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A LOCAL LIMIT THEOREM FOR COEFFICIENTS OF MODIFIED BORWEIN'S METHOD

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Abstract. The paper extends the study of the modified Borwein method for the calculation of the Riemann zeta-function. It presents an alternative perspective on the proof of a local limit theorem for coefficients of the method. The new approach is based on the connection with the limit theorem applied to asymptotic enumeration.

1. Introduction

In [1] we introduced a modification of Borwein's method for the calculation of the Riemann zeta-function and proposed an asymptotic expression for the coefficients of the method. The asymptotic modification of the algorithm proved to be more than three times faster than the original one ([1]). Borwein's method for calculating Riemann zeta-function is based on the alternating series convergence ([4]). It applies to complex numbers $s = \sigma + it$ with $\sigma \geqslant 1/2$.

Let

$$d_{nk} = n \sum_{i=0}^{k} \frac{(n+i-1)!4^i}{(n-i)!(2i)!}, \quad n \in \mathbb{N}, \ \ 0 \leqslant k \leqslant n,$$

then the Riemann zeta-function

$$\zeta(s) = \frac{1}{d_{nn}(1-2^{1-s})} \sum_{k=0}^{n-1} \frac{(-1)^k (d_{nn} - d_{nk})}{(k+1)^s} + \gamma_n(s),$$

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where

$$|\gamma_n(s)| \leqslant \frac{3}{(3+\sqrt{8})^n} \frac{(1+2|t|)e^{\frac{\pi|t|}{2}}}{|1-2^{1-s}|}.$$

It is challenging to compute coefficients d_{nk} for large n directly (because of factorials in the definition). Therefore we have introduced a modification of the method. Let $c_{nk} = 1 - d_{nk}/d_{nn}, \quad 0 \leqslant k \leqslant n-1$. Now

$$\zeta(s) = \sum_{k=0}^{n-1} \frac{(-1)^k c_{nk}}{(k+1)^s} + \gamma_n(s).$$

Let

$$u_{nk} = n\frac{(n+k-1)!4^k}{(n-k)!(2k)!}, \quad n \in \mathbb{N},\ \ 0 \leqslant k \leqslant n. \tag{1.1}$$

Now we can calculate d_{nk} recurrently, i.e. $d_{nk} = d_{n,k-1} + u_{nk}$, $d_{n0} = 1$, and

$$c_{nk} = 1 - \sum_{i=0}^{k} a_{ni},$$

where

$$a_{nk} = \frac{u_{nk}}{\sum_{i=0}^{n} u_{ni}}. \tag{1.2}$$

In [1] we proved a local limit theorem for coefficients of modified Borwein's method. Note that throughout the paper, all limits, whenever unspecified, will be taken as $n \to \infty$.

Theorem 1.1 (I. Belovas, L. Sakalauskas [1]). *Let* $\mu_n = \frac{n}{\sqrt{2}}$, $\sigma_n = \frac{\sqrt{n}}{2\sqrt[4]{2}}$. *Numbers* a_{nk} *satisfy a local limit theorem*

$$\lim_{n\to\infty} \sup_k |a_{nk} - \varphi_{\mu_n,\sigma_n}(k)| = 0,$$

where $\varphi_{\mu,\sigma}(x)$ *is the probability density function of the normal distribution with the mean* μ *and the standard deviation* σ.

The theorem was proved in a "straightforward" way, using Stirling's formula. However, alternative perspective reveals the connection with combinatorial numbers and calls for application of the results of asymptotic enumeration theory ([6]). We will use a general local limit theorem by E. A. Bender, based on the nature of the generating function $\sum u_{nk} z^n w^k$.

Theorem 1.2 (E. A. Bender [3]). *Let* $f(z,w)$ *have a power series expansion*

$$f(z,w) = \sum_{n,k\geqslant 0} u_{nk} z^n w^k \tag{1.3}$$

with non-negative coefficients and let $a < b$ be real numbers. Define

$$R(\varepsilon) = \{z : a \leqslant \Re z \leqslant b, \quad |\Im z| \leqslant \varepsilon\}.$$

Suppose there exists $\varepsilon > 0, \delta > 0$, a non-negative integer m, and functions $A(s)$, $r(s)$ such that

