

A Comparison of Interpolation and Least Squares Methods for the Approximate Solution of Differential Equation



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ABSTRACT: The aim of this article is to assist novice students in understanding and applying numerical analysis techniques. This article presents a comparison between the numerical methods of least squares and Newton's interpolation for solving differential equations with boundary conditions. Two case studies are examined where these methodologies are applied, generating polynomial solutions of degree 20. Both methods demonstrate high accuracy, despite differences in the magnitude and signs of the coefficients for each power forming the polynomial. The solution obtained via interpolation exhibits better accuracy compared to LMS, with an improvement of up to 8 orders of magnitude near the right boundary.

KEYWORDS: Polynomial approximation, numerical analysis, ordinary differential equations, boundary value problems.

I. INTRODUCTION

The advancements in computing have substantially enhanced the significance of numerical methods. The capacity of computers to execute complex calculations rapidly and efficiently has driven the widespread adoption of numerical algorithms across nearly all branches of engineering. In disciplines such as civil engineering, numerical methods are crucial for structural analysis, enabling the evaluation of the behavior of bridges, buildings, and other infrastructures under diverse loading conditions. Similarly, in mechanical and electrical engineering, these methods facilitate the analysis of dynamic systems, optimization of machine design, and the development of circuits and electronic devices, among other applications [1-3].

Additionally, numerical methods are indispensable for simulating complex systems and processes, such as fluid flow, heat transfer, wave propagation, and the dynamics of nonlinear systems. These simulations enable the prediction of system behavior prior to actual implementation, optimizing resource use during the design and construction phases. A key feature of numerical methods is their ability to manage uncertainties and variations in input data. In engineering, models often rely on parameters that may not be fully defined or that can vary within certain ranges. Numerical methods facilitate the simulation of these variations, enabling engineers to make informed decisions and design more robust and efficient systems.

Numerical methods are an essential tool in modern engineering, as they enable the solution of complex problems that cannot be addressed using exact analytical methods [4]. In many cases, the equations that describe physical phenomena, such as differential equations, heat transfer, fluid flow, structural mechanics, and others, do not have exact solutions or are difficult to obtain using traditional methods [1-3]. Numerical methods commonly used to solve differential equations include the Runge-Kutta methods (RKM), Euler's method (EuM), Milne's method (MM), the shooting method (SM), and the finite difference method (FDM),

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among others [4-6]. However, there are also semi-analytical solution methods that can provide algebraic expressions, such as the Classical perturbation method (PM) [7-9], Harmonic balance method (HBM) [10], Modified Taylor method (MTM) [11], Taylor series method coupled with the shooting technique (TSM) [12], Power extended series method (PSEM) [13-15], Rational homotopy perturbation method (RHPM) [16], Leal polynomials method (LPM) [17], Orthogonal collocation method (OCM) [18], and Orthogonal collocation on finite elements (OCFE) [19,20].

In this article, two case studies are presented comparing the least squares method and interpolation to obtain an approximate solution. The paper is organized as follows: Section II provides an overview of the least squares method, while Section III introduces the basics of interpolation. Section IV details the two case studies. In Section V, a detailed discussion of the results is provided. Finally, the conclusions of this work are presented in Section VI.

II. SOME BASICS OF LEAST SQUARES METHOD

Let $(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots, (x_i, y_i)$, represent the coordinates of a data set, where $i = 0, 1, 2, \dots, n$, and the fitting curve is described as $y = f(x, a_0, a_1, a_2, \dots, a_i)$, where $[a_0, a_1, \dots, a_i]$ are adjustment constants. The least squares approximation [17, 21, 22] aims to minimize the sum of the squares of the vertical distances from the y_i values to the ideal model $f(x)$. The objective is to derive the model function $S(a_0, a_1, a_2, \dots, a_i)$ which minimizes the squared error, defined by:

$$S(a_0, a_1, a_2, \dots, a_i) = \sum_{i=1}^n ((y_i) - f(x_i, a_0, a_1, a_2, \dots, a_i))^2. \tag{1}$$

