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An IMT-type Quadrature Formula with the Same Asymptotic Performance as the DE Formula

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1 Introduction

In the family of numerical quadrature formulas obtained by variable transformation, there are the IMT formula [1, 2] and the DE formula [5]. The DE formula has an asymptotic error estimate $O(\exp(-cN/\log N))$, where N is the number of the sampling points, and c is a positive constant independent of N. On the other hand, the asymptotic error of the IMT formula behaves as $O(\exp(-c\sqrt{N}))$. DE formula's performance is therefore better than IMT's. Though the repeated application of the IMT-type transformation [4] is known to give a substantial improvement to the IMT formula, the asymptotic error of the IMT-Double formula including the IMT-type double exponential formula [3], the IMT-Triple formula, the IMT-Quadruple formula, $\cdots$ behaves as $O(\exp(-cN/(\log N)^2))$, $O(\exp(-cN/((\log N)(\log\log N)^2)))$, $O(\exp(-cN/((\log N)(\log\log N)(\log\log\log N)^2)))$, $\cdots$, which do not attain the performance of the DE formula still. We propose in the present paper an IMT-type quadrature formula with the asymptotic error estimate $O(\exp(-cN/\log N))$. The idea of the proposed formula is to optimally choose the parameters of the IMT-type transformation depending on the number N of sampling points.

2 IMT Formula

First of all, we review the IMT formula. The IMT formula consists of a change of variable and the trapezoidal rule with equal mesh size. The trapezoidal rule with equal mesh size is known to be very efficient if applied in the following cases:

1. integration of a periodic smooth function;

2. integration of a smooth function over the entire interval $(-\infty, \infty)$.

The IMT formula uses a variable transformation of the first case. On the other hand, the DE formula uses a variable transformation of the second case.

A typical IMT formula uses the following variable transformation:

$$x = \phi(t) = \frac{1}{Q}\int_0^t \exp\left(-\frac{1}{s} - \frac{1}{1-s}\right) \mathrm{d}s, \quad Q = \int_0^1 \exp\left(-\frac{1}{s} - \frac{1}{1-s}\right) \mathrm{d}s$$

and transforms a given integral

$$I = \int_0^1 f(x)\,\mathrm{d}x$$

into

$$I = \int_0^1 f(\phi(t))\phi'(t)\,\mathrm{d}t,$$

whose integrand becomes a smooth periodic function. Applying the trapezoidal rule with equal mesh size h results in the IMT formula:

$$I_h = h\sum_{n=1}^{N-1} f(\phi(nh))\phi'(nh), \quad h = 1/N.$$

The error of the IMT formula is asymptotically estimated [1, 2, 4] as

$$|I - I_h| = O(\exp(-c\sqrt{N})),$$

where c is independent of N.

3 Proposed IMT-type Quadrature

Let the given integral be

$$I = \int_{-1}^1 f(x)\,\mathrm{d}x. \tag{1}$$

An IMT-type transformation

$$x = \phi_{m,k}(t) = \mathrm{erf}\left(\frac{k}{(1-t)^m} - \frac{k}{(1+t)^m}\right), \quad \mathrm{erf}\,x = \frac{2}{\sqrt{\pi}}\int_0^x \mathrm{e}^{-t^2}\,\mathrm{d}t \tag{2}$$

gives the following formula of IMT-type:

$$I_h = h\sum_{n=1}^{N-1} f(\phi_{m,k}(-1+nh))\phi'_{m,k}(-1+nh), \quad h = 2/N, \tag{3}$$

where m, k are positive parameters which may depend on N. The reason to use the function $\mathrm{erf}\,x$ is that we can easily compute the integral and that the error estimation becomes easier. The feature in this proposal is to choose the optimal parameter depending on $N = 2/h$.