(i) *an $A(s)$ is continuous and non-zero for $s \in R(\varepsilon)$,*
(ii) *an $r(s)$ is non-zero and has a bounded third derivative for $s \in R(\varepsilon)$,*
(iii) *for $s \in R(\varepsilon)$ and $|z| \leqslant |r(s)|(1+\delta)$ function*

$$\left(1 - \frac{z}{r(s)}\right)^m f(z, e^s) - \frac{A(s)}{1 - z/r(s)} \tag{1.4}$$

is analytic and bounded,

(iv) $(r'(\alpha)/r(\alpha))^2 - r''(\alpha)/r(\alpha) \neq 0$ *for* $a \leqslant \alpha \leqslant b$,
(v) $f(z, e^s)$ *is analytic and bounded for*

$$|z| \leqslant |r(\Re s)|(1+\delta), \qquad \varepsilon \leqslant |\Im s| \leqslant \pi.$$

Then we have

$$u_{nk} \sim \frac{n^m e^{-\alpha k} A(\alpha)}{m! r^n(\alpha) \vartheta_\alpha \sqrt{2\pi n}} \tag{1.5}$$

uniformly for $a \leqslant \alpha \leqslant b$, where

$$\frac{k}{n} = -\frac{r'(\alpha)}{r(\alpha)}, \qquad \vartheta_\alpha = \left(\frac{k}{n}\right)^2 - \frac{r''(\alpha)}{r(\alpha)}. \tag{1.6}$$

2. Local limit theorem for the coefficients u_{nk}

First, we prove an auxiliary lemma, identifing the generating function (1.3) of coefficients u_{nk} (1.1).

LEMMA 2.1. *Suppose that*

$$u_{nk} = \begin{cases} 1 & n = k = 0, \\ 0 & k > n, \\ n\frac{(n+k-1)!4^k}{(n-k)!(2k)!} & \textit{otherwise}, \end{cases} \tag{2.1}$$

then the generating function

$$\sum_{n,k \geqslant 0} u_{nk} x^n y^k = \frac{1}{2}\left(1 + \frac{1}{2x^{-1}\Theta(y) - 1} - \frac{1}{2x\Theta(y) - 1}\right). \tag{2.2}$$

Here

$$\Theta(y) = y + \sqrt{y + y^2} + 1/2.$$

Proof. By definition (2.1), we have the recurrent expression

$$u_{nk} = u_{n,k-1} \frac{4(n+k-1)(n-k+1)}{(2k-1)(2k)}. \tag{2.3}$$

Let us consider the generating function (2.2),

$$f(x,y) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} u_{nk} x^n y^k.$$

Taking into account that $u_{n0} = 1$ and (2.3), we obtain the expresion

$$\begin{aligned} f(x,y) &= \sum_{n=0}^{\infty} u_{n0} x^n + \sum_{n=0}^{\infty} \sum_{k=1}^{\infty} u_{n,k-1} \frac{4(n+k-1)(n-k+1)}{(2k-1)(2k)} x^n y^k \\ &= \frac{1}{1-x} + 4 \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} u_{n,k} \frac{(n+k)(n-k)}{(2k+1)(2k+2)} x^n y^{k+1}, \end{aligned} \tag{2.4}$$

yielding the integral equation

$$\begin{aligned} f(x,y) = \frac{1}{1-x} &- y f(x,y) + \frac{3}{2} \int_0^y f(x,t) dt + \\ &+ \int_0^{\sqrt{y}} \int_0^u 4x f_x(x,t^2) + 4x^2 f_{xx}(x,t^2) - f(x,t^2) dt du. \end{aligned}$$

It gives us the linear partial differential equation of the second order,

$$x^2 f_{xx} - (y + y^2) f_{yy} + x f_x - (1/2 + y) f_y = 0.$$

Note that, in view of (2.4), we have initial conditions

$$f(x,0) = \frac{1}{1-x}, \qquad f_y(x,0) = 0.$$

Solving the equation (e.g., by the method of characteristics), we obtain

$$f(x,y) = \frac{1}{2} \left(1 + \frac{1}{2x^{-1}\Theta(y) - 1} - \frac{1}{2x\Theta(y) - 1} \right),$$

which yields us the statement of the lemma. ∎

Now we can proceed with the local limit theorem for coefficients u_{nk} (2.1).

