is itself radial. In this case we use for instance the line-element the projection of which is perpendicular to OF . Its angle τ is the same as the angle of the tangent plane of S . The axis of its corresponding cone C is perpendicular to OF . Hence we have to intersect this cone [its opening is again found from (1)] with the circle $C_1C'_1$ which is done by turning down the plane of the latter.

As soon as we have a point of D we have also its tangent-plane: it coincides with the tangent-plane of the ellipsoid E .

5. Choice of the points on S . The accuracy of our construction depends largely on the accuracy with which the directions of the level-lines and the slopes of the radial sections can be found. If the discontinuity surface in a certain area A is to be found it is therefore advisable to place the recording instruments in several straight lines L_i radiating from the shot-point over A . From each line L_i we obtain the graph of a radial section of the time-distance surface by joining the measured values w on L_i by a smooth curve. From this curve the slopes τ of the tangents can be found graphically. In the map of the area A , the level-lines can be drawn from the measured data.

For each seismometer we obtain one reflection point with its tangent-plane. However, for each intersection of a level-line with one of the lines L_i which occurs in a "new" point (where no instrument was placed) we get another point of the discontinuity surface.

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A NOTE ON NUMERICAL DIFFERENTIATION*

By JOHN W. MILES (*University of California, Los Angeles*)

Summary. Given the matrix $\mathbf{f} = \{f_i\}$, representing $f(x)$ at the set of points $\{x_i\}$, the m th derivatives of $f(x)$ at these points are expressed in terms of all of the f_i according to $\mathbf{f}^{(m)} = \mathbf{C}^{-1}\mathbf{A}^m\mathbf{C}\mathbf{f}$, where $\mathbf{A}$ is the sum of the skew matrix $[(x_i - x_j)^{-1}]$ and the diagonal matrix formed by summing the terms in the corresponding rows of this skew matrix, and $\mathbf{C}$ is the diagonal matrix having as its elements the products of the elements in the corresponding rows of the skew matrix.

1. Introduction. Let $\mathbf{f}$ be the column matrix

$$\mathbf{f} = \{f_i\} = \{f(x_i)\}. \quad (1)$$

We require a square matrix $\mathbf{D}$ such that**

$$\mathbf{f}^{(m)} = \left\{ \frac{d^m f(x)}{dx^m} \right\}_{x=x_i} = \mathbf{D}^m \mathbf{f}. \quad (2)$$

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**The representation of derivatives in matrix form, as in (2), also has been considered by J. Kuntzman in a paper presented at the International Mathematical Congress in Amsterdam (Sept. 1954), but no details have been published. It appears, from private correspondence with Prof. Kuntzman, that the results of Eq. (8) *et seq.* in the present paper are probably new.

It is common practice, especially in working with tabular data, to form derivatives through differencing.¹ The usual differencing procedures, however, are not directly suited to the expression of a derivative at any one of a *limited* number of x_i in terms of *all* of the f_i , as may be necessary in certain applications (*e.g.*, the calculation of the aerodynamic incidence associated with a given deflection mode in the flutter analysis of a highly swept or low aspect ratio wing, where accurate differentiation is important† and the number of control points severely limited). The desired goal of using all the f_i could be achieved by an appropriate combination of forward and backward differencing, just as in interpolation,² but it is more direct to start from the Lagrange interpolation formula††

$$f(x) = \sum_{i=0}^n C_i f_i \prod_{s=0}^n (x - x_s), \quad (3)$$

$$C_i = \prod_{s=0}^n (x_i - x_s)^{-1}, \quad (4)$$

which expresses $f(x)$ as the n th order polynomial prescribed by the $n + 1$ f_i .

2. The first derivative. Differentiating (3) with respect to x and setting $x = x_i$, we have³

$$f'_i = \left(\frac{df}{dx} \right)_{x=x_i} = \sum_{i=0}^n D_{ii} f_i, \quad (5)$$

$$D_{ii} = C_i^{-1} C_i (x_i - x_i)^{-1}, \quad i \neq j, \quad (6a)$$

$$= \sum_{s=0}^n (x_i - x_s)^{-1}, \quad i = j, \quad (6b)$$

where the D_{ii} are the elements of the matrix operator $\mathbf{D}$ introduced in (2). Alternatively, we have the more symmetric form

$$C_i f'_i = \sum_{i=0}^n (x_i - x_i)^{-1} (C_i f_i + C_i f_i). \quad (7)$$

The construction of the matrix $\mathbf{D}$ and its higher powers is facilitated by the *similarity* transformation

