umerical Integration by Bicubic Spline Function

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Abstract

Numerical double integrations are very laborious even for a high speed computer in terms of CPU-time. Furthermore, if the integrand is composed of a product of several functions, more CPU-time is necessary to make the integrand a single function owing to the multiplication of functions. In this paper, we formulate the double integration by which both the multiplication of three functions ($\phi(x)$, $\zeta(x,y)$ and $\psi(y)$) and the integration are executed at a time. The formulation is accomplished with the use of bicubic spline functions.

1. Introdunction

With the development of large and fast digital computers, it has become possible to devise new algorithms for numerical calculations in order to use effectively the computers. One of such devices is a piecewise polinomial spline function, which is applicable to interpolation problems, differential equations, numerical integrations and so on.[1,2]

The purpose of this paper is to formulate the following numerical integration,

$$\int_{x_{min}}^{x_{max}}\int_{y_{min}}^{y_{max}}\phi(x)\zeta(x,y)\psi(y)dxdy,$$

in which the integrand is a product of three functions $\phi(x)$, $\zeta(x,y)$ and $\psi(y)$. The integral is often used in some fields of physics. The formulation is accomplished through the aid of bicubic spline functions. The formula has some advantages. This is expressed in a simple form and adapted to computer programming, and is effective for integrations for a group of many functions $\phi(x)$ and $\psi(y)$. Moreover, the formula will be useful for such a new computer system as an array processor. The integrals $\int\phi(x)dx$ and $\iint\zeta(x,y)dxdy$ are also formulated by spline functions.

2. Spline Interpolation of Integrand

We assume a partition of an interval $[x_{min},x_{max}]$ into M subintervals by mesh point x_m, $x_{min}=x_0<x_1<\dots<x_M=x_{max}$. For simplicity, the interval is assumed to be uniformly partitioned. Let $h=(x_{max}-x_{min})/M$ be the mesh spacing. In a subinterval $[x_m,x_{m+1}]$, the cubic spline function $f_m(x)$ for $\phi(x)$ is given as[2],

$$\phi(x) = f_m(x), \quad x_m < x < x_{m+1}, \quad m=0,1,2,\dots,M-1.$$

$$f_m(x) = (\phi_m - \frac{h^2}{6}\phi_m^{(2)})x_+ + (\phi_{m+1} - \frac{h^2}{6}\phi_{m+1}^{(2)})x_- + \frac{h^2}{6}\phi_m^{(2)}x_+^3 + \frac{h^2}{6}\phi_{m+1}^{(2)}x_-^3, \qquad (2.1)$$

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$$x_+ = (x_{m+1}-x)/h, \quad x_- = (x-x_m)/h, \quad \phi_m = \phi(x_m), \quad \phi_m^{(2)} = d^2\phi(x_m)/dx^2.$$

Here, x_+ and x_- are called normalized distances to the adjacent mesh points. The $f_m(x)$ and its second derivative fit exactly to ϕ_m and $\phi_m^{(2)}$ at the point x_m. Now, in order to obtain a simple expression, we define the following vectors;

$$\vec{\Phi}_m^T = [\phi_m - \frac{h^2}{6}\phi_m^{(2)}, \ \phi_{m+1} - \frac{h^2}{6}\phi_{m+1}^{(2)}, \ \frac{h^2}{6}\phi_m^{(2)}, \ \frac{h^2}{6}\phi_{m+1}^{(2)}],$$

$$\vec{X}_m^T = [x_+, x_-, x_+^3, x_-^3]. \tag{2.2}$$

With the use of eq.(2.2), the cubic spline function eq.(2.1) can be rewritten as

$$f_m(x) = \vec{X}_m^T \cdot \vec{\Phi}_m \qquad \text{or} \qquad = \vec{\Phi}_m^T \cdot \vec{X}_m. \tag{2.3}$$

Similarly, the spline function $g_n(y)$ for $\psi(y)$ is written as

$$g_n(y) = \vec{Y}_n^T \cdot \vec{\Psi}_n \qquad \text{or} \qquad = \vec{\Psi}_n^T \cdot \vec{Y}_n. \tag{2.4}$$

where

$$\vec{\Psi}_n^T = [\psi_n - \frac{h^2}{6}\psi_n^{(2)}, \ \psi_{n+1} - \frac{h^2}{6}\psi_{n+1}^{(2)}, \ \frac{h^2}{6}\psi_n^{(2)}, \ \frac{h^2}{6}\psi_{n+1}^{(2)}],$$