Theorem 2.2. *Let*

$$\mu_n = \frac{n}{\sqrt{2}}, \ \sigma_n^2 = \frac{n\sqrt{2}}{8}, \tag{2.5}$$

then for all k*, such that*

$$|k - \mu_n| = o(\sigma_n^{4/3}), \tag{2.6}$$

we have

$$u_{nk} \sim \frac{(1+\sqrt{2})^{2n}}{2\sqrt{2\pi}\sigma_n} \exp\left(-\frac{(k-\mu_n)^2}{2\sigma_n^2} \right).$$

PROOF. By Lemma 2.1, the generating function

$$f(z,e^s) = \frac{1}{2}\left(1 + \frac{1}{2z^{-1}\Theta(s)-1} - \frac{1}{2z\Theta(s)-1}\right) = \frac{4\Theta^2(s) - 4z^{-1}\Theta(s)+1}{2(2z^{-1}\Theta(s)-1)(2z\Theta(s)-1)},$$

where we write $\Theta(s)$ in place of $\Theta(e^s)$.

Let $r(s)$ (cf. Theorem 1.2) be a root of the function

$$h(z,e^s) = (2z^{-1}\Theta(s)-1)(2z\Theta(s)-1).$$

This function has two roots, $z_1 = 2\Theta(s)$ and $z_2 = (2\Theta(s))^{-1}$. Let us denote

$$r_1(s) = 2\Theta(s), \qquad r_2(s) = \frac{1}{2\Theta(s)}. \tag{2.7}$$

Calculating derivatives, we obtain

$$\frac{r_1'(0)}{r_1(0)} = \frac{1}{\sqrt{2}} > 0, \qquad \frac{r_2'(0)}{r_2(0)} = -\frac{1}{\sqrt{2}} < 0.$$

By Bender ([3, Theorem 1]), the mean $\mu_n = n\mu$ and $\mu = -r'(0)/r(0)$. Note that by definitions (1.1)-(1.2), numbers u_{nk} and a_{nk} are positive. Thus, to obtain positive μ, we choose the root $r_2(s)$, corresponding the negative ratio. Hence, by (2.7), we have

$$r(s) = r_2(s) = \frac{1}{2\Theta(s)} = \frac{1}{2(e^s + \sqrt{e^s + e^{2s}} + 1/2)}. \tag{2.8}$$

Thus,

$$\frac{r'(s)}{r(s)} = -\sqrt{\frac{e^s}{e^s+1}}, \qquad \frac{r'(0)}{r(0)} = -\frac{1}{\sqrt{2}}, \tag{2.9}$$

and

$$\frac{r''(s)}{r(s)} = \frac{e^s}{e^s+1} - \frac{1}{2}\sqrt{\frac{e^s}{(e^s+1)^3}}, \qquad \frac{r''(0)}{r(0)} = \frac{1}{2} - \frac{\sqrt{2}}{8}. \tag{2.10}$$

Next, consider the function $A(s)$ (cf. (1.4) of Theorem 1.2) as the limit

$$A(s) = \lim_{z\to r(s)} f(z,e^s)\left(1 - \frac{z}{r(s)}\right)^{m+1}.$$

Here $m+1$ is the order of the pole. Note that, if the pole is simple, then $m = 0$. Calculating $A(s)$ we obtain

$$A(s) = \lim_{z\to r(s)} \frac{1}{2}\left(1 + \frac{1}{2z^{-1}\Theta(s)-1} - \frac{1}{2z\Theta(s)-1}\right)\left(1 - \frac{z}{r(s)}\right) = \lim_{z\to r(s)} \frac{1}{2}\left(1 + \frac{1}{z^{-1}r^{-1}(s)-1} - \frac{1}{zr^{-1}(s)-1}\right)\left(1 - \frac{z}{r(s)}\right) = \frac{1}{2}.$$

The function (1.4)

$$\left(1-\frac{z}{r(s)}\right)^m f(z,e^s)-\frac{A(s)}{1-z/r(s)}=\frac{\Theta(s)}{2\Theta(s)-z}$$

is analytic and bounded for

$$|s|<\varepsilon, \qquad |z|<|r(0)|+\delta=3-2\sqrt{2}+\delta.$$

Thus, conditions (i)-(iii) and (v) of Theorem 1.2 are satisfied. To verify the condition (iv), we must calculate the expression $(r'(\alpha)/r(\alpha))^2-r''(\alpha)/r(\alpha)$. By (2.9) and (2.10) we have

$$\left(\frac{r'(\alpha)}{r(\alpha)}\right)^2-\frac{r''(\alpha)}{r(\alpha)}=\frac{1}{2}\sqrt{\frac{e^\alpha}{(e^\alpha+1)^3}}\neq 0.$$

