Eberlein Measure and Mechanical Quadrature Formulae. I: Basic Theory*

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A uniform theory of numerical approximation of multiple integrals of arbitrary multiplicity is a long felt need of applied mathematics. In the absence of something better, the Monte Carlo method is the one most commonly used now (see [6] and [7]). For the integration of functions of one variable, for which purpose useful classical formulae exist, the error estimates are unsatisfactory inasmuch as they involve derivatives of high order of the integrand. Moreover, no criteria are available for the comparison of one quadrature method with another per se. In the present paper we construct a theory of mechanical quadrature for k-fold integrals ($k \geqq 1$), and set down a rational basis for the global comparison of different quadrature methods. However, it should be pointed out that the theory yields no error estimates applicable to individual integrands. We discuss the Monte Carlo method at some length, and substantiate the educated guess that the method improves with increasing multiplicity of the integrals. The theory developed here will be used in a future paper to propose some new mechanical quadrature formulae.

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0. Introduction. Real multiple power series

$$\mathbf{x}(t) = \sum x_{n_1 \cdots n_k} (t_1)^{n_1} \cdots (t_k)^{n_k}, \qquad (n_1, \cdots, n_k \geqq 0) \tag{0.1}$$

whose coefficients satisfy the condition

$$||\mathbf{x}||_1 = \sum |x_{n_1 \cdots n_k}| < \infty \tag{0.2}$$

converge uniformly and absolutely for all points t in the k-dimensional Euclidean cube

$$\mathfrak{C} = \{(t_1, \cdots, t_k) = t : -1 \leqq t_j \leqq 1, 1 \leqq j \leqq k\}.$$

The set of all functions defined by (0.1) and (0.2) can be identified with the sequence space l_1, as in [10], and is dense in the Banach space $\mathcal{C}(\mathfrak{C})$ of all real continuous functions on $\mathfrak{C}$ with the uniform norm. We denote the closed unit sphere

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of l_1 by S_∞ and remark that S_∞ absorbs l_1. The integral I defined by

$$I(\mathbf{x}) = 2^{-k} \int_{\mathfrak{C}} \mathbf{x}\, dt$$

and an N-point mechanical quadrature formula J_N defined by

$$J_N(\mathbf{x}) = \sum_{m=1}^{N} A_m \mathbf{x}(t^{(m)}) \tag{0.3}$$

are continuous linear functionals on $\mathcal{C}(\mathfrak{C})$, and so is the error $\mathbf{e}$ defined by

$$\mathbf{e}(\mathbf{x}) = I(\mathbf{x}) - J_N(\mathbf{x}) .$$

In (0.3), the 'weights' A_m ($1 \leqq m \leqq N$) are real numbers and the 'abscissae' $t^{(m)}$ ($1 \leqq m \leqq N$) are points of $\mathfrak{C}$.

The problem of mechanical quadrature is so to choose the weights and the abscissae of J_N that $|\mathbf{e}(\mathbf{x})|$ is minimised in a sense to be made precise. The approach of the present paper, following the lead of [5], is to choose an appropriate subset $\mathcal{A}$ of $\mathcal{C}(\mathfrak{C})$ and to minimise the average of $|\mathbf{e}(\mathbf{x})|^2$ over $\mathcal{A}$. It is clear that we must have a measure over $\mathcal{A}$. Since, in practice, the functions to which one would apply a mechanical quadrature enjoy a certain degree of smoothness, and since such functions form a set of Wiener measure zero, the temptation to identify $\mathcal{A}$ with $\mathcal{C}(\mathfrak{C})$ has to be resisted. We choose $\mathcal{A} = S_\infty$. A countably additive measure on S_∞ is constructed in [10], a generalisation of [4], and is called the Eberlein measure and denoted by $d_E\mathbf{x}$. The corresponding integral over S_∞ is denoted by $E(\cdot)$ or by $\int_{S_\infty} (\cdot)\, d_E\mathbf{x}$. The main results and notation of [10] are summarised in the following section.

