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Research Article

Examining the Mathematica algorithm for general Heun function calculation: a comparative analysis

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Abstract

We investigate the numerical calculation of the general Heun equation using Wolfram Mathematica's functions, comparing the numerical solutions with hypergeometric and explicit solutions. This exploration sheds light on the efficacy and accuracy of the numerical algorithm implemented in Mathematica for computing Heun functions.

Keywords: General Heun function; hypergeometric function; numerical simulations; analytic solution; Wolfram Mathematica

AMS subject classification: 34A25 (Ordinary differential equations, Second-order linear equations); 33C15 (Special functions, Hypergeometric functions); 65L80 (Numerical solution of ordinary differential equations); 33E05 (Computer algebra, Special functions)

1. Introduction

The five Heun equations constitute a class of advanced second-order ordinary differential equations that generalize the equations of the hypergeometric class, as well as many other known equations [1]- [2]. This class emerges from the general Heun equation through the merging of two or more singularities in different combinations, using a coalescence procedure [1], [3]. Due to an additional singularity compared to its predecessor, the Gauss ordinary hypergeometric equation [2], the general Heun equation possesses remarkable potential for diverse applications in physics and mathematics [1]. For instance, the Schrödinger equation for a large number of interaction potentials has been shown to be solvable by reducing it to this equation [4]. Some recent examples include the Laplace equation and the Grad-Shafranov equation for plasma equilibrium [5], [6], [7] in cap-cyclide coordinates, both of which have once again been solved by reducing them to the general Heun equation [8], [9].

Each Heun equation generates a pair of special functions that are now considered a part of the next generation of special functions in mathematical physics. One of these functions is a specialized solution of a Heun equation, while the other is the derivative of that function (in contrast to hypergeometric functions, the derivatives of the Heun functions generally do not belong to the Heun class of functions [10]). These are advanced functions that generalize many known special functions, including Gauss, Kummer, Airy, Bessel, Hermite, Mathieu, Coulomb spheroidal, and spheroidal, among others [2]. These new special functions are currently implemented in computer algebra systems such as Maple [11] and Mathematica [12].

The list of the ten new special functions begins with the general Heun function. It is defined as a particular solution of the general Heun equation that is normalized to unity at the origin. This solution can be constructed through a power-series expansion that converges in a circle centred at the origin, using the Frobenius method [1]:

$$\text{HeunG}(z) = \sum_{n=0}^{\infty} c_n z^n = 1 + \frac{q}{\alpha\gamma} z + \frac{(-a\alpha\beta\gamma + q\,(1+q+\alpha+\beta-\delta+a(\gamma+\delta)))}{2a^2\gamma(1+\gamma)} z^2 + \cdots \tag{1}$$

It turns out that the coefficients c_n of this expansion are governed by a three-term recurrence relation [1], unlike the two-term relation in the hypergeometric case. This difference leads to several complications [1], [3]. For instance, it becomes impossible to derive a general, closed-form expression for the coefficients. In the context of our study, we note that the appearance of the three-term recurrence relation increases computational time and has the potential to cause the accumulation of errors and computational instabilities for some parameters, especially when exploring a close vicinity of a singularity.

In this paper, we test the algorithm of numerical calculation of the Heun function implemented in Mathematica. We use one of Mathematica's functions, NDSolve, which allows us to find numerical solutions to differential equations, in our specific case a second-order general Heun equation. It employs various numerical methods, such as finite difference or finite element methods, to approximate solutions to differential equations.

NDSolve is a versatile tool commonly used in physics, engineering, and other fields to simulate and analyze dynamic systems described by differential equations. More specifically, it utilizes InterpolatingFunction objects to represent numerical approximations of the solutions for the functions. These objects provide approximations for y_i across the range of the independent variable$x$ values from x_{min} to x_{max}. The process of constructing solutions is iterative: starting at a specific x value, NDSolve takes a series of steps to gradually cover the entire span from x_{min} to x_{max}. To initiate this process, NDSolve requires appropriate initial or boundary conditions for y_i and their derivatives. These conditions define the values of $y_i(x)$, and possibly their derivatives y_i', at specific points x. Typically, for ordinary differential equations, these conditions can be specified at any x, and NDSolve will automatically extend its solution across the entire x range from x_{min} to x_{max}.

