COMPOSITE RULES FOR IMPROPER INTEGRALS

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1. Introduction. In this note we consider how composite rules for approximate integration may be applied to certain types of improper integrals. Recall that composite rules are based on piecewise polynomials, e.g. the composite trapezoid rule is based on piecewise linear interpolation.

From approximation theory we know that if p_n is the piecewise linear function which interpolates a function $f \in C^2[0,1]$ at the points $\{i/n \ : \ 0 \leq i \leq n\}$ then

$$\|p_n - f\|_\infty = O(n^{-2}).$$

In [1] de Boor considers what happens when f is taken to be the square root function. The rate of convergence deteriorates:

$$\|p_n - f\|_\infty = O(n^{-1/2}).$$

However, if, rather than using a uniform mesh, we concentrate more mesh points toward the origin, then the optimal rate of convergence $O(n^{-2})$ can be recovered. In particular, if $p_{q,n}$ is the piecewise linear polynomial interpolating $f(x) = x^{1/2}$ at the points

$$x_i := \left(\frac{i}{n}\right)^q, \ 0 \leq i \leq n, \tag{1}$$

then

$$\|p_{q,n} - f\|_\infty = O(n^{-2}),$$

provided that $q \geq 4$. It follows that if $q \geq 4$ then the optimal order of convergence holds for the corresponding composite trapezoid rule, i.e.

$$\left| \int_0^1 p_{q,n}(x) - f(x)dx \right| = O(n^{-2}). \tag{2}$$

From numerical experiments however, it appears that the same rate of convergence holds for q as small as $4/3$. In the following figure

$$t = \log_2 \left(\left| \int_0^1 p_{q,n}(x) - f(x)dx \right| / \left| \int_0^1 p_{q,2n}(x) - f(x)dx \right| \right),$$

with $n = 8192$. If the rate of convergence is $O(n^{-m})$ then

$$t \approx \log_2(C/n^{-m})/(C/(2n)^{-m}) = m.$$

Points (q,t) are plotted for various values of q. These points appear to lie on or very near to the curve $t = \min\{(3/2)q, 2\}$, whose graph is included in the figure.

2. A Composite Trapezoid Rule. By considering similar empirical results for the functions x^α with various values of α we guess that a more general result holds. We assume here and throughout that $-1 < \alpha < 1$. In Theorem 1 below we show that a Trapezoid Rule may be applied with optimal rate of convergence in the numerical integration of functions which behave like the function x^α up to and including the second derivative. Our definition of "behave like the function x^α up to and including the mth derivative" is given by

$$\begin{aligned} C_\alpha^m(0,1] := \{u \in C^m(0,1] :\ & \text{for } k = 0,1,\ldots,m, |x^{k-\alpha}u^{(k)}(x)| \\ & \text{is bounded for } x \in (0,1]\}. \end{aligned}$$

For $u \in C_\alpha^m(0,1]$, let

$$M_k := \sup_{x\in(0,1]} |x^{k-\alpha}u^{(k)}(x)|,\ 0 \le k \le m.$$

We first prove a lemma about the meshes given in (1).

Lemma. Let $q > 1$. For $i > 1$,

$$x_i - x_{i-1} \le \frac{1}{n} q 2^{q-1}\left(\frac{i-1}{n}\right)^{q-1}.$$

Proof. By the Mean Value Theorem $x_i - x_{i-1} = \frac{1}{n}q\gamma^{q-1}$, $\gamma \in (\frac{i-1}{n}, \frac{i}{n})$. Note that

$$\gamma^{q-1} < \left(\frac{i}{n}\right)^{q-1} = \left(\frac{i}{i-1}\right)^{q-1}\left(\frac{i-1}{n}\right)^{q-1} \le 2^{q-1}\left(\frac{i-1}{n}\right)^{q-1}.$$

The lemma now follows.

We modify slightly our previous definition of $p_{q,n}$ on the interval $[0, x_1]$, now taking it to be identically zero there.

Theorem 1. If $f \in C^2_\alpha(0,1]$ then, for $q > 2/(1+\alpha)$, equation (2) holds.

Proof. By hypothesis $|f(x)| \le M_0 x^\alpha$. Hence,

$$\int_0^{x_1} |p_{q,n}(x) - f(x)| dx = \int_0^{x_1} |f(x)| dx \le M_0 \frac{x_1^{\alpha+1}}{\alpha+1}$$

$$= \frac{M_0}{\alpha+1}\left(\frac{1}{n}\right)^{q(\alpha+1)} \le \frac{M_0}{\alpha+1}\left(\frac{1}{n}\right)^2. \qquad (3)$$