1. The Eberlein Integral. Let

$$\mathbf{x} = \{x_{n_1 \cdots n_k}\}$$

be an element of l_1; and P_n the projection operator on l_1 into l_1, defined by requiring that the k-fold sequence $P_n\mathbf{x}$ be obtained from the k-fold sequence $\mathbf{x}$ through replacing by 0 every $x_{n_1 \cdots n_k}$ with $n_1 + \cdots + n_k > n$. We introduce the abbreviations

$$c_i = \frac{(k+i-1)!}{(k-1)!i!}, \qquad \sigma_n = \sum_{i=0}^{n} c_i ,$$

$$\mu_n = \prod_{i=0}^{n} (c_i!) , \qquad \phi_n(x) = \prod_{i=1}^{n} (1 - \|P_{i-1}\mathbf{x}\|_1)^{c_i} .$$

If f is any weak* continuous real function or any bounded real weak* Baire function, then the Eberlein integral, $E(f)$, of f is defined as the limit, when $n \to \infty$, of

$$\frac{\mu_n}{2^{\sigma_n}} \int \cdots \cdots \int_{\|P_n\mathbf{x}\|_1 \leqq 1} \frac{f(P_n\mathbf{x})}{\phi_n(\mathbf{x})} , \tag{1.1}$$

the integration in (1.1) being with respect to all the real variables $x_{n_1 \cdots n_k}$ with $n_1 + \cdots + n_k \leqq n$. Thus defined, the integral E is linear and positive; and $E(1) = 1$. Moreover,

$$\int_{S_\infty} (x_{n_1\cdots n_k})^p d_E \mathbf{x} = 0 \quad \text{if } p \text{ is odd}\,, \tag{1.2}$$

$$\int_{S_\infty} x_{m_1\cdots m_k} x_{n_1\cdots n_k} d_E \mathbf{x} = 0 \quad \text{if } (m_1, \cdots, m_k) \neq (n_1, \cdots, n_k) \tag{1.3}$$

and

$$\int_{S_\infty} (x_{n_1\cdots n_k})^2 d_E \mathbf{x} = \frac{1}{3} \frac{2n_1 + \cdots + n_k}{\prod_{i=1}^n (c_i + 1)(c_i + 2)}.$$

Now, if

$$\mathbf{y} = \{y_{n_1\cdots n_k}\}$$

is a bounded k-fold sequence of real numbers, and if we write

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum x_{n_1\cdots n_k} y_{n_1\cdots n_k}\,,$$

the summation being over all nonnegative integers $n_1, \cdots, n_k$, then $\langle \mathbf{x}, \mathbf{y} \rangle$ is a weak* continuous real function of $\mathbf{x}$ defined on S_∞. A routine calculation using (1.2), (1.3), and (1.4) shows that

$$\int_{S_\infty} \langle \mathbf{x}, \mathbf{y} \rangle^p d_E \mathbf{x} = 0 \quad \text{if } p \text{ is odd}\,, \tag{1.5}$$

and that

$$\int_{S_\infty} \langle \mathbf{x}, \mathbf{y} \rangle^2 d_E \mathbf{x} = \frac{1}{3} \sum_{n=0}^{\infty} \frac{2^n \sum_n' (y_{n_1\cdots n_k})^2}{\prod_{i=1}^n (c_i + 1)(c_i + 2)}\,, \tag{1.6}$$

where $\sum_n'$ denotes, here and in the rest of this paper, a summation over all nonnegative integers $n_1, \cdots, n_k$ with $n_1 + \cdots + n_k = n$.

2. Optimal Quadrature Formulae. For all k-tuples $(n_1, \cdots, n_k)$ of nonnegative integers, define the functions

$$T_{n_1\cdots n_k}(t) = (t_1)^{n_1} \cdots (t_k)^{n_k}, \qquad t \in \mathfrak{C},$$

and denote $\mathbf{e}(T_{n_1\cdots n_k})$ by $e_{n_1\cdots n_k}$. The sequence $\{e_{n_1\cdots n_k}\}$ may be identified with $\mathbf{e}$ on S_∞. It is easily seen that,

$$\begin{aligned} e_{n_1\cdots n_k} &= (I - J_N) T_{n_1\cdots n_k} \\ &= 2^{-k} \prod_{i=1}^{k} \frac{1 + (-1)^{n_i}}{n_i + 1} - \sum_{m=1}^{N} A_m (t_1^{(m)})^{n_1} \cdots (t_k^{(m)})^{n_k}\,, \\ |e_{n_1\cdots n_k}| &\leqq 1 + \sum_{m=1}^{N} |A_m|\,; \end{aligned} \tag{2.1}$$

and it follows that $\mathbf{e} \in m = (l_1)^*$.

