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Original article

A Second-Order Difference Scheme for Solving a Class of Fractional Differential Equations

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Abstract

Introduction. Increasing accuracy in the approximation of fractional integrals, as is known, is one of the urgent tasks of computational mathematics. The purpose of this study is to create and apply a second-order difference analog to approximate the fractional Riemann-Liouville integral. Its application is investigated in solving some classes of fractional differential equations. The difference analog is designed to approximate the fractional integral with high accuracy.

Materials and Methods. The paper considers a second-order difference analogue for approximating the fractional Riemann-Liouville integral, as well as a class of fractional differential equations, which contains a fractional Caputo derivative in time of the order belonging to the interval (1, 2).

Results. To solve the above equations, the original fractional differential equations have been transformed into a new model that includes the Riemann-Liouville fractional integral. This transformation makes it possible to solve problems efficiently using appropriate numerical methods. Then the proposed difference analogue of the second order approximation is applied to solve the transformed model problem.

Discussion and Conclusions. The stability of the proposed difference scheme is proved. An a priori estimate is obtained for the problem under consideration, which establishes the uniqueness and continuous dependence of the solution on the input data. To evaluate the accuracy of the scheme and verify the experimental order of convergence, calculations for the test problem were carried out.

Keywords: Fractional differential equation, Caputo derivative, Riemann-Liouville integral, Difference scheme.

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Научная статья

Разностная схема второго порядка для решения класса дифференциальных уравнений дробного порядка

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Аннотация

Введение. Повышение точности при аппроксимация дробных интегралов, как известно, является одной из актуальных задач вычислительной математики. Цель настоящего исследования — создание и применение разност-

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ного аналога второго порядка для аппроксимации дробного интеграла Римана-Лиувилля. Его применение исследуется при решении некоторых классов дифференциальных уравнений дробного порядка. Разностный аналог предназначен для аппроксимации дробного интеграла с высокой точностью.
Материалы и методы. В работе рассматривается разностный аналог второго порядка для аппроксимации дробного интеграла Римана-Лиувилля, а также класс дифференциальных уравнений дробного порядка, который содержит дробную производную Капуто по времени порядка, принадлежащего интервалу (1, 2).
Результаты исследования. Для решения вышеупомянутых уравнений преобразованы исходные дифференциальные уравнения дробного порядка в новую модель, которая включает дробный интеграл Римана-Лиувилля. Это преобразование позволяет эффективно решать задачи с использованием соответствующих численных методов. Затем предложенный разностный аналог второго порядка аппроксимации применяется для решения преобразованной модельной задачи.
Обсуждение и заключения. Доказана устойчивость предложенной разностной схемы. Получена априорная оценка для рассматриваемой задачи, которая устанавливает единственность и непрерывную зависимость решения от входных данных. Для оценки точности схемы и проверки экспериментального порядка сходимости проведены расчеты для тестовой задачи.

Ключевые слова: дифференциальное уравнение дробного порядка, производная Капуто, интеграл Римана-Лиувилля, разностная схема.

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Introduction. Fractional calculus (FC) is a branch of mathematics that investigates and applies derivatives and integrals of real and complex order. While the concept originated centuries ago, it gained significant interest in the late 1960s among engineers who realized its potential for accurately modeling real-world systems compared to conventional integer order calculus [1]. The delay in its adoption can be attributed to various factors such as the lack of a clear interpretation for fractional derivatives, the perceived adequacy of integer calculus, and the inherent complexity of FC [2]. Nowadays, FC has become a well-established field, finding extensive applications across various fields, including science, engineering, and mathematics. The extensive literature highlights the broad usage of FC in numerous subject areas such as control systems, acoustics, medical and biological sciences, optics, waves, finance, economics, signal processing, and more [3, 4].

Mathematical models based on differential equations with integer order derivatives have proven useful in studying the dynamics of real-world systems. However, these models have limitations in capturing long-range temporal memory or long-range spatial interactions that are inherent in many real-world phenomena. This restriction arises due to the omission of these features in integer order derivatives [5]. In contrast, FDEs offer a significant advantage as they exhibit nonlocal behavior. This implies that fractional calculus serves as a powerful tool for capturing the memory and evolutionary properties exhibited by a wide range of physical phenomena and complex systems [6, 7]. Consequently, mathematical models based on FDE are more realistic and practical compared to classical integer-order models [8].