In addition, because the solutions obtained in the various cases studied in this paper can be written in terms of generalized hypergeometric functions ${}_pF_q(a_1, \cdots, a_p; b_1, \cdots, b_q; z)$ (see [8]), we compared, via Mathematica, the numerical and the hypergeometric results. Finally, we compared these two results with the explicit solution obtained using the general Heun function $HeunG(a, q, \alpha, \beta, \gamma, \delta, z)$ recently implemented in Mathematica [13].

2. Analytical background

Consider the general Heun equation [1]- [2] given by

$$\frac{d^2u}{dz^2} + \left(\frac{\gamma}{z} + \frac{\delta}{z-1} + \frac{\epsilon}{z-a}\right)\frac{du}{dz} + \frac{\alpha\beta z - Q}{z(z-1)(z-a)}u = 0 \tag{2}$$

with parameters corresponding to the solution of the two-dimensional Laplace equation in cap-cyclide coordinates [8]:

$$\gamma = 1 + 2\sigma, \quad \delta = \epsilon = \frac{1}{2}, \quad \alpha\beta = \frac{1}{4} + \sigma, \quad \sigma = \pm\frac{q}{2}, \tag{3}$$

$$a = \frac{1}{k^2}, \quad Q = \frac{\sigma(a+1)}{2} + \frac{(1+a)q^2 + ap^2}{4}, \tag{4}$$

where p and q are arbitrary constants. The parameters α and β are determined here by applying the Fuchsian condition:

$$1 + \alpha + \beta = \gamma + \delta + \epsilon. \tag{5}$$

In this paper, we consider the solutions of the general Heun equation in terms of the generalized hypergeometric functions which are achieved if the parameter γ is a non-positive integer [8]. These specific values of γ are of particular computational interest. The reason is that for a negative integer γ, the standard Frobenius series solution of the general Heun equation in the vicinity of the singular point $z = 0$ provides only one independent solution, leading to complications when constructing the second solution. Nevertheless, there exists a countable set of specific cases for which the general solution of the Heun equation can be solved in terms of generalized hypergeometric functions. In these cases, the accessory parameter Q should obey a special polynomial equation of the degree $-\gamma + 1$ [14]- [15].

We start with the simplest case $\gamma = 0$ achieved if $q = 1$ ($\sigma = -\frac{q}{2}$). The accessory parameter of the equation (2) should then satisfy the equation $Q = 0$, which occurs when $p = 0$. The Fuchsian condition reduces to $\alpha + \beta = 0$ and using equation (3) , we obtain $\alpha = -\frac{1}{2}, \quad \beta = \frac{1}{2}$. In this case, the general Heun equation admits the following general solution in terms of the Gauss hypergeometric functions:

$$u(z) = c_1 \cdot {}_2F_1\left(\alpha, \beta; \epsilon; \frac{z-a}{1-a}\right) + c_2 \cdot {}_2F_1\left(\alpha, \beta; \delta; \frac{z-1}{a-1}\right), \quad c_1, c_2 \in \mathbb{C}. \tag{6}$$

Next, we examine the special case $\gamma = -1$, which is obtained if $\sigma = \frac{q}{2}$ $q = -2$ or $\sigma = -\frac{q}{2}$ $q = 2$. In this case, if the accessory parameter Q satisfies the quadratic equation

$$2Q^2 - (1 + a)Q + 2a\alpha\beta = 0, \tag{7}$$

so that $\alpha = -\frac{3}{2}, \quad \beta = \frac{1}{2}$, the general solution to equation (2) admits the following representation in terms of the Clausen generalized hypergeometric functions [16]:

$$u(z) = c_1 \cdot {}_3F_2\left(1 + e_1, \alpha, \beta; e_1, \epsilon; \frac{z-a}{1-a}\right) + c_2 \cdot {}_3F_2\left(1 + s_1, \alpha, \beta; s_1\delta; \frac{z-1}{a-1}\right), \tag{8}$$

