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ON IGNORING THE SINGULARITY*

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Abstract. Conditions are given, weaker than those previously known, under which one can ignore a singularity while carrying out a numerical quadrature. The conditions apply in all (finite) dimensions. A special case concerns the theory of uniformly distributed sequences.

Key words. numerical quadrature, endpoint singularity, uniform distribution

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1. The problem, a solution, and previous work. We are concerned with applying quadrature rules to functions with endpoint singularities. For $n = 1, 2, \cdots$, let Q_n be the quadrature rule given by

$$Q_n(f) = \sum_{k=1}^{n} w_{nk} f(x_{nk}),$$

where the weights w_{nk} are real or complex numbers, and the nodes x_{nk} are in $(0,1]$ and are nondecreasing in k. We shall assume throughout that

$$\lim_{n\to\infty} Q_n(f) = \int_0^1 f(x)\,dx$$

for all f continuous on $[0,1]$.

Let R be the class of all functions for which the Riemann integrals $\int_a^1 f(x)\,dx$ exist for all a in $(0,1]$ and converge to a finite limit as a approaches zero. Let M denote the class of functions in R that are monotone, and BM the class of functions in R that are bounded in absolute value by a member of M. We wish to integrate functions in BM numerically by applying the quadrature rules Q_n—this is known as "ignoring the singularity." Miller [4] and Rabinowitz [6] gave a simple condition on the weights and nodes that guarantees convergence of $Q_n(f)$ to $\int_0^1 f(x)\,dx$ for f in BM. We shall refer to this condition, which we state below, as "the standard hypothesis." We present an equally simple and strictly weaker condition for convergence.

We write $\sum^{(a)}$ for a sum over all k such that x_{nk} is less than a.

THEOREM 1. *If there is a positive constant c such that $\sum^{(a)} |w_{nk}| \le ca$ for all $a < a_0$ and all $n > n_0$, then*

$$\lim_{n\to\infty} Q_n(f) = \int_0^1 f(x)\,dx$$

for all f in BM.

We defer the proof, as the theorem will follow from a more general result given below. We pause to demonstrate that the hypothesis in Theorem 1 is strictly weaker than the standard hypothesis.

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The standard hypothesis is the existence of positive constants c and a such that $x_{nk} < a$ implies

$$|w_{nk}| \le c(x_{nk} - x_{n,k-1})$$

for all $n > n_0$. Summing on k, it is clear that this hypothesis implies that of Theorem 1. Now let Q_n be the quadrature rule given by

$$w_{nk} = \frac{1}{n}, \quad x_{n1} = \frac{1}{n}, \quad x_{nk} = \frac{k-1}{n-1} \quad \text{for } 2 \le k \le n.$$

It is clear that $Q_n(f)$ tends to $\int_0^1 f(x)\,dx$ for all f continuous on $[0,1]$. Taking $k = 2$ in the standard hypothesis, we find that c must satisfy $1/n \le c/n(n-1)$, which is impossible for large n. On the other hand, $\#\{k : x_{nk} < a\} \le 2na$, as we readily establish, so

$$\sum^{(a)} w_{nk} = \frac{1}{n}\#\{k : x_{nk} < a\} \le 2a$$

and the quadrature rule satisfies the hypothesis of Theorem 1, with $c = 2$.

2. Higher dimensions, main theorem, and proof. Theorem 1 generalizes easily to functions of any number of variables, the most difficult problem being to find congenial notation.

Write H_m for $(0,1]^m$. A quadrature rule Q_n is given by

$$Q_n(f) = \sum_{k=1}^{n} w_{nk} f(\mathbf{x}_{nk}),$$

where the weights w_{nk} are real or complex numbers, and the nodes $\mathbf{x}_{nk}$ are in H_m.

Let $\mathbf{a} = (a_1, \cdots, a_m)$ and $\mathbf{b} = (b_1, \cdots, b_m)$ be in H_m. We adopt the following notation:

$$\begin{aligned}
&\mathbf{a} < \mathbf{b} := a_j < b_j \quad \text{for } 1 \le j \le m;\\
&\mathbf{a} \le \mathbf{b} := a_j \le b_j \quad \text{for } 1 \le j \le m;\\
&|\mathbf{a}| := a_1 a_2 \cdot \ldots \cdot a_m;\\
&m(\mathbf{a}) := \min_j (a_j);\\
&B(\mathbf{a},\mathbf{b}) := \{\mathbf{x} : \mathbf{a} \le \mathbf{x} \le \mathbf{b}\};\\
&\int_{\mathbf{a}}^{\mathbf{b}} f(\mathbf{x})\,dV := \int_{B(\mathbf{a},\mathbf{b})} f(\mathbf{x})\,dV.
\end{aligned}$$