Writing (0.1) in the form

$$\mathbf{x}(t) = \sum_{n=0}^{\infty} \sum_n' x_{n_1\cdots n_k} T_{n_1\cdots n_k}(t)\,,$$

we obtain

$$(I - J_N)(\mathbf{x}) = \sum_{n=0}^{\infty} \sum_n{}' x_{n_1\cdots n_k}(I - J_N)(T_{n_1\cdots n_k})$$
$$= \sum_{n=0}^{\infty} \sum_n{}' x_{n_1\cdots n_k} e_{n_1\cdots n_k}$$
$$= \langle \mathbf{x}, \boldsymbol{e} \rangle .$$

Writing $\sigma^2(I - J_N)$ for $\int_{S_\infty} \langle \mathbf{x}, \boldsymbol{e}\rangle^2 d_E\mathbf{x}$, and evaluating the integral with the help of (1.6), (1.7) and (2.1), we get

$$\sigma^2(I - J_N) = \sum_{n=0}^{\infty} \frac{2^n}{3\lambda_n} S_n , \tag{2.2}$$

where we have used the abbreviations

$$\lambda_0 = 1 , \qquad \lambda_n = \prod_{i=1}^{n} (c_i + 1)(c_i + 2) \quad \text{for} \quad n > 0 \text{ and } S_n = \sum_n{}' (e_{n_1\cdots n_k})^2 .$$

$\sigma^2(I - J_N)$ will be used as a measure for the error of the quadrature formula J_N over the space S_∞ equipped with the measure $d_E\mathbf{x}$. Using the expression (2.2), we shall seek to minimize $\sigma^2(I - J_N)$ as a function of the weights A_m and the abscissae $\boldsymbol{t}^{(m)}$.

Remark I. There is no J_N for which $\sigma^2(I - J_N) = 0$. In fact, the existence of such a J_N implies, in particular, that

$$(2p + 1) \sum_{m=1}^{N} A_m(t_1^{(m)})^{2p} = 1 , \qquad p \geqq 0 ,$$

which leads to a contradiction when we let $p \to \infty$.

Definitions. An N-point mechanical quadrature formula J_N is *completely optimal* if $\sigma^2(I - J_N)$ is an absolute minimum as a function of the weights and the abscissae of J_N. With prescribed abscissae, a J_N for which $\sigma^2(I - J_N)$ is a minimum in the weights is *optimal in the weights.* We shall denote such a formula by W_N.

THEOREM I. *For each* $N \geqq 1$, *there exists a* W_N *corresponding to any preassigned distinct abscissae* $\boldsymbol{t}^{(1)}, \boldsymbol{t}^{(2)}, \cdots, \boldsymbol{t}^{(N)}$ *in* $\mathfrak{C}$.

Proof. Consider the k-fold sequences

$$\boldsymbol{f} = \left\{ \left(\frac{2^n}{3\lambda_n}\right)^{1/2} 2^{-k} \prod_{i=1}^{k} \frac{1 + (-1)^{n_i}}{n_i + 1} \right\}$$

and

$$\boldsymbol{g}_l = \left\{ \left(\frac{2^n}{3\lambda_n}\right)^{1/2} (t_1^{(l)})^{n_1} \cdots (t_k^{(l)})^{n_k} \right\}, \qquad 1 \leqq l \leqq N ,$$

where $n = n_1 + \cdots + n_k$ and each n_i assumes all nonnegative integer values. Observing that $c_n \geqq 1$ and hence that $\lambda_n \geqq 2^n 3^n$ for all $n \geqq 0$, we see that

$$\|\boldsymbol{f}\|_2^2 = \sum_{n=0}^{\infty} \left[\frac{2^n}{3\lambda_n} \sum_n{}' \left\{ 2^{-2k} \prod_{i=1}^{k} \frac{[1 + (-1)^{n_i}]}{(n_i + 1)^2} \right\} \right]$$
$$\leqq \sum_{n=0}^{\infty} \frac{2^n}{3\lambda_n} c_n < \sum_{n=0}^{\infty} (2/3^{n+1}) < \infty ;$$

and similarly that

$$\|g_l\|_2^2 < \sum_{n=0}^{\infty} \frac{2^n}{3\lambda_n} c_n < \infty\,, \qquad 1 \leqq l \leqq N\,.$$

