QUADRATURE FORMULAE FOR FUNCTIONS OF TWO VARIABLES AND APPLICATIONS

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1. Introduction.

A numerical approximation to the integral of a continuous function f(x) over the interval [a,b] can generally be written in the form

$$(1) \qquad \sum_{i=0}^{p} W_i \; f(x_i)$$

where $\{W_i\}$ is a set of quadrature weights and $x_i \varepsilon I$ with

$$I = \{x_i : \; a \leq x_0 \leq x_1 \leq --- \leq x_p \leq b\}$$

If the integrand were expressed in the form f(x,y(x)) then the expression in (1) would become

$$\sum_{i=0}^{p} W_i \; f(x_i, \; y(x_i))$$

In this report we shall consider quadrature rules for approximating the integral of a nonlinear function of two variables over a finite interval [a,b]. In addition, conditions for these methods to be convergent will be established. These formulae become useful when the function varies more rapidly with respect to one variable than with respect to the other. From an efficiency point of view, it means that fewer approximations need be made in the

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direction of the slowly varying variable. The development of such quadrature rules was considered in [2] for the case $f(x,y(x)) = g(x)\ y(x)$ and a subsequent paper applied the rules in solving linear Fredholm integral equations [3]. Other applications arise in connection with the numerical solution of non-linear differential, integral and, in this paper, integro-differential equations. The property of A-stability has been considered for methods of solving differential and integral equations. We shall illustrate an application of A-stability in solving integro-differential equations.

2. Computation of the Coefficients.

Let $f(x,y(x))$ be a continuous function defined for all $x \in [a,b]$ and let J be another partition of $[a,b]$ given by

$$J = \{t_i : \ a \le t_0 \le t_1 \le \cdots \le t_q \le b\} \quad , \quad q > 0$$

A polynomial approximation to the function $f(x,y(x))$ takes the form

$$\sum_{i=0}^{p} \sum_{j=0}^{q} \ell_i(x)\ L_j(x)\ f(t_j,y_i)$$

where $\ell_i(x) = Q(x)/(x-x_i)\,Q'(x_i)$, $Q(x) = \prod_{i=0}^{p} (x-x_i)$

and $L_j(x) = P(x)/(x-t_j)\,P'(t_j)$, $P(x) = \prod_{j=0}^{q} (x-t_j)$

In particular, weights $\{W_{ij}\}$ can be defined by

$$(2) \quad W_{ij} = \int_a^b \ell_i(x)\ L_j(x)\ dx$$

and an approximation to $\int_a^b f(x,y(x))\,dx$ takes the form

$$(3) \quad \sum_{i=0}^{p} \sum_{j=0}^{q} W_{ij}\ f(t_j,y(x_i))$$

3. Theoretical Results.

Definition 1. A quadrature formula is said to be convergent if for any continuous function $f(x,y(x))$ defined for all $x \in [a,b]$,

$$\left| \int_a^b f(x,y(x))\,dx - \sum_{i=0}^{p}\sum_{j=0}^{q} W_{ij}\, f(t_j,y(x_i)) \right| \to 0$$

as $p \to \infty$, $q \to \infty$ such that $t_q \leq b$ and $x_p \leq b$.

Definition 2. Let $E(f) = \int_a^b f(x,y(x))\,dx - \sum_{i=0}^{p}\sum_{j=0}^{q} W_{ij}\, f(t_j,y(x_i))$ be the error term associated with a quadrature formula. The formula is said to be exact for a given function f if $E(f) = 0$.

Theorem 1. Let $\sum_{i=0}^{p}\sum_{j=0}^{q} b_{ij}\, f(t_j,y(x_i))$ be an approximation to $\int_a^b f(x,y(x))\,dx$ obtained by integrating a polynomial which interpolates $f(x,y(x))$ at the points $(t_j,x_i) \in J \times I$. Let $E(f)$ denote the error term. Then $E(f) = 0$ for all pairs of polynomials $(g,h) \in \pi_p \times \pi_q$ where $f = gh$.

Proof: The proof follows immediately using the definition of and the uniqueness of interpolating polynomials.

Theorem 2. The quadrature rule defined by (3) is uniquely determined by the interval of integration [a,b] and the partitions I and J.

Proof: Let $\int_a^b f(x,y(x))\,dx = \sum_{i=0}^{p}\sum_{j=0}^{q} W_{ij}\, f(t_j,y(x_i)) + E(f)$

where the weights $\{W_{ij}\}$ are given by equation (2) and $E(f)$ is the error term.