where c_1, c_2 are arbitrary constants and

$$e_1 = -\frac{a\alpha\beta}{Q}, \quad s_1 = -\frac{\alpha\beta}{Q}. \tag{9}$$

We note that for specific parameters (3) this solution reduces to quasi-polynomials:

$$u(z) = c_1\sqrt{1-z}\,(6 - p^2(1 + 2z)) + c_2\sqrt{1-k^2z}\,(4 - (2 + p^2)z), \quad c_1, c_2 \in \mathbb{C}. \tag{10}$$

with

$$p = \pm\sqrt{-1 - k^2 \pm \sqrt{1 + 14k^2 + k^4}}, \tag{11}$$

where any combination of signs is admissible. Observe that the condition (7) is equivalent to

$$Q = \frac{2 + 2k^2 + p^2}{4k^2}. \tag{12}$$

Alternative representations for the analytic solution (8) can be obtained by using the 192 solutions to the general Heun equation presented by Maier [17]. In order to reformulate solution (8), two appropriate linearly independent solutions should be chosen. We apply the following representation:

$$\begin{aligned} u(z) = {} & C_1\, z^{1-\gamma} H(1-a, -Q + \alpha\beta + (a-1)(\gamma-1)\delta, 1 + \alpha - \gamma, 1 + \beta - \gamma, \delta, 2 - \gamma; 1 - z) \\ & + C_2\, z^{1-\gamma} H(a, Q - (\gamma-1)(1 + \alpha + \beta - \gamma + (a-1)\delta), 1 + \alpha - \gamma, 1 + \beta - \gamma, 2 - \gamma, \delta; z), \quad C_1, C_2 \in \mathbb{C}. \end{aligned} \tag{13}$$

Observe that this formula is well-defined because δ and $2 - \gamma$ are not negative integers.

We also consider the case where $\gamma = -2$, which occurs when either $\sigma = \frac{q}{2}$ $q = -3$ or $\sigma = -\frac{q}{2}$ $q = 3$. In this instance, we have $\alpha\beta = -\frac{5}{4}$ and applying the Fuchsian condition (5) we obtain $(\alpha, \beta) = (-\frac{5}{2}, \frac{1}{2})$. In this case, if the accessory parameter Q satisfies the third-degree equation

$$2Q^3 - 5(1 + a)Q^2 - (8a - 3)Q + 5a(a + 1) = 0, \tag{14}$$

the solution of the general Heun equation (2) can be expressed using the generalized hypergeometric function:

$$u(z) = c_1 \cdot {}_4F_3\left(1+e_1, 1+e_2, \alpha, \beta; e_1, e_2, \epsilon; \frac{z-a}{1-a}\right) + c_2 \cdot {}_4F_3\left(1+s_1, 1+s_2, \alpha, \beta; s_1, s_2\delta; \frac{z-1}{a-1}\right), \tag{15}$$

where the expressions for the parameters e_1, e_2, s_1, s_2 are:

$$e_{1,2} = \frac{Q-a-2 \mp \sqrt{1+7a-2a^2+(3a+1)Q-Q^2}}{2}, \tag{16}$$

$$s_{1,2} = \frac{Q-2a-1 \mp \sqrt{7a-2+a^2+(3+a)Q-Q^2}}{2}. \tag{17}$$

For the specific values of the involved parameters defined by equations (3), (4), the solution (15) again reduces to a quasi-polynomial function:

$$u(z) = c_1\sqrt{1-z}\,P_1(z) + c_2\sqrt{1-k^2z}\,P_2(z), \quad c_1, c_2 \in \mathbb{C}. \tag{18}$$

with the following two quadratic polynomials:

$$\begin{aligned} P_1(z) = {} & (160+22p^2+p^4+2k^2(p^2-16)) - 2(4(5+22k^2+5k^4)+12(k^2+1)p^2+p^4)z \\ & +(160k^4+2p^2+p^4+k^2(22p^2-32))z^2, \end{aligned} \tag{19}$$

$$\begin{aligned} P_2(z) = {} & (160k^4+2p^2+p^4+k^2(22p^2-32)) - 2k^2(4(5+22k^2+5k^4)+12(k^2+1)p^2+p^4)z \\ & +k^4(160+22p^2+p^4+2k^2(p^2-16))z^2, \end{aligned} \tag{20}$$

where p satisfies the relation (14).

