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Lagrange Interpolation in Matrix Form for Numerical Differentiation and Integration

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Abstract: Numerical differentiation has been widely applied in engineering practice due to its remarkable simplicity in the approximation of derivatives. Existing formulas rely on only three-point interpolation to compute derivatives when dealing with irregular sampling intervals. However, it is widely recognized that employing five-point interpolation yields a more accurate estimation compared to the three-point method. Thus, the objective of this study is to develop formulas for numerical differentiation using more than three sample points, particularly when the intervals are irregular. Based on Lagrange interpolation in matrix form, formulas for numerical differentiation are developed, which are applicable to both regular and irregular intervals and can use any desired number of points. The method can also be extended for numerical integration and for finding the extremum of a function from its samples. Moreover, in the proposed formulas, the target point does not need to be at a sampling point, as long as it is within the sampling domain. Numerical examples are presented to illustrate the accuracy of the proposed method and its engineering applications. It is demonstrated that the proposed method is versatile, easy to implements, efficient, and accurate in performing numerical differentiation and integration, as well as the determination of extremum of a function.

Keywords: Numerical Derivative, Numerical Integration, Extrema of a Function

1. Introduction

Differentiation is a well-studied subject, see, e.g. [1–3]; however, there are still a number of challenging problems in this field. Numerical differentiation refers to methods of approximating or computing the rate of change of a function or process at a specific point using the sampling data. It is widely applied in many engineering disciplines, such as determining deflections, strains, bending moments, shears in structural analysis, and responses and reactions in dynamic analysis.

Besides numerical differentiation, there are two other methods that are popular in the computation of derivatives using computer programs, i.e., symbolic differentiation and the so-called automatic differentiation. It is challenging to determine which method is the most superior method as each approach has its own distinct advantages.

Symbolic differentiation involves the automated manipulation of expressions to compute derivatives [4]. This method uses established rules of differentiation along with the known derivatives of common functions to derive a symbolic expression for the derivative of a given function. Symbolic computational software, such as Mathematica [5] and Maple [6], has been extensively developed to implement symbolic differentiation. Although symbolic differentiation can provide exact solutions, which could be particularly useful in many applications, it has some drawbacks. The essential problem is that computing the full analytical expression can sometimes result in expression swelling, which can produce very large symbolic expressions due to the application of the product rule and chain rule in differentiation [7]. Furthermore, in most engineering applications, only the evaluation of derivatives at several points is needed [8]; hence, symbolic differentiation is not favoured for efficiency considerations in these applications.

With the rapid development of Artificial Intelligence and deep learning, automatic differentiation has gained great popularity in computing derivatives. In contrast to symbolic differentiation, automatic differentiation excels in efficiency while maintaining accuracy [9, 10]. Automatic differentiation computes the partial derivatives of a sequence of elementary arithmetic operations for which derivatives are known. These derivatives are then combined through the chain rule to obtain the derivative of the main function [11]. As a result, it allows for finding the derivatives of more general functions than symbolic differentiation. Additionally, the computations can be significantly simplified because it stores only the numerical values of intermediate sub-expressions in memory.

Unlike symbolic differentiation and automatic differentiation which rely on fundamental differentiation rules, numerical differentiation is the finite difference approximation of derivatives using values of the main function evaluated at some sample points [8]. Despite the inherent errors in truncation and rounding errors in finite difference approximation, numerical differentiation is still widely used due to its convenience [12]. The most important advantage of numerical differentiation is that it can deal with situations when the main function is unavailable or, in other words, when the function is defined by a set of discrete samples. This flexibility sets it apart from the other two methods that require the explicit expression of the main function. Furthermore, numerical differentiation plays a crucial role in solving differential equations [13], making it particularly advantageous in certain engineering applications, such as dynamic vibration analysis.

In numerical differentiation, the derivative of a function $y(x)$ can be approximated by

$$y'(x) = \frac{y(x+h) - y(x)}{h} + \mathcal{O}(h), \tag{1}$$

where $h > 0$ is a small step size, and $\mathcal{O}(h)$ is known as the truncation error. Equation (1) is also known as the forward finite difference approximation [14]. Various techniques have been developed to reduce the truncation errors in numerical differentiation, such as using a central difference approximation

$$y'(x) = \frac{y(x+h) - y(x-h)}{2h} + \mathcal{O}(h^2). \tag{2}$$

In equation (2), the truncation error is reduced from first-order to second-order in h. The corresponding second-order derivative based on equation (2) is

$$y''(x) = \frac{y(x+h) - 2\,y(x) + y(x-h)}{h^2} + \mathcal{O}(h^2). \tag{3}$$

It should be mentioned that equations (2) and (3) are based on three-point approximation, which means that three points are used to compute the derivatives.

Estimations of y' and y'' by using five points or samples are known to be more accurate than by using three points or samples. If five points are used, the first-order and second-order derivatives can be evaluated as

$$y'(x) = \frac{-y(x+2h) + 8\,y(x+h) - 8\,y(x-h) + y(x-2h)}{12h}, \tag{4}$$

and

$$y''(x) = \frac{-y(x+2h) + 16\,y(x+h) - 30\,y(x) + 16\,y(x-h) - y(x-2h)}{12h^2}. \tag{5}$$

Equations (2) to (5) are based on the assumption that the intervals between sample points are consistent. However, in practice, the intervals could be unevenly spaced. In this case, the existing formulas use only three points $(x-\delta,\ x,\ x+\Delta)$, for example,

$$y'(x) = \left[\frac{y(x+\Delta) - y(x)}{\Delta}\right] \cdot \left(\frac{\delta}{\Delta + \delta}\right) + \left[\frac{y(x) - y(x-\delta)}{\delta}\right] \cdot \left(\frac{\Delta}{\Delta + \delta}\right), \tag{6}$$

$$y''(x) = \left[\frac{y(x+\Delta) - y(x)}{\Delta}\right] \cdot \left(\frac{2}{\Delta + \delta}\right) - \left[\frac{y(x) - y(x-\delta)}{\delta}\right] \cdot \left(\frac{2}{\Delta + \delta}\right). \tag{7}$$

Although five points give a better estimate than three points, there are no five-points formulas available when the intervals are irregular.