The need to accurately model and understand various phenomena and processes, coupled with the effectiveness of FDE models in capturing long-range memory and non-local interactions, has propelled the quest for efficient numerical or analytical solution techniques. Researchers strive to develop innovative methods that can handle the complexities and challenges associated with FDEs, enabling a deeper comprehension of the systems under investigation. However, obtaining analytical solutions for FDEs is generally challenging and exact solutions often involve infinite series representations such as the Mittag-Leffler function, the Fox H-function, or the hyperbolic geometry function, which can pose computational difficulties during evaluation [9]. Consequently, there is a growing interest in the development of computationally efficient numerical algorithms for solving FDEs. These methods include a variety of high-performance computing techniques such as finite difference methods:

– predictor-corrector methods;
– finite element methods, spectral methods;
– boundary particle methods;
– implicit meshless methods;
– Galerkin methods, finite volume methods;
– local radial basis function methods (see [10] and the citations provided within).

In the past few years, there has been a significant focus on the development of numerical methods for solving one-dimensional time FDEs. Numerous studies have been published in order to investigate and advance these numerical approaches [11, 12, 13]. Yand et al. [14] applied the Lubich's fractional multistep method for numerical solution of fractional diffusion-wave equation by transforming the original model into a equivalent integro-differential equation. They demonstrated that their method achieves a temporal order of accuracy of α for $1 \le \alpha \le 1.71832$. In [15], the authors presented a method of order 3-α for $0 < \alpha < 1$ to approximate the Caputo derivative. They then proposed a discrete difference scheme by introducing two new variables to transform the original equation into a lower-order system of equations. Two alternating direction implicit schemes for solving two-dimensional time fractional nonlinear super-diffusion equations is introduced in [16]. These schemes are based on the equivalent partial integro-differential equations of the original problem. The Riemann-Liouville fractional integral is discretized using the classical first-order approximation. The authors prove that both schemes exhibit first-order accuracy in time, ensuring convergence of the numerical solutions. Khibiev et al. [13] developed a second-order difference analog to approximate the generalized Caputo derivative. They successfully applied this difference analog for numerically solving the generalized time-fractional diffusion equation, specifically focusing on cases with smooth solutions.

Based on the insights gained from the discussion and the comprehensive review of relevant literature in this Section, our objective is to develop a second-order difference analog for approximating the Riemann-Liouville fractional integral and then apply this difference analog to solving a class of FDEs. The paper is organized as follows. In Section 2, we introduce the class of FDEs that contain a fractional Caputo derivative of order $\alpha + 1$, where $0 < \alpha < 1$. We transform the FDE model into a form that includes the Riemann-Liouville fractional integral, and present an a priori estimate for the solution of the differential model in subsection 2.1. In Section 3, we propose a difference analog for approximating the Riemann-Liouville fractional integral. We also estimate the truncation error of the method and apply it to solve the new FDE model. Additionally, we investigate the stability of the numerical method in the subsection 3.1. In Section 4, we perform numerical simulations to validate the accuracy and efficiency of the proposed method for solving the considered FDE. We also investigate the method's experimental order of convergence. Finally, in Section 5, we provide a brief conclusion summarizing the key findings and contributions of our study.

Materials and Methods. In this section, we present a specific class of initial-value FDEs and propose a methodology to effectively solve these models. In this study, a new effective and precise numerical scheme is being sought to approximate the solutions of the following initial-value FDEs:

$$\partial_{0t}^{\alpha+1} y(t) + \varkappa y(t) = g(t), \tag{1}$$

$$y(0) = y_0, \; y_t(0) = y_1, \tag{2}$$

In which $\varkappa$ is a positive constant, $0 < \alpha < 1$ and $0 < t \le T$.