Then $g_1, \cdots, g_N$ and f are elements of the sequential Hilbert space l_2. As the abscissae $t^{(l)}$ are preassigned, the g_l are fixed vectors of l_2. It is clear from (2.2) that $\sigma^2(I - J_N)$ is the square of the distance between f and a variable vector in the linear manifold spanned by $g_1, \cdots, g_N$. Let us call this manifold $M(N, t)$. This manifold, being of dimension $\leqq N$, is closed; and there is a unique vector $g_0 \in M(N, t)$.

$$\|f - g_0\|_2 \leqq \|f - g\|_2\,, \qquad g \in M(N, t)\,, \tag{2.3}$$

(see, for instance, [1, p. 11]). Writing $g_0 = \sum_{m=1}^{N} A_m{}^0 g_m$ we see that the weights $A_1{}^0, A_2{}^0, \cdots, A_N{}^0$ minimise $\sigma^2(I - J_N)$ for the fixed abscissae $t^{(1)}, \cdots, t^{(N)}$. Q.E.D.

The uniqueness of this representation of W_N is not obvious until we establish the linear independence of $g_1, \cdots, g_N$.

THEOREM II. *The dimension of the linear manifold $M(N, t)$ is strictly less than N if and only if some two abscissae of J_N coincide.*

Proof. The 'if' part is obvious. To prove the 'only if' part, assume dim $M(N, t) < N$. Then there are real constants $a_1, a_2, \cdots, a_N$, not all zero, such that $\sum_{l=1}^{N} a_l g_l = 0$. This means that

$$\sum_{l=1}^{N} a_l (t_1{}^{(l)})^{n_1} \cdots (t_k{}^{(l)})^{n_k} = 0$$

for all nonnegative integers $n_1, \cdots, n_k$. In particular, for an arbitrary choice of $n_1, \cdots, n_k$, we have

$$\sum_{l=1}^{N} a_l (t_1{}^{(l)})^{(p-1)n_1} \cdots (t_k{}^{(l)})^{(p-1)n_k} = 0\,, \qquad p = 1, 2, \cdots, N\,.$$

As the a's are not all zero, the determinant of this system of linear equations vanishes; viz.,

$$\prod_{i<j=2}^{N} [(t_1{}^{(i)})^{n_1} \cdots (t_k{}^{(i)})^{n_k} - (t_1{}^{(j)})^{n_1} \cdots (t_k{}^{(j)})^{n_k}] = 0$$

(see, for instance, [2, p. 41]). Then, for some pair of indices i, j ($i \neq j$), we have

$$(t_1{}^{(i)})^{n_1} \cdots (t_k{}^{(i)})^{n_k} = (t_1{}^{(j)})^{n_1} \cdots (t_k{}^{(j)})^{n_k}\,.$$

As this argument can be repeated an infinity of times—say, each n_i either zero or odd—whereas there are only $\frac{1}{2}N(N - 1)$ index pairs (i, j), we conclude that, for some fixed index pair (i, j),

$$(t_l{}^{(i)})^{n_l} = (t_l{}^{(j)})^{n_l}\,, \qquad 1 \leqq l \leqq k\,,$$

for an infinity of odd values of n_l; and hence that

$$t^{(i)} = t^{(j)}\,. \qquad \text{Q.E.D.}$$

COROLLARY. *With prescribed distinct abscissae, the representation of a W_N is unique. If only M ($<N$) of the abscissae are distinct, then the W_N reduces to a W_M and, as such, has a unique representation again.*

Remark II. Referring to the notation of Theorem I, we note that $\boldsymbol{f}$ is nearer to $\boldsymbol{g}_0$ than to any other point of $M(N, \boldsymbol{t})$. Consequently $\boldsymbol{f} - \boldsymbol{g}_0$ is orthogonal to $M(N, \boldsymbol{t})$. Using the representation $\boldsymbol{g}_0 = \sum_{m=1}^{N} A_m \boldsymbol{g}_m$, we obtain

$$(2.4) \qquad \sum_{m=1}^{N} A_m(\boldsymbol{g}_m, \boldsymbol{g}_l) = (\boldsymbol{f}, \boldsymbol{g}_l), \qquad 1 \leqq l \leqq N,$$

where (,) is the inner product in l_2. It may be noted that these equations are identical with the equations

$$\frac{\partial}{\partial A_l} \sigma^2(I - J_N) = 0, \qquad 1 \leqq l \leqq N.$$

