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The Modified Adaptive Quadrature Method for Line Integrals

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Abstract

In this paper, we present one of the interesting applications on the predictor curve tracing method which is the line integrals. We give a modification for the Simpson's rule and the adaptive quadrature method. Results of some numerical experiments for evaluating the line integral of a vector field over an implicitly defined curve are presented. Moreover, we give some error estimates for our modified rules. Finally, we present some numerical experiments.

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1 Introduction

The predictor methods for numerically tracing implicitly defined curves have been developed and investigated in a number of papers and books. For recent surveys see, *e.g.*, [1]. One of the interesting application of the continuation methods is calculating the line integrals over implicitly defined curves. In order to handle this case for an implicitly defined curve, it is necessary to develop reliable numerical methods for determining when the curve has been completely traversed.

In Section 2 we review the main ideas of a predictor continuation method. One of the most important aspects which has to be faced is how to deal with the lack of an explicit parametrization of the curve in the numerical quadrature for the line integral.

In Section 3, we present the modified Simpson's rule for evaluating the line integral as a vector field over an implicitly defined curve. Also, we give some error estimates for this modified rule. Moreover, the proofs of these error estimates are presented.

In Section 4, we present the modified adaptive quadrature method. Finally, in Section 5, we present some of our numerical experiments and their analysis.

2 Continuation methods

We shall mean that a map is smooth if it has as many continuous derivatives as the discussion requires.

Definition 2.1 Let A be an $n \times (n+1)$ matrix with $\operatorname{rank}(A) = n$. The unique vector $t(A) \in \Re^{n+1}$ satisfying the three conditions:

1. $At = 0$;
2. $\|t\| = 1$;
3. $\det \begin{bmatrix} A \\ t^T \end{bmatrix} > 0$;

is called the *tangent vector induced by* A. We shall denote the transpose of A by A^T.

Definition 2.2 Let A be an $n \times (n+1)$ matrix with maximal rank. Then the *Moore-Penrose inverse* of A is defined by $A^+ = A^T(AA^T)^{-1}$.

Now assume that A is an $n \times (n+1)$ matrix with $\operatorname{rank}(A) = n$, and that a decomposition

$$A^T = Q \begin{bmatrix} R \\ 0^T \end{bmatrix}$$

is given, where Q is an $(n+1) \times (n+1)$ orthogonal matrix, and R is an $n \times n$ nonsingular upper triangular matrix. If z denotes the last column of Q, then $Az = 0$ and $\|z\| = 1$, the remaining task is to choose the sign of z so that

$$\det \begin{bmatrix} A \\ z^T \end{bmatrix} > 0.$$

Now

$$\left(A^T\, z\right) = Q \begin{bmatrix} R & 0 \\ 0^T & 1 \end{bmatrix}$$

implies

$$\det \begin{bmatrix} A \\ z^T \end{bmatrix} = \det(A^T,\, z) = \det(Q)\ \det(R).$$

Hence, $t(A) = \pm\, z$ in dependence on whether the determinant is positive or negative. Since

$$A^T = Q \begin{bmatrix} R \\ 0^T \end{bmatrix} \qquad \text{and} \qquad A = (R^T,\, 0)\, Q^T,$$

one can easily show that

$$A^{+} = Q \begin{bmatrix} (R^T)^{-1} \\ 0^T \end{bmatrix}.$$

Next, assume that

1. $H : \Re^{n+1} \longrightarrow \Re^n$ is a smooth map;
2. There is a point $u \in \Re^{n+1}$ such that:
   I) $H(u) = 0$;
   II) The Jacobian matrix $H'(u)$ has maximum rank, *i.e.*, $\operatorname{rank}(H'(u)) = n$.

Then it follows from the Implicit Function Theorem that there exists a smooth curve $C : J \longrightarrow \Re^{n+1}$ for some open interval J containing the zero such that for all $a \in J$:

1. $C(0) = u$;
2. $H(C(a)) = 0$;
3. $\operatorname{rank}(H'(C(a))) = n$;
4. $C'(a) \neq 0$.

