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DERIVATION MATRIX IN MECHANICS – DATA APPROACH

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Abstract:

Existence of data allows use of solution methods for differential equations that would otherwise be inapplicable. The solution process for this is formalized by using derivation matrices that reduce the time necessary for derivation and solving of differential equations. Derivation matrices are formulated by applying numerical methods in matrix notation, like finite difference schemes. In this work, a novel formulation is developed based on Lagrange polynomials with special care taken at boundary points in order to persevere a uniform precision. The main advantage of the approach is straightforward formulation, clear engineering insight into the process and (almost) arbitrary precision through choice of the interpolation order. The result of this procedure is the derivation matrix of the dimension [n×n], where 'n' is the number of data points. The resulting matrix is singular (of rank 'n-1') until boundary/initial conditions are introduced. However, that does not prevent the user to successfully differentiate its unknown function represented with the recorded data points. Derivation matrix approach is easily applicable to a wide range of engineering problems. This methodology could be extended to dynamic systems with multiple degrees of freedom and adapted when velocities or accelerations are recorded instead of displacements.

1 Introduction

Differential equations have a long history and are widely used in the description of engineering problems. They can be solved analytically or numerically; for various reasons, the second approach is much more commonly used by engineers [1]. There are many ways to develop a procedure for numerical differentiation, which can generally be divided into single-step and multistep methods [2]. There are also explicit (such as Euler's forward procedure) and implicit (such as Euler's backward procedure) procedures. Moreover, one can distinguish between local formulations, where the derivative at a point depends on the value of some neighbouring points (as in finite differences), and global formulations, where the derivative at a point depends on the value of all points in a scheme (as in Pade derivatives) [3]. Global schemes require the solution of a system of linear equations, which naturally leads to the formulation of the derivative matrix.

The Pade derivative scheme is global and is formulated using the derivative matrix and achieves 'spectral accuracy' (accuracy comparable to analytical solutions) [4]; it is described in [5] where it is used in solving an engineering problem in strong formulation. Another global scheme based on the weak formulation and finite elements was developed in [6] and applied to the flux calculation in transport differential equations. In this paper we present the formulation and use of differentiation matrices based on Lagrange polynomials for the solution of simple engineering differential equations. The first advantage of such an approach is simplicity, since we use familiar operations of linear algebra to solve a differential equation [3]. The second advantage

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could be the suitability of the method for data analysis problems, where we collect a large amount of (experimental) data that needs further processing [7]. Often the data need to be differenced, which can be easily done using the derivative matrix.

The alternative is to regress the collected data, which introduces an additional error. The proposed method has comparable or better accuracy than most single-step methods, but does not have the spectral accuracy property. We estimate that the main application could be the computation of derivatives from numerical or experimental results, i.e., the computation of the flux from the scalar field (e.g., in temperature problems) and the computation of the strain or stress field (or moments) from the computed or measured displacement data. Since the solution of the differential equation is now reduced to a linear algebra procedure, the method is also suitable for training engineers who are traditionally well trained in linear algebra. Numerical examples illustrate the procedure.

2 Formulation of the derivation matrix

However, finite difference scheme is the basic method for the numerical differentiation (see e.g., [2]). One way to form the scheme is through polynomial interpolation based on Lagrange polynomials.

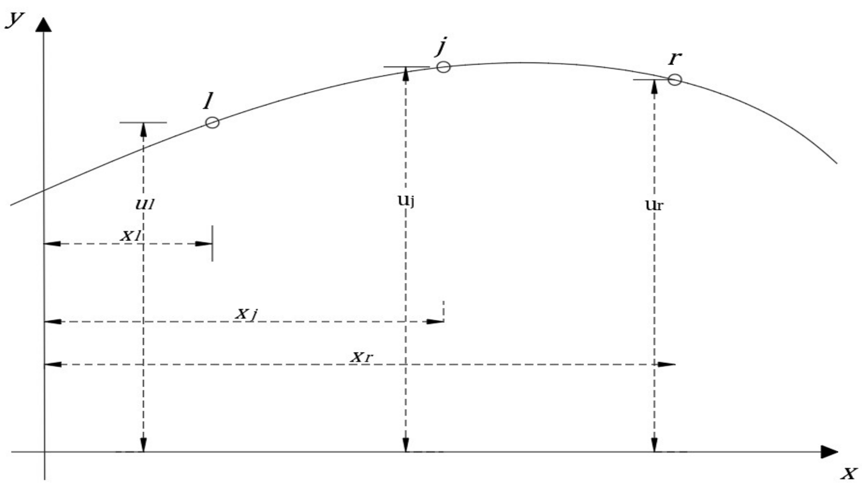

Figure 1. Discretization of the domain.