In order to estimate the error, we assume that f is analytic in some complex domain which contains $(-1, 1)$. By the error analysis in Appendix 1, the error terms of the quadrature (3) are given as $|I - I_h| \sim E_1 + E_2$,

$$\begin{aligned} E_1 &= A_1 \exp\left(-\left(\alpha' k^2\right)^{\frac{1}{2m+1}} \left(\frac{\pi N}{2m}\right)^{\frac{2m}{2m+1}} \cdot (2m+1) \sin\frac{\pi/2}{2m+1}\right), &(4)\\ E_2 &= A_2 \exp\left(-\frac{\pi^{3/2}\beta' N}{4mk}\right), &(5)\end{aligned}$$

where α', β' are positive constants depending on singularities of f, and A_1, A_2 are positive constants depending on f. We first choose the parameters so that E_1 equals E_2, and approximately optimize the order of E_1, E_2 in addition. Then, the parameters are

$$m = \frac{1}{2}\log N, \quad k = \frac{\mathrm{e}\beta'}{\sqrt{\pi}} \tag{6}$$

and the error terms are evaluated asymptotically as follows

$$\log E_1 \sim \log E_2 \sim -\frac{\pi^2 N}{2\mathrm{e}\log N}, \quad N \to \infty.$$

In fact,

$$\left(\frac{\pi N}{2m}\right)^{\frac{2m}{2m+1}} = \frac{\pi N}{2m}\left(\frac{2m}{\pi N}\right)^{\frac{1}{2m+1}} = \frac{\pi N}{\log N}\left(\frac{2m}{\pi \mathrm{e}^{2m}}\right)^{\frac{1}{2m+1}} = \frac{\pi N}{\log N}\left(\frac{1}{\mathrm{e}} + o(1)\right),$$

and

$$(2m+1)\sin\frac{\pi/2}{2m+1} = \frac{\pi}{2} + o(1), \quad m \to \infty.$$

Therefore, when the parameters are chosen as in (6), the error of our formula is estimated as

$$|I - I_h| = O(\exp(-cN/\log N)). \tag{7}$$

This order is the same as that of the DE Formula.

4 Numerical Examples

We computed the following integrals

$$\begin{aligned} I_1 &= \int_{-1}^{1} \sqrt{1-x^2}\,\mathrm{d}x,\\ I_2 &= \int_{-1}^{1} \frac{\mathrm{d}x}{1+x^2},\\ I_3 &= \int_{-1}^{1} \log(1+x)\,\mathrm{d}x,\end{aligned}$$

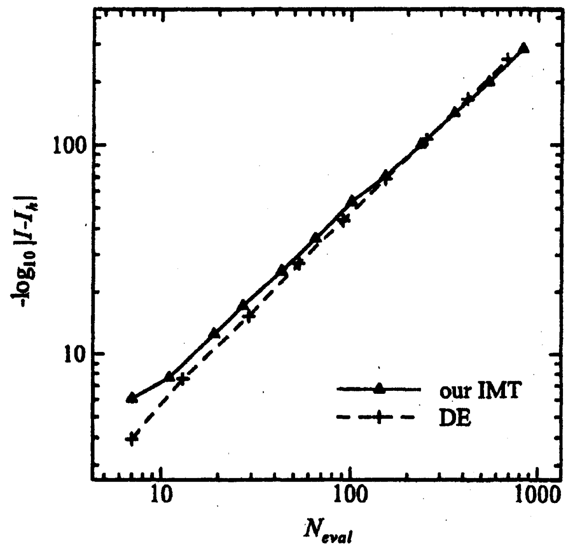
$$
\begin{aligned}
I_4 &= \int_{-1}^{1} \frac{\mathrm{d}x}{(2+x)(1-x)^{3/4}(1+x)^{1/4}}, \\
I_5 &= \int_{-1}^{1} \frac{\cos \pi x}{\sqrt{1-x}}\, \mathrm{d}x, \\
I_6 &= \int_{-1}^{1} \frac{\mathrm{d}x}{\sqrt{1.00000001 - x^2}}
\end{aligned}
$$

by using the transformations:

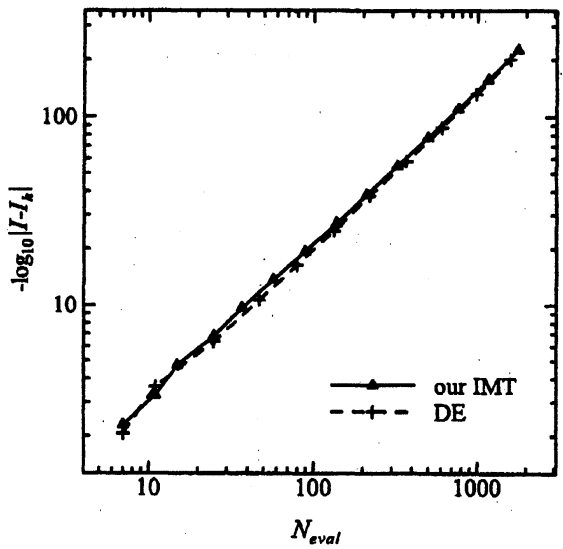
1. Our transformation: $\phi_{m,k}(t) = \mathrm{erf}(k(1-t)^{-m} - k(1+t)^{-m})$, $m = (1/2)\log N$, $k = 2.2$;