LEMMA. *Let the abscissae and optimal weights of a W_N be $\boldsymbol{t}^{(1)}, \cdots, \boldsymbol{t}^{(N)}$ and $\alpha_1, \cdots, \alpha_N$ respectively. Let the abscissae and optimal weights of a W_{N+1} be $\boldsymbol{t}^{(1)}, \cdots, \boldsymbol{t}^{(N)}, \boldsymbol{t}^{(N+1)}$ and $\beta_1, \cdots, \beta_N, \beta_{N+1}$ respectively. Then $\sigma^2(I - W_{N+1}) < \sigma^2(I - W_N)$, unless $\beta_{N+1} = 0$ and $\beta_i = \alpha_i$ for $1 \leqq i \leqq N$.*

Proof. The relation

$$\sigma^2(I - W_{N+1}) \leqq \sigma^2(I - W_N)$$

is obvious. Suppose equality holds. The point of $M(N, \boldsymbol{t})$ nearest to $\boldsymbol{f}$ is $\boldsymbol{g}' = \sum_{i=1}^{N} \alpha_i \boldsymbol{g}_i$, and the point of $M(N + 1, \boldsymbol{t})$ nearest to f is $g'' = \sum_{i=1}^{N+1} \beta_i g_i$. The parallelogram law (see [9, p. 23]) implies that $\boldsymbol{g}^* = \frac{1}{2}(\boldsymbol{g}' + \boldsymbol{g}'')$ is no farther from $\boldsymbol{f}$ than is $\boldsymbol{g}''$. But $M(N, \boldsymbol{t}) \subset M(N + 1, \boldsymbol{t})$. This gives rise to a contradiction unless $\boldsymbol{g}' = \boldsymbol{g}''$—i.e. unless $\beta_{N+1} = 0$ and $\beta_i = \alpha_i$ for $1 \leqq i \leqq N$. Q.E.D.

THEOREM III. *Given a W_N, there is a properly better W_{N+1}—i.e. one such that*

$$\sigma^2(I - W_{N+1}) < \sigma^2(I - W_N).$$

Proof. Let the distinct abscissae of W_N be $\boldsymbol{t}^{(1)}, \cdots, \boldsymbol{t}^{(N)}$ and let the optimal weights be $\alpha_1, \cdots, \alpha_N$. Then the α's satisfy the system of linear equations

$$(2.5) \qquad \sum_{i=1}^{N} \alpha_i(\boldsymbol{g}_i, \boldsymbol{g}_j) = (\boldsymbol{f}, \boldsymbol{g}_j), \qquad 1 \leqq j \leqq N.$$

Choose the abscissae of W_{N+1} as those of W_N augmented by $\boldsymbol{t}^{(N+1)}$, as yet undetermined except that we require

$$(2.6) \qquad \boldsymbol{t}^{(N+1)} \neq \boldsymbol{t}^{(i)}, \qquad 1 \leqq i \leqq N.$$

Let the optimal weights of W_{N+1} be $\beta_1, \cdots, \beta_N, \beta_{N+1}$—functions of $\boldsymbol{t}^{(N+1)}$. On the strength of the Lemma, it is enough to show that $\boldsymbol{t}^{(N+1)} \in \mathfrak{C}$ can be so chosen as to satisfy (2.6) and the condition: $\beta_{N+1} \neq 0$. The β's satisfy the linear equations

$$(2.7) \qquad \sum_{i=1}^{N+1} \beta_i(\boldsymbol{g}_i, \boldsymbol{g}_j) = (\boldsymbol{f}, \boldsymbol{g}_j), \qquad 1 \leqq j \leqq N + 1.$$

For $1 \leqq p \leqq N + 1$, let Δ_p denote the Gram determinant

$$\det [(\boldsymbol{g}_i, \boldsymbol{g}_j)], \qquad i, j = 1, 2, \cdots, p.$$

As $\boldsymbol{t}^{(1)}, \boldsymbol{t}^{(2)}, \cdots, \boldsymbol{t}^{(N)}, \boldsymbol{t}^{(N+1)}$ are distinct, Theorem II shows that $\boldsymbol{g}_1, \boldsymbol{g}_2, \cdots, \boldsymbol{g}_N, \boldsymbol{g}_{N+1}$ are linearly independent, and hence that no Δ_p vanishes. Solving the system (2.7), we get

$$\beta_{N+1} = \Delta / \Delta_{N+1}$$

where the first N columns of Δ and Δ_{N+1} are identical, and the (jth row, $(N+1)$th column) element of Δ is $(\boldsymbol{f}, \boldsymbol{g}_j)$. Subtract $\sum_{i=1}^{N} \alpha_i$ (ith column of Δ) from the $(N+1)$th column of Δ, use relations (2.5), abbreviate $\boldsymbol{f} - \sum_{i=1}^{N} \alpha_i \boldsymbol{g}_i$ as $\boldsymbol{f}^\circ$, and see that

$$\beta_{N+1} = \frac{\Delta_N}{\Delta_{N+1}} (\boldsymbol{f}^\circ, \boldsymbol{g}_{N+1}) .$$