Suppose that the domain is discretized and labeled according to the image above (Figure 1.) where x are the coordinate labels, u are the unknown function values and h is the distance between successive points, i.e. constant throughout the whole domain (the indexes are labeled according to the finite difference method, l - 'left' and r - 'right'). Unknown values are interpolated using Lagrange interpolation polynomials.

2.1. Scheme in the central point

Starting with quadratic interpolation, Lagrange polynomial for values in three points looks:

$$p_j(x)=u_l \cdot L_l(x)+u_j \cdot L_j(x)+u_r \cdot L_r(x) \tag{1}$$

In the interpolation equation 'u' are the unknown values of the function in the previously defined points (l, j and r) and $L(x)$ are the Lagrange polynomials of the second order for those same points. The derivative w_j of the interpolation polynomial p_j at point x_j will give a scheme for the interpolation of the derivation at point x_j. This method of obtaining an interpolation scheme is not common but has several advantages: it is clear that the scheme is not accurate but only interpolates the derivation value, boundary point schemes are easily obtained and schemes of higher order of accuracy are easily obtained. The derivative of the interpolation polynomial is:

$$w_j(x)=p'_j(x) \tag{2}$$

$$p'_j(x)=u_l \cdot L'_l(x)+u_j \cdot L'_j(x)+u_r \cdot L'_r(x) \tag{3}$$

The differentiations of the Lagrange polynomials in points l, j and r are:

$$L'_l(x)=\frac{(x_j\text{-}x_r)}{2h^2} \tag{4}$$

$$L'_j(x)=\frac{(x_l\text{-}2x_j+x_r)}{h^2} \tag{5}$$

$$L'_r(x)=\frac{(x_j\text{-}x_l)}{2h^2} \tag{6}$$

Therefore, the differentiation of the polynomial interpolation at point x_j is:

$$p'_j(x_j)=\frac{u_l(x_j\text{-}x_r)+2u_j(x_l\text{-}2x_j+x_r)+u_r(x_j\text{-}x_l)}{2h^2} \tag{7}$$

$$w_j(x_j)=\frac{-u_l+u_r}{2h} \tag{8}$$

The expression (8) represents the differentiation scheme in the central point with the 2nd order of accuracy according to the finite difference method.

2.2. Linear scheme at boundary points

The differentiation scheme at the boundary points should satisfy the boundary conditions. It is obtained by calculating Lagrange polynomials at those point, instead of that at the central point. However, if boundary points were to be calculated using the same scheme as before, only two points would end up being included in the interpolation – the observed point and the first neighbouring point. This would result with a differentiation of the 1st order of accuracy and would stray from the rest of the domain which is of the 2nd order of accuracy. This is improved by correcting the original expression for the parabola and include Lagrange polynomials for three adjacent points on the same side.

The polynomial interpolation when x_j is on the left boundary is:

$$p_l(x)=u_j \cdot L_j(x)+u_r \cdot L_r(x)+u_{r2} \cdot L_{r2}(x) \tag{9}$$

and the differentiations of the Lagrange polynomials are now:

$$L'_j(x_j)=\frac{(2x_j\text{-}x_r\text{-}x_{r2})}{2h^2} \tag{10}$$

$$L'_r(x_j)=\frac{(x_j\text{-}x_{r2})}{-h^2} \tag{11}$$

$$L'_{r2}(x_j)=\frac{(x_j\text{-}x_r)}{2h^2} \tag{12}$$

The differentiation scheme at the left boundary point is:

$$w_j(x_j)=\frac{u_j(-3h)\text{-}2u_r(-2h)+u_{r2}(h)}{2h^2} \tag{13}$$

For the right boundary by analogy (with x_j being x_n):

$$w_j(x_n)=\frac{-3u_n+4u_{n-1}\text{-}u_{n-2}}{2h} \tag{14}$$

Now three points participate in the calculation of the boundary derivative and the accuracy is of the 2nd order.