Numerical integration is a fundamental mathematical technique employed to approximate definite integrals, offering a practical and versatile approach for solving problems where analytical solutions are challenging or impossible to obtain [15, 16]. By discretizing the integration process into manageable steps, numerical integration methods enable the efficient calculation of areas under curves, cumulative sums, and other essential mathematical operations. Most importantly, in some practical engineering problems, the direct measurement of a certain parameter might be not available. Instead, the derivative of it can be easily collected. In such cases, numerical integration can be applied to determine the required parameter approximately.

For example, the measurement of deflection of some structures, such as long-span bridges and transmission towers, may be sometimes challenging. It is more practical to measure the slope using inclinometers or tilt censors than directly measuring the deflection at certain locations. Subsequently, numerical integration can be used to integrate the slope with respect to the position along the building to obtain the deflection at any positions. The intervals can be irregular when the tilt censors are not equally spaced.

In the field of structural engineering, the measurement of bending moment is important. However, the direct measurement of it requires specialized instrumentation such as bending moment sensors or transducers, which is more complex and less common than sensors used for shear force measurement. Consequently, a preferred approach involves obtaining the bending moment by numerically integrating shear force data.

Another example of the application of numerical integration is to determine material hardness through indentation. To conduct the indentation test, a variable load is applied to the material, and the resulting indentation depth under each load step is recorded. Using the acquired force-displacement data, the total work done during the indentation process can be calculated through numerical integration, which is further used together with the indentation depth to obtain material hardness.

When the intervals are regular, a definite integral is computed by using the trapezoidal rule or Simpson's rule as

$$\int_a^b y(x)\,\mathrm{d}x = \frac{h}{2}\Big(y_0 + 2\sum_{k=1}^{k=n-1} y_k + y_n\Big), \tag{8}$$

$$\int_a^b y(x)\,\mathrm{d}x = \frac{h}{3}\Big(y_0 + 4\sum_{k=1}^{k=n/2} y_k + 2\sum_{k=1}^{k=n/2-1} y_k + y_n\Big), \tag{9}$$

where the interval $(a,\, b)$ of integration is divided into n sub-intervals of equal length $h = (b-a)/n$: $y_0 = a,\, y_1,\, y_2,\, \ldots,\, y_n = b$. However, a formula is not available when the intervals are irregular.

A possible approach for performing numerical differentiation and integration with irregular intervals using five points stencil is the Lagrange's interpolation formula, because it can be differentiated or integrated. For a given set of n samples at $x_1,\, x_2,\, \ldots,\, x_n$, Lagrange's interpolation formula is

$$y(x) = \sum_{k=1}^{n}\left[\prod_{\substack{j=1\\ j\neq k}}^{n}\left(\frac{x-x_j}{x_k-x_j}\right)y_k\right]. \tag{10}$$

Differentiating equation (10) with respect to x once and twice gives the first-order and second-order derivatives:

$$y'(x) = \sum_{k=1}^{n}\frac{\mathrm{d}}{\mathrm{d}x}\left[\prod_{\substack{j=1\\ j\neq k}}^{n}\left(\frac{x-x_j}{x_k-x_j}\right)y_k\right], \quad y''(x) = \sum_{k=1}^{n}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[\prod_{\substack{j=1\\ j\neq k}}^{n}\left(\frac{x-x_j}{x_k-x_j}\right)y_k\right]. \tag{11}$$

Integrating equation (10) with respect to x from a to b gives the definite integral:

$$\int_a^b y(x)\,\mathrm{d}x = \sum_{k=1}^{n}\int_a^b\left[\prod_{\substack{j=1\\ j\neq k}}^{n}\left(\frac{x-x_j}{x_k-x_j}\right)y_k\right]\mathrm{d}x. \tag{12}$$

However, it is obvious that each process is very tedious and such an operation is seldom applied.

As estimates of derivatives based on five points have better accuracy than those by using three points, the objective of this study is to derive a formula for numerical differentiation which can use any desired number of sample points when the intervals are irregular. In Section 2, the formulation of the method based on Lagrange interpolation in matrix form is presented. The method can be applied in performing numerical differentiation and numerical integration, and finding extreme values of a function from its samples. In the proposed formula, the target point need not be at a sampling point, insofar as it is within the sampling domain. Four numerical examples are presented in Section 3 to illustrate the proposed method, and some conclusions are drawn in Section 4.

2. Formulation

2.1. Lagrange Interpolation in Matrix Form

Let $y(x)$ be a single-valued smooth function of variable x. n samples are taken at n distinct points $x_1 < x_2 < \cdots < x_n$ to obtain the corresponding values $y_1,\, y_2,\, \ldots,\, y_n$ of the function. A polynomial of degree $(n-1)$ is used to match function $y(x)$ in the interval $x_1 \le x \le x_n$:

$$y(x) = \sum_{i=0}^{n-1} a_i\, x^i = \begin{Bmatrix} 1 & x & x^2 & \dots & x^{n-1} \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1} \end{Bmatrix}. \tag{13}$$

$y(x)$ is to be matched at the n sampling points (x_1, y_1), (x_2, y_2), $\dots$, (x_n, y_n). By collocation, the coefficients a_i of the polynomial of degree $(n-1)$ can be determined as

$$\begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{Bmatrix} = \mathbf{V}_{\mathrm{s}} \begin{Bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{Bmatrix} \quad \Longrightarrow \quad \begin{Bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{Bmatrix} = \mathbf{V}_{\mathrm{s}}^{-1}\, \mathbf{y}_{\mathrm{s}} \tag{14}$$

where $\mathbf{V}_{\mathrm{s}}$ is the Vandermonde matrix of dimension $n \times n$ that depends on the x values of the sampling points, and $\mathbf{y}_{\mathrm{s}}$ denotes the column vector of dimension n of values of y at the sampling points given by

$$\mathbf{V}_{\mathrm{s}} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} \end{bmatrix}, \qquad \mathbf{y}_{\mathrm{s}} = \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{Bmatrix}, \tag{15}$$

where the subscript "s" stands for "sample".

Substituting equation (14) into equation (13), function $y(x)$ is given by

$$y(x) = \begin{Bmatrix} 1 & x & x^2 & \cdots & x^{n-1} \end{Bmatrix} \mathbf{V}_{\mathrm{s}}^{-1}\, \mathbf{y}_{\mathrm{s}}, \tag{16}$$

in which x is the target point and it can be any value satisfying $x_1 \le x \le x_n$. Equation (16) is Lagrange interpolation in matrix form.