$$\mathbf{D} = \mathbf{C}^{-1} \mathbf{A} \mathbf{C}, \quad (8)$$

where $\mathbf{C}$, which we designate as the *conditioning* matrix, is diagonal and comprises the C_i , while $\mathbf{A}$ is the *antisymmetric* matrix formed by eliminating the factor of $C_i^{-1} C_i$ from D_{ii} . If $\mathbf{A}$ is resolved into a *skew* matrix $^{(0)}\mathbf{A}$ and a *diagonal* matrix $^{(e)}\mathbf{A}$ according to

¹E. Whittaker and A. Robinson, *The calculus of observations*, Blackie and Son, London, 1949, pp. 62-68.

†It generally is necessary to consider at least the first and second derivatives of the wing deflection in calculating the wing incidence.

²Whittaker and Robinson, *loc. cit.* pp. 47-50.

††The prime on the product symbol, and subsequently the summation symbol, implies the omission of the term $j = s$.

³W. E. Milne, *Numerical analysis*, Princeton Univ. Press, 1949, pp. 93-100.

$$\mathbf{A} = {}^{(0)}\mathbf{A} + {}^{(*)}\mathbf{A}, \quad (9)$$

we have the construction sequence

$${}^{(0)}\mathbf{A} = [(1 - \delta_i^i)(x_i - x_i)^{-1}], \quad (10)$$

$${}^{(*)}\mathbf{A} = \left[\delta_j^i \sum_{s=0}^n {}^{(0)}A_{is} \right], \quad (11)$$

$$\mathbf{C} = \left[\delta_j^i \prod_{s=0}^n {}^{(0)}A_{is} \right]. \quad (12)$$

We remark that, in the interests of convenience, $\mathbf{C}$ may be modified by the introduction of any constant, normalizing factor.

3. The higher derivatives. It follows from the known properties of the similarity transformation, or otherwise directly from (7), that

$$\mathbf{D}^m = \mathbf{C}^{-1} \mathbf{A}^m \mathbf{C}. \quad (13)$$

Few applications demand derivatives higher than the second, but we emphasize that, in consequence of its generation from the n th order polynomial (3), $\mathbf{A}$ must satisfy the equation

$$\mathbf{A}^{n+1} = 0. \quad (14)$$

We also remark that, in virtue of the Cayley-Hamilton theorem, (14) implies that the $n + 1$ latent roots of $\mathbf{A}$ all vanish.

The elements of $\mathbf{A}^2$ may be constructed directly from the product law

$$A_{ij}^{(2)} = \sum_{s=0}^n A_{is} A_{sj}. \quad (15)$$

Substituting the A_{ij} from (10) and (11), we find

$$A_{ij}^{(2)} = 2A_{ii}(A_{ii} - A_{ij}), \quad i \neq j, \quad (16a)$$

$$= \frac{1}{2} \sum_{s=0}^n A_{is}^{(2)}, \quad i = j, \quad (16b)$$

which affords a relatively direct construction of $\mathbf{A}^2$ from $\mathbf{A}$. We note that the diagonal elements of $\mathbf{A}^2$ still follow from the summation of the remaining elements of a given row, but that $\mathbf{A}^2$ no longer is characterized by any direct symmetry.

4. The case of equal intervals. We now suppose that the x_i are separated by equal intervals of length h — viz.,

$$x_i = x_0 + ih \quad (17)$$

so that the interpolation coefficients defined by (4) become

$$C_i = (-)^{n-i}/h^n j!(n-j)!, \quad (18a)$$

$$= (-)^{n-i} \binom{n}{j} n! h^{-n}, \quad (18b)$$

where $\binom{n}{i}$ denotes the binomial coefficient. It is expedient to remove the constant factor $n! (-h)^{-n}$ in forming the conditioning matrix, however, and we adopt the modified form

$$\mathbf{C} = \left[\delta_i^j (-h)^i \binom{n}{i} \right]. \quad (19)$$

Factoring out h , the $\mathbf{A}$ matrix is given by

$$h\mathbf{A} = \left[(1 - \delta_i^j)(i - j)^{-1} + \delta_i^j \sum_{s=0}^n (i - s)^{-1} \right]. \quad (20)$$