It remains to show that there is a $\boldsymbol{t}^{(N+1)} \in \mathfrak{C}$ satisfying (2.6) and such that $(\boldsymbol{f}^\circ, \boldsymbol{g}_{N+1}) \neq 0$. Suppose, on the contrary, that

$$(\boldsymbol{f}^\circ, \boldsymbol{g}_{N+1}) = 0 \tag{2.8}$$

for every choice of $\boldsymbol{t}^{(N+1)}$ satisfying (2.6). Then (2.8) holds on some neighbourhood in $\mathfrak{C}$. Rewriting the left-hand side of (2.8) as

$$\sum_{n=0}^{\infty} \left[\frac{2^n}{3\lambda_n} \sum_{n}{}' a_{n_1 \cdots n_k} (t_1^{(N+1)})^{n_1} \cdots (t_k^{(N+1)})^{n_k} \right], \tag{2.9}$$

where

$$a_{n_1 \cdots n_k} = 2^{-k} \prod_{i=1}^{k} \frac{1 + (-1)^{n_i}}{n_i + 1} - \sum_{m=1}^{N} \alpha_m (t_1^{(m)})^{n_1} \cdots (t_k^{(m)})^{n_k} ,$$

we see that the multiple power series (2.9) vanishes for all $\boldsymbol{t}^{(N+1)}$ in some neighbourhood in $\mathfrak{C}$. Since (2.9) may be regarded as a complex convergent power series in $t_1^{(N+1)}, \cdots, t_k^{(N+1)}$ restricted to a real environment, all the $a_{n_1 \cdots n_k}$ vanish (see [3, p. 34]). But this means

$$I(T_{n_1 \cdots n_k}) = W_N(T_{n_1 \cdots n_k})$$

for all $n_1, \cdots, n_k \geqq 0$, and hence that

$$I(\mathbf{x}) = W_N(\mathbf{x})$$

for all $\mathbf{x} \in S_\infty$ contradicting Remark I. Q.E.D.

3. Monte Carlo Quadratures. The N-point Monte Carlo quadrature formula is

$$M_N(\mathbf{x}) = \frac{1}{N} \sum_{m=1}^{N} \mathbf{x}(\boldsymbol{t}^{(m)})$$

where $\boldsymbol{t}^{(1)}, \cdots, \boldsymbol{t}^{(N)}$ are random points in $\mathfrak{C}$. The variance of the error associated with this method of quadrature is given by

$$\sigma_M{}^2 = 2^{-kN} \int_{-1}^{1} \cdots \int_{-1}^{1} \left\{ \int_{S_\infty} [I(\mathbf{x}) - M_N(\mathbf{x})]^2 d_E \mathbf{x} \right\} \prod_{i,j} dt_i{}^{(j)}$$

where $\prod_{i,j} dt_i{}^{(j)}$ denotes the product of all the differentials $dt_i{}^{(j)}$ $(1 \leqq i \leqq k, 1 \leqq j \leqq N)$. Using Fubini's theorem, we rewrite this as

$$\sigma_M{}^2 = 2^{-kN} \int_{S_\infty} \{ \quad \} d_E \mathbf{x} , \tag{3.1}$$

where

$$(3.2) \qquad \{\quad\} = \int_{-1}^{1} \cdots \int_{-1}^{1} \left[I(\mathbf{x}) - \frac{1}{N} \sum_{m=1}^{N} \mathbf{x}(t^{(m)}) \right]^2 \prod_{i,j} dt_i^{(j)},$$

which reduces to

$$(2^{kN}/N)\{I(\mathbf{x}^2) - [I(\mathbf{x})]^2\}.$$

Substituting this evaluation in (3.1), we get

$$(3.3) \qquad N\sigma_M{}^2 = \int_{S_\infty} I(\mathbf{x}^2) d_E\mathbf{x} - \int_{S_\infty} [I(\mathbf{x})]^2 d_E\mathbf{x}.$$

