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NUMERICAL EVALUATION OF LINE INTEGRALS*

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Abstract. In this paper, some simple methods for the calculation of line integrals over smooth curves are considered, where an explicitly differential parametrization for the curve is either not available or is inconvenient to differentiate explicitly. The method consists in first replacing a parametrization of the curve by a piecewise polynomial interpolant of it, and then using a Newton-Cotes formula for the integration of the resulting integral. The surprising result is that the order of convergence of the resulting quadrature is higher than would be expected on the basis of interpolation theory alone. Indeed, an interpolation polynomial of order p (degree $p-1$), reproduces the derivatives of the parametrization function, needed for line integrals, only up to order $p-1$. But on using on each subinterval an interpolation formula of order p coupled with a Newton-Cotes quadrature rule using p nodes, the resulting integration method has the same order as would be obtained by applying only the Newton-Cotes formula with the original parametrization of the curve.

Key words. numerical integration, quadrature formulas, interpolation

AMS subject classifications. primary 65D30; secondary 65D05

1. Introduction. The numerical evaluation of line integrals is of interest because many planar boundary value problems of mathematical physics can be reformulated as boundary integral equations. Recently, in Chien (1991), boundary integral equations were considered for three-dimensional boundary value problems, with the resulting integral equation being formulated over a surface. This integral equation was discretized via a triangulation of the surface, with both the surface and the unknown being approximated by piecewise polynomial interpolation. The resulting numerical scheme was found to possess a higher order of convergence than expected a priori. Here then, we want to investigate whether results of a similar nature hold also for problems formulated over curves in two dimensions.

One situation in which these results might be useful is for planar boundary integral equations, when the boundary is known, but where there is not an explicitly differentiable parametrization for it. Our results also could find application in computer graphics. The only paper that we have located that is somewhat related to the method presented here is Lyness (1968). But his problem, numerical method, and analysis of it are different than what is done here.

We define the numerical method in § 2; in § 3 the general theorem is proved. We give a simple numerical example in § 4.

2. The numerical scheme. Let $r(t)$, $a \le t \le b$, be a smooth parametrization of the curve γ in $\mathbb{R}^2$, with $r'(t) \neq 0$. The problem we want to address here is the evaluation of the line integral

$$\int_\gamma f(r)\, ds = \int_a^b f(r(t))|r'(t)|\, dt, \tag{2.1}$$

where f represents a given smooth function, defined on γ. It is usually assumed that an explicitly differentiable parametrization $r(t)$ is given. The above integral is calculated by analytically evaluating $r'(t)$ and then discretizing the integral via a quadrature,

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yielding

$$\int_a^b f(r(t))|r'(t)|\,dt \cong \sum_{i=1}^{Q} w_i f(r(x_i))|r'(x_i)|. \tag{2.2}$$

We will modify this by also approximating $r(t)$, and thus the curve γ.

In many problems of mathematical physics, f represents a differentiable function that is defined in a domain Ω containing the curve γ in its interior. In other words, f can be assumed to be defined in a neighborhood of γ, not only on γ itself, so that it can be evaluated at nearby points as well. The existence of such an extension of f to an open neighborhood Ω, with preservation of differentiability, can be established rigorously; but we omit it here. This remark is of fundamental importance for our later derivations.

In what follows, we analyze a different procedure than (2.2), one based on piecewise polynomial interpolation of the curve γ. Let us consider a uniform partition of the interval $[a, b]$, given by the breakpoints $t_j, j=0,\dots,n$, with $t_j = a+jh$, $h=(b-a)/n$. On each subinterval $[t_{j-1}, t_j]$, $j=1,\dots,n$, we approximate the parametrization $r(t)$ by using polynomial interpolation of order $p \geq 2$ (degree $p-1$) in each component of $r(t)$. We denote by $r_p(t)$ the resulting piecewise polynomial function of order p. Next we replace $r(t)$ by $r_p(t)$ in the above integral, and then a quadrature is applied to the latter. This yields

$$\int_a^b f(r(t))|r'(t)|\,dt \cong \sum_{j=1}^{n}\sum_{k=1}^{q} w_{kj} f(r_p(s_{kj}))|r_p'(s_{kj})|, \tag{2.3}$$

where the w_{kj} represent the quadrature weights appropriate for the quadrature in use, and s_{kj} are the quadrature nodes in the subinterval $[t_{j-1}, t_j]$ of the partition.

