ON IGNORING THE SINGULARITY IN NUMERICAL QUADRATURE

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*This research was supported in part by the National Aeronautics Space Administration under Grant No. NGL-40-002-015, and in part by the Air Force Office of Scientific Research under Grant No. AF-AFOSR-67-0693A.

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1. Introduction

Davis and Rabinswitz [1] recently studied the question of "ignoring the singularity" in numerical quadrature. That is, if f(t) becomes singular at a point ξ where $a \leq \xi \leq b$ then one defines $f(\xi) = 0$ (or any other finite value) and then approximates the integral.

$$I = \int_a^b f(t)dt$$

by a usual numerical quadrature rule. They show that this procedure is not valid in general. However if $\xi = a$ (or some other rational point of [a,b]), then compound quadrature rules do approximate I when f is monotone near ξ. Certain of the positive results in [1] where generalizied by Rabinswitz [2]. Gautschi [3] has applied a result in [2] to two other quadratures of interpolatory type.

The purpose of this paper is to generalize some of the convergence theorems in [1] and [2]. We shall replace the assumption of monotonicity of f(t) near $t = \xi$ by the more general condition that f(t) can be dominated by a monotone, integrable function. We shall also establish some theorems on error bounds and convergence rates which are similar to those obtained in [4].

2. General Quadratures

Let M be the set

$$M = \{f \in C(0,T] \cap L^1(0,T) : f \text{ is nonnegative and non-increasing on } 0 < t \leq T\}.$$

Define M_d to be the set of all functions $f \in C(0,T]$ such that f can be majorizied by a function in M,

$$M_d = \{f \in C(0,T] : \exists\, F \in M \text{ with } |f(t)| \leq F(t) \text{ on } 0 < t \leq T\}.$$

For any function $f \in M_d$ assign the arbitrary value $f(t) = 0$ when $t = 0$.

Given any numerical quadrature rule

$$Q(f) = \Sigma_{j=0}^{n} \; W(j)\, f(T(j)), \; f \in C[0,T]$$

let Q(f,S) be the modified quadrature rule obtained from Q by redefining $f(0) = 0$,

$$Q(f,S) = \Sigma_{j=0}^{n} \; W(j) f(T(j)), \; f(0) := 0$$

Then $Q(f,S)$ ignores possible singularities at $t = 0$ and is well defined for all functions $f \in M_d$. In general $Q(f,S) \neq Q(f)$ for all functions $f \in C[0,T]$. With these preliminaries we are ready to generalize the lemma [2]. First consider rules which are open at $t = 0$.

Lemma 1. Consider a sequence of rules

$$Q_n(f) = \Sigma_{j=0}^{n} W_n(j)\, f(T_n(j))$$

where

$$0 < T_n(0) < T_n(1) < \ldots < T_n(m_n) \leq T$$

and $W_n(j)>0$ for all j. Define $T_n(-1) = 0$.

Suppose there exist positive constants C and A such that uniformly for all positive integers n, if $j = 0(1)m_n$ and if $|T_n(j)| < A$ then

(2.1) $\quad W_n(j) \leq C\{T_n(j) - T_n(j-1)\}$.

($j = 0(1)m_n$ means $j = 0,1,2,\ldots,m_n$.)

