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Sinc-collocation solution for nonlinear two-point boundary value problems arising in chemical reactor theory

J. Rashidinia^a and M. Nabati^{b,*}

^{a,b} Iran University of Science and Technology, Narmak, 1684613114, Tehran, Iran.

Abstract

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Numerical solution of nonlinear second order two-point boundary value problems based on Sinc-collocation method, developed in this work. We first apply the method to the class of nonlinear two-point boundary value problems in general and specifically solved special problem that is arising in chemical reactor theory. Properties of the Sinc-collocation method are utilized to reduce the solution of nonlinear two-point boundary value problem to some nonlinear algebraic equations. By solving such system we can obtain the numerical solution. We compared the obtained numerical result with the previous methods so far, such as Adomiad method, shooting method, Sinc Galerkin method and contraction mapping principle method.

Keywords: Sinc-collocation, nonlinear, boundary value problems, chemical.

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1 Introduction

Boundary value problems arise in a variety of the fields in applied mathematics, theoretical physics, chemical reaction and engineering. These categories of the problems have been handled by a reasonable number of researches who are working both numerically and analytically. The majority of these problems cannot be solved analytically, so we have to use the numerical methods, but there is not unified method to handle all types of problems.

In this paper, we consider the nonlinear differential equations:

$$au''(x) + bu'(x) + F(u(x), x) = 0, (1.1)$$

with boundary conditions:

$$\begin{cases} a_0 u(0) + a_1 u'(0) = 0, \\ b_0 u(1) + b_1 u'(1) = 0, \end{cases}$$
(1.2)

where $a_0, a_1, b_0, b_1, b, a \neq 0$ are given constant, F is analytic function in (0, 1) and may be singular in 0 or 1 or both. The special class of (1.1)-(1.2) arises in chemical reactor theory. This differential equation is the mathematical model for an adiabatic tubular chemical reactor which processes an irreversible exothermic chemical reaction. For steady state solutions this model can be reduce to the following ordinary differential equation given in [7] by

$$u''(x) - \lambda u'(x) + F\left(u(x), \mu, \beta, \lambda\right) = 0, \qquad (1.3)$$

with boundary conditions

$$u'(0) = \lambda u(0), u'(1) = 0, \tag{1.4}$$

*Corresponding author.

E-mail addresses: rashidinia@iust.ac.ir (J. Rashidinia) and mohamad_nabati@yahoo.com (M. Nabati)

where $F(u(x), \mu, \beta, \lambda) = \lambda \mu(\beta - u) \exp(u)$.

The unknown u represents the steady state temperature of the reaction, and the parameters λ, μ and β represent the Peclet number, the Damkohler number and the dimensionless adiabatic temperature rise, respectively. The existence solution of this problem has been considered in [4]. This problem has been studied by several authors [5], [7], [8], [11] who have demonstrated numerically the existence of solutions for particular ranges.

Recently equation (1.3) with conditions (1.4) have been consider by Modbouly et. al [7], first by using Green function technique, converted the problem into a Hammerestein integral equation and then solve the problem by Adomian's method. The Galerkin method, based on Sinc function is reported in [11].

Sinc methods have increasingly been recognized as powerful tools for problems in applied physics, chemistry and engineering. The Sinc methods are easily implemented and given good accuracy for problem not only in regular equations but also for problem with singularities. Approximation by Sinc functions are typified by errors of the form $O(\exp(-\frac{c}{h}))$ where c > 0 is constant and h is an step size [13], [14]. This property is good reason for many authors to use these approximation for solving problems. Numerical solutions of boundary value problems by using Sinc functions have been studied first by Frank Stenger more than thirty years ago [12]. The efficiency of the method has been formally proved by many researchers. Bialecki [1] used Sinc-collocation method to solve a linear two point boundary value problems. Lund [6] applied symmetrization Sinc-Galerkin for boundary value problems. Dehghan and Saadatmandi [2] used Sinc-collocation method for solving nonlinear system of second order. El-Gamel [3] solving a class of linear and nonlinear two point boundary value problem by Sinc-Galerkin method. The books by Stenger [13], [14] and by Lund and Bowers [6] provide excellent over wive of existing methods based on Sinc function for solving integral equations, ordinary and partial differential equations. In our pervious work we applied Sinc collocation method for solution of linear and nonlinear integral equations [9] [10].