$$\vec{Y}_n^T = [y_+, y_-, y_+^3, y_-^3], \qquad h = (y_{n+1}-y_n), \tag{2.5}$$

$$y_+ = (y_{n+1}-y)/h, \quad y_- = (y-y_n)/h, \quad y_n < y < y_{n+1}.$$

Here, the uniform partition of an interval $[y_{min}, y_{max}]$ is assumed as,

$$y_{min} = y_0 < y_1 < y_2 < \dots < y_N = y_{max}.$$

The first derivative of $f_m(x)$ is easily calculated as ; $f_m^{(1)}(x) = (d\vec{X}_m^T/dx) \cdot \vec{\Phi}_m$. Matching first derivatives $f_m^{(1)}(x)$ and $f_{m-1}^{(1)}(x)$ at x_m yields

$$h(\phi_{m+1} - 2\phi_m + \phi_{m-1}) = (h^3/6) \cdot (\phi_{m+1}^{(2)} + 4\phi_m^{(2)} + \phi_{m-1}^{(2)}). \tag{2.6}$$

The second derivatives $\phi_m^{(2)}$ $(m=1,2,\dots,M-1)$ can be determined by eq.(2.6) with ϕ_m $(m=0,1,\dots,M)$, $\phi_0^{(2)}$ and $\phi_M^{(2)}$.[2] Hereafter, we assume that the second derivatives have already been given in any ways.

There is no unique way of writing the bicubic spline function for $\zeta(x,y)$.[4] Our procedure of a spline interpolation is an improvement on the piecewise cubic interpolation procedure in eq.(2.1). The uniform partition of the interval $[x_{min}, x_{max}] \times [y_{min}, y_{max}]$ is assumed in a same way as in eq.(2.2) and (2.5). Then, the bicubic spline function $z_{m,n}(x,y)$ for $\zeta(x,y)$ is written as,

$$\zeta(x,y) = z_{m,n}(x,y), \quad x_m < x < x_{m+1}, \quad y_n < y < y_{n+1},$$

$$z_{m,n}(x,y) = \vec{X}_m^T \cdot F_{m,n} \cdot \vec{Y}_n. \tag{2.7}$$

Here, the matrix $F_{m,n}$ is given as,

$$F_{m,n} = \begin{bmatrix} \alpha_{m,n}, & \alpha_{m,n+1}, & \alpha_{m,n}^{(0,2)}, & \alpha_{m,n+1}^{(0,2)} \\ \alpha_{m+1,n}, & \alpha_{m+1,n+1}, & \alpha_{m+1,n}^{(0,2)}, & \alpha_{m+1,n+1}^{(0,2)} \\ \alpha_{m,n}^{(2,0)}, & \alpha_{m,n+1}^{(2,0)}, & \alpha_{m,n}^{(2,2)}, & \alpha_{m,n+1}^{(2,2)} \\ \alpha_{m+1,n}^{(2,0)}, & \alpha_{m+1,n+1}^{(2,0)}, & \alpha_{m+1,n}^{(2,2)}, & \alpha_{m+1,n+1}^{(2,2)} \end{bmatrix} \tag{2.8}$$

The matrix elements of $F_{m,n}$ are shown in appendix (see Appendix).

3. Formulation of Numerical Integration

Owing to the assumption of the uniform partition, we can obtain the constant vector $\vec{a}$; $\vec{a}^T = \int_{x_m}^{x_{m+1}} \vec{X}_m^T dx = \int_{y_n}^{y_{n+1}} \vec{Y}_n^T dy$. Here, $\vec{a} = [h/2, h/2, h/4, h/4]$. By the integration of eq.(2.3), the following formula is obtained,

$$\int_{x_{min}}^{x_{max}} \phi(x)dx = \sum_{m=0}^{M-1} \vec{a}^T \cdot \vec{\Phi}_m . \tag{3.1}$$

And also, by the integration of eq.(2.7), we can obtain the following formula,

$$\int_{x_{min}}^{x_{max}} \int_{y_{min}}^{y_{max}} \zeta(x,y)dxdy = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \vec{a}^T \cdot F_{m,n} \cdot \vec{a} . \tag{3.2}$$

By rewriting eq.(3.1) under the assumption $h^2\phi_m^{(2)} \simeq (\phi_{m+1} - 2\phi_m + \phi_{m-1})$, $h^2\phi_0^{(2)} = h^2\phi_M^{(2)} = 0$, we have the following formula similar to Duran's[3].

$$\int_{x_{min}}^{x_{max}} \phi(x)dx = h\left[\frac{5}{12}(\phi_0 + \phi_M) + \frac{13}{12}(\phi_1 + \phi_{M-1}) + \sum_{m=2}^{M-2} \phi_m\right] .$$