2.2. Numerical Differentiation

The derivatives of $y(x)$ can be easily obtained by differentiating equation (16) with respect to x:

$$y'(x) = \begin{Bmatrix} 0 & 1 & 2x & 3x^2 & \cdots & (n-1)x^{n-2} \end{Bmatrix} \mathbf{V}_{\mathrm{s}}^{-1}\, \mathbf{y}_{\mathrm{s}}, \tag{17}$$

$$y''(x) = \begin{Bmatrix} 0 & 0 & 2 & 6x & \cdots & (n-1)(n-2)x^{n-3} \end{Bmatrix} \mathbf{V}_{\mathrm{s}}^{-1}\, \mathbf{y}_{\mathrm{s}}. \tag{18}$$

It should be emphasized that equations (16) to (18) are applicable for any $n \ge 3$. For numerical differentiation, $n = 5$ offers great efficiency and sufficient accuracy.

If only three sampling points are used, equations (17) and (18) reduce to

$$y'(x) = \begin{Bmatrix} 0 & 1 & 2x \end{Bmatrix} \mathbf{V}_{\mathrm{s}}^{-1}\, \mathbf{y}_{\mathrm{s}}, \qquad y''(x) = \begin{Bmatrix} 0 & 0 & 2 \end{Bmatrix} \mathbf{V}_{\mathrm{s}}^{-1}\, \mathbf{y}_{\mathrm{s}}, \tag{19}$$

where

$$\mathbf{V}_{\mathrm{s}} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix}, \qquad \mathbf{y}_{\mathrm{s}} = \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix}. \tag{20}$$

Equation (19) can be easily evaluated to give

$$y'(x) = \frac{(2x - x_2 - x_3)\, y_1}{(x_1 - x_2)(x_1 - x_3)} + \frac{(2x - x_1 - x_3)\, y_2}{(x_2 - x_1)(x_2 - x_3)} + \frac{(2x - x_1 - x_2)\, y_3}{(x_3 - x_1)(x_3 - x_2)}. \tag{21}$$

At the point $x = x_2$, the derivative of $y(x)$ is

$$y'(x_2) = \frac{\Delta \cdot y_3}{(\Delta+\delta)\,\delta} - \frac{\delta \cdot y_1}{(\Delta+\delta)\,\Delta} - \frac{(\Delta-\delta)\,y_2}{(\Delta+\delta)\,\Delta}, \tag{22}$$

where $\Delta = x_2 - x_1$ and $\delta = x_3 - x_2$. Equation (22) can be further simplified to

$$y'(x_2) = \left(\frac{\Delta}{\Delta+\delta}\right) \cdot \left(\frac{y_3 - y_2}{\delta}\right) + \left(\frac{\delta}{\Delta+\delta}\right) \cdot \left(\frac{y_2 - y_1}{\Delta}\right). \tag{23}$$

Therefore, the proposed method reproduces equation (6) when only three points are selected.

Similarly, for the second-order derivative, evaluating equation (20) at $x = x_2$ yields

$$y''(x_2) = \frac{2y_1}{(\Delta+\delta)\,\Delta} - \frac{2y_2}{\Delta\,\delta} + \frac{2y_3}{(\Delta+\delta)\,\delta}. \tag{24}$$

Equation (24) can be expressed as

$$y''(x_2) = \frac{2}{\Delta+\delta}\left(\frac{y_3 - y_2}{\delta} - \frac{y_2 - y_1}{\Delta}\right), \tag{25}$$

which is the same as equation (7).

2.3. Numerical Integration

To evaluate the definite integral of $y(x)$ between a and b, the interval $[a,\, b]$ is divided into sub-intervals. Interpolate the function $y(x)$ in each sub-interval by a polynomial as in equations (13) and (16), and then sum the results over all sub-intervals. For example, considering a typical sub-interval $[x_1,\, x_n]$ with n sampling points $(x_1,\, y_1)$, $(x_2,\, y_2)$, $\ldots$, $(x_n,\, y_n)$, function $y(x)$ is given by equation (16). Integrating equation (16) with respect to x from x_1 to x_n yields

$$\int_{x_1}^{x_n} y(x)\,\mathrm{d}x = \begin{Bmatrix} x_n - x_1 & \frac{x_n^2 - x_1^2}{2} & \frac{x_n^3 - x_1^3}{3} & \cdots & \frac{x_n^n - x_1^n}{n} \end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\,\mathbf{y}_\mathrm{s}. \tag{26}$$

Similar to numerical differentiation, the case when $n = 5$ offers great efficiency and sufficient accuracy in numerical integration.

2.4. Extrema of a Function

Equations (17) and (18) can be used to find the extremum of a function from its sample values. The critical points of function $y(x)$ given by equation (16) can be determined by setting equation (17) to zero:

$$y'(x) = \begin{Bmatrix} 0 & 1 & 2x & 3x^2 & \cdots & (n-1)x^{n-2} \end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\,\mathbf{y}_\mathrm{s} = 0, \tag{27}$$

which is a polynomial equation of degree $(n-2)$. The roots of equation (27) in the interval $[x_1,\, x_n]$ are the critical points.

In our context, a critical point is a location where the slope is equal to zero. The nature of a critical point x^* depends on the value $y''(x^*)$, which can be evaluated using equation (18). If $y''(x^*) < 0$, then $y(x^*)$ is a relative maximum; whereas if $y''(x^*) > 0$, then $y(x^*)$ is a relative minimum.

3. Numerical Examples

In this section, four examples are presented to illustrate the superiority of the proposed method.

3.1. Example 1 – Numerical Differentiation

Consider function $y(x) = \sqrt{x}$. Sample the function at five points with irregular intervals as listed in Table 1.

Table 1. *Five sampling points with irregular intervals.*

x	1.0	1.2	1.5	1.9	2.4
y	1.00000	1.09545	1.22475	1.37841	1.54919

The point $x = 1.5$ is chosen as the target; the exact derivatives are $y'(1.5) = 0.40825$ and $y''(1.5) = -0.13606$. These values will be used to check the accuracy of the results using the proposed method.

