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Improvement of Numerical Integration Formulas by Iterated Cubic Splines

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Abstract

We improve numerical integration with a fixed number of evaluation points based on iterated cubic splines. Some numerical examples are given to illustrate usefulness of our methods.

1. Introduction and Description of Methods

Iterated cubic splines are useful for order-preserving approximation to a given function. There is computational evidence that they give better results than a single spline ([1], [3]). Recently we have considered an application of the iterated cubic splines to evaluation of integrals on subintervals $[x_j, x_{j+1}]$ or the ratios to the whole interval [0, 1] required in statistics:

$$(1) \qquad \int_{x_j}^{x_{j+1}} f(x)\,dx \ \text{ or } \ \int_{x_j}^{x_{j+1}} f(x)\,dx \Big/ \int_0^1 f(x)\,dx \ \text{ for some or all } j \ \ (0 \leq j \leq n-1)$$

where let $n \geq 1$, $x_j = jh$ $(=j/n)$ ([5]). Use the notation: $f_j = f(x_j)$, $s_{m,j} = s_m(x_j)$, $s'_{m,j} = s'_m(x_j)$ and $f_{j+1/2} = f((x_j + x_{j+1})/2)$. Then, the iterated cubic splines s_m $(m \geq 0)$ are recursively defined as follows. First, let s_0 be the usual cubic spline interpolant of f on the uniform partition of [0, 1] with knots x_j, i.e.,

$$(2) \qquad s_{0,j} = f_j \ \ (0 \leq j \leq n) \ \text{ subject to } \ \Delta^k s'_{0,0} = \nabla^k s'_{0,n} = 0$$

where from now on, $k \in \{0, 1, \ldots, n-1\}$ is fixed and Δ (∇) is the forward (backward) difference operator. Next, let s_m $(m \geq 1)$ be the cubic spline interpolant of s'_{m-1} on the same uniform partition, i.e.,

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(3) $$s_{m,j}=s'_{m-1,j} \quad (0\leq j\leq n) \quad \text{subject to} \quad \Delta^k s'_{m,0}=\nabla^k s'_{m,n}=0.$$

In computation of the iterated cubic splines s_m $(m\geq 0)$, it is convenient to rewrite the end condition $\Delta^k s'_{m,0}=0$ as follows:

(4) $$c_k s'_{m,0}+s'_{m,1}=L_k(d_1, d_2, \ldots, d_{k-1})$$

where for c_k, L_k and computational comment, see [3] or [5]. The end condition $\Delta^9 s'_{m,0}=0$ used in the numerical examples is equivalent to

(5) $$(71/265)s'_{m,0}+s'_{m,1}=(92017d_1-24637d_2+6567d_3-1715d_4+419d_5-87d_6 +13d_7-d_8)/57240$$

where d_j is the right hand side of the consistency relation for the cubic spline:

(6) $$(s'_{m,j+1}+4s'_{m,j}+s'_{m,j-1})/6=(s_{m,j+1}-s_{m,j-1})/(2h) \quad (=d_j).$$

For a periodic function f, the end conditions (2)–(3) are to be replaced by

(7) $$s^{(r)}_{m,0}=s^{(r)}_{m,n} \quad (0\leq r\leq 2,\ m\geq 0).$$

The following asymptotic error estimates for the m-th derivative $f^{(m)}$ by the m-th iterated cubic spline s_m are based on results in [3] (nonperiodic) and [6] (periodic) where $C^q_p[0, 1]$ denotes the set of periodic functions in $C^q(-\infty, \infty)$ with period one.

Lemma ([3]–[6]). *For $1\leq m\leq 9$ and $f\in C^{10}_p[0, 1]$ (periodic case) and $1\leq m\leq k\leq n-1$, $k\leq 9$ and $f\in C^{10}[0, 1]$ (nonperiodic case), then*

(8) $$s_{m,j}=f^{(m)}_j-m\left\{\frac{h^4}{180}f^{(m+4)}_j-\frac{h^6}{1512}f^{(m+6)}_j\right\}-c_m h^8 f^{(m+4)}_j+O(h^L) \quad (0\leq j\leq n)$$

where $c_1=1/25920$, $L=10-m$ or $L=k+1-m$ for periodic case or nonperiodic case. Note that the h^8 term is absorbed into the order term for $m\geq 2$.