Therefore, equation (1) is designed to minimize the error with respect to the sample set. To achieve this, partial derivatives are taken with respect to each adjustment constant, resulting in a system of nonlinear equations given by:

$$\begin{aligned} \frac{\partial S}{\partial a_0} &= \frac{\partial}{\partial a_0} \left(\sum_{i=1}^n ((y_i) - f(x_i, a_0, a_1, a_2, \dots, a_i))^2 \right) = 0, \\ \frac{\partial S}{\partial a_1} &= \frac{\partial}{\partial a_1} \left(\sum_{i=1}^n ((y_i) - f(x_i, a_0, a_1, a_2, \dots, a_i))^2 \right) = 0, \\ \frac{\partial S}{\partial a_2} &= \frac{\partial}{\partial a_2} \left(\sum_{i=1}^n ((y_i) - f(x_i, a_0, a_1, a_2, \dots, a_i))^2 \right) = 0, \\ &\vdots \\ \frac{\partial S}{\partial a_n} &= \frac{\partial}{\partial a_n} \left(\sum_{i=1}^n ((y_i) - f(x_i, a_0, a_1, a_2, \dots, a_i))^2 \right) = 0. \end{aligned} \tag{2}$$

By solving the system in equation (2) for the adjustment constants, a model can be obtained that provides the best fit to the data set. This method allows the creation of a continuous function in space with minimized error relative to the samples [31]. Consequently, various models can be tested, and the one providing the best fit can be selected. Figure. 1 illustrates the methodology, where the asterisk symbol represents the data set. For each datum, a value (x_i, y_i) is given (where $i = 1, 2, 3, \dots$) The best-fitting function, represented by the blue line, can then be obtained.

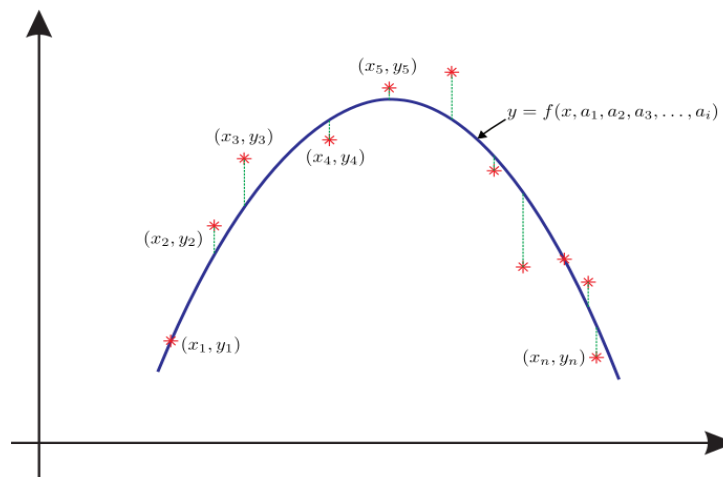


Figure 1. The least squares method.

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III. SOME BASICS OF NEWTON INTERPOLATION METHOD

The Newton Interpolation method (NIM) are denoted by Newton polynomials as ω_i , where $i = 0, \dots, n$. The Newton polynomials are defined as follows:

$$\begin{aligned}\omega_0(x) &= 1, \\ \omega_1(x) &= (x - x_0), \\ \omega_2(x) &= (x - x_0)(x - x_1), \\ &\vdots \\ \omega_n(x) &= (x - x_0)(x - x_1) \cdots (x - x_{n-1}),\end{aligned}\tag{3}$$

using a product notation, we have

$$\omega_i(x) = \prod_{k=0}^{i-1} (x - x_k).\tag{4}$$

The expansion for Newton interpolation is given by

$$p(x) = \sum_{i=0}^n c_i \omega_i(x).\tag{5}$$

In this polynomial representation, the polynomial interpolation problem leads to the following observations. Starting with a single node x_0 , we have $f(x_0) = p(x_0) = c_0$. Considering two nodes x_0 and x_1 , we find that $f(x_0) = p(x_0) = c_0$ and $f(x_1) = p(x_1) = c_0 + c_1(x_1 - x_0)$. This implies that the coefficient

$$c_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}.\tag{6}$$

For three nodes, x_0, x_1, x_2 we have the coefficients c_0, c_1 and $f(x_2)$ given by

$$f(x_2) = p(x_2) = c_0 + c_1(x_2 - x_0) + c_2(x_2 - x_0)(x_2 - x_1).\tag{7}$$

The coefficient c_2 is given by

$$c_2 = \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}.\tag{8}$$

This procedure can be continued and results in a so-called triangular system that allows for the definition of the remaining coefficients c_3, \dots, c_n . It is evident that the coefficients c_k depends only on the interpolation points $(x_0, y_0), \dots, (x_k, y_k)$, where $y_i = f(x_i)$ for $i = 0, \dots, n$. Figure 2 shows the interpolation points.