2. DE transformation: $\phi_{\mathrm{DE}}(t) = \tanh((\pi/2)\sinh t)$.

We chose the parameter k empirically: We computed $\int_{-1}^{1}(1-x^2)^{\alpha}\,\mathrm{d}x$, $\alpha = 0.25, 0.5, 0.75$ with k beginning from 1.4 to 3.0 with each 0.2. We found that $k = 2.2$ committed the least error. With this empirical fact, we chose $k = 2.2$ throughout our experiments. The result is shown in Fig. 1, Fig. 2 and Fig. 3.



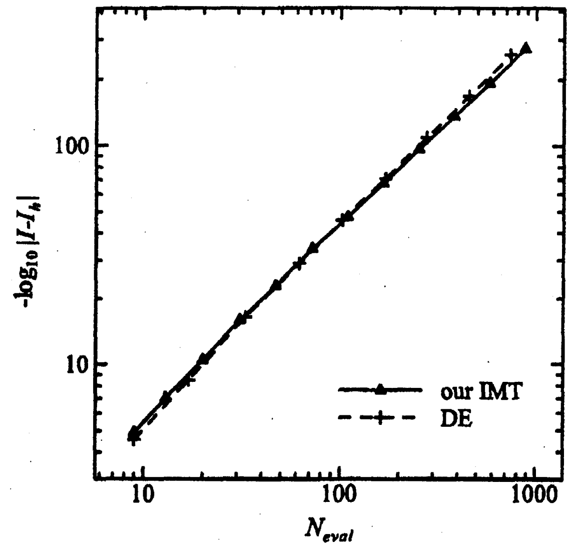
Errors in the case of
$I_1 = \int_{-1}^{1} \sqrt{1-x^2}\,\mathrm{d}x$



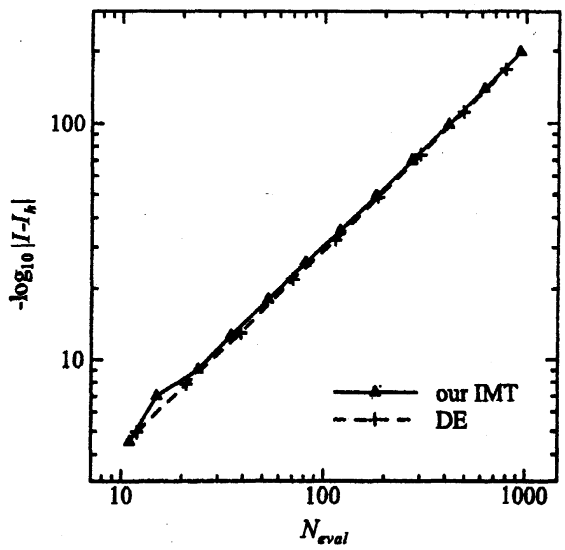
Errors in the case of
$I_2 = \int_{-1}^{1} \frac{\mathrm{d}x}{1+x^2}$

Fig. 1: Comparison between our formula and the DE formula for I_1 and I_2

The horizontal axis is the number of sampling points actually computed by which we mean that we count only those N sampling points such that $|f(\phi_{m,k}(-1+nh))\phi'_{m,k}(-1+nh)|$ is greater than $|I - I_h|$. The vertical axis represents $-\log_{10}|I - I_h|$. From these figures we see that our formula has almost as high degree of the performance as the DE formula. In addition, maximal precisions obtained by our formula are higher than those by the DE formula (the symbol $\triangle$ in the uppermost position).