Using Three Sampling Points

When three sampling points are used at $x = 1.2, 1.5, 1.9$, the corresponding vector $\mathbf{y}_\mathrm{s}$ and the Vandermonde matrix $\mathbf{V}_\mathrm{s}$ are

$$\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 1.09545 \\ 1.22475 \\ 1.37841 \end{Bmatrix}, \quad \mathbf{V}_\mathrm{s} = \begin{bmatrix} 1 & 1.2 & 1.44 \\ 1 & 1.5 & 2.25 \\ 1 & 1.9 & 3.61 \end{bmatrix} \Longrightarrow \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 0.457779 \\ 0.611707 \\ -0.066929 \end{Bmatrix}.$$

Applying equation (19), the first-order and second-order derivative can be computed

$$y'(1.5) = \begin{Bmatrix}0 & 1 & 3\end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = 0.41092,$$

$$y''(1.5) = \begin{Bmatrix}0 & 0 & 2\end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = -0.13386.$$

If equations (6) and (7) are used, then the first-order and second-order derivatives are obtained as

$$y'(1.5) = \left(\frac{1.37841 - 1.22475}{0.4}\right) \cdot \left(\frac{0.3}{0.7}\right) + \left(\frac{1.22475 - 1.09545}{0.3}\right) \cdot \left(\frac{0.4}{0.7}\right) = 0.41092.$$

$$y''(1.5) = \left(\frac{1.37841 - 1.22475}{0.4}\right) \cdot \left(\frac{2}{0.7}\right) - \left(\frac{1.22475 - 1.09545}{0.3}\right) \cdot \left(\frac{2}{0.7}\right) = -0.13386.$$

Therefore, the proposed method agrees with the existing formula for computing the first and second derivatives using three points when intervals are irregular.

Using Five Sampling Points

When five sampling points are used at $x = 1.0, 1.2, 1.5, 1.9, 2.4$, the corresponding vector $\mathbf{y}_\mathrm{s}$ and the Vandermonde matrix $\mathbf{V}_\mathrm{s}$ are

$$\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 1.00000 \\ 1.09545 \\ 1.22475 \\ 1.37841 \\ 1.54919 \end{Bmatrix}, \quad \mathbf{V}_\mathrm{s} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1.44 & 1.728 & 2.0736 \\ 1 & 1.5 & 2.25 & 3.375 & 5.0625 \\ 1 & 1.9 & 3.61 & 6.859 & 13.0321 \\ 1 & 2.4 & 5.76 & 13.824 & 33.1776 \end{bmatrix} \Longrightarrow \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 0.33111 \\ 0.89787 \\ -0.29707 \\ 0.07671 \\ -0.00862 \end{Bmatrix}.$$

Applying equations (17) and (18), the first-order and second-order derivatives can be determined

$$y'(1.5) = \begin{Bmatrix}0 & 1 & 3 & 6.75 & 13.5\end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = 0.40803,$$

$$y''(1.5) = \begin{Bmatrix}0 & 0 & 2 & 9 & 27\end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = -0.13661.$$

The relative errors between the estimated first-order and second-order derivatives using 5 sampling points and the exact values are 0.054% and 0.386%, respectively; whereas the corresponding errors using 3 sampling points are 0.655% and 1.635%, respectively, which are significantly higher. This indicates that the estimates from five-point interpolation are more accurate as expected.

3.2. Example 2 – Numerical Integration

This example is used to show that the definite integral of the error function is

$$\mathrm{erf}(1) = \frac{2}{\sqrt{\pi}} \int_0^1 \mathrm{e}^{-x^2}\,\mathrm{d}x = 0.8427007929.$$

The integrand is $y(x) = \mathrm{e}^{-x^2}$. The domain of integration $[0,\ 1]$ is divided into two sub-intervals $[0, 0.5]$ and $[0.5, 1]$.

Sub-Interval $[0, 0.5]$

Select five sampling points in this interval: $x = 0, 0.125, 0.25, 0.375, 0.5$. The corresponding vector $\mathbf{y}_\mathrm{s}$ of sampling values of the integrand and the Vandermonde matrix $\mathbf{V}_\mathrm{s}$ are

$$\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 1 \\ 0.9844964 \\ 0.9394131 \\ 0.8688151 \\ 0.7788008 \end{Bmatrix}, \quad \mathbf{V}_\mathrm{s} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0.125 & 0.015625 & 0.0019531 & 0.0002441 \\ 1 & 0.250 & 0.062500 & 0.0156250 & 0.0039063 \\ 1 & 0.375 & 0.140625 & 0.0527344 & 0.0197754 \\ 1 & 0.500 & 0.250000 & 0.1250000 & 0.0625000 \end{bmatrix},$$

which gives

$$\mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 0 \\ 0.0010648 \\ -1.0169995 \\ 0.0866474 \\ 0.3469972 \end{Bmatrix}.$$

Hence, the integral in the first sub-interval $[0,\ 0.5]$ can be found using equation (26)

$$I_1 = \int_0^{0.5} \mathrm{e}^{-x^2}\mathrm{d}x = \begin{Bmatrix} 0.5 & \frac{0.5^2}{2} & \frac{0.5^3}{3} & \frac{0.5^4}{4} & \frac{0.5^5}{5} \end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\,\mathbf{y}_\mathrm{s} = 0.4612807.$$

Sub-Interval $[0.5, 1]$

Select five sampling points in this interval: $x = 0.5, 0.625, 0.75, 0.875, 1$. The corresponding vector $\mathbf{y}_\mathrm{s}$ of sampling values of the integrand and the Vandermonde matrix $\mathbf{V}_\mathrm{s}$ are

$$\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 0.7788008 \\ 0.6766338 \\ 0.5697828 \\ 0.4650432 \\ 0.3678794 \end{Bmatrix}, \quad \mathbf{V}_\mathrm{s} = \begin{bmatrix} 1 & 0.500 & 0.250000 & 0.1250000 & 0.0625000 \\ 1 & 0.625 & 0.390625 & 0.2441406 & 0.1525879 \\ 1 & 0.750 & 0.562500 & 0.4218750 & 0.3164063 \\ 1 & 0.875 & 0.765625 & 0.6699219 & 0.5861816 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix},$$

which gives

$$\mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 0.9581345 \\ 0.3048297 \\ -1.8724796 \\ 1.2045461 \\ -0.2271513 \end{Bmatrix}.$$

Hence, the integral in the second sub-interval $[0.5,\ 1]$ can be found using equation (26)

$$I_2 = \int_{0.5}^{1} \mathrm{e}^{-x^2} \mathrm{d}x = \left\{ 1-0.5 \quad \frac{1-0.5^2}{2} \quad \frac{1-0.5^3}{3} \quad \frac{1-0.5^4}{4} \quad \frac{1-0.5^5}{5} \right\} \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = 0.2855434.$$

Therefore, the definite integral of the error function is

$$\mathrm{erf}(1) = \frac{2}{\sqrt{\pi}} \int_0^1 \mathrm{e}^{-x^2}\,\mathrm{d}x = \frac{2}{\sqrt{\pi}}\,(I_1 + I_2) = 0.8427008,$$

which is the same as the exact solution to the 7th decimal.

