi i n^2\right)+\text{sign}(n)Q\left(1-\tfrac{s}{2};-\pi i n^2\right)\right], \tag{9}$$

where $Q\left(a;x\right)=\frac{\Gamma(a,x)}{\Gamma(x)}$ is the normalized incomplete Gamma function (see Gradshteyn & Ryzhik (2000)). If $n=0$ the term in the sum should be replaced by $-\pi^{\frac{1-s}{2}}e^{-i\theta(t)+\frac{\pi i}{4}(s-1)}/\Gamma\left(\frac{3-s}{2}\right)$. Equation (9) was derived using the following integral

$$\int\limits_{\epsilon i+\mathbb{R}}\frac{e^{-\frac{x^2}{2}}x^{s-1}}{x+bi}dx=\pi i e^{\frac{b^2}{2}+\frac{\pi i s}{2}(1-\hat{b})}(ib)^{s-1}\left[\hat{b}Q\left(\tfrac{1-s}{2};\tfrac{b^2}{2}\right)-Q\left(1-\tfrac{s}{2};\tfrac{b^2}{2}\right)\right], \tag{10}$$

where the argument of $ib$ is between $(-\pi;\pi]$ and $\hat{b}=sign(Re(b))$. To obtain (10) we separate $(x+bi)^{-1}$ into real and imaginary parts and use Gradshteyn & Ryzhik (2000) to evaluate each integral.

Now we have to approximate $\Upsilon_3(s)$. First we perform a change of variables, $w=\sqrt{2\pi i}x+w_0$, and obtain

$$\Upsilon_3(s)=\frac{1}{\sqrt{\pi i}}2^{-1-\frac{s}{2}}t^{\frac{s-1}{2}}e^{-\frac{ti}{2}}\Gamma\left(\frac{1-s}{2}\right)\int\limits_{\mathbb{R}}e^{-x^2}g(t,x)F_{N,\delta}\left(\sqrt{2\pi i}x+w_0\right)dx, \tag{11}$$

where function $g(t,x)$ is defined as

$$g(t,x)=e^{\frac{x^2}{2}-\sqrt{ti}x}\left(1+\frac{x}{\sqrt{ti}}\right)^{-\frac{1}{2}+ti}=e^{\frac{x^2}{2}-\sqrt{ti}x+\left(-\frac{1}{2}+ti\right)\ln\left(1+\frac{x}{\sqrt{ti}}\right)}.$$

Expanding $\ln\left(1+\frac{x}{\sqrt{ti}}\right)$ in a Taylor series we find that (for every $x$) $g(t,x)\to 1$ as $t\to\infty$ and we obtain the following asymptotic expansion

$$\begin{aligned}g(t,x) &= e^{\frac{1}{\sqrt{ti}}\left(\frac{x^3}{3}-\frac{x}{2}\right)-\frac{1}{ti}\left(\frac{x^4}{4}-\frac{x^2}{4}\right)+O\left(t^{-\frac{3}{2}}\right)} = \\ &= 1+\left(-\tfrac{1}{2}x+\tfrac{1}{3}x^3\right)\tfrac{1}{\sqrt{ti}}+\left(\tfrac{3}{8}x^2-\tfrac{5}{12}x^4+\tfrac{1}{18}x^6\right)\tfrac{1}{ti}+O\left(t^{-\frac{3}{2}}\right).\end{aligned} \tag{12}$$

As a next step we substitute (12) into (11) and integrate term by term. To achieve this we need to compute functions $f_n(\tau,\delta) = \int_{\mathbb{R}} e^{-x^2} x^n F_{N,\delta}\left(\sqrt{2\pi i}x + w_0\right) dx$, where $\tau = \sqrt{\frac{t}{2\pi}} - N$. We follow the steps of the derivation of the RS formula in Titchmarsh (1986) and compute the exponential generating function for $f_n(\tau,\delta)$