In this study, we first apply Sinc-collocation method for solving (1.1)-(1.2) and also (1.3)-(1.4). Our method reduce the solution (1.1)-(1.2) to a set of nonlinear algebraic equations. By solving this algebraic equations we can find the approximation solution based on Sinc function.

In section 2 we give the relevant properties of Sinc function such as definitions, notations and some theorems. In section 3 we start the treatment on the boundary conditions and then used Sinc-collocation method find approximation solution for (1.1)-(1.2). In section 4 we solve one test example with various parameters and demonstrate the accuracy of the proposed numerical scheme by considering this special example.

2 Preliminaries and Fundamentals

In this section , some definitions, notations and theorems from [6] are presented. The Sinc function is defined on the whole real line $-\infty < x < \infty$ by

$$Sinc(x) = \begin{cases} \frac{\sin(\pi x)}{\pi x}, & x \neq 0\\ 1, & x = 0. \end{cases}$$

For h > 0 and $k = 0, \pm 1, \pm 2, ...$ the translated Sinc function with evenly space nodes are given as follow

$$S(k,h)(x) = Sinc\left(\frac{x-kh}{h}\right) = \begin{cases} \frac{\sin((\pi/h)(x-kh))}{(\pi/h)(x-kh)}, & x \neq kh\\ 1, & x = kh. \end{cases}$$

The Sinc function form for the interpolating points $x_j = jh$ is given by

$$S(k,h)(jh) = \delta_{kj}^{(0)} = \begin{cases} 0, & k \neq j \\ 1, & k = j \end{cases}$$

If a function f(x) is defined on the real line, then for h > 0 the series

$$C(f,h)(x) = \sum_{k=-\infty}^{\infty} f(kh) Sinc(\frac{x-kh}{h}),$$

is called the Whittaker cardinal expansion of f whenever this series converges. The properties of Whittaker cardinal expansion have been extensively studied on [15].

These properties are derived in the infinite strip D_d of the complex w-plane, where for d > 0

$$D_d = \{w = \xi + i\eta : |\eta| < d \le rac{\pi}{2}\}.$$

Many problems that arise in applied mathematics do not have the whole real line as their natural domain. There are two point of view. One is to change variables in the problem so that, in the new variables, the problem has a domain corresponding to that of the numerical process. A second procedures is to move the numerical process and to study it on the new domain. The latter approach is the method chosen here. The development for transform Sinc method from one domain to another is accomplished via conformal mapping. Approximation can be constructed for infinite, semi-infinite and finite interval.

Definition 2.1. Let D be a domain in the w = u + iv plane with boundary points $a \neq b$, let $z = \phi(w)$ be a one-to-one conformal map of D onto the infinite strip D_d where $\phi(a) = -\infty$, $\phi(b) = +\infty$. Denote by $w = \psi(z)$ inverse of the mapping ϕ and let

$$\Gamma \equiv \left\{ w\epsilon C : w = \psi(x), x\epsilon(-\infty, \infty) \right\} = \psi((-\infty, \infty)),$$

$$\Gamma_a \equiv \left\{ w\epsilon \Gamma : w = \psi(x) \quad , \ x\epsilon(-\infty, 0) \right\} = \psi((-\infty, 0)),$$

$$\Gamma_b \equiv \left\{ w\epsilon \Gamma : w = \psi(x) \quad , \ x\epsilon[0, \infty) \right\} = \psi([0, \infty)).$$

Definition 2.2. Let B(D) denote the class of analytic functions F in D which satisfy for some constant α with $0 \leq \alpha < 1$,

$$\int_{\psi(x+\Gamma)} |F(w)dw| = O(|x|^{\alpha}) \qquad x \to \pm \infty,$$

where $\Gamma = \{iy : |y| < d\}$ and for γ a simple closed contour in D

$$N(F,D) \equiv \lim_{\gamma \to \partial D} \int_{\gamma} |F(w)dw| < \infty$$

Further, for h > 0, define the nodes

$$w_k = \psi(kh)$$
 $k = 0, \pm 1, \pm 2, \pm 3, \dots$ (2.1)