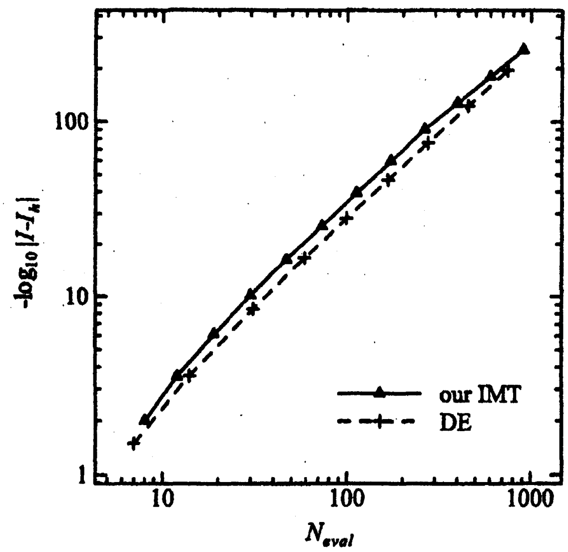


Errors in the case of
$I_3 = \int_{-1}^{1} \log(1+x)\,\mathrm{d}x$

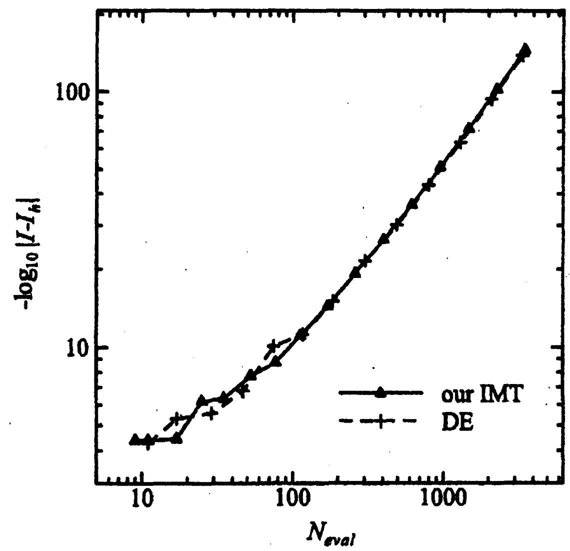


Errors in the case of
$I_4 = \int_{-1}^{1} \frac{\mathrm{d}x}{(2+x)(1-x)^{3/4}(1+x)^{1/4}}$

Fig. 2: Comparison between our formula and the DE formula for I_3 and I_4



Errors in the case of
$I_5 = \int_{-1}^{1} \frac{\cos \pi x}{\sqrt{1-x}}\,\mathrm{d}x$



Errors in the case of
$I_6 = \int_{-1}^{1} \frac{\mathrm{d}x}{\sqrt{1.00000001-x^2}}$

Fig. 3: Comparison between our formula and the DE formula for I_5 and I_6

Appendix 1 Error Analysis

We assume that $f(z)$ is analytic on a complex domain including the real interval $(-1,1)$ and has singularities which behave as

1. $f(z) = a(1-z^2)^\alpha + o(|1-z^2|^\alpha), \quad z \to \pm 1, \quad \alpha > -1;$

2. $f(z) = b(z-z_\mathrm{p})^{-1}(z-\bar{z}_\mathrm{p})^{-1} + O(1), \quad z \to z_\mathrm{p}.$

We also assume that $\mathrm{Im}\, z_\mathrm{p} > 0$ and that z_p is the singularity which is closest to $(-1,1)$. The error of (3) is estimated [1, 2, 4] by

$$I - I_h = -\sum_{j=1}^{\infty}(-1)^{jN}(C_{jN} + C_{-jN}),$$

where C_n are Fourier coefficients:

$$C_n = \int_{-1}^{1} g(x)\mathrm{e}^{\pi i n x}\,\mathrm{d}x, \quad g(x) = f(\phi_{m,k}(x))\phi'_{m,k}(x).$$

Since $2|\mathrm{Re}\, C_N|$ is dominant in $|I - I_h|$, it suffices for our purpose to calculate C_N. The singularities of $g(z)$ are as follows:

1. $g(z) \sim 4am\left(\frac{k}{2\sqrt{\pi}}\right)^{1-\alpha}(1\mp z)^{-m(1-\alpha)-1}\exp(-(1+\alpha)k^2((1-z)^{-m}-(1+z)^{-m})^2),$
   $z \to \pm 1;$