Now, we proceed to the integration $\iint \phi(x)\zeta(x,y)\psi(y)dxdy$. Using eqs.(2.3), (2.4) and (2.7), we have

$$\phi(x)\zeta(x,y)\psi(y) = \vec{\Phi}_m^T \cdot \vec{X}_m \vec{X}_m^T \cdot F_{m,n} \cdot \vec{Y}_n \vec{Y}_n^T \cdot \vec{\Psi}_n . \tag{3.3}$$

Owing to the assumption of the uniform partition, we can obtain the constant matrix A: $A = \int_{x_m}^{x_{m+1}} \vec{X}_m \vec{X}_m^T dx = \int_{y_n}^{y_{n+1}} \vec{Y}_n \vec{Y}_n^T dy$. The matrix A is explicitly written as,

$$A = \begin{bmatrix} h/3 & h/6 & h/5 & h/20 \\ h/6 & h/3 & h/20 & h/5 \\ h/5 & h/20 & h/7 & h/140 \\ h/20 & h/5 & h/140 & h/7 \end{bmatrix}$$

By the double integration of eq.(3.3), the following result is obtained,

$$\int_{x_{min}}^{x_{max}} \int_{y_{min}}^{y_{max}} \phi(x)\zeta(x,y)\psi(y)dxdy = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \vec{\Phi}_m^T A \cdot F_{m,n} \cdot A\vec{\Psi}_n . \tag{3.4}$$

In eqs.(3.1) and (3.4), for effeciency, it is better to treat the factors $(\vec{a}\vec{\Phi}_m^T)$, $(A\vec{\Phi}_m^T)$ and $(A\vec{\Psi}_n^T)$ as a single factor. Moreover, you had better take common factors about the mesh spacing h out of the vector $\vec{a}$ or the matrix A in a process of numerical integration, and multiply the final results by h at the last step.

4. Conclusion and Discussion

The formulae obtained in section 3 are effective for a computer system, for example, an array processor which can calculate fast a matrix multiplication or addition. When we integrate many sets of functions $\phi(x)$ and $\psi(y)$, eq.(3.4) is advantageous over eq.(3.2). In eq.(3.4), the integrand is left to be a product of three functions, so that the integration can immediately be executed with the multiplication of three spline functions at a time. Then, the integration is executed through the following two steps:

$$\vec{J}_n = \sum_{m=0}^{M-1} (\vec{\Phi}_m^T A) \cdot F_{m,n} , \quad \text{Integral} = \sum_{n=0}^{N-1} \vec{J}_n \cdot (A\vec{\Psi}_n).$$

With the second equation, the integral for $\psi(y)$ can be obtained by one-dimensional integration.

Error bounds are given as

$$(h^5/360)\Sigma\|\phi_m^{(4)}\|,\qquad \text{for eq.(3.1)}$$

$$(h^6/360)\Sigma\Sigma\{\|\zeta_{m,n}^{(0,4)}\| + \|\zeta_{m,n}^{(4,0)}\|\},\qquad \text{for eq.(3.2)}$$

$$(h^6/360)\Sigma\Sigma\{\|\phi_m\|\cdot\|\zeta_{m,n}\|\cdot\|\psi_n^{(4)}\| + \|\phi_m^{(4)}\|\cdot\|\zeta_{m,n}\|\cdot\|\psi_n\| + \|\phi_m\|(\|\zeta_{m,n}^{(0,4)}\| + \|\zeta_{m,n}^{(4,0)}\|)\|\psi_n\|\}.\qquad \text{for eq.(3.4)}$$

where $\|\phi_m\|$ is a maximum value of $|\phi(x)|$ in a subinterval $[x_m,x_{m+1}]$, and $\|\zeta_{m,n}\|$ a maximum value of $|\zeta(x,y)|$ in a subinterval $[x_m,x_{m+1}]\times[y_n,y_{n+1}]$. Here,

$$\zeta_{m,n}^{(4,0)} = \partial^4\zeta(x,y)/\partial x^4,\quad \zeta_{m,n}^{(0,4)} = \partial^4\zeta(x,y)/\partial y^4,\quad \phi_m^{(4)} = \partial^4\phi(x)/\partial x^4,$$

$$\psi_n^{(4)} = \partial^4\psi(y)/\partial y^4,\quad x = x_m,\quad y = y_n.$$

These error bounds are derived from the assumption of differentiability of $\phi(x)$, $\psi(y)$ and $\zeta(x,y)$.