Theorem 2.1. [6] Let $\phi' F \in B(D)$ and h > 0. Let ϕ be a one-to-one conformal map of the domain D onto D_d . Let $\psi = \varphi^{-1}$, $w_k = \psi(kh)$, furthermore assume that there are positive constant α, β and C so that

$$|F(\zeta)| \le C \begin{cases} \exp(-\alpha |\phi(\zeta)|), & \zeta \in \Gamma_a \\ \exp(-\beta |\phi(\zeta)|), & \zeta \in \Gamma_b \end{cases}$$

If the selections

$$N = [|\frac{\alpha}{\beta}M + 1|], \tag{2.2}$$

$$h = \left(\frac{\pi d}{\alpha M}\right)^{1/2},\tag{2.3}$$

are made, then, for all $\zeta \in \Gamma$

$$\varepsilon = F(\zeta) - \sum_{k=-M}^{N} F(w_k) Sinc(\frac{\phi(\zeta) - kh}{h}),$$

is bounded by

$$\|\varepsilon\|_{\infty} \le KM^{1/2} \exp(-(\pi d\alpha M)^{1/2}).$$

and K is a constant depending on F, d, ϕ and D.

To construct approximation on the interval (0, 1), which is used in this paper, consider the conformal map:

$$\phi(z) = \log\left(\frac{z}{1-z}\right). \tag{2.4}$$

The map ϕ carries the eye-shaped region

$$D = \Big\{ z = x + iy : |\arg(\frac{z}{1-z})| < d \le \frac{\pi}{2} \Big\},\$$

onto the infinite strip D_d . The basis function on the interval $\Gamma = (0, 1)$ for $z \in D$ are derived from the composite translated Sinc functions

$$S_k(z) = S(k,h)o\phi(z) = Sinc\left(\frac{\phi(z) - kh}{h}\right), \quad z \in D.$$
(2.5)

The inverse map of $w = \phi(z)$ is

$$z = \phi^{-1}(w) = \psi(w) = \frac{\exp(w)}{1 + \exp(w)}.$$
(2.6)

The collocation method requires derivatives of composite Sinc function evaluated at the node so that we need to use the following lemma.

Lemma 2.1. [6] Let ϕ be the conformal one-to-one mapping of the simply connected domain D onto D_d given by (8) then

$$\delta_{jk}^{(0)} = S(j,h)o\phi(z_k) = \begin{cases} 1, & j = k, \\ 0, & j \neq k, \end{cases}$$
$$\delta_{jk}^{(1)} = \frac{d}{d\phi}[S(j,h)o\phi(z)](z_k) = \frac{1}{h} \begin{cases} 0, & j = k, \\ \frac{(-1)^{k-j}}{k-j}, & j \neq k, \end{cases}$$
$$\delta_{jk}^{(2)} = \frac{d^2}{d\phi^2}[S(j,h)o\phi(z)](z_k) = \frac{1}{h^2} \begin{cases} \frac{-\pi^2}{3}, & j = k, \\ \frac{-2(-1)^{k-j}}{(k-j)^2}, & j \neq k. \end{cases}$$

For the assembly of discrete system, it is convenient to define the following matrices:

$$I^{(r)} = [\delta_{jk}^{(r)}] \qquad r = 0, 1, 2 \quad , \tag{2.7}$$

where $\delta_{jk}^{(r)}$ denotes the (j,k)th element of the matrix $I^{(r)}$.

3 Discretization of Problem by Sinc-Collocation Method:

For discretization of the following problem

$$au''(x) + bu'(x) + F(u(x), x) = 0, (3.1)$$

with boundary conditions:

$$\begin{cases} a_0 u(0) + a_1 u'(0) = 0, \\ b_0 u(1) + b_1 u'(1) = 0. \end{cases}$$
(3.2)

Since $\frac{d}{dx}[S(k,h)o\phi(x)]$ is undefined at x = 0 and x = 1 (by $\phi(x)$ in (2.4)) and because the mixed boundary conditions must be handled at endpoints by the approximation solution, thus we consider the approximation solution as follows

$$u_m(x) = c_{-M-1}w_a(x) + \frac{1}{\phi'(x)} \sum_{k=-M}^N c_k S_k(x) + c_{N+1}w_b(x), \qquad m = M + N + 1.$$
(3.3)