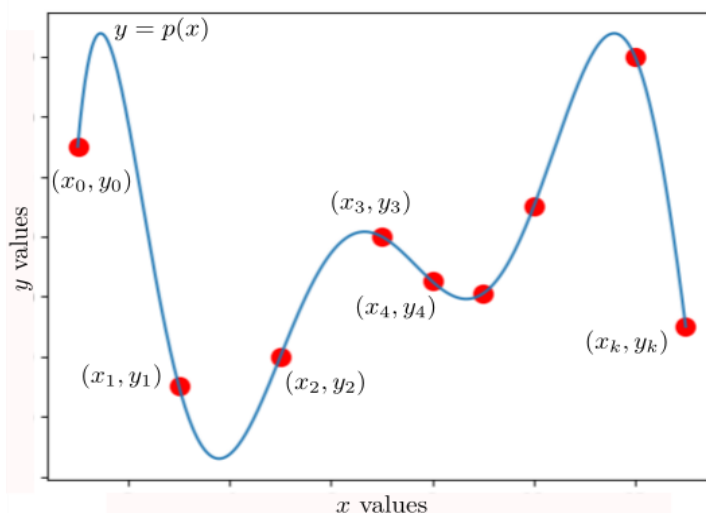


Figure 2. Points for obtain Newton interpolation $p(x)$.

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We will use the following so-called finite difference notation for a function f . The 0th-order finite difference is defined as $f[x_0] = f(x_0)$. The first order finite difference is given by

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}. \quad (9)$$

The second order finite difference is defined by

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}. \quad (10)$$

In general, the n th-order finite difference of the function f , also known as the n th Newton divided difference, is defined recursively by

$$f[x_0, \dots, x_n] = \frac{f[x_1, \dots, x_n] - f[x_0, \dots, x_{n-1}]}{x_n - x_0}. \quad (11)$$

Newton's method for solving the polynomial interpolation problem can be summarized as follows. Given $n + 1$ interpolation points $(x_0, y_0), \dots, (x_n, y_n)$ where $y_i = f(x_i)$, the n th-order interpolation polynomial is expressed in Newton's form as

$$p_n(x) = c_n(x - x_0)(x - x_1) \cdots (x - x_{n-1}) + c_{n-1}(x - x_0)(x - x_1) \cdots (x - x_{n-2}) + \cdots + c_1(x - x_0) - c_0, \quad (12)$$

the coefficients are given by

$$c_k = f[x_0, \dots, x_k], \quad (13)$$

for $k = 0, \dots, n$. The recursion is

$$p_n(x) = p_{n-1}(x) + f[x_0, \dots, x_n](x - x_0)(x - x_1) \cdots (x - x_{n-1}). \quad (14)$$

The finite differences are commonly arranged in a table format. For $n = 3$. Figure 3 shows the schematic of Newton divided difference

| | | | | |
|-------|----------|---------------|--------------------|-------------------------|
| x_0 | $f[x_0]$ | $f[x_0, x_1]$ | $f[x_0, x_1, x_2]$ | $f[x_0, x_1, x_2, x_3]$ |
| x_1 | $f[x_1]$ | $f[x_1, x_2]$ | $f[x_1, x_2, x_3]$ | |
| x_2 | $f[x_2]$ | $f[x_2, x_3]$ | | |
| x_3 | $f[x_3]$ | | | |

Figure 3. Schematic of Newton divided difference.

IV. STUDY CASES

LINEAR DIFFERENTIAL EQUATION

Solve using LMS and NIM for the second order linear differential equation given by

$$\frac{d^2}{dx^2}y(x) - 2\frac{d}{dx}y(x) + 1 = 0, \quad (15)$$

with boundary conditions given by

$$y(0) = 0, \quad y(1) = 1. \quad (16)$$

Solving eq. (15) with analytical methods [1-3] we obtain the exact solution given by

$$y(x) = \frac{e^{2x} - 1}{2(e^2 - 1)} + \frac{x}{2}. \quad (17)$$

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To numerically solve eq. (15), FDM [4-6, 26] was used with $\Delta x = 0.05$. substituting in eq. (15) the centered finite difference equation given by