For the nodes and weights on each subinterval $[t_{j-1}, t_j]$, we assume that they are based on a Newton-Cotes formula

$$\int_0^1 g(t)\,dt \cong \sum_{k=1}^{q} \nu_k g(\eta_k)$$

with $\eta_k = (k-1)/(q-1)$, $k=1,\dots,q$. Define the nodes and weights in (2.3) by

$$s_{kj} = t_{j-1} + \eta_k h, \quad w_{kj} = \nu_k h, \qquad k=1,\dots,q, \quad j=1,\dots,n. \tag{2.4}$$

For the interpolation nodes, we use

$$x_{ij} = t_{j-1} + \frac{i-1}{p-1}h, \qquad i=1,\dots,p \quad j=1,\dots,n. \tag{2.5}$$

The results in Theorem 1 generalize to other composite quadrature schemes, but the main application appears to be to the evenly spaced case, and thus our work is restricted to that case.

It is well known that

$$\|r'-r_p'\|_\infty = O(h^{p-1}), \tag{2.6}$$

and thus we would ordinarily expect the errors in (2.3) to also be $O(h^{p-1})$. In fact, we can do better than this.

THEOREM 1. *Let $p \geq 2$ and $q \geq 1$ be integers as used in the above definitions of the interpolation and quadrature rules. Define*

$$\tilde{p} = \begin{cases} p, & p \text{ even}, \\ p+1, & p \text{ odd} \end{cases}$$

and define $\tilde{q}$ similarly. Assume the curve γ has a parametrization $r \in C^{p+2}[a, b]$ with $r'(t) \neq 0$. For $f \in C(\gamma)$, assume the composition map $f \circ r \in C^{\tilde{q}}[a, b]$. Furthermore, without loss of generality, assume f is the restriction to γ of a twice continuously differentiable function of several variables, also called f, which is defined in an open neighborhood U of γ. Then for the error in (2.3), *denoted by* $E_n(f)$,

$$E_n(f) = O(h^{\text{Min}\{\tilde{p},\tilde{q}\}}). \tag{2.7}$$

A proof based on asymptotic expansions could be provided, case by case, but its length and difficulty led us rather to present a general proof in § 3 using a less direct approach. Some numerical illustrations are given in § 4. As a remark, note that if we use a composite q-point Newton-Cotes quadrature formula and if $p = q$ with p odd, then the convergence rate is $O(h^{p+1})$, which is much better than was expected on the basis of (2.6). In addition, for the general case of $q = p$, (2.7) implies that the order of convergence is the same as if the exact derivative $r'(t)$ had been used. Also, when $q = p$, the quadrature nodes $\{s_{kj}\}$ and interpolation nodes $\{x_{kj}\}$ are the same, and thus the function values of f that are used for the quadrature will satisfy

$$f(r_p(s_{kj})) = f(r(x_{kj})).$$

Therefore, f is being evaluated at points only on the original curve γ.

3. Proof of Theorem 1. We prove Theorem 1 with a sequence of lemmas, given below. The error is examined on a single prototype subinterval $[0, h]$, which is to correspond to a small section of the curve γ; and this is then applied to each subinterval $[t_{j-1}, t_j]$ to obtain the final result in (2.7). Consider the error

$$E_h \equiv \int_0^h f(r(t))|r'(t)|\,dt - h\sum_{k=1}^{q} \nu_k f(r_p(u_k))|r_p'(u_k)| \tag{3.1}$$

with

$$u_k = \eta_k h, \qquad k = 1, \ldots, q,$$

by analogy with (2.4). Decompose E_h as

$$E_h = E_{h1} + E_{h2} + E_{h3}, \tag{3.2}$$

$$E_{h1} = \int_0^h [f(r(t)) - f(r_p(t))]|r'(t)|\,dt, \tag{3.3}$$

$$E_{h2} = \int_0^h f(r_p(t))[|r'(t)| - |r_p'(t)|]\,dt, \tag{3.4}$$

$$E_{h3} = \int_0^h f(r_p(t))|r_p'(t)|\,dt - h\sum_{k=1}^{q} \nu_k f(r_p(u_k))|r_p'(u_k)|. \tag{3.5}$$

In defining the interpolation function $r_p(t)$, the interpolation nodes are

$$v_i = \frac{i-1}{p-1}\,h, \qquad i = 1, \ldots, p,$$

by analogy with (2.5). For the error in the interpolation function $r_p(t)$, use the Newton divided difference form

$$r(t) - r_p(t) = (t - v_1) \cdots (t - v_p) r[v_1, \ldots, v_p, t]. \tag{3.6}$$

We will later differentiate this formula to obtain the error in $r_p'(t)$. Also, note that

$$\max_{0\le t\le h} |(t-v_1)\cdots(t-v_p)| = O(h^p). \tag{3.7}$$

LEMMA 1. *Assume $f\in C^2(U)$, as in Theorem 1, and assume $r\in C^{p+1}[0,h]$. Then*

$$E_{h1} = O(h^{\hat p}), \qquad \hat p = \begin{cases} p+1, & p \text{ even},\\ p+2, & p \text{ odd}. \end{cases} \tag{3.8}$$