<u>Suppose for each function</u> $g \in C[0,T]$ <u>one has</u>

(2-2) $\lim Q_n(g) = \int_0^T g(t)dt, n\to\infty.$

<u>Then for any function</u> $f \in M_d$

(2-3) $\lim Q_n(f,S) = \int_0^T f(t)dt, \ n\to\infty.$

<u>In particular if</u> $0<B<A$, <u>if one defines</u>

$$f_B(t) = f(t) \text{ on } B \le t \le T; = f(B) \text{ or } 0 \le t \le B,$$

<u>and if</u>

$$\delta(t) = \sup \{|f(s) - f_B(s)| : t \le s \le T\},$$

<u>then the error</u>

$$E_s(f,Q_n) = \int_0^T f(t)dt - Q_n(f,S)$$

<u>satisfies the estimate</u>

(2-4) $|E_s(f,Q_n)| \le |E(f_B,Q_n)| + |\int_0^B \{f(t) -$

$f(B)\}dt| + C\int_0^B \delta(t)dt.$

Proof. Write $E = E_s(f, Q_n)$ in the form

$$E = \int_0^T \{f(t) - f_B(t)\}dt + E(f_B, Q_n) + \Sigma_{j=0}^{m_n} W_n(j)$$

$$\{f_B(T_n(j)) - f(T_n(j)\}$$

$$= \int_0^B \{f(t) - f(B)\}dt + E(f_B, Q_n) + \varepsilon_n.$$

Then for any n

$$|\varepsilon_n| \le \Sigma_{j=0}^{m_n} W_n(j) \; |f(T_n(j)) - f_B(T_n(j))|$$

$$\le \Sigma_{j=0}^{m_n} W_n(j) \; \delta \; (T_n(j)) = Q_n(\delta, S)$$

Since $f \in M_d$, there exists a majorizing function $F \in M$. Then for s in the range $b < t \le s < B$ one has

$$|f(s) - f_B(s)| \le F(s) + F(B) \le 2F(t).$$

Therefore

$$\delta\,(t) \le 2F(t) \text{ on } 0 < t \le B, \; \delta(t) = 0$$

on $B \le t \le 1$, and hence $\delta \in L^1(0,1)$. Note also that $\delta(t)$ is continuous, nonnegative and nonincreasing. This together with (2.1) implies that

$$Q_n(\delta,S) = \Sigma_{T_n(j)<B} W_n(j)\delta(T_n(j)) \leq C\Sigma\{T_n(j) - T_n(j-1)\}\delta(T_n(j) \leq C\ \Sigma \int_{T_n(j-1)}^{T_n(j)} \delta(t)dt = C \int_0^B \delta\ (t)dt.$$

This completes the proof of (2.4).

Line (2.3) follows immediately from (2.4) and the estimate $\delta(t) \leq 2\ F(t)$. Indeed by first choosing B small and then choosing n large one can make the right hand side of (2.4) as small as desired. Q.E.D.

Almost the same result is true for quadratures which are closed at t = 0.

Lemma 2. _Suppose a sequence of quadrature rules_ Q_n _satisfies the two conditions_

$$0 = T_n(0) < T_n(1) < \ldots < T_n(m_n) \leq T\ ,\ W_n(j)>0.$$

Suppose there exist positive constants C _and_ A _such that if_ $|T_n(j)| < A$ _and if_ $j = 1(1)m_n$ then (2.1) _is true uniformly in n._ _If_ (2.2) _is also true then_ (2.3) _follows._ _In particular if_ $f_b \in C[0,T]$ _and_ $\delta \in M_d$ _are the functions defined in Lemma_ 1 _and if_ $0 < B < A$, _then_

$$(2.5)\qquad |E_s(f,Q_n)| \le |E(f_B, Q_n)| + |\int_0^B\{f(t) - f(B)\}dt| + C\int_0^B \delta(t)dt + W_n(0)\,|f(B)|.$$

Proof. The proof is the same as that of Lemma 1 except for the estimates of ε_n. In this case

$$\varepsilon_n = \Sigma_{j=0}^{m_n} W_n(j)\,\{f(T_n(j)) - f_B(T_n(j)\},$$

and

$$|\varepsilon_n| \le Q_n(\delta,S) + W_n(0)\,|f(B)|$$

$$\le C\int_0^B\delta(t)dt + W_n(0)\,|f(B)|$$

where we define $\delta(0) = 0$. Our hypotheses easily imply that $W_n(0) \to 0$ as $n \to \infty$. Therefore Lemma 2 is proved.