$$\begin{aligned}\frac{d^2}{dx^2}y(x) &= \frac{y_{n-1} - 2y_n + y_{n+1}}{\Delta x^2}, \\ \frac{d}{dx}y(x) &= \frac{y_{n+1} - y_{n-1}}{2\Delta x},\end{aligned}\tag{18}$$

we obtain the discretized differential equation

$$1.05y_{n-1} - 2y_n + 0.95y_{n+1} + 0.0025 = 0.\tag{19}$$

Solving eq. (19) with Newton--Raphson [4-6] for $n = 1, 2, \dots, 19$, we have the values for y_0, y_1, \dots, y_{20} . In this way, we obtain two vectors, one for the x values with $\Delta x = 0.05$ and another vector for the y values. To determine the polynomials with LMS and NIM, the commands `PolynomialInterpolation(xvalues,yvalues,x,form=Newton)` and `NonlinearFit(model,xvalues,yvalues,x)` were used. Solutions with NIM and LMS are given by (21) and (20) respectively.

$$\begin{aligned}y_{NIM}(x) &= 0.65634620332952489x + 0.15647668760744599x^2 + 0.104404854076063767x^3 + \\ &0.052245990764358680x^4 + 0.020915879239471301x^5 + 0.0069774472352329308x^6 + \\ &0.0019971744246553435x^7 + 0.00049095663402249044x^8 + 0.00013951996689741758x^9 - \\ &0.000054328078982673909x^{10} + 0.00016596782772293354x^{11} - 0.00026934238666747823x^{12} + \\ &0.00035404217233024993x^{13} - 0.00036168509841020129x^{14} + 0.00028393027783503974x^{15} - \\ &0.0001671194126926049x^{16} + 0.00007095382283679825x^{17} - 0.000020361180370863256x^{18} + \\ &3.49470451741379606E(-6)x^{19} - 2.65925791431640295E(-7)x^{20}.\end{aligned}\tag{20}$$

$$\begin{aligned}y_{LMS}(x) &= 0.656346513382579125x + 0.156459602911968266x^2 + 0.104784791468578457x^3 + \\ &0.0476482723508768372x^4 + 0.0549705437514139503x^5 - 0.155579321698876588x^6 + \\ &0.505139420961254787x^7 - 0.947814158934797258x^8 + 0.758753375844371384x^9 + \\ &0.976404503225633651x^{10} - 3.53301356498850142x^{11} + 4.24597785468251586x^{12} - \\ &2.06443844344329328x^{13} - 0.283757957797020728x^{14} + 0.498674010581991772x^{15} - \\ &0.0231816009320996083x^{16} + 0.430016023803910945x^{17} - 0.826428454459058115x^{18} + \\ &0.507509106413305178x^{19} - 0.108470517127701000x^{20}.\end{aligned}\tag{21}$$

Figure 4 shows the solution of Eq. (21) and Eq. (22) compared with the exact solution provided by Eq. (17).

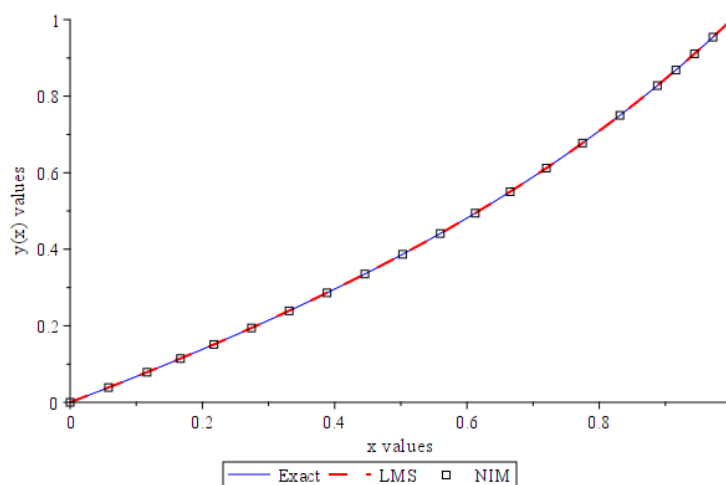


Figure 4. Solution with LMS and NIM vs exact solution.