An alternative formulation for solution (15) can be constructed through the utilization of two suitable linearly independent general Heun solutions (13).

3. Numerical simulations

We now compare the above analytic solutions with the numerical solution obtained using the NDSolve function in Wolfram Mathematica 13.2 for different values of the parameter k. In addition, we will investigate how these solutions differ from the solution ((13)) expressed in terms of general Heun functions. NDSolve requires appropriate initial or boundary conditions for the function and its derivatives. The accuracy of the numerical solution heavily depends on these conditions being correctly specified. The step size and the numerical method used (e.g., explicit vs. implicit methods) are crucial for accuracy and stability. Smaller step sizes can lead to more accurate results but at the cost of increased computational time. Mathematica allows the user to specify method options to control these aspects. The values of the parameters in the Heun equation, particularly those near singularities, can significantly affect the stability and accuracy of the numerical solution. Near singularities, numerical solutions are prone to instabilities and increased error accumulation. We validated the effectiveness of NDSolve by comparing its numerical solutions with analytic solutions expressed in terms of generalized hypergeometric functions and explicit solutions written through the general Heun function itself. We focused on three specific cases defined by distinct non-positive integer values of the characteristic exponent for a singularity of the general Heun equation. For each case, we observed that Mathematica's numerical solutions closely matched the analytic solutions over the domain $0 < z < 1$. This consistency across different parameter values demonstrated the robustness and reliability of the NDSolve algorithm for computing Heun functions. One of the main challenges when using NDSolve for Heun functions is dealing with the vicinity of singularities. Singularities can cause computational instabilities and error accumulation. The Heun equation involves a three-term recurrence relation for the series coefficients, unlike the two-term relation in the hypergeometric case, leading to increased computational complexity and potential numerical instability. To mitigate these challenges, we carefully chose specific parameter values that allow expressing the Heun function as a combination of a finite number of hypergeometric functions. This approach facilitated more stable and accurate numerical comparisons. However, we acknowledged that further investigation is necessary to explore the performance of NDSolve for a broader set of parameter combinations, particularly near singularities.