Proof. Applying Taylor's theorem to f and using (3.6)-(3.7),

$$\begin{aligned} f(r(t))-f(r_p(t)) &= \nabla f(r(t))\cdot[r[t]-r_p(t)]+O(h^{2p})\\ &= [\nabla f(r(0))+t\alpha(t)]\cdot\{(t-v_1)\cdots(t-v_p)r[v_1,\ldots,v_p,t]\}\\ &\quad + O(h^{p+2}). \end{aligned} \tag{3.9}$$

$\alpha(t)$ is a continuous vector-valued function, obtained in the Taylor expansion of $\nabla f(r(t))$ as a function of t about $t=0$. Also consider the expansions

$$\begin{aligned} r[v_1,\ldots,v_p,t] &= r[v_1,\ldots,v_p,0]+tr[v_1,\ldots,v_p,\zeta,\zeta], \qquad \zeta\in[0,h],\\ |r'(t)| &= |r'(0)|+t\beta(t) \end{aligned} \tag{3.10}$$

with $\beta(t)$ continuous on $[0,t]$.

Using these expansions in (3.9), we obtain

$$E_{h1} = \left\{\int_0^h (t-v_1)\cdots(t-v_p)\,dt\right\}\nabla f(r(0))\cdot r[v_1,\ldots,v_p,0]|r'(0)|+O(h^{p+2}).$$

If p is odd, then the above integral is zero. Considering separately the cases of p even or odd, the above formula yields directly a proof of (3.8). □

LEMMA 2. *Assume $r\in C^{p+2}[0,h]$, $p\ge 2$; and assume $r'(t)\ne 0$, $0\le t\le h$. Assume $f\in C^2(U)$, as in Theorem 1. Then*

$$E_{h2} = O(h^{\hat p}), \qquad \hat p = \begin{cases} p+1, & p \text{ even},\\ p+2, & p \text{ odd}. \end{cases} \tag{3.11}$$

Proof. We begin by examining the error in $|r_p'(t)|$. Write

$$|r'(t)|-|r_p'(t)| = \frac{|r'(t)|^2-|r_p'(t)|^2}{|r'(t)|+|r_p'(t)|}. \tag{3.12}$$

From (3.6), it is straightforward to show that

$$\|r'-r_p'\|_\infty = O(h^{p-1}). \tag{3.13}$$

From this, we obtain the expansion

$$\begin{aligned} \frac{1}{|r'(t)|+|r_p'(t)|} &= \frac{1}{2|r'(t)|+O(h^{p-1})} = \frac{1}{2|r'(t)|}+O(h^{p-1})\\ &= \frac{1}{2|r'(\frac12 h)|}-\frac{r'(\frac12 h)\cdot r''(\frac12 h)}{2|r'(\frac12 h)|^3}(t-\tfrac12 h)+O(h^2), \qquad p\ge 3. \end{aligned} \tag{3.14}$$

For the case $p=2$, we will later use

$$\frac{1}{|r'(t)|+|r_p'(t)|} = \frac{1}{2|r'(\frac12 h)|}+O(h). \tag{3.15}$$

By the assumption that $r'(t) \neq 0$ on $[0, h]$, we nave that the denominator on the right side of (3.12) is bounded away from zero.

For the numerator in (3.12),

$$|r'(t)|^2 - |r_p'(t)|^2 = r'(t) \cdot r'(t) - r_p'(t) \cdot r_p'(t). \tag{3.16}$$

Write (3.6) as

$$r_p(t) = r(t) - \omega(t) r[v_1, \ldots, v_p, t] \tag{3.17}$$

with

$$\omega(t) = (t - v_1) \cdots (t - v_p).$$

Differentiate (3.17) to obtain

$$r_p'(t) = r'(t) - \omega'(t) r_1(t) - \omega(t) r_2(t) \tag{3.18}$$

with

$$r_1(t) \equiv r[v_1, \ldots, v_p, t], \qquad r_2(t) \equiv r[v_1, \ldots, v_p, t, t].$$

Substituting into (3.16), we obtain

$$|r'(t)|^2 - |r_p'(t)|^2 = 2\omega'(t) r'(t) \cdot r_1(t) + 2\omega(t) r'(t) \cdot r_2(t) + O(h^{2p-2}). \tag{3.19}$$