We will use the predictor continuation method to numerically trace the solution curve C. The predictor step we will use is called the *Runge-Kutta predictor of order three* which is given by

$$v = u + \frac{h}{9}\left(2K_1 + 3K_2 + 4K_3\right),$$

where u is a point lying along the solution curve C, $h > 0$ represents a stepsize,

$$K_1 = t(H'(u)),$$
$$K_2 = t(H'(u + \tfrac{h}{2}K_1)),$$

and

$$K_3 = t(H'(u + \frac{3h}{4}K_2)).$$

One of the most important issues in the predictor continuation method is the stopping criterion. We modified a stopping criterion for determining when an implicitly defined closed curve has been completely traversed. We have implemented and tested the modified stopping criterion on many different examples. The results obtained indicate that it is efficient and works properly in higher dimensions. For more details, see [2]–[4].

3 The modified Simpson's rule

For a smooth curve C with a parametrization, say $\beta: [0,1] \longrightarrow \Re^{n+1}$ and $C = \{\beta(s): 0 \le s \le 1\}$, the line integral $\int_C f \cdot dC$ can be written as an ordinary integral, *i.e.*,

$$\int_C f \cdot dC = \int_0^1 f(\beta(s)) \cdot \beta'(s)\, ds.$$

For the latter integral the Simpson's rule is given by

$$\int_C f \cdot dC \approx \frac{1}{6}[f(\beta(0)) \cdot \beta'(0) + 4\ f(\beta(\frac{1}{2})) \cdot \beta'(\frac{1}{2}) + f(\beta(1)) \cdot \beta'(1)]. \tag{3.1}$$

For the section C_i of the curve C with endpoints u_i and u_{i+1}, the modified Simpson's rule is given by

$$\int_{C_i} f \cdot dC_i \approx \frac{1}{3}[f(u_i) + 4\ f(\frac{u_i + u_{i+1}}{2}) + f(u_{i+1})] \cdot [u_{i+1} - u_i]. \tag{3.2}$$

To find the line integral $\int_C f \cdot dC$, we divide the curve C into finite number of subcurves according to the points generated along the oriented curve C while traversing, then we use Equation (3.2) to approximate the line integral on each subcurve and then we add the approximate values to get an approximate value for the integral on the whole curve.

It is well known that the global discretization error of the standard Simpson's rule is $\bigcirc(h^4)$. In this paper, we prove that the modified Simpson's rule has the same global discretization error. This result is given in the following theorem.

Theorem 3.1 *The global discretization error of the modified Simpson's rule is* $\bigcirc(h^4)$.

Proof. Let $f: \Re^n \longrightarrow \Re$ be a smooth map. Let C_i be a subcurve of the closed curve C for which u_i and u_{i+1} are its endpoints. Let $\{0, h, 2h, \ldots, nh = 1\}$ be a uniform partition of $[0,1]$. Let $\sigma_j = [jh, (j+1)h]$ for $j = 0, 1, \ldots, n-1$. Let $\alpha_i: [0,1] \longrightarrow C_i$ be a smooth map such that it isomorphically maps $[0,1]$ onto C_i. This map will divide C_i into subdivisions $C_i^j = \alpha_i(\sigma_j)$ for $j = 0, 1, \ldots, n-1$. Let T_i^j be the line segment for which $v_j = \alpha(jh)$ and $v_{j+1} = \alpha((j+1)h)$ are its endpoints. Let $d_i^j(x)$ denote the distance of a point $x \in \Re^{n+1}$ from C_i^j in the direction of the normal n_i^j of T_i^j and $\gamma_i^j: [0,1] \longrightarrow T_i^j$ denote the parametrization of the line segment T_i^j defined by

$$\gamma_i^j(t) = (1-t)v_j + t\, v_{j+1}.$$

Furthermore, we parametrize C_i^j via $\beta_i^j : T_i^j \longrightarrow C_i^j$ by

$$\beta_i^j(v) = v + d_i^j(v)\, n_i^j.$$

Thus,

$$\int_{C_i^j} f \cdot dC = \int_{\sigma_j} f(\beta_i^j(\gamma_i^j(t))) \mid (\beta_i^j \circ \gamma_i^j)'(t) \mid dt. \tag{3.3}$$

Now,

$$\begin{aligned} dC &= \mid (\beta_i^j \circ \gamma_i^j)'(t) \mid dt \\ &= \mid (\gamma_i^j + d_i^j(\gamma_i^j) n_i^j)' \mid dt \\ &= \mid (\gamma_i^j)' + (\bigtriangledown d_i^j \cdot (\gamma_i^j)') n_i^j \mid dt \\ &\leq \mid (\gamma_i^j)' \mid (1+ \parallel \bigtriangledown d_i^j \parallel)\, dt. \end{aligned}$$