We obtain the parameter α by solving the equation

$$\frac{k}{n}=-\frac{r'(\alpha)}{r(\alpha)}.$$

Using (2.9) we get

$$\frac{k}{n}=\frac{1}{\sqrt{1+e^{-\alpha}}}.$$

Hence,

$$e^\alpha=\frac{k^2}{n^2-k^2}.$$

Next (cf. (1.6) and (2.8)),

$$\vartheta_\alpha^2=\frac{1}{2}\sqrt{\frac{e^\alpha}{(e^\alpha+1)^3}}=\frac{1}{2e^\alpha}\left(\frac{e^\alpha}{e^\alpha+1}\right)^{3/2},$$

$$r^n(\alpha)=(2(e^\alpha+\sqrt{e^\alpha+e^{2\alpha}}+1/2))^{-n}.$$

Now we can calculate (1.5) of Theorem 1.2,

$$\begin{aligned} u_{nk} &\sim \frac{e^{-\alpha k}\frac{1}{2}}{r^n(\alpha)\vartheta_\alpha\sqrt{2\pi n}} \\ &= \frac{(2(e^\alpha+\sqrt{e^\alpha+e^{2\alpha}}+1/2))^n}{2\sqrt{\pi n}e^{\alpha(k-1/2)}\left(\frac{e^\alpha}{e^\alpha+1}\right)^{3/4}} = \frac{\left(\frac{n+k}{n-k}\right)^n\left(\frac{k}{n}\right)^{-3/2}}{2\sqrt{\pi n}\left(\frac{k^2}{n^2-k^2}\right)^{k-1/2}} \\ &= \frac{(1+\sqrt{2})^{2n}}{2\sqrt{2\pi}\sigma_n}\frac{\sqrt[4]{2}}{2}\frac{\left(\frac{1+\frac{k}{n}}{1-\frac{k}{n}}\right)^n}{(1+\sqrt{2})^{2n}}\frac{\left(\left(1-\frac{k}{n}\right)\left(1+\frac{k}{n}\right)\right)^{k-1/2}}{\left(\frac{k}{n}\right)^{2k+1/2}} \qquad (2.11) \\ &= \frac{(1+\sqrt{2})^{2n}}{2\sqrt{2\pi}\sigma_n}\underbrace{\frac{\sqrt[4]{2}/2}{\sqrt{\left(1-\frac{k}{n}\right)\left(1+\frac{k}{n}\right)\frac{k}{n}}}}_{=\theta_{nk}}\underbrace{\frac{\left(1+\frac{k}{n}\right)^{n+k}\left(1-\frac{k}{n}\right)^{-n+k}}{(1+\sqrt{2})^{2n}\left(\frac{k}{n}\right)^{2k}}}_{=\delta_{nk}}. \end{aligned}$$

Note that by (2.5) and (2.6), we have

$$\left|\frac{k}{n}-\frac{1}{\sqrt{2}}\right|=o\left(\frac{1}{\sqrt[3]{n}}\right), \tag{2.12}$$

hence $k/n \to 1/\sqrt{2}$, while $n \to \infty$. Thus, $\theta_{nk} \to 1$.