Consider a second quadrature formula with weights $\{b_{ij}\}$ obtained by integrating any polynomial which interpolates $f(x,y(x))$

at the points $(t_j, x_i) \in J \times I$. Denoting the error term for this rule by $E_1(f)$, we have

$$\int_a^b f(x,y(x))dx = \sum_{i=0}^{p} \sum_{j=0}^{q} b_{ij} f(t_j, y(x_i)) + E_1(f)$$

By Theorem (1) $E(f) = E_1(f) = 0$ for all $(g,h) \in \pi_p \times \pi_q$

In particular, choose $g(x)\,h(x) = \ell_i(x)\,L_j(x)$. Then

$$\int_a^b \ell_i(x)\,L_j(x)\,dx = \sum_{i=0}^{p} \sum_{j=0}^{q} b_{nm}\,\ell_i(x_m)\,L_j(x_n) + E(\ell_i L_j)$$

$$= b_{ij}$$

But $\int_a^b \ell_i(x)\,L_j(x)\,dx = W_{ij}$ by equation (2). Hence the quadrature rule is unique.

Theorem 3. Let $f(x,y(x))$ be a function which is continuously differentiable on $[a,b]$ $q+1$ times with respect to x and $p+1$ times with respect to y. Let I and J be partitions of $[a,b]$. Then the error term for a quadrature rule defined by equation (3) is given by

$$(4) \quad E(f) = \frac{P(x)}{(q+1)!}\,\frac{\partial^{q+1} f(\xi,y)}{\partial x^{q+1}} + \frac{Q(x)}{(p+1)!}\,\frac{\partial^{p+1} f(x,\eta)}{\partial y^{p+1}} - \frac{P(x)\,Q(x)}{(q+1)!\,(p+1)!}\,\frac{\partial^{q+p+2} f(\xi',\eta')}{\partial x^{q+1}\,\partial y^{p+1}}$$

where $\eta = y(\xi_1)$, $\eta' = y(\xi_2)$, $\xi, \xi_1, \xi_2, \xi' \in (a,b)$ and $P(x)$ and $Q(x)$ were defined in section 2.

Proof: The proof is analogous to that for finding the error term in an interpolating polynomial for a function of one variable. In particular, the integrated form of the error for the case $f(x,y(x)) = g(x)\,y(x)$ is given in [2].

If the partitions I and J are chosen to be equispaced with $x_i = a + ih_2$ and $t_j = a + jh_1$, then equation (4) takes the form

$$E(f) = \frac{h_1^{q+1}}{(q+1)!} \frac{\partial^{q+1} f(\xi,y)}{\partial x^{q+1}} \prod_{j=0}^{q} (u_1-j) + \frac{h_2^{p+1}}{(p+1)!} \frac{\partial^{p+1} f(x,\eta)}{\partial y^{p+1}} \prod_{i=0}^{p} (u_2-i)$$

$$- \frac{h_1^{q+1} h_2^{p+1}}{(q+1)!(p+1)!} \frac{\partial^{p+q+2} f(\xi',\eta')}{\partial x^{q+1} \partial y^{p+1}} \prod_{j=0}^{q} (u_1-j) \prod_{i=0}^{p} (u_2-i)$$

where $u_1h_1 = x-t_0$ and $u_2h_2 = x-x_0$.

Corollary 1. Let h_1 and h_2 be the steps in the partitions J and I, respectively. Then $E(f) \to 0$ as $\max (h_1,h_2) \to 0$ such that $qh_1 \leq b$ and $ph_2 \leq b$.

In particular, for the case $h_1 = h_2 = h$ we have

Corollary 2 $|E(f)| \leq Mh^r$ where M is a positive constant and $r = \min (p+1,q+1)$.

4. Applications

The quadrature rules defined can be used in finding numerical approximations to the solution of ordinary differential, integro-differential and integral equations ([3], [4], [8], [11]).

In this section we shall find numerical solutions to an integro-differential equation of the form

(5) $\quad y'(x) = F(x,y(x), z(x)) \qquad y_0 = \eta$

$$\text{where } z(x) = \int_0^a K(x,t,y(t))\, dt \quad 0 \leq x \leq a$$

Conditions for such an equation to have a unique and continuous solution are contained in ([6], [12]). In addition, numerical procedures have been discussed in ([7],[14]).