$$\begin{aligned} \sum_{n\geq 0} \frac{f_n(\tau,\delta)}{n!} u^n &= \int_{\mathbb{R}} e^{-x^2+xu} F_{N,\delta}\left(\sqrt{2\pi i}x + w_0\right) dx = \\ &= \int_{\mathbb{R}} \frac{e^{-x^2+xu}}{\sinh\left(\frac{1}{2}(\sqrt{2\pi i}x + w_0)\right)} dx - \sum_{n=N+1-\delta}^{N+\delta} 2(-1)^n \int_{\mathbb{R}} \frac{e^{-x^2+xu}}{\sqrt{2\pi i}x + w_0 - 2\pi i n} dx = \\ &= (-1)^N \sqrt{2\pi i} e^{\frac{u^2}{4}} \tilde{\Psi}\left(\tau + \tfrac{1}{\sqrt{2\pi i}}\tfrac{u}{2}, \delta\right) \end{aligned} \tag{13}$$

where the function $\tilde{\Psi}(\tau,\delta)$ is defined as

$$\tilde{\Psi}(\tau,\delta) = \frac{\sqrt{2}e^{\frac{3\pi i}{8}} \sin(\pi\tau) - e^{-2\pi i(\tau^2-\tau)}}{\cos(2\pi\tau)} - \sum_{k=1-\delta}^{\delta} (-1)^k e^{-2\pi i(\tau-k)^2} \left[\operatorname{sign}\left(k - \tfrac{1}{2}\right) + \Phi\left(\sqrt{\tfrac{2\pi}{i}}(\tau - k)\right)\right], \tag{14}$$

and $\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$ is the error function (see Gradshteyn & Ryzhik (2000)). The first integral in (13) is one of the Mordell integrals (see Ramanujan (1915), Mordell (1933), Kuznetsov (2006)) and can be computed using the method described in Titchmarsh (1986). The second integral can be found in Gradshteyn & Ryzhik (2000).

Taking $n$-th derivative of both sides of (13) we obtain

$$f_n(\tau,\delta) = (-1)^N \sqrt{2\pi i}\, (8\pi)^{-\frac{n}{2}} e^{-\frac{\pi i n}{4}} \sum_{k=0}^{\left[\frac{n}{2}\right]} \frac{n!}{k!(n-2k)!} (2\pi i)^k\, \tilde{\Psi}^{(n-2k)}(\tau,\delta). \tag{15}$$

Now we use (15), (12) and (11) to obtain the following asymptotic formula for $\Upsilon_3(s)$:

$$\Upsilon_3(s) = \frac{1}{2}(-1)^N 2^{\frac{1-s}{2}} t^{\frac{s-1}{2}} e^{-\frac{ti}{2}} \Gamma\left(\frac{1-s}{2}\right) \left[\tilde{S}_0 + \left(\tfrac{2\pi}{t}\right)^{\frac{1}{2}} \tilde{S}_1 + \left(\tfrac{2\pi}{t}\right) \tilde{S}_2 + O\left(t^{-\frac{3}{2}}\right)\right], \tag{16}$$

where the correction terms are

$$\begin{aligned} \tilde{S}_0 &= \tilde{\Psi}(\tau,\delta) \\ \tilde{S}_1 &= -\tfrac{1}{96\pi^2} \tilde{\Psi}^{(3)}(\tau,\delta) \\ \tilde{S}_2 &= \tfrac{i}{96\pi} \tilde{\Psi}(\tau,\delta) + \tfrac{1}{64\pi^2} \tilde{\Psi}^{(2)}(\tau,\delta) + \tfrac{1}{18432\pi^4} \tilde{\Psi}^{(6)}(\tau,\delta). \end{aligned}$$

Finally, we combine (4), (7), (8), (9) and (16) to obtain the following expression for $Z(t)$:

$$\begin{aligned} Z(t) &= 2\sum_{k=1}^{N-\delta} \frac{\cos(\theta(t) - t\ln(n))}{\sqrt{n}} + \\ &+ \operatorname{Re}\left\{ \sum_{n=N+1-\delta}^{N+\delta} \frac{e^{i(\theta(t) - t\ln(|n|))}}{\sqrt{|n|}} \left[Q\left(\tfrac{1}{4} + \tfrac{it}{2}; \pi i n^2\right) + \operatorname{sign}(n) Q\left(\tfrac{3}{4} + \tfrac{it}{2}; \pi i n^2\right)\right]\right\} + \\ &+ (-1)^N \left(\tfrac{2\pi}{t}\right)^{\frac{1}{4}} \operatorname{Re}\left\{ e^{-i\theta(t)} \left(\tfrac{t}{2\pi e}\right)^{\frac{it}{2}} \left[\tilde{S}_0 + \left(\tfrac{2\pi}{t}\right)^{\frac{1}{2}} \tilde{S}_1 + \left(\tfrac{2\pi}{t}\right) \tilde{S}_2 + O\left(t^{-\frac{3}{2}}\right)\right]\right\}. \end{aligned} \tag{17}$$

We have also used the fact that $\pi^{s-\frac{1}{2}}\frac{\Gamma\left(\frac{1-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right)} = e^{-2i\theta(t)}$ which follows from the definition of $\theta(t)$ (see (1)).