- Case $\gamma = 0$

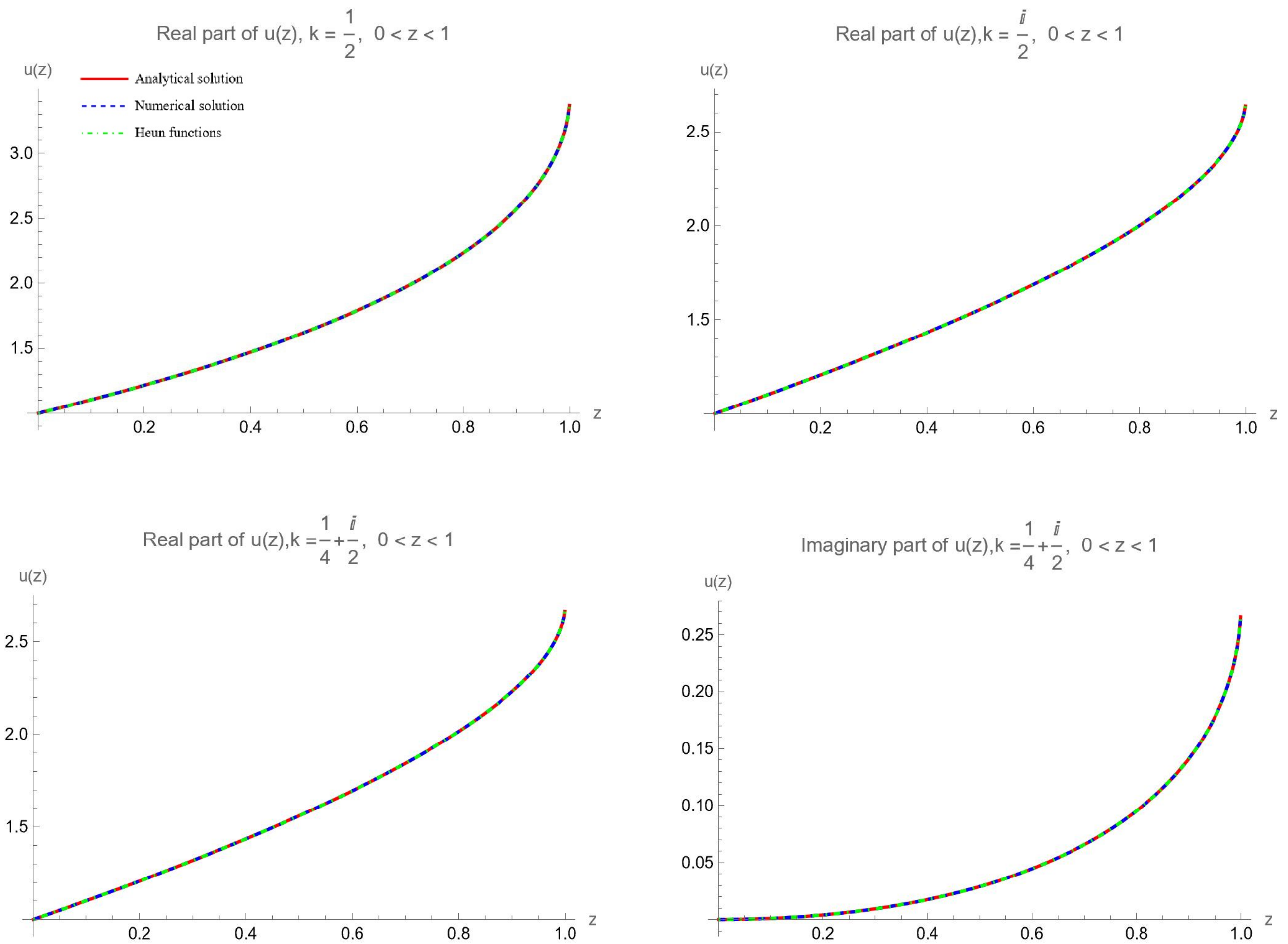
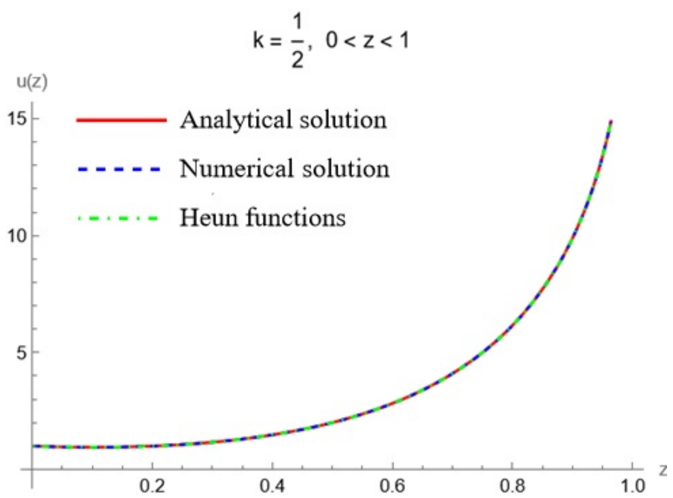


Figure 1. Comparison of analytical and numerical solutions of the general Heun equation in the case $\gamma = 0$, in the $0 < z < 1$ domain for different values of k.

