Higher-order Numerical Differentiation of Experimental Information

Cubic-spline and discrete-quadratic polynomials are described for numerically computing up through third-order derivatives. Concept is demonstrated by stress analyzing, from moiré and holographically recorded displacements, loaded plates and beams

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ABSTRACT—Cubic-spline and discrete-quadratic polynomial techniques are presented for reliably computing up to third-order derivatives of experimental information. The concept is demonstrated by stress analyzing from measured displacements, a transversely loaded plate and a beam under four-point bending. The respective displacement fields were recorded using holography and moiré. The accuracy of the employed numerical-differentiation techniques is indicated.

List of Differentiation Symbols

\[ x = \text{independent variable} \]
\[ y = y(x) = \text{theoretical relationship} \]
\[ y', y'', y''' = \text{analytical derivatives from theoretical coordinates } (x, y) \]
\[ R(Y; x) = \text{cubic-spline polynomial} \]
\[ I(Y; x) = \text{cubic-spline interpolation polynomial} \]
\[ L(Y; x) = \text{discrete-quadratic polynomial} \]
\[ R'(x, y), L'(x, y) = \text{numerical derivatives from theoretical coordinates } (x, y) \]
\[ R', L' = \text{numerical derivatives from smoothed input data represented by } R(Y; x) \text{ or } L(Y; x), \text{ respectively} \]
\[ R'', L'' = \text{numerical second derivatives from smoothed } R' \text{ or } L' \text{ input data, respectively} \]
\[ \frac{\partial^2 R}{\partial x^2}, \frac{\partial^2 L}{\partial x^2} = \text{numerical second derivatives computed directly from smoothed input data represented by } R(Y; x) \text{ or } L(Y; x), \text{ respectively} \]

Introduction

The solution of real-world problems often requires the differentiation of numerically discrete rather than analytical information. This is particularly true if the information is obtained experimentally. Classical examples include the membrane analogy as applied to fluid flow and torsion problems, finite-element and moiré strain analysis, scattered-light photoelasticity and transversely loaded plates. Applications perhaps less familiar to the mechanic occur in diffusion, heat and mass transfer, acoustics, the determination of entropy and partial specific volumes in chemistry, plus logistic population and dose-response analyses in the life and health sciences. In experimental solid mechanics, first-order derivatives have been obtained optically, and mechanically. While Stetson proposed an optical technique for displaying second partial derivatives directly, Boone found the method to be insufficiently accurate. Limited numerical differentiation of experimental data has been reported by Swinson, Berghaus, Olson, Boone and Brandt and their respective colleagues.

Mechanical differentiation is tedious, subjective and time consuming. Optical-differentiation techniques, when applicable, typically necessitate high fringe densities and laboratory-type conditions. They are consequently unsuitable for many practical applications. On the other hand, numerical processing of data has been stimulated greatly by the availability of computers. However, heretofore numerical-differentiation approaches have been essentially limited to lower-order derivatives and, in many cases, these have not been sufficiently reliable.

In this paper, the utilization of piecewise polynomials (particularly cubic-spline and discrete-quadratic functions) for obtaining higher-order derivatives of experimental information is presented and the accuracy demonstrated. Both numerical and hand smoothing of the experimental data are employed. Derivatives through the third order are evaluated and compared with theory. For demonstrative purposes, the numerical-differentiation methods are used, together with optically measured deflections, to stress analyze a uniformly loaded, circular plate and a beam under four-point bending. The respective displacement fields were recorded using...
Numerical Differentiation

General Comments

The determination of derivatives from experimentally obtained information is a frequently encountered difficulty. Fitting tangents to hand-plotted curves is essentially limited to first-order derivatives. If the data are available at equal intervals of the independent variable, simple finite-difference techniques can be employed. An alternative is to curve-fit (perhaps by least squares) a mathematical expression to the data and subsequently differentiate this expression. Modern computational facilities permit representing arbitrary curves—in particular, those suggested by experimental data—by relatively simple formulas. Until recently, the fitting of analytical expressions to discrete information typically utilized a single expression over the entire interval of interest. Commonly employed functions involve combinations of polynomials, exponentials and logarithms. Because of their simplicity, $n^{th}$ degree polynomials are often employed. While a sufficiently high-degree polynomial can interpolate the data well, highly erroneous derivatives may occur. The reliability of the derivatives can be improved substantially by employing piecewise polynomials, two classes of which are employed herein and described below.

Cubic Spline

Piecewise cubic polynomials have long been used by draftsmen and engineers in the form of “mechanical splines” to fair in smooth curves between specific points. These splines are thin beams loaded at particular locations. Such mechanical splines act as analog computers of the classical Bernoulli–Euler theory. The mathematical cubic spline is a continuous function having continuous first and second derivatives, but is discontinuous in the third derivative at the junction (input) points. This corresponds to the draftsman’s spline having continuous curvature but discontinuities in the rate of curvature where the loads are applied.

The cubic spline is a piecewise interpolation polynomial defined over the interval $a \leq x \leq b$ which is divided by a mesh of points $x_j$ such that:

$$ a = x_0 < x_1 < \ldots x_j < \ldots < x_n = b. $$

An associated ordinate is prescribed at each of the abscissa mesh points:

$$ Y: y_0, y_1, \ldots, y_n. $$

Motivated by beam theory, an interpolation function $I(Y; x)$ is obtained which is continuous together with its first and second derivatives over the entire interval $[a, b]$. It is a cubic expression in each subinterval $x_i \leq x \leq x_{i+1}$ ($j = 0, \ldots, n - 1$) and satisfies $I(Y; x_j) = y_j$ ($j = 0, \ldots, n$) at each mesh point. In practice, the coordinates $(x_j, y_j)$ of the discrete mesh points may arise from experiment.

While spline functions have received considerable application for interpolation, it is often advantageous to replace strict interpolation of discrete points by some kind of smoothing. This may be particularly true if the isolated coordinates show appreciable scatter as experimental data sometimes do. Reinsch obtained a smoothing cubic-spline function $R(Y; x)$ which minimizes the integral

$$ V = \int_{a}^{b} \left[ g''(x) \right]^2 \, dx \quad (1) $$

among all functions $g(x)$ subject to the condition

$$ \sum_{j=0}^{n} \left[ \frac{g(x_j) - y_j}{\delta y_j} \right]^2 \leq S, \quad \delta y_j \in C^{2}[x_0, x_n] \quad (2) $$

where $y_j$ are the ordinates of the discrete points $x_j$, and $\delta y_j > 0$ are the estimated errors or the individual data-point smoothing parameter of the individual $y_j$, and $S \equiv 0$ is an overall (redundant) smoothing index which controls the extent of smoothing. Reinsch suggests that, if possible, one should employ for $\delta y_j$ an estimate of the standard deviation of ordinates $y_j$, whereas $S$ may be taken equal to the number of mesh points, $n + 1$. For $S = 0$, smoothing is eliminated and the previously discussed interpolation results. By introducing the Lagrange-multiplier technique, Reinsch obtained from eqs (1) and (2) the following smoothing function $R(Y; x)$:

$$ R(Y; x) = a_1 + b_1(x - x_j) + c_1(x - x_j)^2 + d_1(x - x_j)^3, \quad x_j \leq x \leq x_{j+1} \quad (3) $$

The continuity conditions are such that the cubic expressions of eq (3) join at the mesh points $x_j$ so that $R$, $\frac{dR}{dx}$ and $\frac{d^2R}{dx^2}$ are continuous throughout.

Equation (3) therefore describes a piecewise smoothing cubic-polynomial $R(Y; x)$ which is continuous

Fig. 1—First-order derivative

holography and moiré.