The derivation matrix is formed according to previously obtained schemes. For a 2nd order accuracy derivation matrix schemes are obtained for the points on the left and right boundaries and for all other points.

$$\mathbf{M}=\frac{1}{2h}\begin{bmatrix} -3 & 4 & -1 & \dots & 0 & 0 & 0 \\ -1 & 0 & 1 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & -1 & 0 & 1 \\ 0 & 0 & 0 & \dots & 1 & -4 & 3 \end{bmatrix} \tag{15}$$

The derivation matrix allows us to convert the entire vector of value points of a function into a vector of derivatives of that function,

$$w=M\cdot p \tag{16}$$

where w is the vector of points with derivation values, M is the derivation matrix and p is the vector of points containing the values of the function. An expanded derivation matrix for five point interpolation is obtained using the same procedure and is of the 4th order of accuracy:

$$\mathbf{M}=\frac{1}{12h}\begin{bmatrix} -25 & 48 & -36 & 16 & -3 & & 0 & 0 & 0 & 0 & 0 \\ -3 & -10 & 18 & -6 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 1 & -8 & 0 & 8 & -1 & & 0 & 0 & 0 & 0 & 0 \\ & & \vdots & & & \ddots & & & \vdots & & \\ 0 & 0 & 0 & 0 & 0 & & 1 & -8 & 0 & 8 & -1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 6 & -18 & 10 & 3 \\ 0 & 0 & 0 & 0 & 0 & & 3 & -16 & 36 & -48 & 25 \end{bmatrix} \tag{17}$$

2.3. An example of using the derivation matrix

Using derivation matrix, the derivative of the function

$$y=\sqrt{x}\cdot e^{\sin(x)} \tag{18}$$

is calculated both analytically and numerically. The observed interval (from 0.5 to 9.5) is divided in desired number of points and the impact of point distribution on the accuracy of interpolation will be observed. Firstly, the values of the function and the values of the analytical derivative in all points are obtained. The next step is to construct a derivation matrix *M* for the observed number of points. The derivation matrix has the same number of rows and columns. The values of numerical differentiation are obtained by multiplying the derivation matrix with the vector containing values of the function.

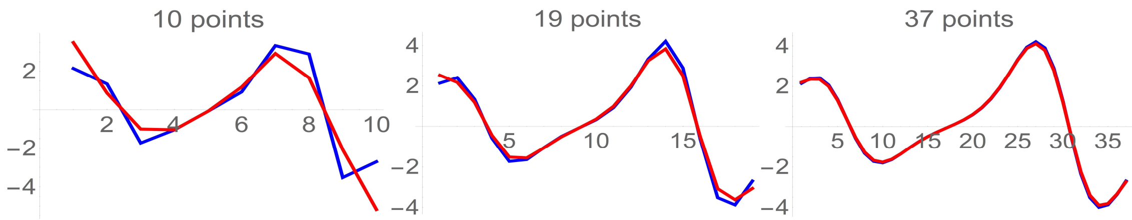

Figure 2. Results of numerical and analytical differentiation (2nd order of accuracy).

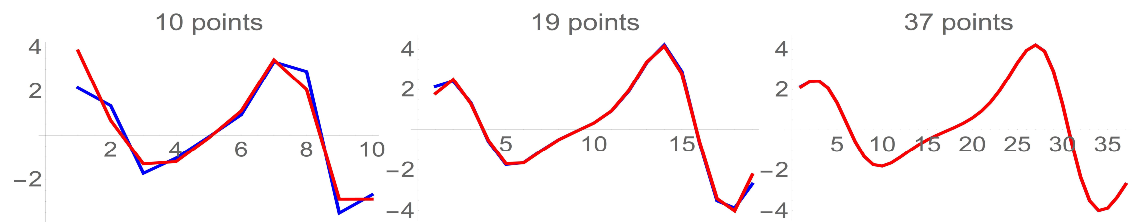

Figure 3. Results of numerical and analytical differentiation (4th order of accuracy).

The blue line in Figures 2. and 3. represents analytical (exact) differentiation i.e. values obtained by differentiating the function and the red line represents numerical differentiation that is obtained by multiplying the derivation matrix with the vector containing the values of the function. In this example the interval was divided into 10, 19 and 37 points. The biggest errors were observed on the boundaries and a higher level of interpolation should be used for those boundary points. It is concluded that the division of the interval into 37 points is satisfactory.

3 Examples

3.1. Solving a differential equation using derivation matrix

Solving a differential equation in the domain of numerical mathematics means calculating the values of the function in discrete points using known values of the derivatives in those same points. When the values of the derivatives are known and presented as a vector of value points *w* it is sufficient to invert the derivation matrix *M* and the original function vector should be obtained. This way expression (16) becomes the expression (19) and the same steps as in the previous example are applied.

$$p=M^{-1}\cdot w \tag{19}$$

Multiplying the values of the derivatives with the inverse of the matrix *M* results in values of the function in selected points. However, the derivation matrix is singular and its inverse is not defined. Therefore, in order to calculate the differential equation of the first order, function value in at least one point must be known. Usually those values are on the boundaries and when those are embedded in the matrix *M*, it is no longer singular and the calculation can be computed.