- Case $\gamma = -1$



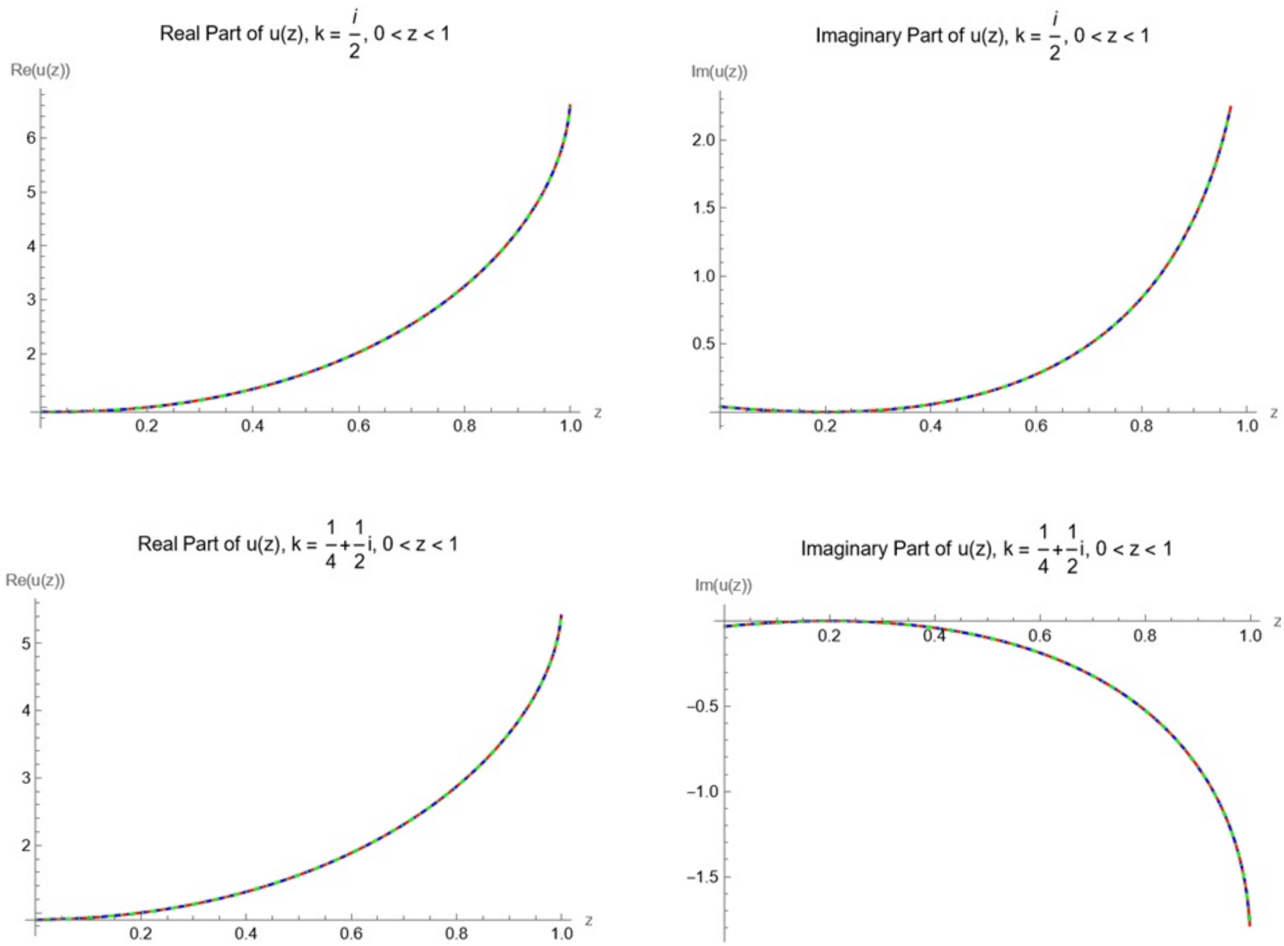


Figure 2. Comparison of analytical and numerical solutions of the general Heun equation in the case $\gamma = -1$, in the $0 < z < 1$ domain for different values of k.