There exist multiple definitions for derivatives and integral operators in the context of fractional calculus. Some widely used definitions include the Caputo derivative and the Riemann-Liouville derivative. These definitions differ in the way they capture the fractional order behavior of a function. In the Caputo derivative, the fractional derivative is defined by considering the fractional order differentiation of the function while preserving the initial conditions. This makes it particularly suitable for modeling real-life processes where the initial conditions are crucial in determining the behavior of the system [17, 1]. For this reason, in our study, we adopt the fractional derivative in equation (1) in the Caputo sense. This choice is motivated by the compatibility of the Caputo derivative with real-life applications and its ability to accurately capture the initial conditions of the system. The Caputo derivative is defined as follows:

$$\partial_{0t}^{\alpha+1} y(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\eta)^{-\alpha} y''(\eta) d\eta, \; 0 < \alpha < 1,$$

where α represents the fractional order, and Γ(·) denotes the gamma function. By utilizing the Caputo derivative, we are able to effectively capture the fractional order behavior of the system and account for the influence of past history on the current state. This definition allows us to model various real-life phenomena where the initial conditions play a crucial role in determining the system's dynamics [18, 2].

Applying the Riemann-Liouville fractional integration operator of order α, denoted by $D_{0t}^{-\alpha} y(t)$ to the both sides of the model (1), we reach:

$$\frac{dy}{dt} + \varkappa D_{0t}^{-\alpha} y = f(t), \ 0 < t \le T, \tag{3}$$

where $f(t) = D_{0t}^{-\alpha} g(t) + y_1$ and the Riemann-Liouville fractional integration operator is defined as:

$$D_{0t}^{-\alpha} y(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} y(\xi) d\xi. \tag{4}$$

The model (3) is subject to the initial condition $y(0)=y_0$. In Eq. (3), as t approaches 0, we have $y_t(0)=f(0)=y_1$. Therefore, the second initial condition in Eq. (2) can be derived.

A priori estimate for the solution of the differential problem. The following theorem presents an a priori estimate for the solution of the differential problem (3), which provides valuable insights into the behavior and properties of the solution, allowing for a better understanding and analysis of the model. Before presenting the main theorem, it is essential to introduce the following corollary, which is derived from the results presented in [19].

Corollary 1. For any function $y(t)$ absolutely continuous on $[0,T]$ the following inequality takes place:

$$\int_0^t y(s) D_{0s}^{-\alpha} y(s) ds \ge 0, \ 0 < \alpha < 1.$$

Theorem 1. The solution $y(t)$ of the problem (3) satisfies the following a priori estimate:

$$y^2(t) \le C_1 \left(y_0^2 + \int_0^t f^2(s) ds \right), \ C_1 = \max\{2, 4T\}.$$

Proof. Multiplying Eq. (3) by $y(t)$, then changing the variable t to s and integrating over the time variable s from 0 to t, we get:

$$\int_0^t y(s) y'(s) ds + \varkappa \int_0^t y(s) D_{0s}^{-\alpha} y(s) ds = \int_0^t y(s) f(s) ds. \tag{5}$$

From corollary 1 and the fact that $\varkappa > 0$, the second term of left-hand side of (5) is non-negative and can be omitted. In this way we have:

$$\frac{1}{2}(y^2(t) - y_0^2) \le \int_0^t \left(\varepsilon y^2(s) + \frac{1}{4\varepsilon} f^2(s) \right) ds,$$

$$y^2(t) \le 2\varepsilon \int_0^t y^2(s) ds + y_0^2 + \frac{1}{2\varepsilon} \int_0^t f^2(s) ds. \tag{6}$$

To complete the proof, we need to estimate the integral $\int_0^t y^2(s) ds$. For this purpose, we integrate (6) with respect to the variable t form 0 to t. Set $\varepsilon = \frac{1}{(4T)}$, taking into account the following inequality:

$$\int_0^t d\xi \int_0^\xi y^2(s) ds = \int_0^t (t-s) y^2(s) ds \le T \int_0^t y^2(s) ds,$$

we can reach the following conclusion:

$$\int_0^t y^2(s) ds \le 2T y_0^2 + 4T^2 \int_0^t f^2(s) ds. \tag{7}$$

Now, by substituting equation (7) into equation (6) and setting $\varepsilon = \frac{1}{(4T)}$, one can complete the proof.

Derivation of the difference scheme for approximation FDE. The objective of this subsection is to introduce a difference analog that effectively approximates the Riemann-Liouville fractional integral. Subsequently, we employ this difference analog to devise a robust and accurate second-order difference scheme specifically developed for approximating the model (3).