3.3. Example 3 – Extrema of a Function

Consider function $y(x) = \mathrm{e}^{x/3}\sin x$. In the interval $[0,\ 7]$, the maximum value is $y_{\max} = 1.78277$ at $x = 1.89255$, and the minimum value is $y_{\min} = -5.08028$ at $x = 5.034140$. These results are used to assess the efficiency and accuracy of the results obtained using the proposed method.

Sample the function at ten points with irregular intervals as listed in Table 2 and shown in Figure 1.

Table 2. *Ten sampling points with irregular intervals.*

x	0.1	0.8	1.5	2.3	3.0
x	0.1	0.8	1.5	2.3	3.0
x	3.6	4.1	4.6	5.5	6.4
y	-1.469219	-3.209491	-4.604363	-4.412943	0.9840206

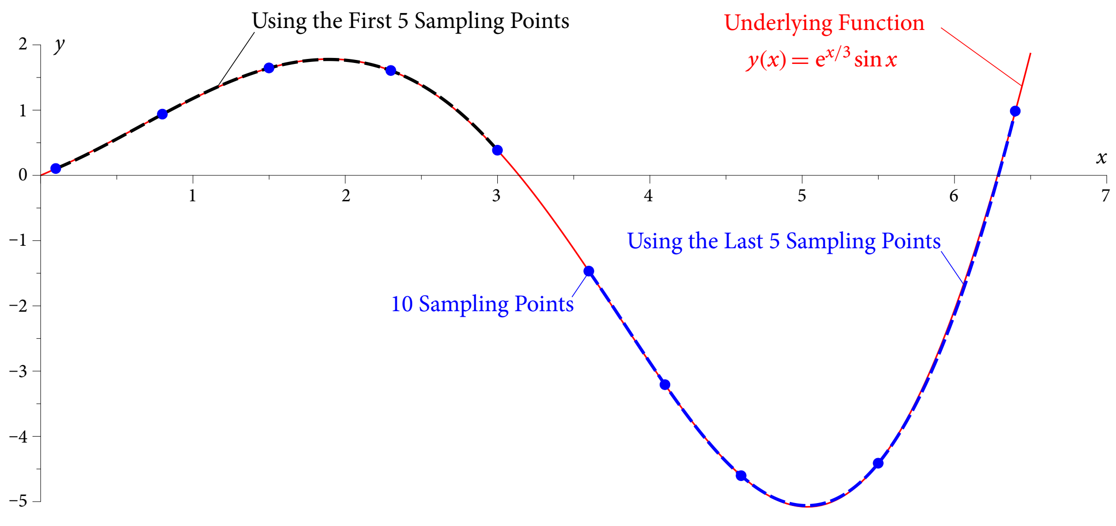

Figure 1. *Finding extremum of a function.*

Using the First Five Sampling Points

When the first five sampling points are used, i.e, $x = 0.1, 0.8, 1.5, 2.3, 3.0,$ the corresponding vector $\mathbf{y}_\mathrm{s}$ of sampling values and the Vandermonde matrix $\mathbf{V}_\mathrm{s}$ are

$$\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 0.1032173 \\ 0.9365838 \\ 1.6445912 \\ 1.6051894 \\ 0.3836040 \end{Bmatrix}, \quad \mathbf{V}_\mathrm{s} = \begin{bmatrix} 1.0 & 0.1 & 0.01 & 0.001 & 0.0001 \\ 1.0 & 0.8 & 0.64 & 0.512 & 0.4096 \\ 1.0 & 1.5 & 2.25 & 3.375 & 5.0625 \\ 1.0 & 2.3 & 5.29 & 12.167 & 27.9841 \\ 1.0 & 3.0 & 9.00 & 27.000 & 81.0000 \end{bmatrix} \Longrightarrow \mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = \begin{Bmatrix} 0.0122629 \\ 0.8459374 \\ 0.6736215 \\ -0.3780205 \\ 0.0244134 \end{Bmatrix}.$$

Equations (27) becomes

$$\begin{aligned} y'(x) &= \begin{Bmatrix} 0 & 1 & 2x & 3x^2 & 4x^3 \end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\,\mathbf{y}_\mathrm{s} \\ &= 0.8459374 + 1.3472430\,x - 1.1340615\,x^2 + 0.0976538\,x^3 = 0, \end{aligned}$$

which has one root $x = 1.8902812$ in the interval $[0.1, 3.0]$. The second-order derivative is given by equation (18)

$$y''(x) = \begin{Bmatrix} 0 & 0 & 2 & 6x & 12x^2 \end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\,\mathbf{y}_\mathrm{s} = 1.3472430 - 2.2681230\,x + 0.2929614\,x^2.$$

The value of the second-order derivative at the critical point is

$$y''(1.8902812) = -1.8933487 < 0 \Longrightarrow \text{relative maximum.}$$

The value of $y(x)$ is given by equation (16)

$$\begin{aligned} y(x) &= \begin{Bmatrix} 1 & x & x^2 & x^3 & x^4 \end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\,\mathbf{y}_\mathrm{s} \\ &= 0.0122629 + 0.8459374\,x + 0.6736215\,x^2 - 0.3780205\,x^3 + 0.0244134\,x^4. \end{aligned}$$

The relative maximum is then obtained:

$$y_\mathrm{max} = y(1.8902812) = 1.7767229,$$

with a relative error of 0.339%, which is very small, as compared to the exact result.