- Case $\gamma = -2$

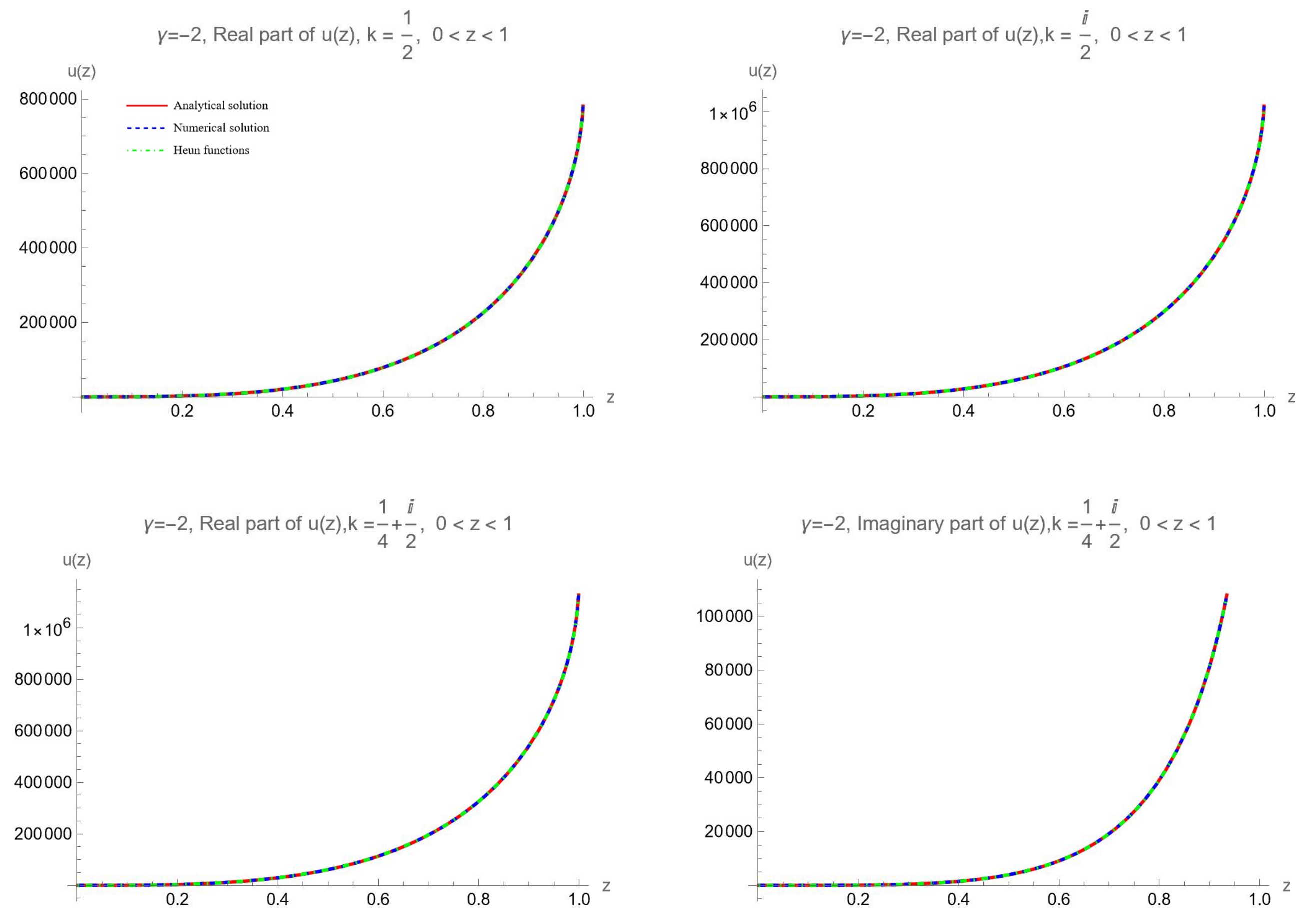


Figure 3. Comparison of analytical and numerical solutions of the general Heun equation in the case $\gamma = -2$, in the $0 < z < 1$ domain for different values of k.