It is well known that $d_i^j = \bigcirc(h^4)$ and hence $\bigtriangledown d_i^j = \bigcirc(h^3)$ since we use Runge-Kutta method of order three to generate the point along the solution curve. Thus, $dC = \mid (\gamma_i^j)' \mid \bigcirc(1 + h^3)\ dt$. Since γ_i^j is a linear parametrization of T_i^j, $dC = \bigcirc(1 + h^3)\, dt$. Therefore, from Equation (3.3) we get

$$\int_{C_i^j} f \cdot dC = \int_{\sigma_j} f \circ \beta_i^j \, dt \bigcirc (1 + h^3)$$

and hence,

$$\int_{C_i} f \cdot dC = (\sum_j \int_{\sigma_j} f \circ \beta_i^j \, dt) \bigcirc (1 + h^3). \tag{3.4}$$

The conclusion of the proof of Theorem 3.1 follows from the standard arguments. Note that each integral in the right-hand side of Equation (3.4) is taken over a closed interval . Hence, we can apply the well known error estimate for the Simpson's rule to get the result of Theorem 3.1. □

Also, we note that the exact value of the line integral can be written as a sum of the approximate value of the line integral and the expansion of terms of h^2. This result is given by the following theorem.

Theorem 3.2 *If $I_n(h)$ denotes the approximation of the line integral $I_0 = \int_C f \cdot dC$ using the modified Simpsons's rule, then $I_n(h)$ can be expanded in terms of h^2 as follows*

$$I_n(h) = I_0 + h^4\ I_1 + \cdots + h^{4+2k}\, I_{k+1} + \bigcirc(h^{5+2k}). \tag{3.5}$$

Proof. It is similar to the proof of Syam [5] for the modified trapezoidal rule. □

In the next section, we want to discuss the modified adaptive quadrature method for approximating the line integrals over an implicitly defined closed curves.

4 The modified adaptive quadrature method

Modified adaptive quadrature is a process designed to use the modified Simpson's rule to approximate the line integral $\int_C f \cdot dC$ to within a given error tolerance, $\epsilon > 0$. To explain the total procedure, let us assume that f is badly behaved only on some small subcurve Γ of C. The composite modified Simpson's rule with relatively few points will produce fairly accurate approximation for $\int_{C\setminus\Gamma} f \cdot dC$ although the entire estimate for $\int_C f \cdot dC$ may be badly in error. If we were to take the seemingly natural course of halving the step size over C, we would no appreciably increase the accuracy estimate for $\int_C f \cdot dC$. Thus the new work done in $C \setminus \Gamma$ is essentially wasted whereas more refinement may still be necessary on Γ.

Let Γ be a subcurve of C for which its endpoints are u and v. Then,

$$\int\limits_\Gamma f \cdot d\Gamma = S(u,v) + \gamma_1 h^5, \tag{4.1}$$

where γ_1 is constant, and $S(u,v) = \frac{1}{3}[f(u) + 4f(\frac{u+v}{2}) + f(v)] \cdot [v-u]$. Moreover, we can predict a point w using a stepsize $\frac{h}{2}$ and the Runge-Kutta method of order three from u. Write the integral in equation (4.1) as

$$\begin{aligned} \int\limits_\Gamma f \cdot d\Gamma &= [S(u,w) + \gamma_2 \left(\tfrac{h}{2}\right)^5] + [S(w,v) + \gamma_3 \left(\tfrac{h}{2}\right)^5] \\ &= S(u,w) + S(w,v) + \gamma_4\, \frac{h^5}{16}, \end{aligned} \tag{4.2}$$

where $\gamma_4 = \frac{\gamma_2+\gamma_3}{2}$. Assume that $\gamma_1 \approx \gamma_4$. The success of the technique depends on the accuracy of this assumption. If it is accurate, then using equation (4.1) and (4.2) we get

$$\left| \int\limits_\Gamma f \cdot d\Gamma - [S(u,w) + S(w,v)] \right| < \epsilon$$

if

$$|S(u,v) - [S(u,w) + S(w,v)]| < 15\epsilon.$$

The following algorithm explain how this method works.

Algorithm 4.1 Approximate the integral $\int\limits_\Gamma f \cdot d\Gamma$, where Γ is a subcurve of C with endpoints u and v to within a given tolerance ϵ.

INPUT: The points u and v; tolerance ϵ limit N to number of levels.

OUTPUT: Approximation I or message than N is exceeded.