Using the Last Five Sampling Points

When the last five sampling points are used, i.e, $x = 3.6, 4.1, 4.6, 5.5, 6.4,$ the corresponding vector $\mathbf{y}_\mathrm{s}$ of sampling values and the Vandermonde matrix $\mathbf{V}_\mathrm{s}$ are

$$\mathbf{y}_\mathrm{s} = \begin{Bmatrix} -1.4692196 \\ -3.2094912 \\ -4.6043630 \\ -4.4129437 \\ 0.9840206 \end{Bmatrix}, \quad \mathbf{V}_\mathrm{s} = \begin{bmatrix} 1.0 & 3.6 & 12.96 & 46.656 & 167.9616 \\ 1.0 & 4.1 & 16.81 & 68.921 & 282.5761 \\ 1.0 & 4.6 & 21.16 & 97.336 & 447.7456 \\ 1.0 & 5.5 & 30.25 & 166.375 & 915.0625 \\ 1.0 & 6.4 & 40.96 & 262.144 & 1677.7216 \end{bmatrix},$$

which gives

$$\mathbf{V}_\mathrm{s}^{-1}\mathbf{y}_\mathrm{s} = \begin{Bmatrix} -70.7709347 \\ 66.5021899 \\ -21.3663164 \\ 2.6754802 \\ -0.1073216 \end{Bmatrix}.$$

Equations (27) becomes

$$\begin{aligned} y'(x) &= \begin{Bmatrix} 0 & 1 & 2x & 3x^2 & 4x^3 \end{Bmatrix} \mathbf{V}_\mathrm{s}^{-1}\,\mathbf{y}_\mathrm{s} \\ &= 66.5021899 - 42.7326328\,x + 8.0264407\,x^2 - 0.4292866\,x^3 = 0, \end{aligned}$$

which has one root $x = 5.0298711$ in the interval $[3.6, 6.4]$. The second-order derivative is given by equation (18)

$$y''(x) = \{0 \quad 0 \quad 2 \quad 6x \quad 12x^2\} \, \mathbf{V}_\mathrm{s}^{-1} \, \mathbf{y}_\mathrm{s} = -42.7326328 + 16.0528815\,x - 1.2878597\,x^2.$$

The value of the second-order derivative at the critical point is

$$y''(5.0298711) = 5.4289529 > 0 \Longrightarrow \text{relative minumum.}$$

The value of $y(x)$ is given by equation (16)

$$\begin{aligned} y(x) &= \{1 \quad x \quad x^2 \quad x^3 \quad x^4\} \, \mathbf{V}_\mathrm{s}^{-1} \, \mathbf{y}_\mathrm{s} \\ &= -70.7709347 + 66.5021899\,x - 21.3663164\,x^2 + 2.6754802\,x^3 - 0.1073216\,x^4. \end{aligned}$$

The relative maximum is then obtained:

$$y_\mathrm{max} = y(5.0298711) = -5.061298,$$

with a relative error of 0.374%, which is very small, as compared to the exact result.

3.4. Example 4 – Deformation, Bending Moment, and Shear Force of a Beam-Column

Consider an Euler-Bernoulli beam-column AB, which is clumped at end A and supported by a pin at end B, as shown in Figure 2. The beam-column is subjected to an axial compressive load P at end B and a parabolically distributed lateral load $q(x) = q_0\,x^2$. The length of the beam-column is L, the moment of inertia is I, and the Young's modulus is E.

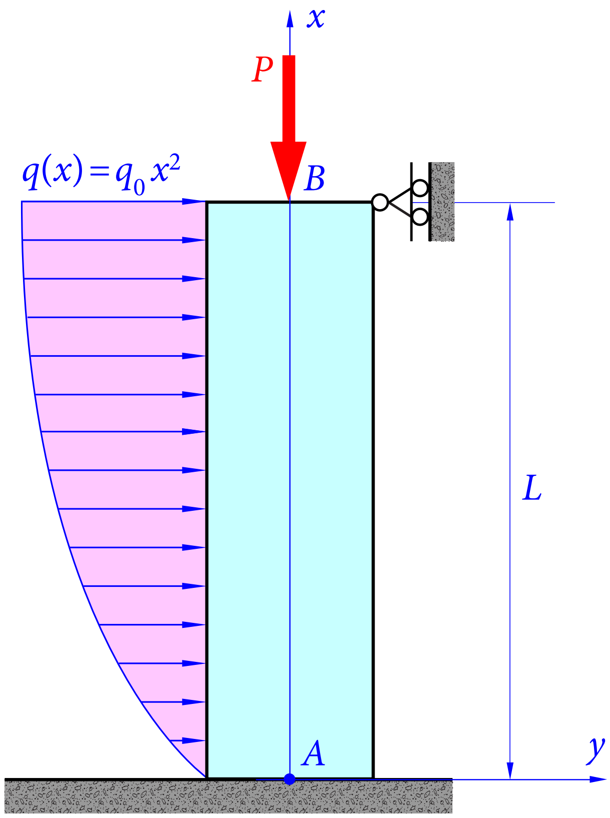

Figure 2. *Clamped-pinned beam-column.*

The differential equation that governs the transverse deflection $y(x)$ is

$$\frac{\mathrm{d}^4 y(x)}{\mathrm{d}x^4} + \alpha^2\,\frac{\mathrm{d}^2 y(x)}{\mathrm{d}x^2} = \frac{q_0\,x^2}{EI}, \qquad \alpha^2 = \frac{P}{EI}. \tag{28}$$

The transverse deflection $y(x)$, which is the general solution of differential equation (28), is

$$y(x) = C_0 + C_1 x + A\cos\alpha x + B\sin\alpha x + \frac{q_0}{P}\Big(\frac{x^4}{12} - \frac{x^2}{\alpha^2}\Big), \tag{29}$$

where A, B, C_0, and C_1 are determined from the boundary conditions.

The bending moment and shear force are given by

$$M(x) = EI\,\frac{\mathrm{d}^2 y(x)}{\mathrm{d}x^2}, \qquad V(x) = -\frac{\mathrm{d}M(x)}{\mathrm{d}x} - P\,\frac{\mathrm{d}y(x)}{\mathrm{d}x}. \tag{30}$$

The boundary conditions are

$$\begin{aligned}&\text{At the clamped support } A,\ x=0: && y(0)=0, \quad y'(0)=0,\\ &\text{At the pin support } B,\ x=L: && y(L)=0, \quad M(L)=0.\end{aligned}$$

Using the boundary conditions, the constants are obtained as

$$\begin{aligned}A = -C_0 &= -\frac{q_0\big(\alpha^4L^4\sin\alpha L - 12\,\alpha^3L^3 + 24\,\alpha L - 24\sin\alpha L\big)}{12\,\alpha^4 P\,\big(\alpha L\cos\alpha L - \sin\alpha L\big)},\\ B = -\frac{C_1}{\alpha} &= \frac{q_0\big(\alpha^4L^4\cos\alpha L - 12\,\alpha^2L^2 + 24 - 24\cos\alpha L\big)}{12\,\alpha^4 P\,\big(\alpha L\cos\alpha L - \sin\alpha L\big)}.\end{aligned}$$

As a numerical example, the following parameters are used: Young's modulus $E = 100\,\text{GPa}$, the thickness, width, and height of the beam-column are $b = 1\,\text{m}$, $h = 10\,\text{m}$, $L = 20\,\text{m}$. The moment of inertia is $I = \frac{1}{12}bh^3$. The loadings are $P = 2$ GN and $q = 2\,\text{MN/m}^2$. Note that very large loadings are applied to create substantial deflection of the beam-column for the purpose of illustration.