To construct a difference method to approximate the Riemann-Liouville fractional integral (4), for an integer number N and a given time T, we discretize the interval $[0,T]$ into equally spaced $t_j=j\tau$, $j=0,1,\ldots,N$, where $\tau = \frac{T}{N}$ is the temporal step length. For notational brevity, we denote the numerical solution of $y(t_j)$ at the point t_j by y^j. To approximate the Riemann-Liouville fractional integral at $t=t_{j+1}$, where $j=1,2,\ldots,N$, we employ a generalized trapezoidal formula. This formula is utilized in the following manner:

$$D_{0t_{j+1}}^{-\alpha} y(t) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{j+1}} (t_{j+1}-\xi)^{\alpha-1} y(\xi) d\xi = \frac{1}{\Gamma(\alpha)} \sum_{s=0}^{j} \int_{t_s}^{t_{s+1}} (t_{j+1}-\xi)^{\alpha-1} y(\xi) d \approx$$
$$\approx \frac{1}{\Gamma(\alpha)} \sum_{s=0}^{j} \int_{t_s}^{t_{s+1}} (t_{j+1}-\xi)^{\alpha-1} \left(y(t_{s+1}) \frac{\xi - t_s}{\tau} + y(t_s) \frac{t_{s+1}-\xi}{\tau} \right) = \tag{8}$$
$$= \frac{\tau^{\alpha}}{\Gamma(\alpha+2)} \left(\sum_{s=0}^{j} c_{j-s}^{(\alpha)} y^{s+1} + c_{j+1}^{-(\alpha)} y^0 \right) = \Delta_{0t_{j+1}}^{-v} y,$$

in which $c_0^{(\alpha)}=1$ and

$$c_s^{(\alpha)} = (s+1)^{\alpha+1} - 2s^{\alpha+1} + (s-1)^{\alpha+1},$$
$$c_s^{-(\alpha)} = (\alpha+1)(s+1)^{\alpha} - ((s+1)^{\alpha+1} - s^{\alpha+1}).$$

The truncation error of the operator $\Delta_{0t_{j+1}}^{-v}$ in (8) is characterized by the following lemma.

Lemma 1. Suppose $y(t) \in c^2[0,t_{j+1}]$. For any $\nu \in (0,1)$, $\Delta_{0t_{j+1}}^{-v}$ is defined in (8). Then we have:

$$\left| D_{0t_{j+1}}^{-v} y(t) - \Delta_{0t_{j+1}}^{-v} y \right| = O(\tau^2).$$

Proof. By using the Lagrange interpolation remainder formula, it follows that:

$$\left| D_{0t_{j+1}}^{-v} y(t) - \Delta_{0t_{j+1}}^{-v} y \right| \le \sum_{s=0}^{j} \int_{t_s}^{t_{s+1}} (t_{j+1}-\xi)^{v-1} \left| \frac{C^2}{2} (t_{s+1}-\xi)(\xi - t_s) \right| d\xi \le$$
$$\le \frac{C_2}{8} \tau^2 \sum_{s=0}^{j} \int_{t_s}^{t_{s+1}} (t_{j+1}-\xi)^{v-1} d\xi = \frac{C_2}{8} \tau^2 \int_0^{t_{j+1}} (t_{j+1}-\xi)^{v-1} d\xi \le \frac{C_2 T^v}{8} \tau^2 = O(\tau^2),$$

here $C_2 = \max_{0 \le t \le T} \left| y''(t) \right|$.

The validity of this approximation can be readily confirmed through the application of Taylor's Theorem.

In the uniform domain $\Omega=\{t_j: j=0,1,\ldots,N\}$, we consider the fractional differential model (3) at the point t_{j+1}, with $j=1,2,\ldots,N-1$. Applying the proposed difference scheme (8) as well as the approximation (9) to the model (3), we propose the following difference scheme:

$$\frac{3y^{j+1} - 4y^j + y^{j-1}}{2\tau} + \varkappa \Delta_{0t_{j+1}}^{-\alpha} y = f(t_{j+1}), \tag{10}$$

$$y^0 = y_0. \tag{11}$$

At the initial time step t_1, we estimate the value of y^1 by employing Taylor's theorem as follows:

$$y^1 = y_0 + \tau y_1 + O(\tau^2). \tag{12}$$

Taking into account Lemma 1 and equation (9) and (12), one can conclude that if the solution of the differential model (3) satisfies the smoothness condition $y(t) \in C_t^2(\Omega)$, then the difference scheme (10)–(11) demonstrates an order of accuracy of $O(\tau^2)$.