Bratu's problem in 1D

In this example, we will derive an analytical approximate solution for Bratu's equation using LMS and NIM. This equation holds significant importance due to its numerous applications in science and engineering, where it is utilized to model physical and

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chemical systems. The Bratu model is applied in thermal combustion theory to describe fuel ignition, in chemical reactions, nanotechnology, and radiative heat transfer. Additionally, it plays a key role in the Chandrasekhar model for the expansion of the universe, among other applications [23, 24]. Given these diverse applications, substantial research has been devoted to addressing this problem. Consequently, Bratu’s problem [23, 25] is formulated as follows:

$$\frac{d^2}{dx^2}y(x) + \Phi e^{y(x)} = 0, \tag{22}$$

with boundary conditions given by

$$y(0) = 0, \quad y(1) = 0. \tag{23}$$

and $\Phi = 2.513830719$.

To solve eq. (22) we will use FDM con $\Delta x = 0.05$, and eq. (18) to second derivative. In this way, we obtain

$$y_{n-1} + 0.0062845767975e^{y_n} - 2y_n + y_{n+1} = 0. \tag{24}$$

Solving eq. (24) with Newton-Raphson [4-6] for $n = 1, 2, \dots, 19$, we have the values for y_0, y_1, \dots, y_{20} . In this way, we obtain two vectors, one for the x values with $\Delta x = 0.05$ and another vector for the y values. To determine the polynomials with LMS and NIM, the commands PolynomialInterpolation and NonlinearFit were used. Solutions with NIM and LMS are given by (25) and (26) respectively.

$$y_{NIM}(x) = 1.720128443640218971729x - 1.256827439055559072x^2 - 0.72083475057662646986x^3 - 0.063997951230578387052x^4 + 0.44904256145860782486x^5 - 1.4575435642920005015x^6 + 10.149096189764743420x^7 - 48.735409281849964039x^8 + 180.87693496605174027x^9 - 530.0891431448260701x^{10} + 1231.9009868168424306x^{11} - 2275.6165269680280965x^{12} + 3334.9710726083557611x^{13} - 3850.4687198689967788x^{14} + 3456.7764916743046149x^{15} - 2361.4645323584113059x^{16} + 1185.2770646817245494x^{17} - 411.87736257175880927x^{18} + 88.477866620304638370x^{19} - 8.8477866634463355022x^{20}. \tag{25}$$

$$y_{LMS}(x) = 1.7201282335470655244x - 1.2568107473298733526x^2 - 0.72140933519745738235x^3 - 0.052551792715395086718x^4 + 0.30009456473054326404x^5 - 0.10216016748404672583x^6 + 1.1392186387655841546x^7 - 3.6575836605990399622x^8 + 7.5668358034003122753x^9 - 10.726304212583515470x^{10} + 7.919659034731444185x^{11} + 2.4460831347265027027x^{12} - 12.056599767896566556x^{13} + 10.091818126794679516x^{14} + 2.2311124553067428326x^{15} - 12.170125764543474918x^{16} + 11.943972598591827211x^{17} - 6.0795338487795569033x^{18} + 1.6546897924578650277x^{19} - 0.19053308580514839778x^{20}. \tag{26}$$

Figure 5 shows the solution of Eq. (25) and Eq. (26) compared with the numerical solution provided FDM.

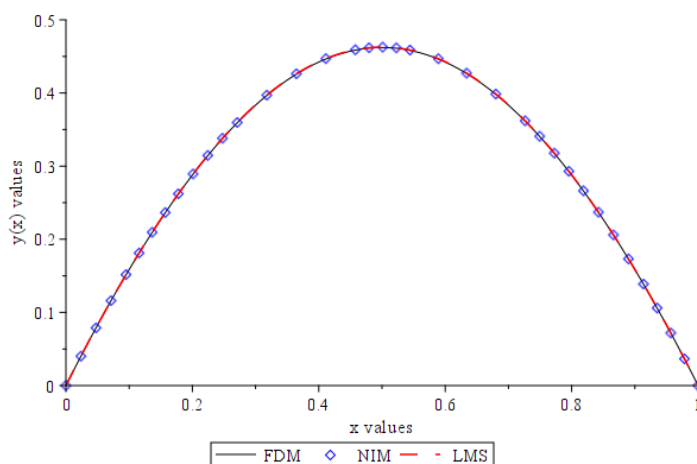


Figure 5. Solution with LMS and NIM vs FDM.