The correction terms in the above equation (17) can be simplified if we use the asymptotic formula (3) to rewrite the factor $e^{-i\theta(t)}\left(\frac{t}{2\pi e}\right)^{\frac{it}{2}}$ as

$$e^{-i\theta(t)}\left(\frac{t}{2\pi e}\right)^{\frac{it}{2}} = e^{\frac{\pi i}{8}-\frac{i}{48t}-\frac{7i}{5760t^3}+\dots}.$$

Thus we introduce the new function $\Psi(\tau,\delta) = -\text{Re}\left\{e^{\frac{\pi i}{8}}\tilde{\Psi}(\tau,\delta)\right\}$, use (14) to simplify the expression for $\Psi(\tau,\delta)$ and present all the results in the following theorem:

**Theorem 1.** *Let $t$ be a real positive number. Define $N = \left[\sqrt{\frac{t}{2\pi}}\,\right]$ and $\tau = \sqrt{\frac{t}{2\pi}} - N$. Fix an integer number $\delta \geq 0$. Then*

$$\begin{aligned} Z(t) &= 2\sum_{k=1}^{N-\delta}\frac{\cos(\theta(t)-t\ln(n))}{\sqrt{n}} + \\ &+ Re\left\{\sum_{n=N+1-\delta}^{N+\delta}\frac{e^{i(\theta(t)-t\ln(|n|))}}{\sqrt{|n|}}\left[Q\left(\tfrac{1}{4}+\tfrac{it}{2};\pi i n^2\right)+sign(n)Q\left(\tfrac{3}{4}+\tfrac{it}{2};\pi i n^2\right)\right]\right\} + \\ &+ (-1)^{N-1}\left(\tfrac{2\pi}{t}\right)^{\frac{1}{4}}\left[\sum_{j=0}^{m-1}\left(\tfrac{2\pi}{t}\right)^{\frac{j}{2}}S_j + O\left(t^{-\frac{m}{2}}\right)\right], \end{aligned} \tag{18}$$

*where the first three correction terms are:*

$$\begin{aligned} S_0 &= \Psi(\tau,\delta) \\ S_1 &= -\tfrac{1}{96\pi^2}\Psi^{(3)}(\tau,\delta) \\ S_2 &= \tfrac{1}{18432\pi^4}\Psi^{(6)}(\tau,\delta) + \tfrac{1}{64\pi^2}\Psi^{(2)}(\tau,\delta). \end{aligned} \tag{19}$$

*and*

$$\Psi(\tau,\delta) = (-1)^{\delta}\frac{\cos\left(2\pi\left(\tau^2-\tau-\frac{1}{16}\right)\right)}{\cos(2\pi\tau)}\cos(4\pi\delta\tau) + \sum_{k=1-\delta}^{\delta}(-1)^k Re\left\{e^{\frac{\pi i}{8}-2\pi i(\tau-k)^2}\Phi\left(\sqrt{\tfrac{2\pi}{i}}(\tau-k)\right)\right\}.$$

*Here $Q(a,z) = \frac{\Gamma(a,z)}{\Gamma(a)}$ is the normalized incomplete Gamma function and $\Phi(x) = \frac{2}{\sqrt{\pi}}\int\limits_0^x e^{-t^2}dt$ is the error function. If $\delta > N$ the $n = 0$ term in the second sum in equation (18) should be replaced by*

$$-\frac{2\pi^{\frac{1}{4}}e^{\frac{\pi i}{8}-\frac{\pi t}{4}}}{\left(\frac{1}{2}+it\right)|\Gamma\left(\frac{1}{4}+\frac{it}{2}\right)|}.$$

.

**Remark 2:** Note that the correction terms (19) have the same form as in the classical RS formula (see equation (2)). This can be explained as follows: the coefficients in front of derivatives of $\Psi(\tau,\delta)$ are obtained from the expansion (12) of $g(t,x)$ and thus do not depend on $\delta$. However, when $\delta = 0$ equation (18) must give us the classical RS formula, thus these coefficients must be the same for all $\delta$.