We assume throughout that

$$\lim_{n\to\infty} Q_n(f) = \int_{\mathbf{0}}^{\mathbf{1}} f(\mathbf{x})\,dV$$

for all f continuous on the closure of H_m—of course, $\mathbf{0} = (0, \cdots, 0)$ and $\mathbf{1} = (1, \cdots, 1)$. Let R be the class of all functions for which the Riemann integrals $\int_{\mathbf{a}}^{\mathbf{1}} f(\mathbf{x})\,dV$ exist for all $\mathbf{a}$ in H_m and converge to a finite limit as $\mathbf{a}$ approaches $\mathbf{0}$. Let M be the class of functions in R that are decreasing in each variable, and BM the class of functions in R that are bounded in absolute value by a member of M.

We write $\sum^{(\mathbf{a})}$ for the sum over all k such that $\mathbf{x}_{nk} < \mathbf{a}$.

THEOREM 2. *If there is a positive constant c and a function $\psi(\mathbf{x})$ in M, such that $\sum^{(\mathbf{a})} |w_{nk}| < c|\mathbf{a}|\psi(\mathbf{a})$ provided $m(\mathbf{a}) < a_0$ and $n > n_0$, then*

$$\lim_{n\to\infty} Q_n(f) = \int_{\mathbf{0}}^{\mathbf{1}} f(\mathbf{x})\, dV$$

for all f in R for which $f\psi$ is in BM.

Remark. In the one-variable case, we recover Theorem 1 by taking ψ to be identically 1.

Proof. Given the hypotheses, choose $\mathbf{a} < a_0\mathbf{1}$, let $T = \sum_{\mathbf{x}_{nk} > \mathbf{a}} w_{nk} f(\mathbf{x}_{nk})$, and let $S = Q_n(f) - T$. Now

$$\lim_{\mathbf{a}\to\mathbf{0}} \lim_{n\to\infty} T = \int_{\mathbf{0}}^{\mathbf{1}} f(\mathbf{x})\, dV,$$

so it suffices to show that $\lim_{\mathbf{a}} \lim_n S = 0$.

Write $w(j,a) = 2^{-j}a$ if $j \geq 0$, $w(j,a) = 1$ otherwise. Given an m-tuple of integers $\mathbf{j} = (j_1, \cdots, j_m)$, write $\mathbf{a_j}$ for $\big(w(j_1, a_1), \cdots, w(j_m, a_m)\big)$ and $A_{\mathbf{j}}$ for the box $B(\mathbf{a_j}, \mathbf{a_{j-1}})$. Then

$$S = \sum_{\mathbf{j}=\mathbf{0}}^{\infty}{}' \sum_{\mathbf{x}_{nk}\in A_{\mathbf{j}}} w_{nk} f(\mathbf{x}_{nk}),$$

where $\sum'$ means omit the term $\mathbf{j} = \mathbf{0}$. Writing $\sigma(\mathbf{j})$ for $j_1 + \cdots + j_m$, and taking $n > n_0$, we have

$$\begin{aligned}\left|\sum_{\mathbf{x}_{nk}\in A_{\mathbf{j}}} w_{nk} f(\mathbf{x}_{nk})\right| &\leq \max_{\mathbf{x}\in A_{\mathbf{j}}} |f(\mathbf{x})| \sum^{(\mathbf{a_{j-1}})} |w_{nk}| \\ &\leq \max_{\mathbf{x}\in A_{\mathbf{j}}} |f(\mathbf{x})|\, c\, 2^{-\sigma(\mathbf{j})+m} |\mathbf{a}|\, \psi(\mathbf{a_{j-1}}) \\ &\leq g(\mathbf{a_j})\, c\, 2^{-\sigma(\mathbf{j})+m} |\mathbf{a}|,\end{aligned}$$

where $g(\mathbf{x})$ in M is a bound for $|f\psi|$. Writing $|A|$ for the volume of A, we have

$$\int_{A_{\mathbf{j+1}}} g(\mathbf{x})\, dV \geq |A_{\mathbf{j+1}}| \min_{\mathbf{x}\in A_{\mathbf{j+1}}} g(\mathbf{x}) = 2^{-\sigma(\mathbf{j})-m} |\mathbf{a}|\, g(\mathbf{a_j}).$$