We note that $\mathbf{A}^{(m)}$ is now characterized by the additional symmetry

$$A_{n-i, n-j}^{(m)} = (-)^m A_{ij}^{(m)}. \quad (21)$$

In order to illustrate the foregoing results more specifically, we set $n = 4$ in (19) and (20), whence

$$\mathbf{C} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad (22)$$

$$h\mathbf{A} = \begin{bmatrix} -25/12 & -1 & -1/2 & -1/3 & -1/4 \\ 1 & -5/6 & -1 & -1/2 & -1/3 \\ 1/2 & 1 & 0 & -1 & -1/2 \\ 1/3 & 1/2 & 1 & 5/6 & -1 \\ 1/4 & 1/3 & 1/2 & 1 & 25/12 \end{bmatrix}, \quad (23)$$

$$(h\mathbf{A})^2 = \begin{bmatrix} 35/12 & 13/6 & 19/12 & 7/6 & 11/12 \\ -11/3 & -5/3 & -1/3 & 1/3 & 1/3 \\ -1/2 & -2 & -5/2 & -2 & -1/2 \\ 1/2 & 1/3 & -1/3 & -5/3 & -11/3 \\ 11/12 & 7/6 & 19/12 & 13/6 & 35/12 \end{bmatrix}. \quad (24)$$

Consider, *e.g.*, $*f(x) = \sin(\pi x/4)$ and $h = 1$, for which $\mathbf{f} = \{0, 2^{-1/2}, 1, 2^{-1/2}, 0\}$. Pre-multiplying this column by $\mathbf{C}^{-1}\mathbf{A}\mathbf{C}$ and $\mathbf{C}^{-1}\mathbf{A}^2\mathbf{C}$, as given by (22)–(24), we find $\mathbf{f}' =$

*This example is representative of flutter analysis, in which it often is necessary to introduce wing vibration modes higher (in frequency) than the fundamental and take their first and second derivatives.

$\{0.7712, 0.5572, 0, -0.5572, -0.7712\}$ and $\mathbf{f}'' = \{0.072, -0.443, -0.614, -0.443, -0.072\}$, which differ from the exact results by $\{-1.80, 0.36, 0, -0.36, 1.80\} \%$ and $\{-, -1.4, 0.5, -1.4, -\} \%$ respectively. By way of comparison, we note that the simpler approximations to $\mathbf{D}$ afforded by the use of only first or first and second differences (forward in the first three terms and backward in the last two) yield the much poorer approximations $\mathbf{f}' = \{0.707, 0.293, -0.293, -0.293, -0.707\}$ and $\mathbf{f}'' = \{0.914, 0.586, -0.086, -0.586, -0.914\}$, respectively. In the use of only first differences, central differencing in all but the first and last rows generally would be preferable—*e.g.*,

$$h\mathbf{D} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ -1/2 & 0 & -1/2 & 0 & 0 \\ 0 & -1/2 & 0 & -1/2 & 0 \\ 0 & 0 & -1/2 & 0 & -1/2 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \quad (25)$$

which yields $\mathbf{f}' = \{0.707, 0.500, 0, -0.500, -0.707\}$ for the above example.

NOTE ON THE MANY-PARTICLE PROBLEM*

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1. It was shown by Kato [1] that the symmetric Hamiltonian operator of every quantum mechanical system of particles, having a potential energy of the Coulomb type, is essentially self-adjoint; so that its closure, H , is self-adjoint (or, hypermaximal, in the terminology of von Neumann [4]). In [2], Kato applied this result to prove that the least point, λ_0 , of the spectrum of H for the two-electron system is an eigenvalue, so that λ_0 lies in the point spectrum of H . The corresponding problem in the general many-electron system apparently still remains open. Thus, while the existence of a lower bound for the spectrum of H has been established (see [3], pp. 207–208; also [1], p. 205), no general criterion for the case of $N \geq 3$ electrons guaranteeing that the least point of the spectrum is actually an eigenvalue (or, at least, no criterion which does not depend upon a variational procedure with the attending convergence questions) seems to be known. In this connection, see [3], pp. 196–197, also the remarks of Kato [2], p. 218, and the references cited there.

The object of this note is to point out that λ_0 must be an eigenvalue whenever the atomic number Z is sufficiently large. In fact, it will be shown that *the least point, λ_0 , of the spectrum of the Hamiltonian operator, H , belonging to an atom with N electrons, atomic number Z , and a stationary nucleus, is in the point spectrum whenever*

$$Z \geq 5N(N-1)/8. \quad (1)$$

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