2. $g(z) \sim b(\phi_{m,k}(z)-z_\mathrm{p})^{-1}(\phi_{m,k}(z)-\bar{z}_\mathrm{p})^{-1}\phi'_{m,k}(z), \quad \phi_{m,k}(z) \to z_\mathrm{p},$

and we change the path of integral in the following way:

$$C_N = \int_{-1}^{1} g(x)\mathrm{e}^{\pi i N x}\,\mathrm{d}x = \int_{\Gamma_1+\Gamma_2+\Gamma_3} g(z)\mathrm{e}^{\pi i N z}\,\mathrm{d}z.$$

The path of $\Gamma_1 + \Gamma_2 + \Gamma_3$ is shown in Fig 4, where ζ_p is a pole transformed by $z_\mathrm{p} = \phi_{m,k}(\zeta_\mathrm{p})$ and is closest to the origin.

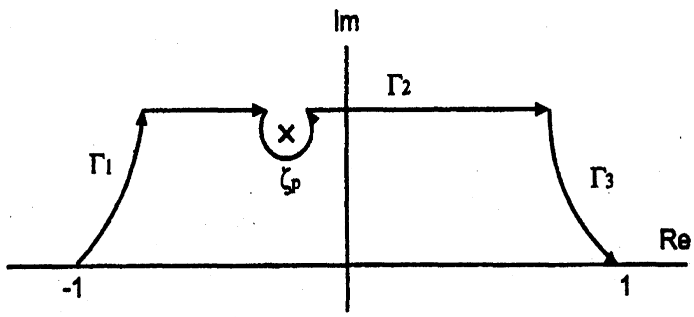


Fig. 4: The path of $\Gamma_1, \Gamma_2, \Gamma_3$

We consider the integral along Γ_1. From the saddle point method [1, 2, 4], we have

$$\log \int_{\Gamma_1} g(z) \mathrm{e}^{\pi \mathrm{i} N z} \, \mathrm{d}z \sim -\left((1+\alpha)k^2\right)^{\frac{1}{2m+1}} (2m+1) \left(\frac{\pi N}{2m} \mathrm{e}^{-\frac{\pi}{2}\mathrm{i}}\right)^{\frac{2m}{2m+1}} - \pi \mathrm{i} N.$$

The estimation on Γ_3 is carried out in the same way and we have

$$\log \int_{\Gamma_3} g(z) \mathrm{e}^{\pi \mathrm{i} N z} \, \mathrm{d}z \sim -\left((1+\alpha)k^2\right)^{\frac{1}{2m+1}} (2m+1) \left(\frac{\pi N}{2m} \mathrm{e}^{+\frac{\pi}{2}\mathrm{i}}\right)^{\frac{2m}{2m+1}} + \pi \mathrm{i} N.$$

By setting $1+\alpha = \alpha' + \varepsilon, \varepsilon > 0$, we obtain (4).

The integral along Γ_2 is estimated as

$$\begin{aligned} \int_{\Gamma_2} g(z) \mathrm{e}^{\pi \mathrm{i} N z} \, \mathrm{d}z &\sim \oint_{|z-z_\mathrm{p}|=\varepsilon} f(z) \mathrm{e}^{\pi \mathrm{i} N \phi^{-1}_{m,k}(z)} \, \mathrm{d}z \\ &= \frac{\pi b}{\operatorname{Im} z_\mathrm{p}} \exp\left(\pi \mathrm{i} N \zeta_\mathrm{p}\right). \end{aligned}$$

Since $\log(1 \pm z)^{-m} = \mp mz + O(m|z|^2)$, we have

$$\zeta_\mathrm{p} = \frac{1}{m} \log \left(\frac{\eta_\mathrm{p}}{2k} + \sqrt{1 + \left(\frac{\eta_\mathrm{p}}{2k}\right)^2} \right) + O\left(\frac{1}{m^2}\right), \quad m \longrightarrow \infty, k = \text{const.},$$

where η_p is a point such that $z_\mathrm{p} = \operatorname{erf} \eta_\mathrm{p}$ and that the quantity

$$\frac{4k}{\sqrt{\pi}} \operatorname{Im} \log \left(\frac{\eta_\mathrm{p}}{2k} + \sqrt{1 + \left(\frac{\eta_\mathrm{p}}{2k}\right)^2} \right) \tag{8}$$

is minimized. Here we assume that $|z_\mathrm{p}|$ is small. From Appendix 2, such a minimizer η_p exists. We then define β as the minimum value of (8). We see that $\beta \approx \operatorname{Im} z_\mathrm{p}$, $z_\mathrm{p} \approx (2/\sqrt{\pi})\eta_\mathrm{p} \approx (4mk/\sqrt{\pi})\zeta_\mathrm{p}$. By setting

$$\beta = \beta' + \varepsilon,$$

we obtain (5).