Let us denote

$$x=\frac{k-\mu_n}{\sigma_n}.$$

By (2.5), we have

$$\frac{k}{n}=\frac{1}{\sqrt{2}}+\frac{x}{2\sqrt[4]{2}\sqrt{n}},$$

and by (2.12), we have

$$|x|=o(\sqrt[6]{n}). \tag{2.13}$$

Calculating the logarithm of δ_{nk} (2.11), we get

$$\begin{aligned}
\log\delta_{nk} &= -2n\log(1+\sqrt{2})-\left(n\sqrt{2}+\frac{x\sqrt{n}}{\sqrt[4]{2}}\right)\log\left(\frac{1}{\sqrt{2}}+\frac{x}{2\sqrt[4]{2}\sqrt{n}}\right)\\
&\quad+\left(n+\frac{n}{\sqrt{2}}+\frac{x\sqrt{n}}{2\sqrt[4]{2}}\right)\log\left(1+\frac{1}{\sqrt{2}}+\frac{x}{2\sqrt[4]{2}\sqrt{n}}\right)\\
&\quad+\left(-n+\frac{n}{\sqrt{2}}+\frac{x\sqrt{n}}{2\sqrt[4]{2}}\right)\log\left(1-\frac{1}{\sqrt{2}}-\frac{x}{2\sqrt[4]{2}\sqrt{n}}\right)\\
&= -2n\log(1+\sqrt{2})\\
&\quad-\left(n\sqrt{2}+\frac{x\sqrt{n}}{\sqrt[4]{2}}\right)\left(\log\frac{1}{\sqrt{2}}+\log\left(1+\frac{x}{\sqrt{2}\sqrt[4]{2}\sqrt{n}}\right)\right)\\
&\quad+\left(\frac{1+\sqrt{2}}{\sqrt{2}}n+\frac{x\sqrt{n}}{2\sqrt[4]{2}}\right)\left(\log\frac{\sqrt{2}+1}{\sqrt{2}}+\log\left(1+\frac{x(\sqrt{2}-1)}{\sqrt{2}\sqrt[4]{2}\sqrt{n}}\right)\right)\\
&\quad+\left(\frac{1-\sqrt{2}}{\sqrt{2}}n+\frac{x\sqrt{n}}{2\sqrt[4]{2}}\right)\left(\log\frac{\sqrt{2}-1}{\sqrt{2}}+\log\left(1-\frac{x(\sqrt{2}+1)}{\sqrt{2}\sqrt[4]{2}\sqrt{n}}\right)\right).
\end{aligned}$$

Using Taylor series expansions for logarithms, we obtain for large enough n,

$$\log\delta_{nk} = -2n\log(1+\sqrt{2}) + \Big(n\sqrt{2} + \frac{x\sqrt{n}}{\sqrt[4]{2}}\Big)\Big(\frac{1}{2}\log 2 - \\ - \frac{x}{\sqrt{2}\sqrt[4]{2}\sqrt{n}} + \frac{x^2}{4\sqrt{2}n} + O\Big(\frac{x^3}{n\sqrt{n}}\Big)\Big) + \Big(\frac{1+\sqrt{2}}{\sqrt{2}}n + \\ + \frac{x\sqrt{n}}{2\sqrt[4]{2}}\Big)\Big(\log\frac{\sqrt{2}+1}{\sqrt{2}} + \frac{x(\sqrt{2}-1)}{\sqrt{2}\sqrt[4]{2}\sqrt{n}} - \frac{x^2(\sqrt{2}-1)^2}{4\sqrt{2}n} + \\ + O\Big(\frac{x^3}{n\sqrt{n}}\Big)\Big) + \Big(\frac{1-\sqrt{2}}{\sqrt{2}}n + \frac{x\sqrt{n}}{2\sqrt[4]{2}}\Big)\Big(\log\frac{\sqrt{2}-1}{\sqrt{2}} - \\ - \frac{x(\sqrt{2}+1)}{\sqrt{2}\sqrt[4]{2}\sqrt{n}} - \frac{x^2(\sqrt{2}+1)^2}{4\sqrt{2}n} + O\Big(\frac{x^3}{n\sqrt{n}}\Big)\Big).$$

By multiplying factors and combining like terms, we obtain

$$\log\delta_{nk} = -\frac{x^2}{2} + O\left(\frac{x^3}{\sqrt{n}}\right),$$

which, combined with (2.11) and (2.13), yields us the statement of the theorem. ∎

Remark 2.3. Theorem 2.2 yields us the asymptotic equivalence

$$\sum_{k=0}^{n} u_{nk} \sim \frac{1}{2}(1+\sqrt{2})^{2n}$$

(cf. [1, Lemma 2.1]).

Remark 2.4. A central limit theorem for the coefficients of modified Borwein's method can be proved analogically, using Bender's central limit theorem applied to asymptotic enumeration (Theorem 1, [2, 3]. However, the approach, based on Hwang's limit theorem ([5]), yields stronger result, enabling us to evaluate the rate of convergence to normal distribution (cf. [1, Theorem 3.1]).

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