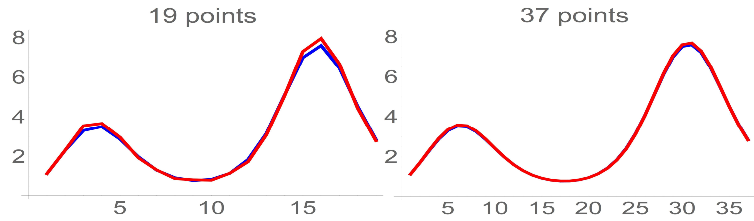

Figure 4. Results of solving a differential equation using derivation matrix (2nd order of accuracy).

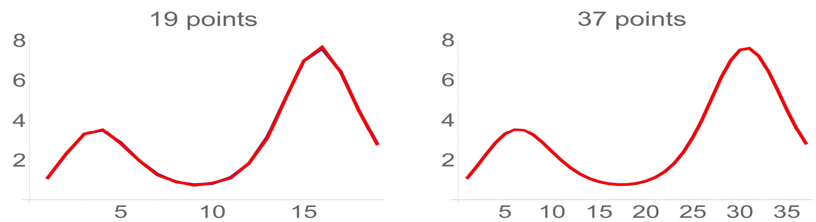

Figure 5. Results of solving a differential equation using derivation matrix (4th order of accuracy).

The blue line in Figures 4 and 5 represent analytically exact solution to the differential equation and the red line represents the numerical solution obtained by including the boundary condition in the vector of derived values and multiplying the inverse of the derivation matrix with the vector of derived values. A better insight into the size of the error can be observed if the calculated values and the exact values are compared numerically (application of the correlation procedure is not suitable here). The error is obtained as a relative dimension (20), where X is a list of calculated results and Y is a list of exact values, and is shown in Figures 6 and 7 (note different scales for the error magnitude).

$$\Delta p\% = \left(\frac{X}{Y} - 1\right) \cdot 100 \tag{20}$$

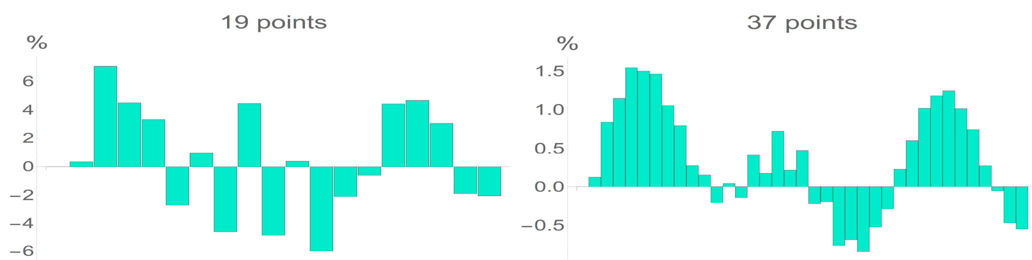

Figure 6. Calculation error (2nd order of accuracy).

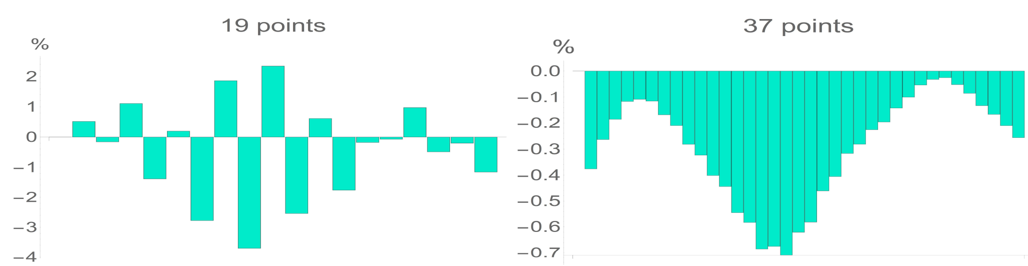

Figure 7. Calculation error (4th order of accuracy).

3.2. Calculation of moments from beam displacements

Beams are probably the most common engineering structure defined with a differential equation relating beam displacements and loads. To solve the beam problem, you must determine the displacements for a given geometry and load. However, the displacements can also be obtained from measurements. Determining the stresses in the beam is equivalent to calculating the bending moments, i.e. the second derivative of the displacements.