**Remark 3:** Note that using the asymptotic expansion (12) of $g(t,x)$ is not the only way to approximate the term $\Upsilon_3(s)$. One could prove that if a constant $a$ satisfies $1 < a \le \sqrt{2}$, then $g(t,x)$ can be expanded in convergent series in the Hermite polynomials $H_n(ax)$. In this way we would obtain a *convergent asymptotic series* for $Z(t)$, where the correction terms would also involve linear combinations of the derivatives of $\Psi(\tau,\delta)$. However we found that such an expansion is certainly more complicated and is not as accurate as (18).

**Remark 4:** When $\delta \to +\infty$ we see that the first sum in (18) vanishes, function $\Psi(\tau,\delta) \to 0$ (this follows from equation (13) and the fact that $F_{N,\delta}(w) \to 0$), thus (18) reduces to the following expansion:

$$Z(t) = 2\mathrm{Re}\left\{ e^{i\theta(t)} \sum_{n\ge 1} n^{-s} Q\left(\frac{s}{2}, \pi i n^2\right) - \frac{\pi^{\frac{1}{4}} e^{\frac{\pi i s}{4}}}{s \mid \Gamma\left(\frac{s}{2}\right) \mid} \right\}, \quad s = \frac{1}{2} + it,$$

which was used in Paris & Cang (1997) to derive an asymptotic expansion for $\zeta\left(\frac{1}{2}+it\right)$.

# 3 Numerical results

Before we can use formula (18) we need to be able to compute efficiently the incomplete Gamma function $Q\left(\sigma + \frac{it}{2}; \pi i n^2\right)$, where $\sigma = \frac{1}{4}, \frac{3}{4}$ and $N+1-\delta \le n \le N+\delta$. In applications, especially when $t$ is large, we will be interested in the case when $\delta \ll N$. But then we find that $\frac{\pi i n^2}{\sigma + \frac{it}{2}} \sim 1$, thus we need to approximate $Q(a,z)$ in the region $\frac{z}{a} \sim 1$. Fortunately we have an excellent approximation to $Q(a,z)$ in this region derived in Temme (1979), see also Dunster et al. (1998). Here we present an approximation to $Q(a,z)$ of order $a^{-\frac{5}{2}}$ which is enough for our purposes (for all the details see Temme (1979)).

**Proposition 2.** *Define* $\mu = \frac{z}{a} - 1$ *and* $\eta = \sqrt{2(\mu - \ln(1+\mu))} = \mu\left(1 - \frac{1}{3}\mu + \frac{7}{36}\mu^2 - \frac{73}{540}\mu^3 + \dots\right)$. *Then*

$$Q(a,z) = \tfrac{1}{2}\, Erfc\left(\sqrt{\tfrac{a}{2}}\,\eta\right) + \frac{e^{-\frac{a}{2}\eta^2}}{\sqrt{2\pi a}}\left[c_0 + c_1 a^{-1} + O\left(a^{-2}\right)\right], \tag{20}$$

*where coefficients* $c_0, c_1$ *are given by*

$$\begin{aligned} c_0 &= -\frac{1}{\eta} + \frac{1}{\mu} = \frac{\mu}{\eta}\left(-\frac{1}{3} + \frac{7}{36}\mu - \frac{73}{540}\mu^2 + \dots\right) \\ c_1 &= \frac{1}{\eta^3} - \frac{1+\mu+\frac{\mu^2}{12}}{\mu^3} = \left(\frac{\mu}{\eta}\right)^3\left(-\frac{1}{540} - \frac{7}{4320}\mu + \dots\right) \end{aligned} \tag{21}$$

**Remark 5:** Note that coefficients $c_k$ have removable singularities at $\mu = 0$, thus when $t$ is close to $2\pi n^2$ and parameters $\mu$ and $\eta$ are close to $0$ we have to use the second set of equations in (21), which do not involve subtracting large numbers.

Below we present the numerical results. An approximation to $Z(t)$ given by equation(18) with $m$ correction terms and fixed $\delta$ will be denoted as RS$[m,\delta]$. The classical RS formula will be denoted as RS$[m,0]$.

