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AN ERROR OF SIMPSON'S QUADRATURE IN THE AVERAGE CASE SETTING

SUNG HEE CHOI AND BUM IL HONG

1. Introduction

Many numerical computations in science and engineering can only be solved approximately since the available information is partial. For instance, for problems defined on a space of functions, information about f is typically provided by few function values, $N(f) = [f(x_1), f(x_2), \dots, f(x_n)]$. Knowing $N(f)$, the solution is approximated by a numerical method. The error between the true and the approximate solutions can be reduced by acquiring more information. However, this increases the cost. Hence there is a trade-off between the error and the cost.

The error between the true solution and the approximation depends on a problem setting. The *worst case setting* is the most commonly studied setting. In this setting, the error of a numerical scheme is defined by its worst performance with respect to the given class of functions. Many results are known in this setting; see [4] and [7] for hundreds of references. In this paper, we concentrate on another setting, the *average case setting*. In this setting, we assume that the class F of input functions is equipped with a probability measure. Then the average case error of an algorithm is defined by its expectation, rather than by its worst case performance. The average case analysis is important and significant number of results have already been obtained (see, e.g., [7] and the references cited therein). There are some justifications of the importance of the average case approach:

(1) **Mathematical interests:** Even if a specific numerical scheme has small worst case error, its average case error provides additional information on the properties of that algorithm. In

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particular, for the *Simpson's quadrature* we show that the average case error is proportional to $n^{-\min\{4,r+1\}}$ if the input function f is r times continuously differentiable. This means that for $r \geq 4$ the worst case and average case behaviors of the quadrature are similar. However, for $r \leq 3$, the average case error is roughly n times smaller than the worst case error. Specifically, for $r = 0$, the average case error is $\Theta(1/n)$,[1] while the problem is unsolvable in the worst case setting.

(2) **Reduction of complexity:** For a number of classes F of functions, some problems are unsolvable in the worst case setting. For instance, this holds for the integration problem with the class $F = \{f \in C[0,1] \mid f \text{ is bounded by } 1\}$. That is, no numerical scheme that uses a finite number of function values can approximate the integral $I(f) = \int_0^1 f(x)dx$ of f with the worst case error less than 1. However, in the average case setting, this problem is solvable. Hence we have the reduction of complexity in the average case setting.

It is well known that the average case setting requires the space of functions to be equipped with a probability measure. In this paper, we choose a probability measure μ_r which is a variant of an *r-fold Wiener measure* ω_r. The reason for choosing the Wiener measure is that it is one of the most commonly assumed probability measures on function spaces. The probability measure ω_r is a *Gaussian measure* with zero mean and correlation function given by $M_{\omega_r}(f(x)\,f(y)) = \int_F f(x)f(y)\,\omega_r(df) = \int_0^1 \frac{(x-t)_+^r}{r!}\frac{(y-t)_+^r}{r!}\,dt$, where $(z-t)_+ = \max\{0,(z-t)\}$. Equivalently, f distributed according to ω_r can be viewed as a Gaussian stochastic process with zero mean and autocorrelation given above. However, since ω_r is concentrated on functions with boundary conditions $f(0) = f'(0) = \cdots = f^{(r)}(0) = 0$, we choose to study a slightly modified measure μ_r that preserves basic properties of ω_r, yet does not require any boundary conditions. More precisely, we assume

[1]The Θ-notation is used for asymptotic equalities. That is, $f(n) = \Theta(g(n))$ means that there are positive constants c_1 and c_2 such that $c_1 g(n) \leq f(n) \leq c_2 g(n)$, $\forall n$. Later on, we will use O and Ω-notations for asymptotic inequalities. More precisely, $f(n) = O(g(n))$ means that $f(n) \leq c_2 g(n)$, $\forall n$; and $f(n) = \Omega(g(n))$ means that $g(n) = O(f(n))$ (i.e., $f(n) \geq c_1 g(n)$, $\forall n$). The o-notation, $f(n) = o(g(n))$, is used to denote the fact that $\lim_n f(n)/g(n) = 0$.

that a function f, as a stochastic process, is given by

$$f(x) = f_1(x) + f_2(1-x), \quad x \in [0,1],$$

where f_1 and f_2 are independent and distributed according to ω_r. Then the corresponding probability measure μ_r is a zero mean Gaussian with the correlation function given by

$$M_{\mu_r}(f(x)\,f(y)) = \int_0^1 \frac{(x-t)_+^r(y-t)_+^r + (t-x)_+^r(t-y)_+^r}{r!\ r!}\,dt.$$

We study the problem of approximating an integral $I(f) = \int_0^1 f(x)\,dx$ for $f \in F = C^r[0,1]$, assuming that the class of integrands is equipped with the probability measure μ_r. In particular, we study *Simpson's quadrature* which is one special case of *Newton-Cotes quadratures*. The error of *Simpson's quadrature* is minimal (modulo a multiplicative constant) when the equally spaced sample points are used in both the worst case and average case settings.