The type of expansions used in the proof of Lemma 1 are also used here.

$$\begin{aligned} f(r_p(t)) &= f(r(t)) + O(h^p) \\ &= f(r(\tfrac{1}{2}h)) + (t - \tfrac{1}{2}h) f_1(r(\tfrac{1}{2}h)) + O(h^2), \end{aligned} \tag{3.20}$$

where $f_1(r(t)) \equiv (d/dt) f(r(t))$. Also, expand $r(t)$, $r_1(t)$ and $r_2(t)$ about $t = \frac{1}{2}h$:

$$\begin{aligned} r(t) &= r(\tfrac{1}{2}h) + (t - \tfrac{1}{2}h) r'(\tfrac{1}{2}h) + O(h^2), \\ r_1(t) &= r_1(\tfrac{1}{2}h) + (t - \tfrac{1}{2}h) r_1'(\tfrac{1}{2}h) + O(h^2), \\ r_2(t) &= r_2(\tfrac{1}{2}h) + O(h). \end{aligned} \tag{3.21}$$

For the cases with $p \geq 3$, combine (3.12), (3.14), and (3.19)-(3.21), and substitute into (3.4), obtaining

$$\begin{aligned} E_{h2} = \int_0^h & \{ f(r(\tfrac{1}{2}h)) + (t - \tfrac{1}{2}h) f_1(r(\tfrac{1}{2}h)) + O(h^2) \} \\ & \cdot \left\{ \frac{1}{2|r'(\tfrac{1}{2}h)|} - \frac{(t - \tfrac{1}{2}h) r'(\tfrac{1}{2}h) \cdot r''(\tfrac{1}{2}h)}{2|r'(\tfrac{1}{2}h)|^3} + O(h^2) \right\} \\ & \cdot \{ 2\omega'(t) [r'(\tfrac{1}{2}h) + (t - \tfrac{1}{2}h) r''(\tfrac{1}{2}h) + O(h^2)] \cdot [r_1(\tfrac{1}{2}h) + (t - \tfrac{1}{2}h) r_1'(\tfrac{1}{2}h) + O(h^2)] \\ & + 2\omega(t) [r'(\tfrac{1}{2}h) + O(h)] \cdot [r_2(\tfrac{1}{2}h) + O(h)] + O(h^{2p-2}) \} \, dt. \end{aligned}$$

When simplified to show the dominant terms, we have

$$\begin{aligned} E_{h2} = & \frac{f(r(\tfrac{1}{2}h)) r'(\tfrac{1}{2}h) \cdot r_1(\tfrac{1}{2}h)}{|r'(\tfrac{1}{2}h)|} \left\{ \int_0^h \omega'(t) \, dt \right\} + \frac{f(r(\tfrac{1}{2}h)) r'(\tfrac{1}{2}h) \cdot r_2(\tfrac{1}{2}h)}{|r'(\tfrac{1}{2}h)|} \left\{ \int_0^h \omega(t) \, dt \right\} \\ & + \left\{ \int_0^h (t - \tfrac{1}{2}h) \omega'(t) \, dt \right\} \\ & \cdot \left\{ \frac{f(r(\tfrac{1}{2}h)) [r''(\tfrac{1}{2}h) \cdot r_1(\tfrac{1}{2}h) + r'(\tfrac{1}{2}h) \cdot r_1'(\tfrac{1}{2}h)]}{|r'(\tfrac{1}{2}h)|} \right. \\ & - \frac{f(r(\tfrac{1}{2}h)) r'(\tfrac{1}{2}h) \cdot r''(\tfrac{1}{2}h)}{|r'(\tfrac{1}{2}h)|^3} [r'(\tfrac{1}{2}h) \cdot r_1(\tfrac{1}{2}h)] + \left. \frac{f_1(r(\tfrac{1}{2}h)) r'(\tfrac{1}{2}h) \cdot r_1(\tfrac{1}{2}h)}{|r'(\tfrac{1}{2}h)|} \right\} \\ & + O(h^{p+2}). \end{aligned} \tag{3.22}$$

For the first term, using $\omega(h)=\omega(0)=0$, we have

$$\int_0^h \omega'(t)\,dt=\omega(h)-\omega(0)=0.$$

For the second term,

$$\int_0^h \omega(t)\,dt=\begin{cases}O(h^{p+1}), & p \text{ even},\\ 0, & p \text{ odd}.\end{cases}$$