In (3.3) $S_k(x)$ is from (2.5) and the boundary bases function w_a, w_b are cubic Hermit functions given by

$$w_a(x) = a_0 x (1-x)^2 - a_1 (2x+1)(1-x)^2,$$

and

$$w_b(x) = b_1(-2x+3)x^2 + b_0(1-x)x^2.$$

These boundary functions interpolate the boundary conditions in (3.2) via the identities

$$w_a(0) = -a_1, w'_a(0) = a_0,$$

 $w_b(1) = b_1, w'_b(1) = -b_0,$

and

$$w_a(1) = w'_a(1) = 0,$$

 $w_b(0) = w'_b(0) = 0.$

For the purpose of illustrating the exposition of our method we define

$$Lu(x) = au''(x) + bu'(x), (3.4)$$

then, (3.1) is now given by

$$Lu(x) = -F(x, u(x)).$$
 (3.5)

In (3.3) the M + N + 3 coefficients $\{c_k\}_{-M-1}^{N+1}$, are determined by substituting $u_m(x)$ into equation (3.1) and evaluating the result at the Sinc points

$$x_j = \frac{\exp(jh)}{1 + \exp(jh)} \qquad j = -M - 1, -M, ..., N, N + 1,$$
(3.6)

where h is defined in (2.3).

For evaluating the result we need to evaluate first and second derivatives from (14), so we first differentiate from $\frac{1}{\phi'(x)}S(k,h)o\phi(x)$ as

$$\frac{d}{dx}\left(\frac{1}{\phi'(x)}S(k,h)o\phi(x)\right) = \left(\frac{1}{\phi'}\right)'S_k(x) + \frac{d}{d\phi}S_k(x),\tag{3.7}$$

so the first derivative of $u_m(x)$ is

$$u'_{m}(x) = c_{-M-1}w'_{a}(x) + \sum_{k=-M}^{N} c_{k} \left[\left(\frac{1}{\phi'}\right)' S_{k}(x) + \frac{d}{d\phi} S_{k}(x) \right] + c_{N+1}w'_{b}(x),$$
(3.8)

similarly by taking the second derivative from $\frac{1}{\phi'(x)}S(k,h)o\phi(x)$ we have

$$u_m''(x) = c_{-M-1}w_a''(x) + \sum_{k=-M}^N c_k \Big[\Big(\frac{1}{\phi'}\Big)'' S_k(x) + \phi'\Big(\frac{1}{\phi'}\Big)' \frac{d}{d\phi} S_k(x) + (\phi')\frac{d^2}{d\phi^2} S_k(x) \Big] + c_{N+1}w_b''(x), \quad (3.9)$$

and we know that

$$u_m(x_j) = \begin{cases} c_{-M-1}w_a(x_j) + \frac{c_j}{\phi'(x_j)} + c_{N+1}w_b(x_j), & j = -M, ..., N, \\ \\ c_{-M-1}w_a(x_j) + c_{N+1}w_b(x_j), & j = -M - 1, N + 1. \end{cases}$$

Substituting (3.3), (3.8), (3.9) in (3.1) and multiplying the resulting equation by $\{\frac{1}{\phi'}\}$ and then setting $x = x_j$ as collocation points in (3.6), finally by using of $u_m(x_j)$ definition above, we obtain the following nonlinear system

$$c_{-M-1} \frac{Lw_a(x_j)}{\phi'(x_j)} + \sum_{k=-M}^{N} c_k \Big[a \frac{d^2}{d\phi^2} S_k(x_j) + g_1(x_j) \frac{d}{d\phi} S_k(x_j) + g_2(x_j) S_k(x_j) \Big] + c_{N+1} \frac{Lw_b(x_j)}{\phi'(x_j)} = -\frac{F(u_m(x_j), x_j)}{\phi'(x_j)}, \qquad j = -M - 1, \cdots, N + 1,$$
(3.10)

where

$$Lw_a = aw_a'' + bw_a', (3.11)$$

$$Lw_b = aw_b'' + bw_b', (3.12)$$

$$g_1(x) = a \left(\frac{1}{\phi'(x)}\right)' + b \left(\frac{1}{\phi'(x)}\right) = a (1 - 2x) + b x (1 - x), \tag{3.13}$$

$$g_2(x) = \left(\frac{1}{\phi'(x)}\right) \left[a \left(\frac{1}{\phi'(x)}\right)'' + b \left(\frac{1}{\phi'(x)}\right)'\right] = x(1-x) \left(-2a + b \left(1-2x\right)\right).$$
(3.14)

Equations (3.10) gives M+N+3 nonlinear algebraic equations which can be solved for the unknown coefficients c_k by using Newton's method. Consequently, $u_m(x)$ given in (3.3) can be calculated.