Next suppose $i > 1$. Using the standard error formula for interpolating polynomials, for each $x \in [x_{i-1}, x_i]$ there is a $\gamma \in (x_{i-1}, x_i)$ such that

$$p_{q,n}(x) - f(x) = \frac{1}{2!} f''(\gamma)(x - x_{i-1})(x - x_i).$$

Note that

$$|f''(\gamma)(x - x_{i-1})(x - x_i)| \le \gamma^{\alpha-2} |\gamma^{2-\alpha} f''(\gamma)| (x_i - x_{i-1})^2$$

$$\le x_{i-1}^{\alpha-2} M_2 (x_i - x_{i-1})^2.$$

It follows that

$$\int_{x_{i-1}}^{x_i} |p_{q,n}(x) - f(x)| dx \le \frac{M_2}{2} \frac{(x_i - x_{i-1})^3}{x_{i-1}^{2-\alpha}}. \qquad (4)$$

Because $q > 2/(1+\alpha)$ there is an $\epsilon > 0$ such that $q = 2/(1+\alpha-\epsilon)$. We write

$$\frac{(x_i - x_{i-1})^3}{x_{i-1}^{2-\alpha}} = \frac{(x_i - x_{i-1})^2}{x_{i-1}^{1-\alpha+\epsilon}} \frac{(x_i - x_{i-1})}{x_{i-1}^{1-\epsilon}}. \qquad (5)$$

Using our Lemma

$$\frac{(x_i - x_{i-1})^2}{x_{i-1}^{1-\alpha+\epsilon}} \leq q^2 2^{2q-2} \left(\frac{1}{n}\right)^2 \left(\frac{i-1}{n}\right)^{q(1+\alpha-\epsilon)-2} = q^2 2^{2q-2} \left(\frac{1}{n}\right)^2. \tag{6}$$

By (4), (5), and (6),

$$\begin{aligned} \left| \int_{x_1}^{1} p_{q,n}(x) - f(x)dx \right| &\leq \sum_{i=2}^{n} \int_{x_{i-1}}^{x_i} |p_{q,n}(x) - f(x)|dx \\ &\leq \frac{q^2 2^{2q-2} M_2}{2} \left(\frac{1}{n}\right)^2 \sum_{i=2}^{n} \frac{(x_i - x_{i-1})}{x_{i-1}^{1-\epsilon}}. \end{aligned} \tag{7}$$

Suppose that $\epsilon < 1$. It is not difficult to show that $x_i^{1-\epsilon} \leq 2^q x_{i-1}^{1-\epsilon}$, for $2 \leq i \leq n$. It follows that

$$\sum_{i=2}^{n} \frac{(x_i - x_{i-1})}{x_{i-1}^{1-\epsilon}} \leq 2^q \sum_{i=2}^{n} \frac{(x_i - x_{i-1})}{x_i^{1-\epsilon}} \leq 2^q \int_0^1 \frac{1}{x^{1-\epsilon}} dx = \frac{2^q}{\epsilon}.$$

If $\epsilon \geq 1$, then

$$\sum_{i=2}^{n} \frac{(x_i - x_{i-1})}{x_{i-1}^{1-\epsilon}} \leq \int_0^1 x^{\epsilon-1} dx = \frac{1}{\epsilon}.$$

Hence,

$$\sum_{i=2}^{n} \frac{(x_i - x_{i-1})}{x_{i-1}^{1-\epsilon}}$$

is bounded in n for any $\epsilon > 0$.

Putting (3) and (7) together we see that the result follows.

If $q < 2/(1+\alpha)$ the proof may be modified to show that $O(n^{-q(1+\alpha)})$ is the rate of convergence in this case.

We note that there are many numerical techniques for the integration of functions with singularities such as those which we describe here. See [3]. In a recent article, Flynn [2] discusses an efficient and easily implemented method for the numerical integration of improper integrals. Adaptive quadrature methods [4] are also used in such cases.

3. General Result on Composite Rules. The next theorem generalizes Theorem 1 and shows that any of the popular composite methods, such as Simpson's rule, may be applied to certain improper integrals without deterioration in the rate of convergence observed in the case of smooth functions, provided that q is chosen sufficiently large. Let

$$0 \le \xi_0 < \xi_1 < \cdots < \xi_r \le 1. \tag{8}$$

For $v\colon [0,1] \to \mathbb{R}$, let Qv be the polynomial of degree r interpolating v at the ξ_i. Define $x_{i,j} := x_{i-1} + \xi_j(x_i - x_{i-1})$, $1 \le i \le n$, $0 \le j \le r$. The proof of the next theorem is very similar to that of Theorem 1.

Theorem 2. Suppose that the ξ_i in (8) are chosen to produce a quadrature rule

$$\int_0^1 v \approx \int_0^1 Qv$$

of precision R. Let $f \in C_\alpha^{R+1}(0,1]$. If $p_{q,n}$ is the piecewise polynomial whose restriction to $[0,x_1]$ is identically zero, and whose restriction to $[x_{i-1},x_i]$, $i > 1$, is the polynomial of degree r which interpolates f at the points $\{x_{i,j}\}$, $0 \le j \le r$, then

$$\left| \int_0^1 p_{q,n}(x) - f(x)dx \right| = O(n^{-(R+1)}),$$

provided that $q > (R+1)/(1+\alpha)$.