By making use of the iterated cubic splines s_m as apporximation to the derivatives in the asymptotic error estimate in Simpson's rule:

(9) $$\int_{x_j}^{x_{j+1}} f(x)\,dx-(h/6)(f_j+4f_{j+1/2}+f_{j+1})=\sum_{k=1}^{3}(-1)^k h^{2k+2} C_k \Delta f^{(2k+1)}_j+O(h^{11}),$$

we can get an improvement of the rule based on the iterated splines:

(10) $$S_{m,j}(h)=(h/6)(f_j+4f_{j+1/2}+f_{j+1})+\sum_{k=1}^{m}(-1)^k h^{2k+2}\bar{C}_k \Delta s_{2k+1,j} \quad (0\leq m\leq 3)$$

where $(C_1, C_2, C_3)=(1/2880, 1/96768, 1/3686400)$ and $(\bar{C}_1, \bar{C}_2, \bar{C}_3)=(1/2880, 1/96768, 67/1059200)$. For the errors in $S_{m,j}(h)$, we obtain

Theorem 1. *Let* $k\in\{2m+3, 2m+4, \ldots, n-1\}$ *and* $k\leq 9$ *be fixed. (This restriction on* k*, defined in* (2) *and* (3)*, is necessary in the nonperiodic case only.) If* $f\in C_p^{10}[0, 1]$ *or* $\in C^{10}[0, 1]$*, then*

$$\int_{x_j}^{x_{j+1}} f(x)\,dx-S_{m,j}(h)=O(h^{2m+5}) \quad (0\leq m\leq 3).$$

Similarly as in Simpson's rule, the asymptotic relation is known for the midpoint one:

(11) $$\int_{x_j}^{x_{j+1}} f(x)\,dx-h/f_{j+1/2}=\sum_{k=1}^{3}(-1)^{k+1}h^{2k}D_k \Delta f_j^{(2k-1)}+O(h^9)$$

from which we get the following formulas:

(12) $$M_{m,j}(h)=hf_{j+1/2}+\sum_{k=1}^{m}(-1)^{k+1}h^{2k}\bar{D}_k \Delta s_{2k-1,j} \quad (0\leq m\leq 3)$$

where $(D_1, D_2, D_3)=(1/24, 7/5760, 31/967680)$ and $(\bar{D}_1, \bar{D}_2, \bar{D}_3)=(1/24, 7/5760, 17/64512)$. For the errors in $M_{m,j}(h)$, we obtain

Theorem 2. *Let* $k\in\{2m+1, 2m+2, \ldots, n-1\}$ *and* $k\leq 7$ *be fixed. (This restriction on* k*, defined in* (2) *and* (3)*, is necessary in the nonperiodic case only.) If* $f\in C_p^8[0, 1]$ *or* $\in C^8[0, 1]$*, then*

$$\int_{x_j}^{x_{j+1}} f(x)\,dx-M_{m,j}(h)=O(h^{2m+3}) \quad (0\leq m\leq 3).$$

Proof. Under the condition on k, m and f in Theorem 2, we have only to check

(13) $$s_{m,j}=f_j^{(m)}-m\left\{\frac{h^4}{180}f_j^{(m+4)}-\frac{h^6}{1512}f_j^{(m+6)}\right\}+O(h^L) \quad (0\leq j\leq n)$$

where $L=8-m$ or $L=k+1-m$ for periodic case or nonperiodic case.

We can also consider improvement of the product trapezoidal rule when $w(x)=x^{\alpha}$ $(\alpha>-1)$ or $\ln(x)$ for which the following asymptotic error formula is obtained:

$$\int_{x_j}^{x_{j+1}} w(x)f(x)\,dx-h\{p_0(j)f_j+q_0(j)f_{j+1}\}$$
$$=\sum_{m=1}^{3} h^{2m}\{p_m(j)f_j^{(2m-1)}+q_m(j)f_{j+1}^{(2m-1)}\}+O(h^{9+\min(0,\alpha)}) \text{ or } O(h^9|\ln(h)|). \tag{14}$$