For the third term, using integration by parts,

$$\int_0^h (t-\tfrac{1}{2}h)\omega'(t)\,dt=-\int_0^h \omega(t)\,dt=\begin{cases}O(h^{p+1}), & p \text{ even},\\ 0, & p \text{ odd}.\end{cases}$$

Combining these results proves (3.11). For the case $p=2$, proceed similarly, using (3.15). □

LEMMA 3. *Assume $r\in C^{p-1}[a,b]$. Then for $0\le k\le p-1$,*

$$\operatorname*{Max}_{1\le j\le n}\ \operatorname*{Sup}_{t_{j-1}<t<t_j} |r_p^{(k)}(t)|<\infty. \tag{3.23}$$

Note also that for $k\ge p$, $r^{(k)}(t)\equiv 0$ because $r_p(t)$ is a polynomial of degree less than p on each subinterval.

Proof. For $t\in(t_{j-1},t_j)$, write $r_p(t)$ using the Newton divided difference formulation:

$$r_p(t)=r(x_{1j})+(t-x_{1j})r[x_{1j},x_{2j}]+\cdots+(t-x_{1j})\cdots(t-x_{p-1,j})r[x_{1j},\ldots,x_{pj}]. \tag{3.24}$$

Differentiate this expression, to find $r_p^{(k)}$ on (t_{j-1},t_j). The result will be a combination of the divided differences of r used in (3.24), and they will be multiplied by various products and sums of $(t-x_{1j}),\ldots,(t-x_{pj})$. Since $r\in C^p[a,b]$, these divided differences are all equal to derivatives of r at intermediate points in (t_{j-1},t_j), and thus these divided differences are bounded. The coefficients are also bounded, since they are multiples of powers of h. □

LEMMA 4. *Assume $q\ge 1$, and $f\circ r\in C^{\tilde q}[0,h]$, where*

$$\tilde q=\begin{cases}q, & q \text{ even},\\ q+1, & q \text{ odd}\end{cases}$$

let $p\ge 2$, and let $r_p(t)$ be the polynomial interpolating $r(t)$ at the nodes $v_k=(k-1/p-1)h$, $k=1,\ldots,p$; and assume $r\in C^{p-1}[0,h]$. Then

$$E_{h3}=O(h^{\tilde q+1}). \tag{3.25}$$

Proof. Using the standard error formula for Newton-Cotes integration,

$$E_{h3}=c_q h^{\tilde q+1} g^{(\tilde q)}(\zeta),\qquad \zeta\in[0,h], \tag{3.26}$$

with

$$g(t)\equiv f(r_p(t))|r_p'(t)|.$$

The function $|r_p'(t)|$ is bounded away from zero for all sufficiently small h, using (3.13) and the assumption $r'(t)\ne 0$ for all t. From Lemma 3, it follows that $g\in C^{\tilde q}[0,h]$. Combined with (3.26), we have (3.25). □

Proof of Theorem 1. Apply Lemmas 1, 2, and 4 to the integration error on each subinterval $[t_{j-1},t_j]$. Note that the hypotheses of these lemmas will be valid, uniformly in h. Adding up the results over these n subintervals leads to the order of convergence given in (2.7). □

TABLE
Empirical orders of convergence for various cases (q, p).

n	(1, 2)	(2, 3)	(3, 3)	(4, 4)	(5, 5)
4	1.70	2.62	3.45	4.29	7.44
8	1.92	2.14	3.94	4.03	6.02
16	1.98	2.02	3.98	4.01	6.05
32	2.00	2.00	4.00	4.00	6.01
64	2.00	2.00	4.00	4.00	5.98
128	2.00	2.00	4.00	4.00	—

4. Numerical examples and discussion. To illustrate our theoretical findings, in this section we present some numerical evidence in support of our claims. The table contains numerical evidence for the following cases: $(q, p) = (1, 2), (2, 3), (3, 3), (4, 4), (5, 5)$. The empirical orders of convergence were obtained using

$$\text{Order} = \log_2 \left[\frac{I_{(1/2)n} - I_{(1/4)n}}{I_n - I_{(1/2)n}} \right],$$

where I_n denotes the integral evaluated using n subintervals. All the computations have been performed on a 80386-based machine, with double precision accuracy. The final entry in the last column was affected by rounding error, and it is omitted.

The integral has been chosen as follows. The curve is a section of an ellipse, given by the parametrization $r(t) = (3 \cos(t), 2 \sin(t))$, $t \in [0, 1]$. For the integrand function, $f(x, y) = \exp(x + y)$, and the true integral is

$$\int_\gamma f(r)\, ds \doteq 73.458567502872.$$

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