Going back to the representation (0.1) of $\mathbf{x}(t)$, we get after a routine calculation,

$$(3.4) \; I(\mathbf{x}^2) = \sum_1 \frac{(x_{n_1\cdots n_k})^2}{(2n_1+1)\cdots(2n_k+1)} + \sum_2 \frac{x_{m_1\cdots m_k} x_{n_1\cdots n_k}}{(m_1+n_1+1)\cdots(m_k+n_k+1)},$$

where $\sum_1$ is a sum over all nonnegative integers $n_1, n_2, \cdots, n_k$; and $\sum_2$ is a sum over all such nonnegative integers $m_1, \cdots, m_k, n_1, \cdots, n_k$ that each of $m_1 + n_1, \cdots, m_k + n_k$ is even and $m_i \neq n_i$ for at least one value of i. If we integrate (3.4) term by term with respect to $d_E\mathbf{x}$ over S_∞, all the terms of $\sum_2$ drop out, and we are left with

$$(3.5) \qquad \begin{aligned} \int_{S_\infty} I(\mathbf{x}^2) d_E\mathbf{x} &= \sum_1 \left[\frac{1}{\prod_{i=1}^k (2n_i+1)} \int_{S_\infty} (x_{n_1\cdots n_k})^2 d_E\mathbf{x} \right] \\ &= \sum_{n=0}^{\infty} \left[\frac{2^n}{3\lambda_n} {\sum_n}' \frac{1}{\prod_{i=1}^k (2n_i+1)} \right], \end{aligned}$$

where we have used the result (1.4). This disposes of the first term on the right-hand side of (3.3). In much the same manner, we find

$$(3.6) \qquad \int_{S_\infty} [I(\mathbf{x})]^2 d_E\mathbf{x} = \sum_{n=0}^{\infty} \left[\frac{2^{2n}}{3\lambda_{2n}} {\sum_n}' \left\{ \prod_{i=1}^k \frac{1}{(2n_i+1)^2} \right\} \right].$$

Substituting from (3.5) and (3.6) into (3.3) we obtain

$$\sigma_M{}^2 = (1/N)\gamma_k$$

where

$$(3.7) \qquad \begin{aligned} \gamma_k = &\sum_{n=0}^{\infty} \left[\frac{2^n}{3\lambda_n} {\sum_n}' \left\{ \prod_{j=1}^k \frac{1}{(2n_j+1)} \right\} \right] \\ &- \sum_{n=0}^{\infty} \left[\frac{2^{2n}}{3\lambda_{2n}} {\sum_n}' \left\{ \prod_{j=1}^k \frac{1}{(2n_j+1)^2} \right\} \right]. \end{aligned}$$

Integrals of high multiplicity occur often enough in applied mathematics to justify a study of the asymptotic behaviour of γ_k for large values of k. We note that the terms for $n = 0$ in the two series in (3.7) cancel out, and that the term for $n = 1$ in the first series is $2k/[9(k+1)(k+2)]$. We write

$$\gamma_k = \frac{2k}{9(k+1)(k+2)} + \alpha_k - \beta_k,$$

where

$$\alpha_k = \sum_{n=2}^{\infty} \left[\frac{2^n}{3\lambda_n} \sum_n{}' \left\{ \prod_{j=1}^{k} \frac{1}{2n_j + 1} \right\} \right]$$

and

$$\beta_k = \sum_{n=1}^{\infty} \left[\frac{2^{2n}}{3\lambda_{2n}} \sum_n{}' \left\{ \prod_{j=1}^{k} \frac{1}{(2n_j + 1)^2} \right\} \right].$$

We note that

$$c_i = c_i(k) \geqq \tfrac{1}{2}k^2, \qquad i \geqq 2,\ k \geqq 1,$$

and that

$$\text{(3.8)} \qquad \sum_n{}' \left\{ \prod_{j=1}^{k} \frac{1}{(2n_j + 1)^2} \right\} \leqq \sum_n{}' \left\{ \prod_{j=1}^{k} \frac{1}{(2n_j + 1)} \right\} \leqq c_n(k).$$