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V. DISCUSSION

In this study, all simulations were performed using Maple 2021 on a computer equipped with 64 GB of RAM, an Intel® Core™ i7-7700 CPU @ 3.60GHz, 4 cores, threads, and an NVIDIA GeForce GTX 1050 Ti video card.

For the case studies presented, polynomial solutions of degree 20 were obtained using both the NIM Method and the LMS method, using on 21 samples derived through finite differences [26]. In both cases, the first three coefficients of the polynomials exhibit a similarity of up to six significant digits. However, as the polynomial degree increases, the precision of the digits tends to diminish. In the first case study, the magnitude of the coefficients derived from LMS is generally larger, while in the second case, the reverse trend is observed. Additionally, there are variations in the signs of the coefficients between the two methods. Despite these differences in sign and magnitude, both methods yield absolute error curves with very similar magnitudes.

Figure 6 illustrates the error curves of the polynomials from equations (20) and (21) compared to the exact solution. The NIM method exhibits a smaller error near the left boundary and in the vicinity of the right boundary compared to the LMS, with an approximate error magnitude on the order of $1E9$.

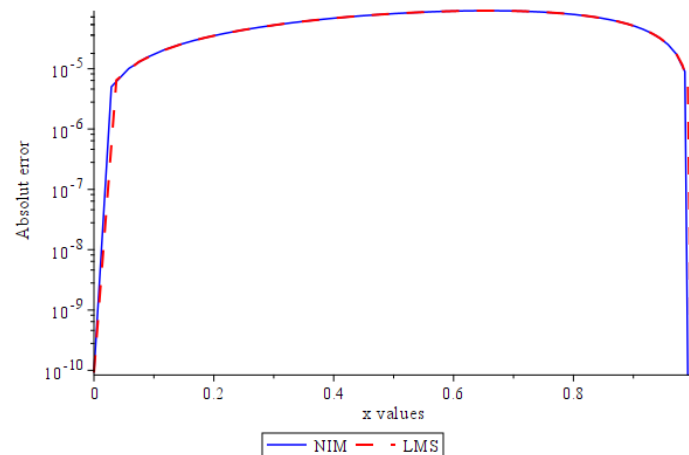


Figure 6. Solution with LMS and NIM vs FDM.

Figure 7 illustrates the error curve for equations (25) and (26) from the second case study. The absolute error curves display behavior similar to that of the previous case study. However, the NIUM method shows superior performance near the right boundary, improving by up to 8 orders of magnitude.

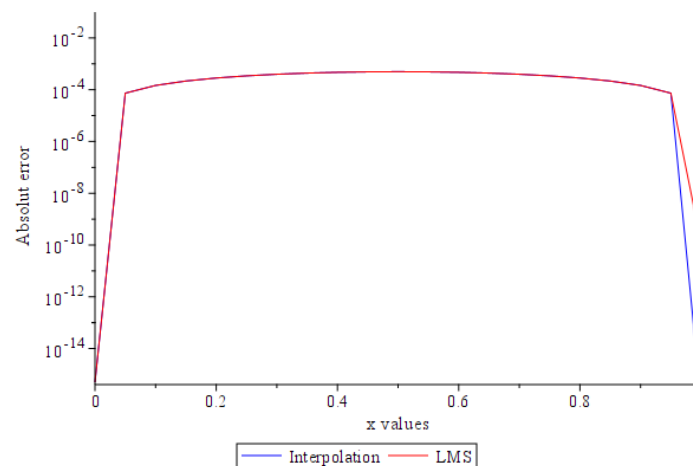


Figure 7. Solution with LMS and NIM vs FDM.

V. CONCLUSIONS

Despite the computational differences between the interpolation method and the least squares method, least squares regression is preferred when there are errors in the data and the goal is to find the curve that best fits the data, approximating the greatest number of points. In contrast, interpolation requires the curve to pass through all given points. Both methodologies used in the case studies presented in this work demonstrated high accuracy, which tends to improve with more significant digits and additional samples. However, NIM exhibited greater precision than LMS at the boundaries because interpolation ensures the curve passes through all data points, forming the polynomial used as the model. On the other hand, LMS offers the flexibility to choose

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different models based on sinusoids, sigmoids, or a combination of functions when the data follows a different distribution, giving it an advantage over interpolation in such cases.

DECLARATION OF INTERESTS STATEMENT

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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