The behavior of *Simpson's quadrature* is well understood in the *worst case setting*. Recall that when $\|f^{(r)}\|_\infty$ is by one, then the *worst case error* of *Simpson's quadrature* is minimized (modulo a multiplicative constant) when n equally spaced points are used and this error is proportional to $n^{-\min\{4,r\}}$. Since the worst case error of any numerical scheme that uses n function values is proportional to n^{-r} (see [1]), *Simpson's quadrature* is almost optimal if and only if $r \leq 4$.

In the *average case setting*, we assume that the space F is endowed with a probability measure μ_r which is a variant of *r-fold Wiener measure*. We show that the *average error* of *Simpson's quadrature* is minimized (modulo a multiplicative constant) when equally spaced points are used. For n such points, the average case error is proportional to $n^{-\min\{4,r+1\}}$. Since the average case error of any numerical scheme that uses n function values is at least proportional to $n^{-(r+1)}$ (see [5]), the *Simpson's quadrature* with equally spaced points is almost optimal in the average case setting if and only if $r \leq 3$.

2. Basic Definitions

In the integration problem, we compute an approximation to the integral $I(f) = \int_0^1 f(x)dx$, where $I : F \to \mathbb{R}$, with $f \in F = C^r[0,1]$. This approximation to $I(f)$ is computed based on n function values. That is, the available *information* $N(f)$ about the integrand f is given by $N(f) = [f(x_1), f(x_2), \dots, f(x_n)]$, $x_i \in [0,1]$. The number n of function values is called the *cardinality* of N, and is denoted by $card(N)$. Formally, the points x_i could be chosen *a priori*, or x_i could be chosen adaptively based on observed values $f(x_1), \dots, f(x_{i-1})$. In the former case, N is said to be *nonadaptive*, and in the latter case, N is said to be *adaptive*. Since adaption does not help (see [9]), without loss of generality, we restrict our attention to nonadaptive information only. Given $y = [y_1, \dots, y_n] = N(f)$, the approximation to $I(f)$ is provided by $\phi(y) = \phi(N(f))$, where $\phi : \mathbb{R}^n \to \mathbb{R}$, called an *algorithm*, is an arbitrary mapping (for more discussion on algorithms and information, see [7]). Numerical quadratures $\phi(y) = \sum_{i=1}^n a_i f(x_i)$ with appropriately chosen weights $a_i \in \mathbb{R}$ are specific examples of algorithms. They include *composite Newton-Cotes quadratures* and, in particular, the *composite Simpson's quadrature*. Since we analyze the *Simpson's quadrature*, we now recall the definition and basic properties of *Simpson's quadrature*, see also e.g., [2]. In composite *Simpson's quadrature*, we have $n = 2k + 1$ with $x_1 = 0$, $x_n = 1$, and $x_{2i} - x_{2i-1} = x_{2i+1} - x_{2i} = h_i$, $i = 1, 2, \dots, k$. On each subinterval $[x_{2i-1}, x_{2i+1}]$, the integral $I_i(f) \equiv \int_{x_{2i-1}}^{x_{2i+1}} f(x)\,dx$ is approximated by

$$S_i(f) = \frac{h_i}{3}\{f(x_{2i-1}) + 4f(x_{2i}) + f(x_{2i+1})\}.$$

Then, $I(f)$ is approximated by $I(f) = \sum_{i=1}^k I_i(f) \approx S(N(f)) = \sum_{i=1}^k S_i(f)$.

The behavior of *Simpson's quadrature* is well understood in the *worst case setting*. Recall that for $F_0 = \{f \in F \mid \|f^{(r)}\|_\infty \le 1\}$, the *worst case error* of an algorithm ϕ that uses N is defined by $e^{worst}(\phi, N) = \sup_{f \in F_0} |I(f) - \phi(N(f))|$. For given n, the worst case error of *Simpson's quadrature* is minimized (modulo a multiplicative constant) when the points x_i are equally spaced, i.e., $N^*(f) = [f(x_1), \dots, f(x_n)]$, $x_i = (i-1)2h$, $h = 1/2(n-1)$, and $e^{worst}(S, N^*) = \Theta\left(n^{-\min\{4,r\}}\right)$. Since due to [1], $\inf\{e^{worst}(\phi, N) \mid \text{for all } (\phi, N) \text{ with } card(N) = n\} = \Theta(n^{-r})$, *Simpson's quadrature* is almost optimal in the worst case setting when $r \leq 4$.