In view of these inequalities, we have the general term in series for α_k

$$= \frac{2^n}{3} \frac{1}{\prod_{i=1}^{n} (c_i + 1)(c_i + 2)} \sum_n{}' \left\{ \prod_{j=1}^{k} \frac{1}{(2n_j + 1)} \right\}$$

$$\leqq \frac{2^n}{3} \frac{c_n}{(c_1 + 1)(c_1 + 2)(c_n + 1)(c_n + 2)\left[\prod_{i=2}^{n-1} (c_i + 1)(c_i + 2) \right]}$$

$$< \frac{2^n}{3} \frac{1}{(k + 1)(k + 2)c_n \left[\prod_{i=2}^{n-1} (c_i)^2 \right]}$$

$$< \frac{2^n}{3} \frac{1}{k^2 \cdot \frac{1}{2}k^2 \cdot (\frac{1}{2}k^2)^{2n-4}} = \frac{k^4}{24} (8/k^4)^n.$$

By a similar argument, the general term of β_k is less than $(k^4/24)(8/k^4)^{2n}$. Hence

$$|\alpha_k - \beta_k| < \frac{8}{3k^4} \left[\frac{k^4}{k^4 - 8} + \frac{k^8}{k^8 - 64} \right] = O(k^{-4}).$$

This proves that, for la.ge values of k,

$$\text{(3.9)} \qquad \gamma_k = \frac{2k}{9(k + 1)(k + 2)} + O(k^{-4}).$$

It is worth noting that the inequalities

$$\text{(3.10)} \qquad 0 < \gamma_{k+1} < \gamma_k$$

hold for $k = 1, 2, \cdots$.

That $\gamma_k > 0$ for all k is obvious. We write $\gamma_k = A_k + B_k$, where

$$A_k = \sum_{n=1}^{\infty} \left[\frac{2^{2n-1}}{3\lambda_{2n-1}} \sum_{2n-1}{}' \left\{ \prod_{j=1}^{k} \frac{1}{(2n_j + 1)} \right\} \right]$$

and

$$B_k = \sum_{n=1}^{\infty} \left[\frac{2^{2n}}{3\lambda_{2n}} \left(\sum_{2n}{}' \left\{ \prod_{j=1}^{k} \frac{1}{(2n_j + 1)} \right\} - \sum_n{}' \left\{ \prod_{j=1}^{k} \frac{1}{(2n_j + 1)^2} \right\} \right) \right].$$

In view of the inequalities (3.8) and the fact that $c_i(k) \geqq k$ for $i \geqq 1$, the general term of the series for A_k is less than $\frac{1}{3}k(2/k^2)^{2n-1}$. Then we have

$$A_k' \equiv \frac{2k}{9(k+1)(k+2)} < A_k < \frac{2k}{9(k+1)(k+2)} + \frac{k}{3}\sum_{n=2}^{\infty}\left[\frac{2}{k^2}\right]^{2n-1}$$
$$= \frac{2k}{9(k+1)(k+2)} + \frac{8}{3k(k^4-4)} \equiv A_k''.$$

It can be verified that $A_k' - A_{k+1}''$ can be expressed as a ratio of two polynomials in $k - 3$ with positive coefficients, and hence that $A_k' - A_{k+1}''$ is positive for $k \geqq 3$. It follows that $A_{k+1} < A_k$ for $k \geqq 3$. Treating B_k in the same manner, we see also that $B_{k+1} < B_k$ for $k \geqq 3$, and conclude that

$$0 < \gamma_{k+1} < \gamma_k, \qquad k \geqq 3.$$

When $k = 1, 2,$ or 3, we evaluate the first two terms of the series for A_k, the first term of the series for B_k, and use estimates for the remaining terms to get

$$\gamma_3 < 0.037,$$
$$0.038 < \gamma_2 < 0.040,$$

and

$$0.042 < \gamma_1,$$

which completes the proof of the assertion (3.10).

To illustrate the utility of the formula (2.1) for the global comparison of quadrature methods, we take $k = 1$ and find $\sigma^2(I - G_2)$ where we denote by G_2 the two-point Gaussian formula. For G_2 we have

$$t^{(1)} = 3^{-1/2}, \qquad A_1 = \tfrac{1}{2}; \qquad t^{(2)} = -3^{-1/2}, \qquad A_2 = \tfrac{1}{2}$$

(see [8, pp. 368, 369]). An easy computation shows $\sigma^2(I - G_2) < (0.07372)3^{-7}$. To match this accuracy with a Monte Carlo formula M_N, one must take $N > 1{,}000$.

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