Combining the two results we have proved:

Theorem 1. <u>Consider a sequence of numerical quadrature rules</u> Q_n <u>where</u>

$$0 \le T_n(0) < T_n(1) <\ldots< T_n(m_n) \le T \text{ and } W_n(j)>0.$$

<u>Suppose</u> (2.1) <u>is true as in Lemma 1 (when</u> $T_n(0)>0$) <u>or Lemma 2</u> ($T_n(0) = 0$). <u>If</u> (2.2) <u>is also true, then for any</u> $f \in M_d$,

$$Q_n(f) \to \int_0^T f(t)dt \text{ as } n \to \infty.$$

Indeed if $0 < B < A$ and if $f_B \in C\,[0,T]$ and $\delta \in M_d$ are the functions defined in Lemma 1 then

$$(2\text{-}6) \quad |E_s(f,Q_n)| \leq |E(f_B,Q_n)| + |\int_0^B\{f(t) - f(B)\}dt| + C\int_0^B \delta(t)dt + \{1 - \operatorname{sgn} T_n(0)\} W_n(0)|f(B)|.$$

One can also generalize the Corollary in [2, p.196] in the obvious way.

3. Compound Rules.

Consider a quadrature rule R defined on the interval $0 \leq t \leq 1$:

$$(R) \quad R(t) = \Sigma_{j=0}^{J} W_j f(t_j)$$

where $J \geq 0$ and

$$(3\text{-}1) \quad 0 \leq t_0 < t_1 < \ldots < t_{J-1}, \; W_j > 0, \; \Sigma_{j=0}^{m} W_j = 1.$$

(If $t_0 > 0$ then define $t_{-1} = 0$.) For any integer $n \geq 1$

and any interval $0 \leq t \leq T$ one can then define a compound rule

$$(n \times R) \qquad R_n(f) = \Sigma_{k=0}^{n-1}\{\Sigma_{j=0}^{J} HW_j \; f(t_j H + Hk)\}$$

where $H = T/n$. Let $C>0$ be any constant satisfying

$$(3.2) \qquad W_j \leq (t_j - t_{j-1})\, C \qquad\qquad (j = 1(1)J)$$

and either

$$(3.3a) \qquad W_0 \leq (t_0 + 1 - t_J)\, C \qquad\qquad (\text{if } t_0 > 0 \text{ or } t_J < 1)$$

or

$$(3.3b) \qquad (W_0 + W_J) \leq (t_J - t_{J-1})\, C \quad (\text{if } t_0=0 \text{ and } t_J=1).$$

Theorem 2. _If_ (R) _satisfies_ (3.1) _then for any_ $f \in M_d$

$$\lim_{n\to\infty} R_n(f,S) = \int_0^T f(t)dt.$$

Proof. The definition (3.2-3) of C implies that (2.1) is true with A=T. Since R integrates constants and $n\to\infty$ then (2.2) is also trival. Therefore Theorem 2 is a corollary of Theorem 1. Q.E.D.

The error estimate (2.6) is rather pessimistie for compound rules. Therefore we shall derive another estimate which is more suitable for many purposes. Let $K>0$ be the smallest constant which satisfies

$$(3.4) \qquad W_j \leq (t_j - t_{j-1})\, K$$

for $j = 1(1)J$ if $t_0=0$ or for $j=0(1)J$ if $t_0>0$.

Theorem 3. Suppose (3.1) and (3.4) are satisfied. Let $H = T/n$ for any function $f \in M_d$ define

$$f_H(t) = f(H) \text{ if } 0 \leq t \leq H; \; f(t) \text{ if } H \leq t \leq T.$$

If $F \in M$ is any majorizing function for f then

$$(3.5) \qquad |E_s(f,R_n)| \leq |E(f_H,R_n)| + \int_0^H F(t)dt + K \int_0^{t_m H} F(t)dt$$

or

$$|E_s(f,R_m)| \leq |E(f_H,R_n)| + (1+K) \int_0^H F(t)dt.$$

Proof. Since (R) integrates constants, then the error may be written in the form

$$E_s(f,R_n) = E(f_H,R_n) + E_0$$

where

$$(3.6) \qquad E_0 = \int_0^H f(t)dt - \Sigma_{j=0}^{J} Hw_j f(t,H).$$

Since $|f(t)| \leq F(t)$ on $0 < t \leq T$, then

$$|\int_0^H f(t)dt| \leq \int_0^H F(t)dt.$$

Let $\alpha = 0$ if $t_0 > 0$ and $\alpha = 1$ if $t_0=0$. Then $f(0) = 0$ and (3.4) imply

$$|\Sigma_{j=0}^{J} Hw_j \; f(t,H)| \leq \Sigma_{\alpha}^{J} Hw_j \; F(t,H)$$

$$\leq K \; \Sigma_{\alpha}^{J} H(t_j - t_{j-1}) \; F(t_j H)$$

$$\leq \quad \Sigma_{\alpha}^{J} \int_{t_{j-1}}^{t_j} F(t)dt = K \int_0^{t_J H} F(t)dt.$$

This proves (3.5) and the theorem.