In the average case setting, we assume that the space $F = C^r[0,1]$ is equipped with a probability measure μ_r which is a variant of the *r-fold Wiener measure*. In order to define it, we first recall basic properties of the classical *r-fold Wiener measure* ω_r, see [3], [6] and [8]. It is a Gaussian measure with zero mean and correlation function given by

$$M_{\omega_r}(f(x)\,f(y)) = \int_F f(x)f(y)\,\omega_r(df) = \int_0^1 \frac{(x-t)_+^r}{r!}\,\frac{(y-t)_+^r}{r!}\,dt,$$

More precisely, we assume that a function f, as a stochastic process, is given by $f(x) = f_1(x) + f_2(1-x)$, where f_1 and f_2 are independent and distributed according to ω_r. Equivalently, this leads to the probability measure μ_r defined on σ-field of the space $C^r[0,1]$ that is zero mean Gaussian with the correlation function given by

$$\begin{aligned} M_{\mu_r}(f(x)\,f(y)) &= \int_0^1 \frac{(x-t)_+^r(y-t)_+^r + (1-x-t)_+^r(1-y-t)_+^r}{r!\,r!}\,dt \\ &= \int_0^1 \frac{(x-t)_+^r(y-t)_+^r + (t-x)_+^r(t-y)_+^r}{r!\,r!}\,dt. \end{aligned}$$

The *average error* of an algorithm ϕ that uses N is defined by

$$\begin{aligned} e^{avg}(\phi, N; \mu_r) &= \left(M_{\mu_r}\left([I(f) - \phi(N(f))]^2 \right) \right)^{1/2} \\ &= \left(\int_F |I(f) - \phi(N(f))|^2 \mu_r(df) \right)^{1/2} \end{aligned}$$

It is known, see [5], that for the *r-fold Wiener measure* ω_r, the average error of any algorithm that uses information of cardinality n is bounded from below by

$$e^{avg}(\phi, N; \omega_r) = \Omega\left(n^{-(r+1)}\right), \quad \forall\phi,\ \forall N,\ card(N) = n.$$

Furthermore, this bound is sharp. Indeed it is attained (modulo a multiplicative constant) by information $N^*(f)$ consisting of function values at equally spaced points and the algorithm $\phi^*(N^*(f))$ that equals the integral of a natural spline of degree $2r+1$ which interpolates f at those equally spaced points and satisfies the same boundary conditions as f does. Similar result holds true for the measure μ_r

3. Average Case Error of Simpson's Quadrature

Recall that the space $F = C^r[0,1]$ is equipped with the probability measure μ_r defined in chapter 2. The error $I(f)-S(N(f))$ of *Simpson's quadrature* equals

$$I(f) - S(N(f)) = \sum_{i=1}^{k} Z_i, \quad \text{where } Z_i = Z_i(f) = I_i(f) - S_i(f).$$

Since f is a zero-mean Gaussian process, Z_i's are zero-mean Gaussian random variables with covariances given in the following lemma.

LEMMA 3.1. *For $i \le j$,*

$$M_{\mu_r}(Z_i Z_j) = \begin{cases} \delta_{ij} \cdot c_r \cdot h_i^{2r+3}, & \text{if } r \le 3, \\ c_{ijr} \cdot h_i^5 h_j^5, & \text{if } r \ge 4, \end{cases}$$

where δ_{ij} is the Kronecker delta. For $r \le 3$, the constant c_r is independent of h_i's and equals respectively: $c_0 = \frac{4}{9}$, $c_1 = \frac{2}{135}$, $c_2 = \frac{1}{945}$, and $c_3 = \frac{1}{4536}$. For $r = 4$, $c_{ii4} = \frac{1}{90^2}(1 - \frac{139}{396}h_i)$ and $c_{ij4} = \frac{1}{90^2}(x_{2i-1} + 1 - x_{2j+1} + h_i + h_j)$. For $r \ge 5$, $c_{ijr} = c_{ijr}(h_i, h_j)$ is bounded from below by

$$a_1 \sum_{p=0}^{r-4} \frac{(x_{2j-1} - x_{2i-1})^p \, x_{2i-1}^{2r-7-p} + (x_{2j+1} - x_{2i+1})^p (1 - x_{2j+1})^{2r-7-p}}{p!\,(r-4-p)!\,(2r-7-p)}$$
$$+ a_2 \left[h_i^{r-3}(x_{2j-1} - x_{2i+1})^{r-4} + h_j^{r-3}(x_{2j-1} - x_{2i+1})^{r-4}\right]$$
$$\ge a_r[x_{2i-1}^{r-3}(x_{2j-1} - x_{2i-1})^{r-4} + x_{2i-1}^{r-3} x_{2j-1}^{r-4} + h_i^{r-3}(x_{2j-1} - x_{2i+1})^{r-4}$$
$$+ (1 - x_{2j+1})^{r-3}(x_{2j+1} - x_{2i+1})^{r-4} + (1 - x_{2j+1})^{r-3}(1 - x_{2i+1})^{r-4}$$
$$+ h_j^{r-3}(x_{2j-1} - x_{2i+1})^{r-4}]$$