Some examples for eqs.(3.2) and (3.4) were calculated by the computer NEAC 2200 series Model 700. In the table 1, a CPU-time and a relative error are shown for each example. For the matrix $F_{m,n}$, the $\zeta_{m,n}^{(2,0)}$, $\zeta_{m,n}^{(0,2)}$ and $\zeta_{m,n}^{(2,2)}$ are calculated by differences of a function $\zeta(x,y)$. The $\phi(x)$, $\psi(y)$ and these derivatives are given within relative errors $O(10^{-10})$. Although the integrand in eq.(3.2) are generated by the multiplication of the $\phi(x)$, $\zeta(x,y)$ and $\psi(y)$, these CPU-time are not included in those of the table. In the computer, a CPU-time is 1.7μsecond for a summation or a substraction, 2.4μsecond for a multiplication, and 3.4μsecond for a division. Floating (real) numbers have relative errors $O(10^{-10})$.

Table 1 Results of numerical integrations by eqs.(3.2) and (3.4). The relative errors and CPU-times are shown for each example and each formula. The following functions are used; $\phi(x)=\sin(x)$, $\psi(y)=\cos(y)$, $x_{min}=y_{min}=0$, $x_{max}=y_{max}=\pi$ and $h=\pi/100$. The function $\zeta(x,y)$ are shown in the table. For eq.(3.2), the integrand is generated by a multiplication of three functions $\phi(x)$, $\psi(y)$ and $\zeta(x,y)$.

		$\zeta(x,y)$ for example $(1+y^2)\cdot\exp(-x\cdot y)$	$\zeta(x,y)$ for example $(1-y^2)\cdot\sin(x\cdot y)$
relative error	by eq.(3.4)	3.70×10^{-7}	1.46×10^{-5}
	by eq.(3.2)	4.28×10^{-5}	1.53×10^{-4}
CPU-time	by eq.(3.4)	3.9 sec.	3.9 sec
	by eq.(3.2)	3.1 sec.	3.1 sec.

References

1) T. N. E. Greville: Mathematical Methods for Digital Computers, Vol.2, John Wiley and Sons.

2) J. L. Blue: Communications of the ACM, Vol.12, No.6, pp327~330, (1969).

3) S. Moriguchi, et al.: SUUGAKU KOUSHIKI I, Iwanamizensho, Japan, p. 67.

4) R. E. Carlson and C. A. Hall: Journal of Approximation Theory, Vol.6, pp.336~377, (1972).

Appendix

Derivation of spline function $z_{m,n}(x,y)$ in eq.(2.7).

In each rectangular element $[x_m,x_{m+1}]\times[y_n,y_{n+1}]$, the spline function $z^{(2,2)}_{m,n}(x,y)$ for $\zeta^{(2,2)}(x,y)$ are linearly interpolated as,

$$\zeta^{(2,2)}(x,y) = z^{(2,2)}_{m,n}(x,y) \equiv \partial^4 z_{m,n}(x,y)/\partial x^2\partial y^2,$$

$$z^{(2,2)}_{m,n}(x,y) = \zeta^{(2,2)}_{m,n}x_+y_+ + \zeta^{(2,2)}_{m+1,n}x_-y_+ + \zeta^{(2,2)}_{m,n+1}x_+y_- + \zeta^{(2,2)}_{m+1,n+1}x_-y_-. \quad \text{(A1)}$$

By executing an indefinite integration of eq.(A1) twice about x and twice about y, the following result is obtained,

$$\begin{aligned} z_{m,n}(x,y) = {} & \alpha^{(2,2)}_{m,n}x_+^3y_+^3 + \alpha^{(2,2)}_{m,n+1}x_+^3y_-^3 + \alpha^{(2,2)}_{m+1,n}x_-^3y_+^3 + \alpha^{(2,2)}_{m+1,n+1}x_-^3y_-^3 \\ & + (\alpha^{(0,2)}_{m,n}y_+^3 + \alpha^{(0,2)}_{m,n+1}y_-^3)x_+ + (\alpha^{(0,2)}_{m+1,n}y_+^3 + \alpha^{(0,2)}_{m+1,n+1}y_-^3)x_- \\ & + (\alpha^{(2,0)}_{m,n}x_+^3 + \alpha^{(2,0)}_{m+1,n}x_-^3)y_+ + (\alpha^{(2,0)}_{m,n+1}x_+^3 + \alpha^{(2,0)}_{m+1,n+1}x_-^3)y_- \\ & + \alpha_{m,n}x_+y_+ + \alpha_{m+1,n}x_-y_+ + \alpha_{m,n+1}x_+y_- + \alpha_{m+1,n+1}x_-y_-. \quad \text{(A2)} \end{aligned}$$