If one knows that $f \in C^1(0,T]$, then the term $E(f_H,R_n)$ may be estimated using Peano's theorem.

That is

$$E(f_H,R_n) = \int_0^1 P_n(s) \; f_m'(s)dt$$

where P_n is the appropriate Peano kernal. Since

$P_n(s+H) = P_n(s)$ on $0 \le s \le T-H$, then $|P_n(s)|$ need be be estimated only on the interval $0 < s < H$. Therefore the following result is an immediate corollary of Theorem 3.

Corollary 1. Assume the hypotheses of Theorem 3. If $f \in C^1(0,T]$ then

$$(3.7) \qquad |E(f,R_n)| \le ||P_n|| \int_H^T |f'(t)|dt + \int_0^H F(t)dt + K \int_0^{t_m H} F(t)dt$$

where $||P_n|| = \sup \{|P_n(s)| = 0 < s < H\}$.

Corollary 1 is useful in estimating convergence rates in certain cases. Following [4] we shall say that a function $f \in C^1(0,T]$ is weakly singular at $t = 0$ if the function

$$\alpha(t,f) = |f(t)| + \int_t^T |f'(s)|ds$$

is in $L^1(0,T)$.

Corollary 2. Suppose the hypotheses of Theorem 3 are true. If f is weakly singular (at $t = 0$) then

$$(3.8) \qquad E_s(f,R_n) = O(\int_0^H \alpha(t,f)dt) \text{ as } H \to 0.$$

Proof. It follows immediately from the definition of weakly singular functions that $f \in M_d$ and $\alpha(t,f) \in M$ is a majorizing function. Thus (3.7) implies

$$|E_s(f,R_n)| \leq ||P_n|| \int_H^T |f'(t)dt + \int_0^H \alpha(t,f)dt + K\int_0^H \alpha(t,f)dt$$

$$\leq ||P_n|| \; \alpha(H,f) + (1 + K) \int_0^H \alpha(t,f)dt.$$

Using the estimate $||P_n|| \leq 2H$ (see for example [4, section II]) and the monotonicity of α one has

$$||P_n|| \; \alpha(H,f) \leq 2H \; \alpha(H,f) \leq 2\int_0^H \alpha(t,f)dt.$$

Therefore for any n $(H = T/n)$ one has

$$|E(f,R_n)| \leq (3 + K) \int_0^H \alpha(t,f)dt.$$

Q.E.D.

For example if $f(t) = t^{-P}$ $(0<p<1)$ then (3.8) predicts that $E_s(f,R_n)$ is at least of order h^{1-P}. If $f(t) = t^{-P} \sin(t^{-q})$ where $0 < p,q < 1$ and $p + q < 1$ then $E_s(f,R_n)$ is at least of order h^{1-p-q}. If $f(t) = t^{-P} \sin(t^{-q})$ where $0 < p < 1$, $q > 0$ and $p + q \geq 1$ then our theory predicts convergence but gives no order estimate.

4. Numerical Example.

The data in [1] will be used to illustrate the theory given above. For the midpoint rule $M(f) = f(\frac{1}{2})$ one has $H = h = T/n$. Since $-P_n(s) = s$ if $0 < s < h/2$; $2-h$ if $h/2 < s < h$, then $||P_n|| = h/2$ and $K = 2$. Therefore (3.2) has the form

$$|E_s(f,M_n)| \leq (h/2) \int_n^T |f'(t)|dt + \int_0^h F(t)dt + 2\int_0^{h/2} F(t)dt.$$

Table 1 contains data for the case

(4.1) $\int_0^1 t^{-1/2} dt = 2.$

The fourth column is the theoretical error computed using (3.7). This error bound is seen to be pessimistic by a factor of 7 to 8. Corollary 2 suggests that the error may be of the approximate form

(4.2) $E_s(f,M_n) = C\sqrt{h}$ $(h=T/n)$

for some constant $C > 0$. The ratios $E_s(f,M_n) / E_s(f,M_{n+1})$ are given in column five. The theoretical ration computed using (4.2) is $\sqrt{2}$ (column six). It can be seen that (4.2) is approximately true with $C = .61$.