4 Numerical Results

To validate the application of Sinc-collocation method to equation (1.1) with conditions (1.2) we camper the solution with numerical results by some classical techniques. We consider the special problem (1.3) with conditions (1.4) that occurs in adiabatic tubular chemical reactor. For this problem, the entire discrete system in (3.10) is constructed as follows.

Define the components of the $(M + N + 3) \times 1$ columns vectors by

$$(\overrightarrow{a}_{-M-1})_j = \frac{Lw_a(x_j)}{\phi'(x_j)},$$
 $(\overrightarrow{b}_{-M-1})_j = w_a(x_j),$ (4.1)

$$(\overrightarrow{a}_{N+1})_j = \frac{Lw_b(x_j)}{\phi'(x_j)}, \qquad (\overrightarrow{b}_{N+1})_j = w_b(x_j), \tag{4.2}$$

$$(\overrightarrow{f})_j = \frac{\lambda\mu}{\phi'(x_j)}, \qquad \qquad \mathbf{1} = (1, 1, \dots, 1, 1)^T, \tag{4.3}$$

then the discrete system (3.10), by using lemma 2.1 can be represented by

$$AC + D(f) \left(diag(\beta . \mathbf{1} - BC) diag(\exp(BC)) \right) \mathbf{1} = 0,$$
(4.4)

where the $(M + N + 3) \times (M + N + 3)$ matrix A is the border matrix

$$A = \begin{bmatrix} \overrightarrow{a}_{-M-1} & A_s & \overrightarrow{a}_{N+1} \end{bmatrix}, \tag{4.5}$$

such that

$$A_s = I^{(2)} + D(g_1)I^{(1)} + D(g_2)I^{(0)}$$
(4.6)

where $\overrightarrow{a}_{-M-1}$, \overrightarrow{a}_{N+1} are vectors defined in (4.1), (4.2) and $I^{(r)}$ is $(M+N+3) \times (M+N+1)$ matrices which are defined in (2.7) and $D(g(x_j))$ denote the $(M+N+3) \times (M+N+3)$ diagonal matrix with

$$D(g(x_j)) = \begin{cases} g(x_i), & j = i, \\ 0, & j \neq i, \end{cases}$$

the $(M + N + 3) \times (M + N + 3)$ matrix B is the border matrix

$$B = \begin{bmatrix} \overrightarrow{b}_{-M-1} & B_s & | & \overrightarrow{b}_{N+1} \end{bmatrix},$$
(4.7)

where $\overrightarrow{b}_{-M-1}$ and \overrightarrow{b}_{N+1} are vectors defined in (4.1), (4.2) and

$$B_{s} = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ (\frac{1}{\phi'})(x_{-M}) & 0 & 0 & \dots & 0 \\ 0 & (\frac{1}{\phi'})(x_{-M+1}) & 0 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \dots & 0 & (\frac{1}{\phi'})(x_{N}) \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}$$

х	(CMP) [7]	(SM) [7]	(AM) [7]	(SGM) [2] (N=20)
0.0	0.006079	0.006048	0.006048	0.006048
0.2	0.018224	0.018192	0.018192	0.018192
0.4	0.030456	0.030424	0.030424	0.030424
0.6	0.042701	0.042669	0.042669	0.042669
0.8	0.054401	0.054371	0.054371	0.054371
1.0	0.061459	0.061458	0.061458	0.061458

Table 1: Comparative of the result from existing methods

Table 2: Result of the Sinc-collocation method

х	N=10	N = 15	N=20
0.0	0.006045	0.006048	0.006047
0.2	0.018189	0.018192	0.018192
0.4	0.030422	0.030424	0.030424
0.6	0.042666	0.042668	0.042669
0.8	0.054367	0.054370	0.054371
1.0	0.061441	0.061455	0.061458

and $C = (c_{-M-1}, c_{-M}, ..., c_N, c_{N+1})^T$ and $exp(C) = (exp(c_{-M-1}), exp(c_{-M}), ..., exp(c_{N+1}))^T$, furthermore diag(C) is the $(M + N + 3) \times (M + N + 3)$ diagonal matrix with

$$diag(C) = \begin{cases} c_i, & j = i, \\ 0, & j \neq i \end{cases}$$

For Sinc-collocation method we use $\alpha = 1$, $d = \frac{\pi}{2}$ and also truncate the numerical results after the sixth decimal points.