Appendix 2 Zeros of $\operatorname{erf} u$

We consider the domain $\{x + \mathrm{i}y \,|\, x \geq 0, y \geq 0\}$, since $\operatorname{erf}(-u) = -\operatorname{erf} u$ and $\operatorname{erf} \bar{u} = \overline{\operatorname{erf} u}$. $\operatorname{erf} u$ has no zeros in the following domain

$$D = \{x + \mathrm{i}y \,|\, x > 0, y > 0, (\sqrt{\pi}/2)\mathrm{e}^{x^2} \operatorname{erf} x > y\mathrm{e}^{y^2}\}.$$

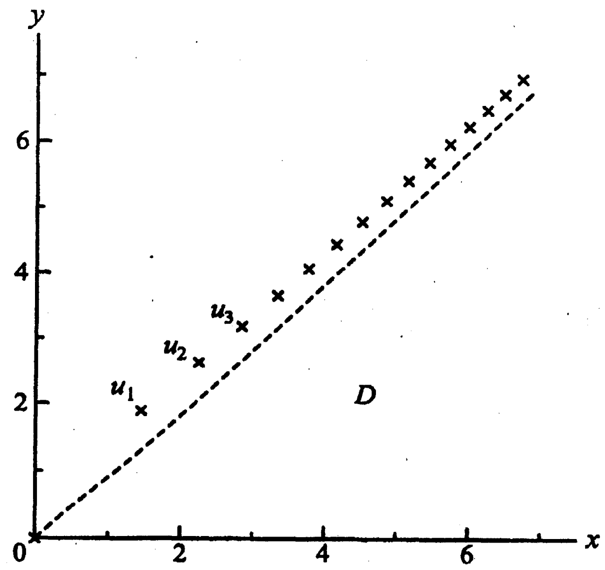


Fig. 5: Domain D and zeros of $\operatorname{erf} u$

In fact, it holds there that

$$\begin{aligned}\left|\int_0^{x+\mathrm{i}y} \mathrm{e}^{-t^2}\,\mathrm{d}t\right| &\geq \left|\int_0^{x} \mathrm{e}^{-t^2}\,\mathrm{d}t\right| - \left|\int_0^{y} \mathrm{e}^{-(x+\mathrm{i}t)^2}\,\mathrm{d}t\right| \\ &\geq \frac{\sqrt{\pi}}{2}\operatorname{erf} x - y\mathrm{e}^{-x^2+y^2} > 0.\end{aligned}$$

The domain D and zeros of $\operatorname{erf} u$ are shown in Fig. 5.

If $|z_\mathrm{p}|$ is assumed to be small enough, $\operatorname{erf} u - z_\mathrm{p}$ has zeros at

$$\eta_0 = \frac{\sqrt{\pi}}{2} z_\mathrm{p} + o(|z_\mathrm{p}|), \quad \eta_j = u_j + \frac{\sqrt{\pi}}{2}\mathrm{e}^{u_j^2} z_\mathrm{p} + o(|z_\mathrm{p}|), \quad j = 1, 2, 3, \cdots,$$

where $0, u_1 \approx 1.45 + 1.88\mathrm{i}, u_2 \approx 2.24 + 2.61\mathrm{i}, \cdots$ are zeros of $\operatorname{erf} u$. Since the asymptote of ∂D is $\{x + \mathrm{i}y \,|\, x > 0, y > 0, x = y\}$, we can estimate $|\mathrm{e}^{u_j^2}| \leq M_1$, $\operatorname{Im}\log \eta_j \geq M_2$, and

$$\frac{4k}{\sqrt{\pi}} \operatorname{Im}\log\left(\frac{\eta_j}{2k} + \sqrt{1 + \left(\frac{\eta_j}{2k}\right)^2}\right) \geq M_3,$$

where M_1, M_2, M_3 are positive constants independent of $j = 1, 2, 3, \cdots$. If $|z_\mathrm{p}|$ is small enough, then $\eta_\mathrm{p} = \eta_0$ and $\beta < M_3$.

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