(Insert table 1 near here)

Table 2 contains similar data for (4.1) using the trapezoid rule (T), Simpson's rule (S) and the Gaussian two point rule (G_2). The theoretical errors are good for the trapezoid rule and progressive worse for Simpson and Gauss two point. In all cases (4.2) is approximately true, $E_s(f,T_n) = 1.5\sqrt{h}$, $E_s(f,S_n) = .89\sqrt{h}$ and $E_s(f,nXG_2) = .35\sqrt{h}$.

(Insert table 2 near here).

One could also analysis the data in [1] for (4.1) using the Gauss 48 - point rule. In this case $E_s(f,n\ X\ G_{48}) = .18\sqrt{h}$ (approximately). It would be very difficult to estimate $||P_n||$ accurately in this case. Thus (3.7) is essentially useless.

Data for the example

$$\int_0^1 t^{-\frac{1}{2}} \sin (t^{-\frac{1}{2}})\, dt = 1.08134$$

is given in table 3 for Simpson's rule and for the Gauss 48 - point rule. For this case our theory predicts convergence but yeilds no useful information on errors or convergence rates. For Simpson's rule the method appears to be convergent. For G_{48} the method starts to converge nicely but blows up at the fourth step.

TABLE 1

n	$M_n(f_0)$	Error	Th.Error	Ratio	Th.Ratio
2^5	1.8931	.1069	.6763	1.414	1.414
2^6	1.9244	.0756	.4815	1.413	1.414
2^7	1.9465	.0535	.4321	1.415	"
2^8	1.9622	.0378	.2427	1.416	"
2^9	1.9733	.0267	.1720	1.413	"
2^{10}	1.9811	.0184	.1218	1.410	"
2^{11}	1.9866	.0134	.0864		

TABLE 2

	Approx.	Error	Th.Error	Ratio	Th.Ratio
2^5 X T	1.7418	.2582	.6031	1.414	1.414
2^6 X T	1.8174	.1826	.4294	1.414	"
2^7 X T	1.8709	.1291	.3055	1.414	"
2^8 X T	1.9087	.0913	.2168	1.415	"
2^9 X T	1.9355	.0645	.1537	1.414	"
2^{10} X T	1.9544	.0456	.1089		
2^5 X S	1.8427	.1573	1.1792	1.413	1.414
2^6 X S	1.8887	.1113	.8735	1.414	"
2^7 X S	1.9213	.0787	.6198	1.415	"
2^8 X S	1.9444	.0556	.4393	1.411	"
2^9 X S	1.9606	.0394	..3113	1.412	"
2^{10} X S	1.9721	.0297	.2203		
2 X G_2	1.7528	.2472	7.6572	1.414	1.414
4 X G_2	1.8252	.1748	5.4012	1.225	1.225
6 X G_2	1.8573	.1427	4.4213	1.155	1.155
8 X G_2	1.8764	.1236	3.8341	1.118	1.118
10 X G_2	1.8894	.1106	3.4328	1.096	1.095
12 X G_2	1.8991	.1009	3.1360	1.080	1.080
14 X G_2	1.9066	.0934	2.9050	1.069	1.069
16 X G_2	1.9126	.0874	1.7640		

TABLE 3

	Approx	Error	Ratio
2^5 X S	1.1234	-.0421	.241
2^6 X S	.9116	.1697	1.562
2^7 X S	.9727	.1086	1.017
2^8 X S	.9745	.1068	1.745
2^9 X S	1.0201	.0612	2.696
2^{10} X S	1.0586	.0227	
1 X G_{48}	.9449	.1346	1.534
2 X G_{48}	.9924	.0889	2.285
3 X G_{48}	1.0402	.0389	.2571
4 X G_{48}	.9300	.1513	

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