Case 1

In this case, in problem (1.3)-(1.4) we use particular value of the parameters, $\lambda = 10$, $\beta = 3$, $\mu = 0.02$. For such value of the parameters, a unique solution is guaranteed by the contraction mapping principle [7] and several authoress solve this problem by these parameters, we compared our results with them. Table (1) gives a comparison of the results from the contraction mapping principle (CMP) [7], the shooting method (SM) [7], the Adomian's method (AM) [7] and the Sinc-Galerkin method (SGM) [2] but in Table (2) numerical results based on our method with N=10, 15, 20 are reported.

As shown in Table (1) and (2), the results using our method with N=20 agree with those of the shooting method, Adomian's method and Sinc-Galerkin method up to sixth decimal place. For this problem the results from the contraction mapping principle agree to at least three decimal place, because by using this method, the required integrations can not be done analytically so are evaluated numerically by using the trapezoidal rule which will involve errors.

Case 2

In problem (1.3)-(1.4) we use another values of the parameters for λ, β, μ that for them the existence of solution is guaranteed by [4]. In Table (3) the numerical results for $\lambda = 5$, $\beta = 0.53$, $\mu = 0.05$, in Table (4) for $\lambda = 5$,

х	N=10	N = 15	N=20	N=30
0.0	0.005214	0.005216	0.005216	0.005216
0.1	0.007814	0.007816	0.007816	0.007816
0.2	0.010394	0.010395	0.010395	0.010395
0.3	0.012943	0.012944	0.012944	0.012944
0.4	0.015446	0.015448	0.015448	0.015448
0.5	0.017879	0.017881	0.017881	0.017881
0.6	0.020199	0.020200	0.020201	0.020201
0.7	0.022336	0.022338	0.022338	0.022338
0.8	0.024175	0.024177	0.024178	0.024178
0.9	0.025527	0.025530	0.025530	0.025530
1.0	0.026076	0.026080	0.026081	0.026081

Table 3: Numerical results for $\lambda = 5$, $\beta = 0.53$, $\mu = 0.05$ by Sinc-collocation method

 $\mu = 0.7$, $\beta = 0.8$ and in Table (5) for $\lambda = 0.05$, $\mu = 0.5$, $\beta = 0.6$ are reported.

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х	N=10	N=15	N=20	N=30
0.0	0.101630	0.101642	0.101645	0.101646
0.1	0.151591	0.151604	0.151607	0.151607
0.2	0.199674	0.199687	0.199690	0.199690
0.3	0.245631	0.245644	0.245647	0.245647
0.4	0.289179	0.289192	0.289195	0.289195
0.5	0.329957	0.329970	0.329973	0.329973
0.6	0.367448	0.367462	0.367465	0.367466
0.7	0.400840	0.400856	0.400860	0.400860
0.8	0.428768	0.428789	0.428794	0.428794
0.9	0.448864	0.448893	0.448900	0.448902
1.0	0.456946	0.456991	0.457001	0.457005

Table 4: Numerical results for $\lambda=5,\,\mu=0.7,\,\beta=0.8$ by Sinc-collocation method

Table 5: Numerical results for $\lambda=0.05,\,\mu=0.5,\,\beta=0.6$ by Sinc-collocation method

x	N=10	N=15	N=20	N=30
0.0	0.2268657	0.2268659	0.2268659	0.2268659
0.1	0.2279443	0.2279445	0.2279445	0.2279445
0.2	0.2289112	0.2289114	0.2289114	0.2289114
0.3	0.2297660	0.2297662	0.2297662	0.2297662
0.4	0.2305083	0.2305085	0.2305085	0.2305085
0.5	0.2311377	0.2311379	0.2311379	0.2311379
0.6	0.2316538	0.2316540	0.2316540	0.2316540
0.7	0.2320561	0.2320563	0.2320563	0.2320563
0.8	0.2323441	0.2323443	0.2323443	0.2323443
0.9	0.2325173	0.2325175	0.2325175	0.2325175
1.0	0.2325752	0.2325754	0.2325754	0.2325754

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