The exact transverse deflection $y(x)$ (m) is given by

$$y(x) = 31.6105067 - 0.9815670\,x - 0.1125\,x^2 + \frac{x^4}{12000} \tag{31}$$

$$- 31.6105067\cos(0.0942809\,x) + 10.4110902\sin(0.0942809\,x). \tag{32}$$

It is found that the maximum deflection is 1.3349 m occurring at $x = 12.2006$ m. The relative maximum bending moment is $M(13.9206) = -11.003$ GN·m at critical point $x = 13.9206$ m, and the bending moment at the base $x = 0$ is $M(0) = 12.5960$ GN·m; hence, the maximum bending moment is $M_{\max} = M(0) = 12.5960$ GN·m. There is no critical point for the shear force, and the shear forces at $x = 0$ and $x = 20$ m are $V(0) = 1.9631$ GN and $V(20) = -3.3702$ GN; hence, the maximum shear force (absolute value) is $V_{\max} = V(20) = -3.3702$ GN.

In an experiment, five sensors are placed at $x = 4, 7, 10, 13, 16$ m, and the measured deflections of the beam-column are listed in Table 3. The purpose of the experiment is to determine the maximal deflection, bending moment, and shear force in the beam-column.

Table 3. *Measured deflections of the beam-column.*

x (m)	4	7	10	13	16
y (m)	0.3503	0.8374	1.2312	1.3200	0.9895

To applied the Lagrange interpolation in matrix form presented in Section 2, the boundary conditions have to be supplemented to cover the deflections of the entire beam-column at $x = 0, 4, 7, 10, 13, 16, 20$ m. The corresponding vector $\mathbf{y}_\text{s}$ of sampling values of deflection and the Vandermonde matrix $\mathbf{V}_\text{s}$ are

$$\mathbf{y}_\text{s} = \begin{Bmatrix}0.\\0.3503\\0.8374\\1.2312\\1.3200\\0.9895\\0.\end{Bmatrix}, \quad \mathbf{V}_\text{s} = \begin{bmatrix}1&0&0&0&0&0&0\\1&4&16&64&256&1024&4096\\1&7&49&343&2401&16807&117649\\1&10&100&1000&10000&100000&1000000\\1&13&169&2197&28561&371293&4826809\\1&16&256&4096&65536&1048576&16777216\\1&20&400&8000&160000&3200000&64000000\end{bmatrix},$$

which gives

$$\mathbf{V}_{\mathrm{s}}^{-1}\mathbf{y}_{\mathrm{s}} = \begin{Bmatrix} 0. \\ 0.0004527 \\ 0.0276852 \\ -0.0013747 \\ -3.0959 \times 10^{-5} \\ 1.3274 \times 10^{-6} \\ 9.6731 \times 10^{-9} \end{Bmatrix}.$$

The deflection (m) of the beam-column given by equations (16) is

$$\begin{aligned} y(x) &= \begin{Bmatrix} 1 & x & x^2 & x^3 & x^4 & x^5 & x^6 \end{Bmatrix} \mathbf{V}_{\mathrm{s}}^{-1}\mathbf{y}_{\mathrm{s}} \\ &= 0.0004527\,x + 0.0276852\,x^2 - 0.0013747\,x^3 - 0.0000310\,x^4 + 1.3277 \times 10^{-6}\,x^5 + 9.6731 \times 10^{-9}\,x^6. \end{aligned}$$

Using equation (30), the bending moment (GN·m) and shear force (GN) are given by

$$M(x) = 12.4583429 - 1.8558023\,x - 0.0835903\,x^2 + 0.0059746\,x^3 + 6.5394 \times 10^{-5}\,x^4,$$

$$V(x) = 1.8548970 + 0.0564398\,x - 0.0096759\,x^2 - 1.3490 \times 10^{-5}\,x^3 - 1.3277 \times 10^{-5}\,x^4 - 1.1608 \times 10^{-7}\,x^5.$$

To find the maximum deflection, equation (27) becomes

$$\begin{aligned} y'(x) &= \begin{Bmatrix} 0 & 1 & 2x & 3x^2 & 4x^3 & 5x^4 & 6x^5 \end{Bmatrix} \mathbf{V}_{\mathrm{s}}^{-1}\mathbf{y}_{\mathrm{s}} \\ &= 0.0004527\,x + 0.0553704\,x - 0.0041240\,x^2 - 0.0001238\,x^3 + 6.6385 \times 10^{-6}\,x^4 + 5.8039 \times 10^{-8}\,x^5 = 0, \end{aligned}$$

which has one root $x = 12.2008$ in the interval $(0, 20)$. The value of maximum $y(x)$ at the critical point is obtained as

$$y_{\max} = y(12.2008) = 1.3348\,\text{m}.$$

with a relative error of 0.0008%, which is negligible in engineering problems, as compared to the exact result.

Set the first-order derivative of the bending moment to zero

$$M'(x) = -1.8558023 - 0.1671807\,x + 0.0179239\,x^2 + 0.0002612\,x^3 = 0,$$

which has a root $x = 13.9313$ m. The bending moments at the critical point and at the base $x = 0$ are

$$M(13.9313) = -11.0050\,\text{GN} \cdot \text{m}, \qquad M(0) = 12.4583\,\text{GN} \cdot \text{m},$$

with relative errors of 0.019% and 1.093%, respectively, as compared to the exact result. Hence, the maximum bending moment occurs at the base of beam-column $M_{\max} = M(0) = 12.4583\,\text{GN} \cdot \text{m}$.

The exact shear force does not have a critical point in $(0, 20)$; however, the shear force from Lagrange interpolation has a critical point at $x = 2.8352$ m, with the shear force being $V(2.8352) = 1.9359$ GN. The shear forces at $x = 0$ and $x = 20$ are

$$V(0) = 1.8549\,\text{GN}, \qquad V(20) = -3.4904\,\text{GN},$$

with relative errors of 5.513% and 6.124%, respectively, as compared to the exact result. The maximum shear force (absolute value) occurs at the top of beam-column $V_{\max} = V(20) = -3.4904\,\text{GN}$.