Sketch of Proof. It is straightforward to show that

$$\int_0^{x_1} |p_{q,n}(x) - f(x)|dx \le \frac{M_0}{\alpha+1}\left(\frac{1}{n}\right)^{R+1}.$$

For $i > 1$ we use a standard formula for the error in the interpolating polynomial

$$f(x) - p_{q,n}(x) = f[x_{i0}, x_{i1}, \ldots, x_{ir}, x] \prod_{j=0}^{r} (x - x_{ij}), \quad x \in [x_{i-1}, x_i].$$

If $R > r$, we continue by writing

$$f[x_{i0}, x_{i1}, \dots, x_{ir}, x]$$

$$= p(x) + f[x_{i0}, x_{i1}, \dots, x_{ir}, x_{i0}, x_{i1}, \dots, x_{iR-r-1}, x] \prod_{j=0}^{R-r-1} (x - x_{ij}),$$

where p is a polynomial of degree $R - r - 1$. Since

$$f[x_{i0}, x_{i1}, \dots, x_{ir}, x_{i0}, x_{i1}, \dots, x_{iR-r-1}, x] = \frac{f^{(R+1)}(\gamma)}{(R+1)!}, \ \gamma \in (x_{i-1}, x_i),$$

we see that $f(x) - p_{q,n}(x)$ equals a sum of the polynomial

$$\tilde{p}(x) = p(x) \prod_{j=0}^{r} (x - x_{ij})$$

and of

$$\frac{f^{(R+1)}(\gamma)}{(R+1)!} \prod_{j=0}^{R-r-1} (x - x_{ij}) \prod_{j=0}^{r} (x - x_{ij}).$$

Note that $\hat{p}(x) := \tilde{p}(x_{i-1} + x(x_i - x_{i-1}))$ has degree R and zeros ξ_j, $0 \le j \le r$. It follows that

$$\int_{x_{i-1}}^{x_i} \tilde{p}(x) dx = (x_i - x_{i-1}) \int_0^1 \hat{p}(x) dx = \int_0^1 Q\hat{p}(x) dx = 0.$$

Since

$$\begin{aligned} |f^{(R+1)}(\gamma)| &= \gamma^{\alpha-R-1} |\gamma^{R+1-\alpha} f^{(R+1)}(\gamma)| \\ &\le x_{i-1}^{\alpha-R-1} |\gamma^{R+1-\alpha} f^{(R+1)}(\gamma)| \\ &\le x_{i-1}^{\alpha-R-1} M_{R+1} \end{aligned}$$

we have

$$\left| \int_{x_{i-1}}^{x_i} p_{q,n}(x) - f(x) dx \right| \leq \frac{M_{R+1}}{(R+1)!} \frac{(x_i - x_{i-1})^{R+2}}{x_{i-1}^{R+1-\alpha}}.$$

An inequality similar to (7) holds with

$$\frac{q^2 2^{2q-2} M_2}{2} \left(\frac{1}{n}\right)^2$$

replaced by

$$\frac{q^{R+1} 2^{(q-1)(R+1)} M_{R+1}}{(R+1)!} \left(\frac{1}{n}\right)^{R+1}.$$

From here the proof follows that of Theorem 1.

4. Numerical Example. For comparison purposes we choose to consider an example found in [2]. We approximate the integral

$$\int_0^1 1/\sqrt{2x - x^2} dx = \int_{1/2}^1 1/\sqrt{x - x^2} dx = 1.5707963267\ldots.$$

We use Simpson's rule, i.e. $\xi_0 = 0$, $\xi_1 = 1/2$, $\xi_2 = 1$, a rule with precision 3. The integrand belongs to $C_\alpha^4(0, 1]$ with $\alpha = -1/2$. Our Theorem 2 predicts convergence at the rate $O(n^{-4})$ provided that $q > 4/(1 + \alpha) = 8$. In the table below the values in the columns labeled "rate" are values of t. Recall from the introduction that t is an empirical measure of m, if the theoretical rate of convergence is $O(n^{-m})$.

	$q = 1$		$q = 4$		$q = 10$	
n	approx.	rate	approx.	rate	approx.	rate
16	1.2154585722	-	1.5674994559	-	1.5728090531	-
32	1.3201997723	0.50	1.5699744101	2.00	1.5709359174	3.85
64	1.3938304725	0.50	1.5705909909	2.00	1.5708055229	3.92
128	1.4457443959	0.50	1.5707450018	2.00	1.5707969168	3.96
256	1.4824001114	0.50	1.5707834961	2.00	1.5707963642	3.98
512	1.5083009511	0.50	1.5707931192	2.00	1.5707963291	3.99

References

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4. D. Kincaid and W. Cheney, *Numerical Analysis*, 2nd edition, Brooks–Cole, Pacific Grove, CA, 1996.

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