Here, first coefficients q_m $(=q_m(j))$ $(0\leq m\leq 3)$ are determined by substitution of $(x-x_j)^{2m}$ $(1\leq m\leq 3)$, $(x-x_j)^7$ into (14) without order terms, and next coefficients p_m $(=p_m(j))$ are successively done by substituting $(x-x_j)^{2m-1}$ $(1\leq m\leq 3)$ as follows:

$$\begin{aligned} &17hq_0=-4c_7+14c_6-35c_4+42c_2,\ 34hq_1=4c_7-14c_6+35c_4-25c_2\\ &204hq_2=-2c_7+7c_6-9c_4+4c_2,\ 12240hq_3=12c_7-25c_6+20c_4-7c_2\\ &17hp_0=4c_7-14c_6+35c_4-42c_2+17c_0,\ 34hp_1=4c_7-14c_6+35c_4-59c_2+34c_1\\ &204hp_2=-2c_7+7c_6-26c_4+34c_3-13c_2,\\ &12240hp_3=17c_7-59c_6+102c_5-65c_4+10c_2 \end{aligned} \tag{15}$$

where $c_m(=c_m(j))=\int_0^1 \theta^m w(x_j+h\theta)\,d\theta$ are successively determined as follows:

for $w(x)=x^{\alpha}$, $h(1+\alpha)c_0=x_{j+1}^{1+\alpha}-x_j^{1+\alpha}$, $h(m+1+\alpha)c_m=x_{j+1}^{1+\alpha}-mjhc_{m-1}$ $(m\geq 1)$;

for $w(x)=\ln(x)$, $hc_0=x_{j+1}\ln(x_{j+1})-x_j\ln(x_j)-h$,

$$h(m+1)c_m=x_{j+1}\ln(x_{j+1})-mjhc_{m-1}+mh/(m+1)\quad (m\geq 1).$$

For $\alpha=0$, $(p_0, p_1, p_2, p_3)=(q_0, -q_1, -q_2, -q_3)=(1/2, -1/12, 1/720, -1/30240)$, i.e., (14) reduces to a special case of the well-known Euler-Machaurin summation formula. Use s_m as an approximation of $f^{(m)}$ to give the following integration formulas:

$$T_{m,j}(h)=h\{p_0(j)f_j+q_0(j)f_{j+1}\}+\sum_{k=1}^{m} h^{2k}\{\overline{p_k(j)}s_{2k-1,j}+\overline{q_k(j)}s_{2k-1,j+1}\}\quad (0\leq m\leq 3) \tag{16}$$

with $(\overline{p_k(j)}, \overline{q_k(j)})=(p_k(j), q_k(j))$ $(k=1, 2)$ and $(\overline{p_3(j)}, \overline{q_3(j)})=(p_3(j), q_3(j))+(p_1(j), q_1(j))/180$. As in the proof of Theorem 2, we have

Theorem 3. *Under the same assumption on k, m and f in Theorem 2,*

$$\int_{x_j}^{x_{j+1}} w(x)f(x)\,dx-T_{m,j}(h)=O(h^{2m+3+\min(0,\alpha)}) \text{ or } O(h^{2m+3}|\ln(h)|)\quad (0\leq m\leq 3)$$

for $w(x)=x^{\alpha}$ $(\alpha>-1)$ *or* $\ln(x)$.

Similarly we improve the trapezoidal rule for integrals of the form $\int_{x_j}^{x_{j+1}} w(x)f(x)\,dx$ with an oscillatory weight $w(x)=\cos(kx)$ or $\sin(kx)$ for a relatively large value of k. For $\cos(kx)$ or $\sin(kx)$, $c_m(=c_m(j))=\int_0^1 \theta^m\, w(x_j+h\theta)\,d\theta$ are determined by

$$
\text{(17)}\quad \begin{aligned} &hkc_0(j)=\sin(kx_{j+1})-\sin(kx_j),\ h^2k^2c_1(j)=hk\sin(kx_{j+1})+\cos(kx_{j+1})-\cos(kx_j),\\ &h^2k^2c_m(j)=hk\sin(kx_{j+1})+m\cos(kx_{j+1})-m(m-1)c_{m-2}(j)\quad (m\ge 2)\end{aligned}
$$

or

$$
\text{(18)}\quad \begin{aligned} &hkc_0(j)=\cos(kx_j)-\cos(kx_{j+1}),\ h^2k^2c_1(j)=-hk\cos(kx_{j+1})-\sin(kx_{j+1})+\sin(kx_j)\\ &h^2k^2c_m(j)=-hk\cos(kx_{j+1})-m\sin(kx_{j+1})+m(m-1)c_{m-2}(j)\quad (m\ge 2).\end{aligned}
$$