Theoretical analysis of the proposed difference scheme. Consider the error $z^j=Y^j-y^j$, with $Y^j=y(t_j)$. Substituting $y^j=z^j+Y$ into the model (3), we obtain the problem for the error as follows:

$$\frac{3z^{j+1}-4z^j+z^{j-1}}{2\tau}+\varkappa\Delta^{-\alpha}_{0t_{j+1}}z=R_i^{j+1}, \tag{13}$$

$$z^0=u_0,\ z^1=\mu,$$

where

$$R_i^{j+1}=-\frac{3Y^{j+1}-4Y^j+Y^{j-1}}{2\tau}-\varkappa\Delta^{-\alpha}_{0t_{j+1}}Y+f(t_{j+1})=O(\tau^2),$$
$$\mu=-y^1+y_0+\tau y_1=O(\tau^2).$$

Before presenting the main theorem for the stability of the proposed difference scheme, it is essential to introduce the following two Lemmas.

Lemma 2 [6]. For any real constants r_0, r_1 such that $r_0\geq\max\{r_1,-3r_1\}$, and $\{v_j\}_{j=0}^{j=N}$ the following inequality holds:

$$v_{j+1}(r_0v_{j+1}-(r_0-r_1)v_j-r_1v_{j-1})\geq E_{j+1}(r_0,r_1)-E_j(r_0,r_1),\ j=1,...,N-1,$$

where

$$E_j(r_0,r_1)=\left(\frac{1}{2}\sqrt{\frac{r_0-r_1}{2}}+\frac{1}{2}\sqrt{\frac{r_0+3r_1}{2}}\right)^2v_j^2+$$
$$+\left(\sqrt{\frac{r_0-r_1}{2}}v_j-\left(\frac{1}{2}\sqrt{\frac{r_0-r_1}{2}}+\frac{1}{2}\sqrt{\frac{r_0+3r_1}{2}}\right)v_{j-1}\right)^2.$$

Lemma 3 [20]. Assume that the sequence $\{a_n\}_{n=0}^{\infty}$ of real numbers is satisfy the following properties:

$$a_n\geq 0,\ a_n-a_n+1\geq 0,\ a_n-2a_{n+1}+a_n+2\geq 0.$$

Let $c_0=\frac{a_0}{2}$ и $c_j=a_j$ for $j\geq 1$. Then:

$$\sum_{s=1}^{n}\sum_{k=1}^{s}c_{s-k}\xi_s\xi_k\geq 0,\ \forall(\xi_1,\xi_2...,\xi_n)\in R^n.$$

Theorem 2. The difference scheme (3) is unconditionally stable and the following a priori estimate is valid for its solution:

$$(z^{j+1})^2\leq C_3\left(\sum_{s=1}^{j}(R^{s+1})^2\tau+\mu^2\right),$$

where C_3 is a positive constant independent of τ and h.

Proof. The proof follows a similar approach to that of Theorem 1. By multiplying equation (13) by $z^{j+1}\tau$ and replacing j with s, we then sum over s from 1 to j and utilize the results from Lemma 2 and Lemma 3. Due to the similarity in methodology, the detailed proof is omitted here for brevity.

Results. To evaluate the performance of the numerical method and gain insights into its convergence behavior, a comprehensive set of numerical experiments is conducted in this section. The primary objective is to analyze the numerical errors by comparing the exact solution with the computed numerical solution. Additionally, the convergence order of the numerical algorithm with respect to the step size τ is investigated. The experimental orders of convergence (EOC) are calculated using the following relations:

$$\mathrm{EOC}=\log_{\tau_1/\tau_2}\frac{E(\tau_1)}{E(\tau_2)},$$

where the maximum absolute error $E(\tau)$ is calculated by:

$$E(\tau)=\max_{1\leq j\leq N}\left|y(t_j)-y^j\right|,$$

with the step size τ.