As we will see, for different choices of parameters $m$ and $\delta$ these approximations have different shapes of the error $Z_{m,\delta}(t) - Z(t)$ as a function of $t$: sometimes the error is smaller for $\tau \sim \frac{1}{2}$ while for other choices of $m$ and $\delta$ the error is smaller at the endpoints $\tau \sim 0$ and $\tau \sim 1$. Thus it is hard to compare the efficiency of approximation RS$[m,\delta]$ at a single point and instead we will present the error graphically for the range of $t$.

First, we compare $\mathrm{RS}[3,0]$ with $\mathrm{RS}[1,3]$, see figure 1. We find that for $10 < t < 70$ approximation $\mathrm{RS}[1,3]$ is actually better and for $200 < t < 600$ both of these approximations have comparable accuracy. For $t$ even larger $\mathrm{RS}[3,0]$ becomes a better approximation, since it has an error term of the order $O\left(t^{-\frac{7}{4}}\right)$ while $\mathrm{RS}[1,3]$ is $O\left(t^{-\frac{3}{4}}\right)$. But we find that even at large $t$ we could increase $\delta$ and make $\mathrm{RS}[1,\delta]$ as good as $\mathrm{RS}[3,0]$: for example at $15000 < t < 17000$ we find that $\delta = 6$ is enough for this purpose.

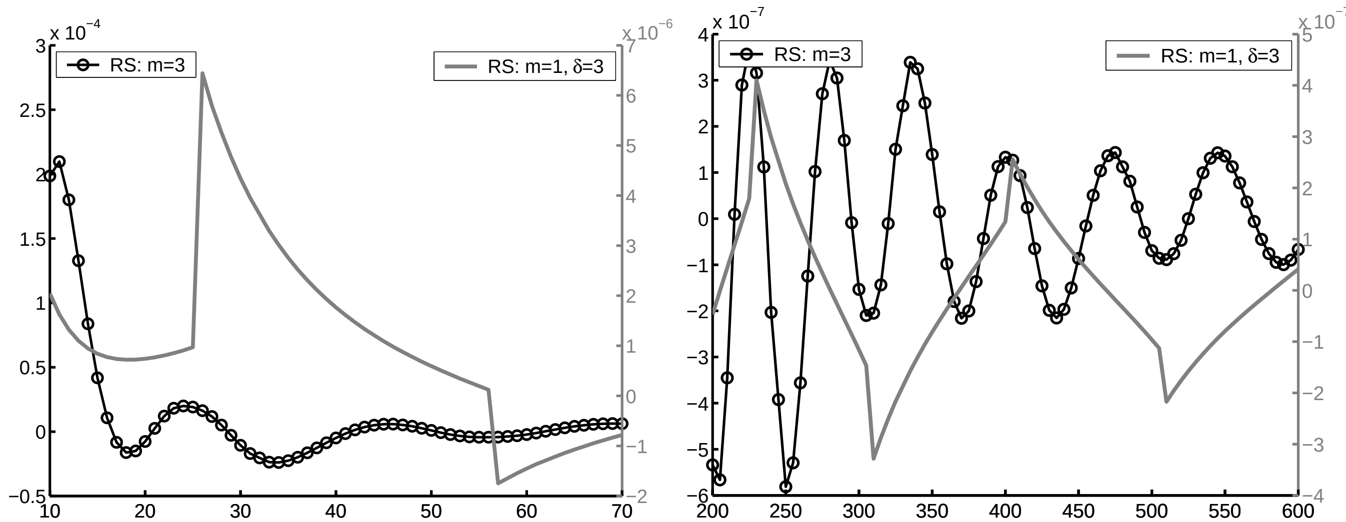


Figure 1: The error for $t \in [10,70]$ $(1 \le N \le 3)$ and $t \in [200,600]$ $(5 \le N \le 9)$.