2. Numerical Examples

First, we consider an application of the above stated numerical formulas $S_{m,j}(h)$ and $M_{m,j}(h)$ by taking two functions $f(x)=\exp(5x)$ and $\sin(4\pi x)$. In Tables 1-4, are given the observed maximum absolute errors in the formulas on subintervals $[x_j,\ x_{j+1}]$ $(0\le j\le n-1)$ and the observed orders of convergence from the numerical results with $n=32$, 64. Figures in parentheses behind the observed orders of convergence are the theoretical ones predicted in Theorems where *a-b* means $a\times 10^{-b}$. For reference, the absolute errors in the composite formulas on the whole interval [0, 1] using $S_{m,j}(1/64)$ (or $M_{m,j}(1/64)$), $0\le m\le 3$ can be improved with a fixed umber of the evaluation points as 3.81-7 → 6.90-11 → 2.85-13 → 1.15-14 (or 7.50-3 → 1.33-6 → 1.76-9 → 1.92-12) where the orders of convergence in the composite rules using $S_{m,j}(h)$ (or $M_{m,j}(h)$) are approximately equal to the theoretical ones, $2m+5$ (or $2m+3$), respectively. Next, we consider an application of the product trapezoidal rule when $w(x)=1/\sqrt{x}$, $\ln(x)$ and 1 to the same functions $\exp(5x)$ and $\sin(4\pi x)$. We use $T_{3,j}(h/2)$ as the unknown exact values to bound the errors in $T_{m,j}(h)$ $(0\le m\le 2)$. In Table 4, note that the theoretical rates of convergence are different from the others since the maximum absolute errors occurred near at $x=0$. Finally we improve the product trapezoidal rule for evaluating two integrals [2]:

$$
\text{(19)}\quad \int_{-1}^{1}(x-2)^{-1}(1-x)^{-1/4}(1+x)^{-3/4}\,dx\ (=-1.944905429166746...)
$$

$$
\text{(20)}\quad \int_0^1 \exp(ux)\cos(kx)\,dx\ (=\exp(u)(u\cos k+k\sin k)-u)(u^2+k^2)^{-1})\quad (u=1,\,5)
$$

The integral (19) whose weight is singular at both end-points is subdivided at $x=0$ producing two integrals with a single end-point singularity. For (19), the absolute observed errors in the composite trapezoidal rule $\sum_{j=0}^{n-1} T_{m,j}(h)$ with $n=32$, i.e., 33 function evaluation points on $[-1, 1]$ were significantly improved as 1.82-5 → 1.43-7 → 4.40-9 → 1.28-10 for $0 \leq m \leq 3$. For (20) with 17 evaluation points, the observed absolute errors in evaluation of $\int_0^1 \exp(ux) \times \cos(kx)\,dx$ with $k=1, 10, 10^2, 10^3, 10^4$ were given in Table 5. Our methods with a fixed number of evaluation points would be useful when finer meshes are not acceptable.

Table 1. Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} f(x)\,dx$ using improved Simpson's rules $S_{m,j}(h)$ $(0 \leq j \leq n-1)$

$f(x)$	nonperiodic $\exp(5x)$				periodic $\sin(4\pi x)$			
$n \backslash m$	0	1	2	3	0	1	2	3
16	2.63-5	5.34-8	2.10-8	1.81-8	7.57-6	1.89-7	5.44-8	5.83-9
32	8.88-7	6.19-10	2.45-11	1.64-11	2.52-7	1.26-9	1.07-10	2.73-12
64	2.88-8	5.21-12	2.77-14	9.66-15	8.02-9	9.40-12	2.09-13	1.31-15
orders	4.9(5)	6.9(7)	9.8(9)	10.7(11)	5.0(5)	7.1(7)	9.0(9)	11.0(11)

Table 2. Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} f(x)\,dx$ using improved midpoint rulse $M_{m,j}(h)$ $(0 \leq j \leq n-1)$