Example 1. Consider the model (3) with an exact analytical solution given by the following expression $y(t)=t^2+t^{3+\alpha}$. The corresponding source term and initial conditions for the given problem can be obtained as follows:

$$f(t) = 2t + (3+\alpha)t^{2+\alpha} + \varkappa \frac{2}{\Gamma(3+\alpha)} t^{\alpha+2} + \varkappa \frac{\Gamma(4+\alpha)}{\Gamma(4+2\alpha)} t^{3+2\alpha}, \; y(0) = y_t(0) = 0.$$

We solve this problem with the presented difference scheme (10).

Table 1 presents the results obtained by varying the values of the step length τ, displaying the maximum error and EOC for different values of α with $\varkappa = 4$, at the time $T = 1$. The Table demonstrates that the method exhibits excellent accuracy even for very small grid sizes, and the EOC consistently reaches the expected value of 2 for all cases.

We proceed with an investigation of the long time performance of the proposed scheme method with the aim of further assessing the precision and reliability of the scheme. Table 2 showcases the maximum error and EOC for different values of a with $\varkappa = 2$, at the time $T = 10$. The Table provides further evidence of the method's high accuracy, even for extended time intervals and very small mesh sizes. The EOC consistently remains at 2, indicating the method's reliability and robustness in accurately solving the problem. These findings confirm the effectiveness and reliability of our numerical scheme in accurately solving the considered problem across different time ranges.

Discussion and Conclusions. In this study, we have presented a second-order numerical analog for approximating the Riemann-Liouville fractional integral and demonstrated its effectiveness in solving a class of ordinary FDEs. By transforming the original FDEs into a model that incorporates the Riemann-Liouville fractional integral, we were able to extend the applicability of our proposed method to solve the model. Furthermore, we established a priori estimates for the solution, which demonstrate the uniqueness and continuous dependence of the solution on the input data. The stability analysis of the proposed difference scheme is also investigated. Numerical simulations are performed to assess the accuracy, efficiency, and long-term reliability of the proposed method. The simulations demonstrate the method's effectiveness in solving FDEs, even for extended time intervals and with small mesh sizes. The experimental order of convergence (EOC) is also investigated, confirming the expected EOC of 2 for different cases.

Table 1

The maximum error and the experimental orders of convergence (EOC) for example 1 with decreasing time-grid size $\tau = T/N$, for $\alpha = 0.1, 0.5, 0.9$, with $\varkappa = 4$, at the time $T = 1$

$\tau = T/N$	$\alpha = 0.1$		$\alpha = 0.5$		$\alpha = 0.9$	
N	$E(\tau)$	CO	$E(\tau)$	CO	$E(\tau)$	CO
80	2.1178e-04		2.2420e-04		3.9043e-04	
160	5.4976e-05	1.9457	5.7336e-05	1.9673	9.8674e-05	1.9843
320	1.4126e-05	1.9604	1.4501e-05	1.9833	2.4799e-05	1.9924
640	3.5885e-06	1.9769	3.6458e-06	1.9918	6.2161e-06	1.9962
1280	9.0518e-07	1.9871	9.1379e-07	1.9963	1.5560e-06	1.9981
2560	2.2750e-07	1.9923	2.2870e-07	1.9984	3.8926e-07	1.9991

Table 2

Long time performance of the proposed scheme for solving example 1 with decreasing time-grid size $\tau = T/N$, for $\alpha = 0.1, 0.5, 0.9$, with $\varkappa = 2$, at the time $T = 10$

	$\alpha = 0.1$		$\alpha = 0.5$		$\alpha = 0.9$	
N	$E(\tau)$	CO	$E(\tau)$	CO	$E(\tau)$	CO
80	3.1602e-02		3.1247e-01		1.1045e+00	
160	8.8350e-03	1.8387	7.9023e-02	1.9834	2.7524e-01	2.0046
320	2.4257e-03	1.8648	1.9915e-02	1.9884	6.8737e-02	2.0016
640	6.5691e-04	1.8846	5.0069e-03	1.9919	1.7177e-02	2.0006
1280	1.7599e-04	1.9002	1.2567e-03	1.9943	4.2936e-03	2.0002
2560	4.6740e-05	1.9128	3.1505e-04	1.9960	1.0733e-03	2.0001

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