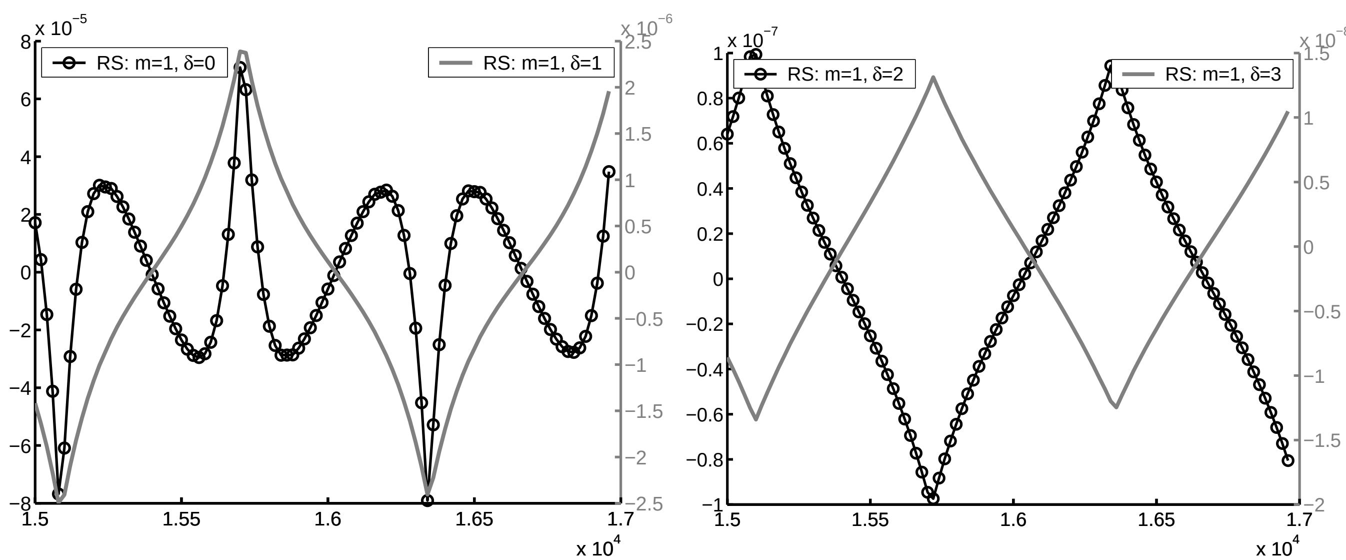


Figure 2: The error for $t \in [15000,17000]$ $(49 \le N \le 52)$. $m = 1$ and $\delta$ increases from $0$ to $3$.