Thus,

$$\left|\sum_{\mathbf{x}_{nk}\in A_{\mathbf{j}}} w_{nk} f(\mathbf{x}_{nk})\right| \leq 4^m c \int_{A_{\mathbf{j+1}}} g(\mathbf{x})\, dV,$$

and

$$|S| \leq \sum_{\mathbf{j}=\mathbf{0}}^{\infty} 4^m c \int_{A_{\mathbf{j+1}}} g(\mathbf{x})\, dV \leq 4^m c \int_{\mathbf{0}}^{\mathbf{a}} g(\mathbf{x})\, dV.$$

It follows that $\lim_{\mathbf{a}} \lim_n S = 0$, as was to be proved.

We applied a similar but rather ad hoc argument to a special case in [5].

3. Uniform distribution.

Let $\mathbf{u} = (\mathbf{u}_1, \mathbf{u}_2, \cdots)$ be a sequence of points in $K_m = [0,1)^m$. We say that $\mathbf{u}$ is uniformly distributed if

$$\lim_{n\to\infty} \frac{1}{n} \#\{\, k \leq n : \mathbf{a} \leq \mathbf{u}_k < \mathbf{b} \,\} = |\mathbf{b} - \mathbf{a}|$$

for all $\mathbf{a}$ and $\mathbf{b}$ with $\mathbf{0} \leq \mathbf{a} < \mathbf{b} \leq \mathbf{1}$. The definition and the following theorem are due to Weyl [8].

THEOREM 3. *If* $\mathbf{u}$ *is uniformly distributed and* f *is Riemann-integrable then*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} f(\mathbf{u}_k) = \int_{\mathbf{0}}^{\mathbf{1}} f(\mathbf{x})\,dV.$$

In the one-variable case, there is a quantitative version of this theorem due to Koksma [2]. We define the *discrepancy* $D_n(u)$ by

$$D_n(u) = \sup_{0<a\le 1} \left| \frac{\#\{\,k \le n : u_k < a\,\}}{n} - a \right|.$$

Bergström and van der Corput were among the pioneers in the study of discrepancy (cf., e.g., [3]).

THEOREM 4. *If* f *is of bounded variation* $V(f)$ *on* $[0,1)$, *then*

$$\left| \frac{1}{n} \sum_{k=1}^{n} f(u_k) - \int_0^1 f(x)\,dx \right| \le D_n(u)V(f).$$

Write $V_a(f)$ for the variation of f on $[a,1]$. Let $\mu(n) = \min\{\,u_k : k \le n\,\}$. It follows from Theorem 4 that if $D_n(u)V_{\mu(n)}(f)$ tends to zero, then $\frac{1}{n}\sum^n f(u_k)$ tends to $\int_0^1 f(x)\,dx$ (as n tends to infinity). This was pointed out by Sobol' [7], without explicit reference to Koksma's Theorem.

Koksma's Theorem can be generalized to higher dimensions. The interested reader may wish to start with the account given by Kuipers and Niederreiter [3] (who write D^* where we have D). In [7] Sobol' generalized his convergence result to higher dimensions. Theorem 2 gives rise to a rather different result. We assume $\mathbf{u}$ is uniformly distributed.

THEOREM 5. *If there is a positive constant* c, *and a function* $\psi(\mathbf{x})$ *in* M, *such that*

$$\#\{\,k \le n : \mathbf{u}_k < \mathbf{a}\,\} \le cn|\mathbf{a}|\psi(\mathbf{a})$$

provided $m(\mathbf{a}) < a_0$ *and* $n > n_0$, *then*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} f(\mathbf{u}_k) = \int_{\mathbf{0}}^{\mathbf{1}} f(\mathbf{x})\,dV$$

for all f *in* R *for which* $f\psi$ *is in* BM.

Proof. Given $\mathbf{u}$, define quadrature rules Q_n by $w_{nk} = 1/n$ and $\mathbf{x}_{nk} = \mathbf{u}_k$. Then

$$\sum^{(\mathbf{a})} w_{nk} = \frac{1}{n}\#\{\,k \le n : \mathbf{u}_k < \mathbf{a}\,\} \le c|\mathbf{a}|\psi(\mathbf{a})$$

provided $m(\mathbf{a}) < a_0$ and $n > n_0$, so Theorem 2 applies. The conclusion of Theorem 2 is precisely that of Theorem 5.

Hardy and Littlewood [1] gave a similar result for the special sequence $u_k = k\theta$, with θ irrational.

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