The deflection, bending moment, and shear force of the beam-column are shown in Figure 3, in which the red solid lines are the exact results, while the blue dashed lines are the results from Lagrange interpolation. It is seen that the results obtained from Lagrange interpolation agree very well with the exact results. Note that, from equation (30), the bending moment $M(x)$ is related to the second-order derivative of the deflection $y(x)$, while the shear force $V(x)$ depends on the third-order derivative of the deflection. As a result, the accuracy of the bending moment from Lagrange interpolation is less than that of the deflection, and the accuracy of the shear force is worse than that of the bending moment.

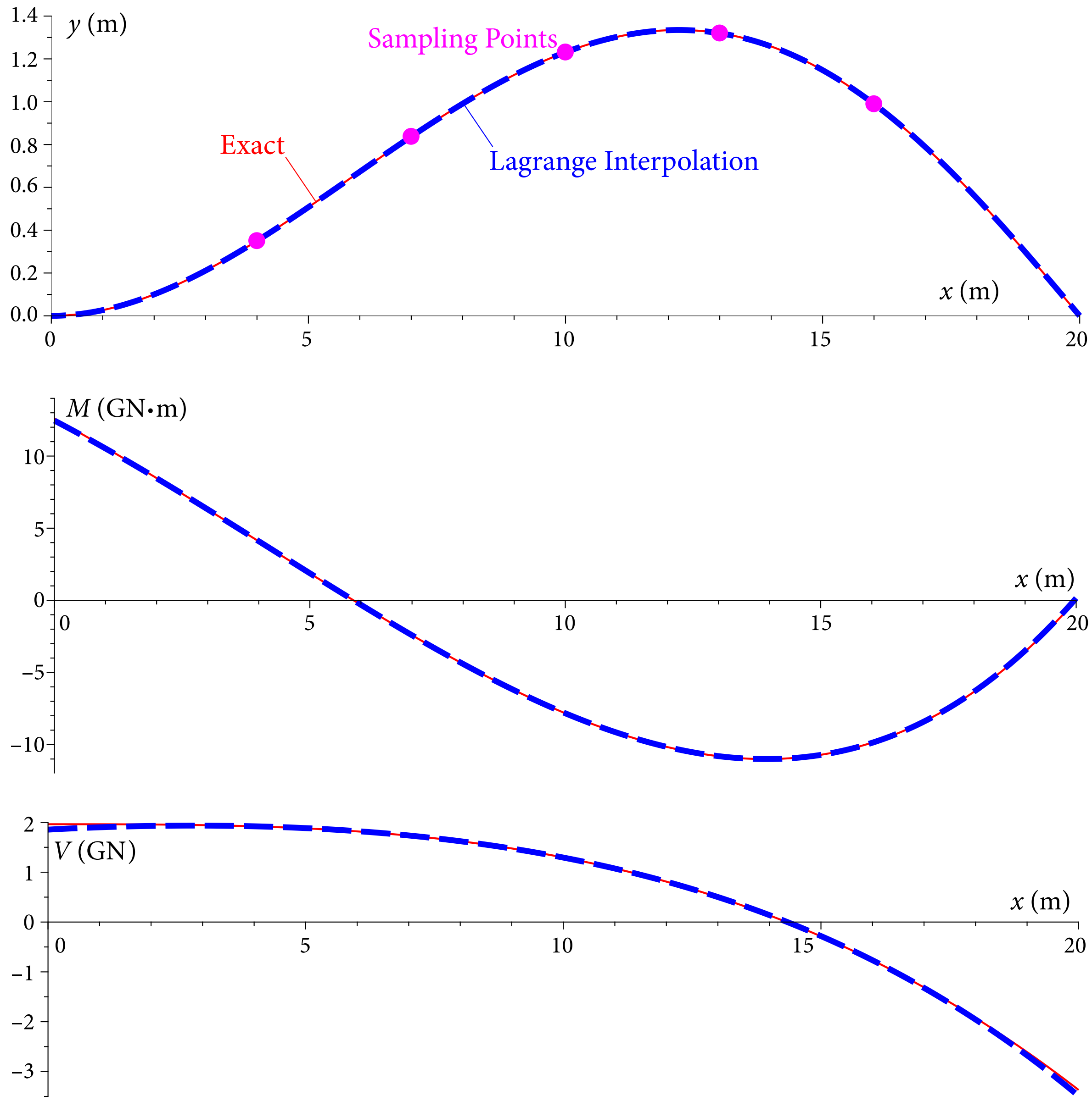

Figure 3. *Deflection, bending moment, and shear force of the beam-column.*

3.5. Discussions

Lagrange interpolation in matrix form, as given by equation (16) for the case of n points, is universal because differentiating the formula once and twice yield the first-order and the second-order derivatives, respectively, whereas integrating it gives the definite integral. The formulation is applicable to both regular and irregular intervals, it can accommodate any $n \geq 3$ sampling points, and it is easy to implement. Because a target point x does not need to be a sampling point, it can be used to determine the extrema of a function from its samples with excellent accuracy, which is essentially a problem of fitting of a set of sampling points using a polynomial and then find the extrema.

Numerical stability and numerical accuracy are first and foremost concerns in numerical analysis. For this reason, it is advisable that the following caveats be adhered to in application:

1. No large discrepancy in the size of the intervals. The intervals are to be as evenly spaced as possible.
2. No large discrepancy in the sample values. The samples are to be more or less of the same order of magnitude.
3. No outlying target point. The target point is to be around the midpoint of the domain.

Although the formulation of Lagrange interpolation in matrix form is applicable for any $n \geq 3$ points, in practice an appropriate (not too large) number of points are to be used for numerical differentiation and integration. This is to minimize roundoff and truncation errors to ensure numerical stability and numerical accuracy. As demonstrated in the numerical examples, the case when $n = 5$ offers great efficiency and accuracy.

4. Conclusions

In this paper, formulas for numerical differentiation based on Lagrange interpolation in matrix form are developed. The formulas derived are applicable to both regular and irregular intervals, and can use any desired number of points. The formulas can be also used for numerical integration and for finding the extremum of a function from its samples. Numerical examples are presented to illustrate the accuracy of the proposed method and its engineering applications. It is demonstrated that the proposed method is versatile, easy to implements, efficient, and accurate.

Conflicts of Interest

The authors declare no conflicts of interest.

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