With the condition that $z_{m,n}(x,y)=\zeta(x,y)$, $z^{(2,0)}_{m,n}(x,y)=\zeta^{(2,0)}(x,y)$, $z^{(0,2)}_{m,n}(x,y)=\zeta^{(0,2)}(x,y)$ and $z^{(2,2)}_{m,n}(x,y)=\zeta^{(2,2)}(x,y)$ at each mesh point (x_m,y_n), the integration constants in eq.(A2) are given as,

$$\begin{aligned} \alpha_{i,j} &= \zeta_{i,j} - \frac{h^2}{6}(\zeta^{(2,0)}_{i,j} + \zeta^{(0,2)}_{i,j}) + (\frac{h^2}{6})^2\zeta^{(2,2)}_{i,j}, \\ \alpha^{(2,0)}_{i,j} &= \frac{h^2}{6}(\zeta^{(2,0)}_{i,j} - \frac{h^2}{6}\zeta^{(2,2)}_{i,j}), \quad \alpha^{(0,2)}_{i,j} = \frac{h^2}{6}(\zeta^{(0,2)}_{i,j} - \frac{h^2}{6}\zeta^{(2,2)}_{i,j}), \\ \alpha^{(2,2)}_{i,j} &= (\frac{h^2}{6})^2\zeta^{(2,2)}_{i,j}, \quad (i=m,m+1;\ j=n,n+1), \quad \text{(A3)} \end{aligned}$$

where

$$\zeta_{i,j} \equiv \zeta(x_i,y_j), \quad \zeta^{(2,0)}_{i,j} \equiv \partial^2\zeta(x_i,y_j)/\partial x^2, \quad \zeta^{(0,2)}_{i,j} \equiv \partial^2\zeta(x_i,y_j)/\partial y^2.$$
$$\zeta^{(2,2)}_{i,j} \equiv \partial^4\zeta(x_i,y_j)/\partial x^2\partial y^2.$$

By rewriting eq.(A2), we obtain the matrix form of the spline function eq.(2.7) for $\zeta(x,y)$. The matrix elements in $F_{m,n}$ are given by eq.(A3).

By matching smoothly the first derivatives $z^{(0,1)}_{m,n}$ or $z^{(1,0)}_{m,n}$ on the both sides of the point (x_m,y_n), the following relations are obtained,

$$\begin{aligned} \frac{h^2}{6}(\zeta^{(2,2)}_{m,n+1} + 4\zeta^{(2,2)}_{m,n} + \zeta^{(2,2)}_{m,n-1}) &= \zeta^{(2,0)}_{m,n+1} - 2\zeta^{(2,0)}_{m,n} + \zeta^{(2,0)}_{m,n-1}, \\ \frac{h^2}{6}(\zeta^{(2,2)}_{m+1,n} + 4\zeta^{(2,2)}_{m,n} + \zeta^{(2,2)}_{m-1,n}) &= \zeta^{(0,2)}_{m+1,n} - 2\zeta^{(0,2)}_{m,n} + \zeta^{(0,2)}_{m-1,n}, \\ \frac{h^2}{6}(\zeta^{(2,0)}_{m+1,n} + 4\zeta^{(2,0)}_{m,n} + \zeta^{(2,0)}_{m-1,n}) &= \zeta_{m+1,n} - 2\zeta_{m,n} + \zeta_{m-1,n}, \\ \frac{h^2}{6}(\zeta^{(0,2)}_{m,n+1} + 4\zeta^{(0,2)}_{m,n} + \zeta^{(0,2)}_{m,n-1}) &= \zeta_{m,n+1} - 2\zeta_{m,n} + \zeta_{m,n-1}. \end{aligned}$$

With the use of the above relations and the values of $\zeta_{m,n}$ $(m=0,1,\ldots,M;\ n=0,1,\ldots,N)$, and $\zeta^{(0,2)}_{m,n}$, $\zeta^{(2,0)}_{m,n}$ and $\zeta^{(2,2)}_{m,n}$ $(m=0,M;\ n=0,N)$, $\zeta^{(0,2)}_{m,n}$, $\zeta^{(2,0)}_{m,n}$ and $\zeta^{(2,2)}_{m,n}$ $(m=1,2,\ldots,M-1;\ n=1,2,\ldots,N-1)$ are calculated. The spline function $z_{m,n}(x,y)$ has the upper error bound $O((h^4/360)(||\zeta^{(0,4)}_{m,n}|| + ||\zeta^{(4,0)}_{m,n}||))$.