In order to simplify the discussion, we shall illustrate using particular quadrature rules and the partitions I and J each with a fixed step h. Integrating (5)over $[x_k, x_{k+2}]$ yields

$$y(x_{k+2}) - y(x_k) = \int_{x_k}^{x_{k+2}} F(x,y(x), Z(x))\,dx$$

Approximating the integral using, for example, Simpson's one-third rule gives

$$(6)\quad y_{k+2} - y_k = \frac{h}{3}\left(F(x_k,y_k,z_k) + 4F(x_{k+1},y_{k+1},z_{k+1}) + F(x_{k+2}, y_{k+2}, z_{k+2})\right)$$

where y_n denotes and approximation to $y(x_n)$ and Z_n denotes an approximation to $Z(x_n)$ where $x_n \varepsilon$ I. An approximation to $Z(x_n)$ can be obtained using the quadrature formulae defined for functions of two variables. Let

$$Z_n = h \sum_{\ell=0}^{N-2} \sum_{i=0}^{2} \sum_{j=0}^{2} b_{nij}^{(2)} K(X_n, X_{2\ell+j}, Y_{2\ell+i}) + h \sum_{i=0}^{m} \sum_{j=0}^{m} b_{ij}^{(m)} K(X_n, X_{n-m+j}, Y_{n-m+i})$$

where N is the integer part of n/2 , m = 2 for n even and m = 3 for n odd. Using equation (2) with the equispaced partition points, one easily finds that

$$b_{ij}^{(2)} = 1/15 \begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}$$

and

$$b_{ij}^{(3)} = 1/35 \begin{bmatrix} 8 & 99/16 & -9/4 & 19/16 \\ 99/16 & 81/2 & -81/16 & -9/4 \\ -9/4 & -81/16 & 81/2 & 99/16 \\ 19/16 & -9/4 & 99/16 & 8 \end{bmatrix}$$

The weights $\{ b_{nij}^{(2)} \}$ are the weights $\{ b_{ij}^{(2)} \}$ used compositely.

We observe that each matrix is symmetric and that adding the columns (or rows) of $\{ b_{ij}^{(2)} \}$ gives the Simpson one-third weights while adding the columns (or rows) of $\{ b_{ij}^{(3)} \}$ give the weights of the Simpson's three-eights rule.

To illustrate, we use the above method to solve the following problem

$$y'(x) = 1 + 2x - y(x) + \int_0^x x(1+2x)e^{t(x-t)}\, y(t)\, dt, \quad 0 \leq x \leq 1.$$

$$y(0) = 1$$

Solution: $y(x) = e^{x^2}$. Results are summarized in Table 1.

TABLE 1

Step Size	| Maximum Error |
.05	7.7×10^{-6}
.10	1.2×10^{-4}

The example was taken from Linz [12] and the results show that the above method gives better accuracy than the block method defined by Linz. Although this is a particular method, it illustrates how one would proceed to define methods which are even more accurate.

A desirable property of methods for solving integro-differential or other types of equations is consistency. It can be argued that methods of the form (6) are in fact consistent - a property based on the convergence of the quadrature formulae.

When the solution tends to zero as x tends to infinity another desirable property of a method is achieved if the approximations $\{ y_n \}$ tend to zero with increasing values of n for a given fixed h. To develop such a procedure greater restrictions are placed on the quadrature rules that can be used. Such restrictions lead to properties of stability, the particular type described above being A-stability. A-stability for differential and integral equations has been discussed by several authors (see, for example [1], [8], [9], [10], [11], [13], [15]). The question of stability for methods used in solving integro-differential equations has barely been touched upon [12].

To illustrate the A-stability property, the following integro-differential equation was solved by a fourth order method using quadrature coefficients as defined in [1] for A-stable methods.

$$y'(x) = xe^{1-y(x)} - \frac{1}{(1+x)^2} - x - \int_0^x \frac{x}{(1+t)^2} e^{1-y(t)}\,dt, \quad 0 \leq x \leq 2$$

$$y(0) = 1$$

Solution: $y(x) = \dfrac{1}{1+x}$. Results are summarized in Table 2.

TABLE 2.

Step Size	| Maximum Error |
.05	4.9×10^{-7}
.10	3.6×10^{-6}

Remarks: This report is a summary of a paper prepared for presentation at the Conference on Computations in Algebra and Number Theory at the University of New Brunswick. The examples were solved using the University's computing facilities (IBM 370-158)

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