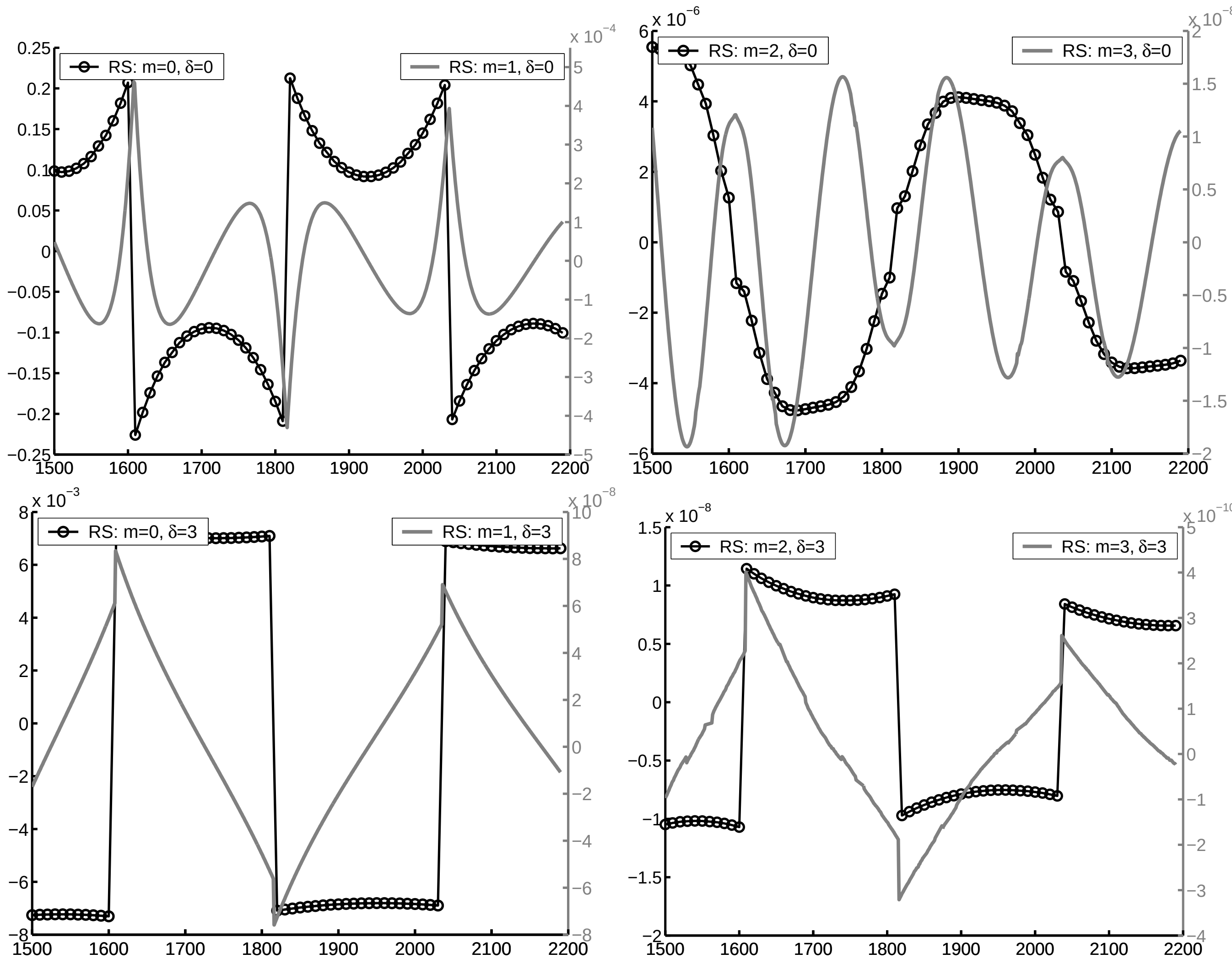


Figure 3: The error for $t \in [1500, 2200]$ ($15 \leq N \leq 18$). $m$ increases from $0$ to $3$, $\delta = 0$ in the top row and $\delta = 3$ in the bottom row.

Second, we examine the effects of increasing $\delta$ while keeping $m = 1$ fixed (see figure 2) in the region $15000 < t < 17000$. We see that increasing $\delta$ by 1 decreases the error roughly by a factor of 10. Also note that the shape of the error (the shape of the graph of the next correction term) becomes more linear as $\delta$ increases. This is easy to explain if we remember that $2\delta$ is the number of subtracted singularities, thus for larger $\delta$ function $\Psi(\tau, \delta)$ and its derivatives become less oscillatory. This fact means that instead of computing $\Psi(\tau, \delta)$ and its derivatives we can efficiently approximate the correction term by just a few terms of its expansion in a Taylor series (or Chebyshev polynomials).

Finally, we examine the effects of increasing the number of correction terms, while keeping $\delta$ fixed (see figure 3). In the top (bottom) row we plot the absolute error of RS$[m, 0]$ (RS$[m, 3]$) when $m$ increases from $0$ to $3$. Note the decrease of 5 orders of magnitude as $m$ goes from $0$ to $1$ in the second row ($\delta = 3$), while in the top row ($\delta = 0$) we have a decrease of 3 orders of magnitude. After this fast initial decrease we gain roughly 1 order of magnitude in the bottom row and 2 orders in the top row. This seems to be a general trend: the error decreases faster with the increase in $m$ for small $\delta$ compared to large $\delta$. Note again that in the bottom row ($\delta = 3$) the correction terms are smoother compared to the top row ($\delta = 0$).