4. Conclusion

In this paper, we investigated the accuracy of the numerical calculation algorithm for the general Heun function implemented in Wolfram Mathematica. We compared the numerical solutions obtained using Mathematicaâ€™s NDSolve function with analytic solutions expressed in terms of (generalized) hypergeometric functions and explicit solutions written through the general Heun function itself. Our analysis focused on three specific cases defined by distinct non-positive integer values of the characteristic exponent for a singularity of the general Heun equation. These cases also involved specific choices for the accessory parameter that allow expressing the Heun function as a combination of a finite number of hypergeometric functions. The comparisons were performed across the domain $0 < z < 1$. The results demonstrate that the Mathematica algorithm accurately reproduces the analytic and explicit solutions for the general Heun function in the examined cases. This suggests the robustness and reliability of the implemented algorithm for a range of parameter values. However, it is important to acknowledge that this study only explored a limited portion of the parameter space. The accurate reproduction of solutions by the Mathematica algorithm can benefit researchers and engineers working with the general Heun equation in various fields, such as quantum mechanics, cosmology, and wave propagation problems. This allows them to efficiently obtain numerical solutions with confidence in their accuracy. Future work could involve investigating the algorithm's performance for a broader set of parameter combinations, especially near singularities where numerical calculations might be more challenging. Additionally, exploring the algorithm's behavior in complex domains of the variable would be valuable. This could provide insights into the solutions' behavior under more realistic conditions, potentially extending the algorithm's applicability to a wider range of problems in various scientific disciplines. Furthermore, investigating the computational efficiency of the Mathematica algorithm compared to alternative methods could be informative.

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Author Contributions

The authors contributed equally to this work. The authors read and approved the final version of the manuscript.

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The authors declare no conflict of interest.

References

1. A. Ronveaux, *Heun's Differential Equations.* Oxford University Press, 1995.
2. F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, *NIST Handbook of Mathematical Functions.* Cambridge University Press, 2010.
3. S. Y. Slavyanov and W. Lay, *Special Functions.* Oxford University Press, 2000.
4. A. M. Ishkhanyan, Schrödinger potentials solvable in terms of the general heun functions, *Annals of Physics*, vol. 388, pp. 456–471, 2018.
5. H. Grad and H. Rubin, Hydromagnetic equilibria and force free fields, *J. Nucl. Energy*, vol. 7, p. 284, 1958.
6. V. D. Shafranov, Equilibrium of a plasma toroid in a magnetic field, *Sov. Phys. JETP*, vol. 37, p. 775, 1960.
7. V. S. Mukhovatov and V. D. Shafranov, Plasma equilibrium in a tokamak, *Nucl. Fusion*, vol. 11, p. 605, 1971.
8. A. Lupica, C. Cesarano, F. Crisanti, and A. Ishkhanian, Analytical solution of the three-dimensional laplace equation in terms of linear combinations of hypergeometric functions, *Mathematics*, vol. 9, p. 3316, 2021.
9. F. Crisanti, C. Cesarano, and A. Ishkhanyan, Grad-shafranov equation in cap-cyclide coordinates: the heun function solution, *Mathematics*, vol. 11(9), p. 3316, 2023.
10. A. M. Ishkhanyan, New solutions of heun's general equation, *J. Phys. A*, vol. 36, p. L81, 2003.
11. Maple Online Help, The five second order linear Heun equations and the corresponding Heun function solutions. Accessed on 30.03.2024.
12. T. A. Ishkhanyan, From sine to Heun: 5 new functions for mathematics and physics in the Wolfram language. Accessed on 30.03.2024.
13. Wolfram Research, HeunG, Wolfram language function.
14. T. A. Ishkhanyan, T. A. Shahverdyan, and A. M. Ishkhanyan, Expansions of the solutions of the general heun equation governed by two-term recurrence relations for coefficients, *Advances in High Energy Physics*, vol. 2018, p. 4263678, 2018.

15. A. M. Ishkhanian, Generalized hypergeometric solutions of the heun equation, *Theor. Math. Phys.*, vol. 202, p. 1, 2020.
16. L. J. Slater, *Generalized Hypergeometric Functions.* Cambridge University Press, 1966.
17. R. S. Maier, The 192 solutions of the heun equation, *Mathematics of Computation*, vol. 76, pp. 811–843, 2007.