In this example, we calculate bending moments from given (i.e., measured) displacements of a statically determinate beam with linear change in height. Note: Statically determinate beams with constant height and variable height have different displacements but equal moments, so the calculation is more challenging, but the result check is simple.

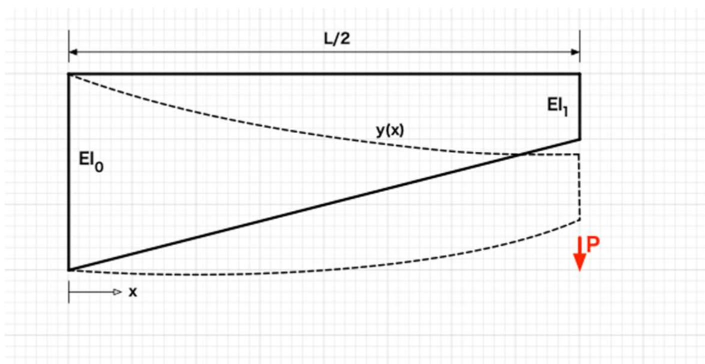

Figure 8. Beam geometry.

We assume a linear change in height, leading to $EI(x)=EI_0-\Delta EIx$ for the moment of inertia. The analytical solution for displacements and moments is [8]

$$y(x)=\frac{1}{4b^3}\left(-cx-b^2LP_0x+b^2P_0x^2+2a^2P_0\mathrm{Log}(a)-c\mathrm{Log}(a-b\frac{L}{2})-2a^2P_0\mathrm{Log}(a-bx)+c\mathrm{Log}(a-bx)\right) \tag{21}$$

$$M(x)=(a-bx)y''(x) \tag{22}$$

with $a=EI_0$, $b=(EI_0-EI_1)x/2L$ and $c=2abP_0x$.

The second derivative is obtained simply by applying Eq.(16) twice, i.e., we multiply the data vector by the square of the derivative matrix.

Note: Although the analytical expression for the moments contains an additional term besides the second derivative of the displacements, it is sufficient to differentiate the displacement data numerically, since they already contain the necessary inertia terms, i.e. one does not need to know the geometrical data of the beam to calculate the bending moments numerically.

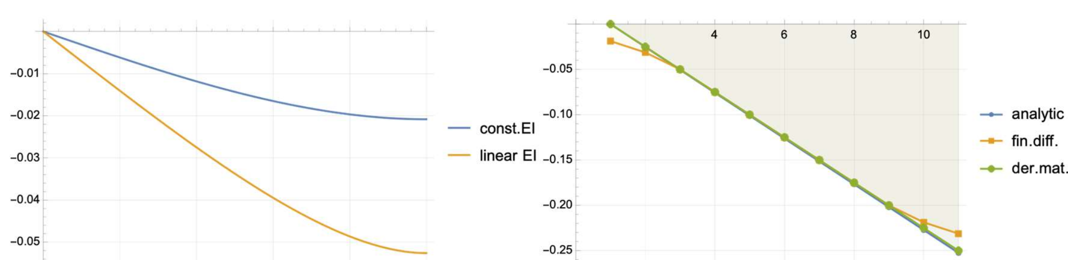

Figure 9. (a) displacements, (b) bending moments.

From Figure 9 it can be seen that the classical finite differences are not suitable for the post-processing of the experimental data and that the derivative matrix from Eq.(17) gives almost identical results to the analytical solution.

4 Conclusion

The formation and use of the derivative matrix to calculate unknown function values was presented. If the function values at discrete points are known, the derivative matrix can be used to obtain the function derivatives at the same points. In the same way, a derivative matrix can solve numerical differential equations, but only with defined and known boundary conditions. However, the main application is the derivation of recorded (experimental) data when we do not have a functional representation of the displacements. For practical use, it is recommended to divide the interval into a number of evenly spaced points. It is also recommended to repeat the calculation with at least two different subdivisions. In this way, the influence of the interval size can be estimated by comparing the two results. It is even possible to improve the accuracy by applying Richardson extrapolation [9].

Computational results for example problems were obtained for three interval divisions (10, 19, and 37 points) and using a 2nd order derivative matrix and a 4th order derivative matrix. It is concluded that setting a larger interval division and using a derivative matrix based on an interpolation scheme involving a higher number of points gives more accurate results. The second example illustrates the applicability of the method in post-processing experimental data and is recommended as a substitute for the commonly used finite differences. The introduction of the derivative matrix reduces the differentiation procedure to one of linear algebra, making the method suitable for training engineers who are traditionally well trained in linear algebra. However, the degree of interpolation and discretization of the domain should be optimised for each given problem.

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