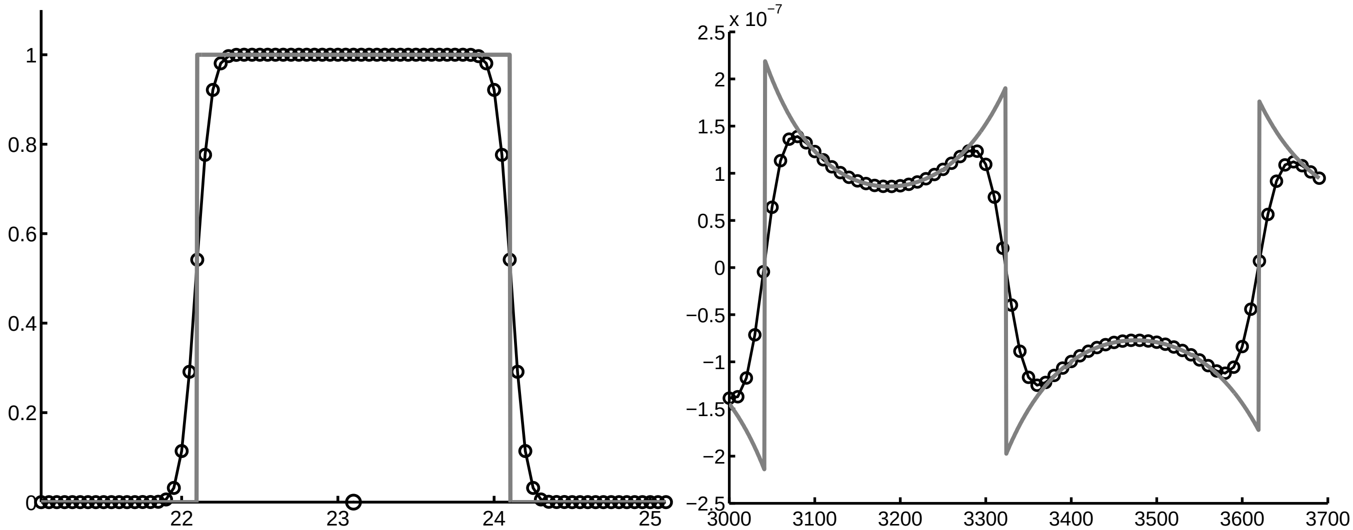


Figure 4: The effect of using a smooth cutoff function. $t \in [3000, 3700]$ ($22 \leq N \leq 24$), $m = 2$ and $\delta = 1$

# 4 Conclusion

In this article we present a generalization of the Riemann-Siegel asymptotic formula, which allows to obtain a significant increase in the accuracy without a lot of extra computational effort. This approximation has an extra free integer parameter $\delta \geq 0$, which corresponds to half of the number of the singularities removed around the critical point. In general increasing $\delta$ results in the decrease of the error.

In this article we compared this new approximation scheme to the classical RS formula, and found that the new formula consistently gives better accuracy even for small $\delta$. We did not compare our approximation to other results, such as approximations by Berry & Keating (1992) or by Paris (1994): while it seems that our approximation can achieve the same accuracy, the question is at what computational cost. To answer this question one would have to optimize approximation schemes. Note that in our scheme there are several things that can be done to reduce the computational cost to just $2\delta$ evaluations of the error function:

1. In equation (18) we have two incomplete gamma functions $Q\left(\sigma + \frac{it}{2}; \pi i n^2\right)$ with $\sigma = \frac{1}{4}, \frac{3}{4}$, but when $t$ is large we can approximate them with just a few terms of the Taylor series around $\sigma_0 = \frac{1}{2}$.

2. The almost linear form of the graphs of correction terms (see figures 2 and 3) suggests an approximation by polynomials: one could use just a few terms of either the Taylor series around $\tau = \frac{1}{2}$ or the Chebyshev series to approximate $S_j$.

An advantage of the Berry & Keating (1992) asymptotic formula is that the approximation terms are smooth functions of $t$; in the approximation by Paris (1994) one can also choose $N \neq \left[\sqrt{\frac{t}{2\pi}}\right]$ and thus have a smooth approximation at the transition points. There is also a simple way to do it in our approximation: instead of completely removing $2\delta$ singularities around the critical point $t_0 = \sqrt{\frac{t}{2\pi}}$, we can assign to every singularity a weight, depending on the distance from the critical point. For example, Theorem 1 could be obtained using the following weights: if the singularity is within the distance of $2\pi\delta$ from the critical point $t_0$, it is assigned the weight of $1$ and is removed completely, otherwise the weight is $0$ (see equation (6)). Note that this scheme is equivalent to using a sharp cutoff function with jumps at $\pm 2\pi\delta$ (see figure 4), and these jumps create discontinuities in the RS formula. However, one could also use a smooth cutoff function, where the weight of each singularity is $1$ if it is close to the critical point $t_0$ and the weight would decrease smoothly to $0$ as the distance to $t_0$ increases (see figure 4). The result of using a smooth cutoff function is that the error at the transition points $t \sim 2\pi n^2$ is certainly smaller, but at the same time the computational complexity is increased: note that on figure 4 the sharp cutoff contains just 2 transition points $n = 23$ and $n = 24$, while the smooth cutoff also contains $n = 22$ and we will need more evaluations of the error function. Another undesirable feature of using the smooth cutoff is that the correction terms become dependent on $t$ and not just on $\tau$ as with the sharp cutoff.

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