$f(x)$	nonperiodic $\exp(5x)$				periodic $\sin(4\pi x)$			
$n \backslash m$	0	1	2	3	0	1	2	3
16	3.23-2	9.02-5	1.98-6	8.45-8	1.47-3	9.97-5	3.90-6	4.56-7
32	4.37-3	3.09-6	1.65-8	8.61-11	1.97-4	9.10-7	3.03-8	8.68-10
64	5.67-4	1.01-7	1.34-10	1.56-13	2.50-5	2.83-8	2.36-10	1.68-12
orders	2.9(3)	4.9(5)	6.9(7)	9.1(9)	3.0(3)	5.3(5)	7.0(7)	9.0(9)

Table 3. Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} w(x)\sin(4\pi x)\,dx$ using improved product trapezoidal rules $T_{m,j}(h)$ $(0 \leq j \leq n-1)$

$w(x)$	$x^{1-\sqrt{2}}$			$\ln(x)$			1		
$n \backslash m$	0	1	2	0	1	2	0	1	2
16	6.51-2	1.03-4	3.56-6	5.00-2	9.09-6	2.88-8	6.47-2	1-02-4	3.81-6
32	8.63-3	3.53-6	3.06-8	6.25-4	2.91-7	2.25-9	8.73-3	3.52-6	3.11-8
64	1.54-3	3.31-7	4.68-10	1.28-4	4.56-8	5.39-11	1.13-3	1.15-7	2.51-10
orders	2.5(2.5)	3.4(4.5)	6.0(6.5)	2.3(2.7)	2.7(4.7)	5.4(6.7)	2.9(3)	4.9(5)	7.0(7)

Table 4. Comparison of the maximum absolute errors in the numerical evaluation of $\int_{x_j}^{x_{j+1}} w(x)\exp(5x)\,dx$ using improved product trapezoidal rules $T_{m,j}(h)$ $(0 \le j \le n-1)$

$w(x)$		$x^{1-\sqrt{2}}$			$\ln(x)$			1	
$n\backslash m$	0	1	2	0	1	2	0	1	2
16	9.55-3	7.99-5	1.32-7	7.15-3	7.08-5	1.01-8	2.92-3	3.68-5	7.23-6
32	1.97-3	2.53-6	1.69-9	8.98-4	2.24-6	8.00-10	3-92-4	1.06-6	5.68-8
64	5.52-4	1.29-7	2.92-11	1.60-4	7.11-8	9.54-12	4.99-5	3.25-8	4.44-10
orders	1.8(2.5)	4.3(4.5)	5.9(6.5)	2.5(2.7)	4.7(4.7)	6.5(6.7)	3.0(3)	5.0(5)	7.0(7)

Table 5. Comparison of the maximum absolute errors in the numerical evaluation of $\int_0^1 \exp(ux)\cos(kx)\,dx$ using composite improved product trapezoidal rules $\sum_{j=0}^{n-1} T_{m,j}(h)$

u		1				5		
$k\backslash m$	0	1	2	3	0	1	2	3
1	3.84-4	2.73-8	3.50-11	2.03-14	1.55-1	2.49-4	8.77-6	3.45-8
10	2.33-4	9.01-9	2.41-11	1.40-14	1.18-1	1.60-4	6.63-6	1.13-7
10^2	1.88-3	6.45-8	1.63-10	9.00-14	2.70-1	2.94-4	1.47-5	1.07-7
10^3	9.30-8	3.10-11	8.61-15	4.88-18	1.61-4	4-36-7	9.05-9	4.19-10
10^4	3.59-8	4.6-15	3.04-15	1.42-18	7.12-6	3.75-10	3.78-10	4.06-12

References

[1] J. Ahlberg, E. Nilson and J. Walsh, Theory of Splines and Their Applications, Academic Press, New York, 1967.

[2] G. Evans, Practical Numerical Integration, John Wiley & Sons, New York, 1993.

[3] M. Sakai and R. Usmani, On consistency relations for cubic splines-on-splines and their asymptotic error estimates, J. Approx. Theory, **55**(1985), 195–200.

[4] M. Sakai and R. Usmani, On spline-on-spline numerical integration formula, J. Approx. Theory, **59** (1989), 350–355.

[5] M. Sakai and R. Usmani, Numerical integration formulas based on iterated cubic splines, Computing, **52**(1994), 309–314.

[6] M. Shelly and G. Baker, On order-preserving approximation to successive derivatives of periodic functions by iterated splines, SIAM J. Numer. Anal., **25**(1988), 1442–1452.