STEP 1: Set $I = 0$; $k = 1$; $\epsilon_k = 10\ \epsilon$; $w_k = (v-u)/2$; $u_k = u$; $fu_k = f(u_k)$; $fr_k = f(u+w_k)$; $fv_k = f(v)$; $S_k = (1/3)*(fu_k + 4*fr_k + fv_k)\cdot w_k$; $L_k = 1$.

STEP 2: while $k > 0$, do steps 3–5.

STEP 3: Set $fy_k = f(u_k + (1/2) * w_k)$; $fz_k = f(u_k + (3/2) * w_k)$; $S1 = (1/6) * (fu_k + 4 * fy_k + fr_k) \cdot w_k$; $S2 = (1/6) * (fr_k + 4 * fz_k + fv_k) \cdot w_k$; $q_1 = u_k$; $q_2 = fu_k$; $q_3 = fr_k$; $q_4 = fv_k$; $q_5 = w_k$; $q_6 = \epsilon_k$; $q_7 = S_k$; $q_8 = L_k$.

STEP 4: $k = k - 1$.

STEP 5: if $|S1 + S2 - q_7| < q_6$, then

set $I = I + S1 + S2$,

elseif $q_8 \geq N$, then

Output ('Level exceeded'); Stop

else set $k = k + 1$;

$u_k = q_1 + q_5$; $fr_k = fz_k$; $fv_k = q_4$; $w_k = \frac{q_5}{2}$; $\epsilon_k = q_k/2$; $S_k = S2$; $L_k = q_8 + 1$.

set $k = k + 1$;

$u_k = q_1$; $fu_k = q_2$; $fr_k = fy_k$; $fv_k = q_3$; $w_k = w_{k-1}$; $\epsilon_k = \epsilon_{k-1}$; $S_k = S1$; $L_k = L_{k-1}$.

STEP 6: Output the approximation I; stop.

In the next section we present some of our numerical examples.

5 Numerical results

In this section the following notation is used.

h: the stepsize which is taken to be fixed during tracing of the solution curve.

ϵ_1: absolute value of the difference between the exact value of the integral and the approximated values by using the modified trapezoidal rule, see [2].

ϵ_2: absolute value of the difference between the exact value of the integral and the approximated values by using the modified Simpson's rule.

δ: the quotient $\frac{\epsilon_2(h)}{\epsilon_2(h/2)}$.

T_1: The computational time in seconds for computing the approximate values by using the modified Simpson's rule.

T_2: The computational time in seconds for computing the approximate values within ϵ_2 by using the adaptive Simpson's rule.

Example 5.1 Let $H = (H_1, H_2, H_3) : \Re^4 \rightarrow \Re^3$ be the smooth map defined by

$$
\begin{aligned}
H_1(x, y, z, w) &= x^2 + \frac{y^2}{4} + \frac{z^2}{9} + \frac{w^2}{16} - 1, \\
H_2(x, y, z, w) &= \frac{1}{1000} x e^y + \frac{1}{1000} y e^z + e^w - 1.001, \\
H_3(x, y, z, w) &= x^2 - y^2 + z^2 - w - 1,
\end{aligned}
$$

and let the integrand $g : \Re^4 \rightarrow \Re^4$ be given by

$$g(x, y, z, w) = \bigtriangledown(x^2 y^2 z^2 w^2).$$

From the fundamental theorem of calculus it is easy to see that $\int_C g \cdot dC = 0$, where C is generated by the smooth map H. The approximation errors of the approximate values of the line integral are given in Table 5.1.

h	ϵ_1	ϵ_2	δ	T_1	T_2
0.128	1.2356*10^{-06}	1.2781*10^{-10}	—	0.36	0.12
0.064	2.9578*10^{-07}	7.8895*10^{-12}	16.2000	0.42	0.14
0.032	7.0779*10^{-08}	4.9279*10^{-13}	16.0100	0.44	0.15
0.016	1.8427*10^{-08}	3.0795*10^{-14}	16.0020	0.50	0.16
0.008	4.6063*10^{-09}	1.9246*10^{-15}	16.0009	0.54	0.17
0.004	1.1515*10^{-09}	1.2028*10^{-16}	16.0003	0.61	0.17
0.002	2.8787*10^{-10}	7.5178*10^{-18}	16.0001	0.70	0.19

Table 5.1

From Table 5.1, we see that the modified Simpson's rule gives better results than the modified trapezoidal rule. Also, the asymptotic error of the modified Simpson's rule is satisfied. Also, we see that the adaptive technique saves many flops and computational time.

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