and from above by

$$a_1 \sum_{p=0}^{r-4} \frac{(x_{2j+1}-x_{2i+1})^p\, x_{2i+1}^{2r-7-p} + (x_{2j-1}-x_{2i-1})^p\,(1-x_{2j-1})^{2r-7-p}}{p!\,(r-4-p)!\,(2r-7-p)}$$
$$+ \quad a_2[h_i^{r-3}(x_{2j+1}-x_{2i-1})^{r-4} + h_j^{r-3}(x_{2j+1}-x_{2i-1})^{r-4}]$$
$$\le a'_r[x_{2i+1}^{r-3}x_{2j+1}^{r-4} + h_i^{r-3}(x_{2j+1}-x_{2i-1})^{r-4}$$
$$+ (1-x_{2j-1})^{r-3}(1-x_{2i-1})^{r-4} + h_j^{r-3}(x_{2j+1}-x_{2i-1})^{r-4}],$$

where $a_1 = \frac{1}{90^2(r-4)!}$, $a_2 = \frac{2(r+2)+(r-4)2^r}{135(r-4)!(r+2)!}$, $a_r = \min\left\{a_2, \frac{a_1}{(r-3)!2^{r-3}}\right\}$, and $a'_r = \max\left\{a_2, \frac{a_1}{(r-3)!}\right\}$.

Proof. Let $Z_{i1} = Z_i(f_1)$ and $Z_{i2} = Z_i(f_2)$. Then $Z_i(f) = Z_{i1} + Z_{i2}$, and due to the independence of f_1 and f_2, we have $M_{\mu_r}(Z_iZ_j) = M_{\omega_r}(Z_{i1}Z_{j1}) + M_{\omega_r}(Z_{i2}Z_{j2})$. For $i \le j$,

$$M_{\omega_r}(Z_{i1}Z_{j1})$$
$$= \int_0^1 \left[\int_{x_{2i-1}}^{x_{2i+1}} \frac{(x-t)_+^r}{r!}\,dx - A_{i1}(t)\right]\left[\int_{x_{2j-1}}^{x_{2j+1}} \frac{(y-t)_+^r}{r!}\,dy - A_{j1}(t)\right] dt$$
$$= \int_0^1 L_{i1}(t)\cdot L_{j1}(t)\,dt,$$

where L_{i1} is the first term and L_{j1} is the second term in the above integral, and $A_{i1}(t) = S_i\left(\frac{(\cdot-t)_+^r}{r!}\right)$. Since $L_{i1}(t) = 0$ when $t \in [x_{2i+1}, 1]$, we have

$$M_{\omega_r}(Z_{i1}Z_{j1}) = \int_0^{x_{2i+1}} L_{i1}(t)\cdot L_{j1}(t)\,dt.$$

Similarly,

$$M_{\omega_r}(Z_{i2}Z_{j2})$$
$$= \int_{x_{2j-1}}^1 \left[\int_{x_{2i-1}}^{x_{2i+1}} \frac{(t-x)_+^r}{r!}\,dx - A_{i2}(t)\right]\left[\int_{x_{2j-1}}^{x_{2j+1}} \frac{(t-y)_+^r}{r!}\,dy - A_{j2}(t)\right] dt$$
$$= \int_{x_{2j-1}}^1 L_{i2}(t)\cdot L_{j2}(t)\,dt,$$

where L_{i2} is the first term and L_{j2} is the second term in the above integral, and $A_{i2}(t) = S_i\left(\frac{(t-\cdot)_+^r}{r!}\right)$. Therefore, we have

$$M_{\mu_r}(Z_iZ_j) = \int_0^{x_{2i+1}} L_{i1}(t)\cdot L_{j1}(t)\,dt + \int_{x_{2j-1}}^1 L_{i2}(t)\cdot L_{j2}(t)\,dt.$$

Consider first $r \leq 3$. Since *Simpson's quadrature* is exact for polynomials of degree ≤ 3, $L_{j1}(t) = 0$ for $t \leq x_{2i+1}$ and $L_{i2}(t) = 0$ for $t \geq x_{2j-1}$. Thus, $M_{\mu_r}(Z_i Z_j) = 0$, and hence, Z_i and Z_j are independent when $i < j$. For $i = j$,

$$M_{\omega_r}(Z_{i1}^2) = \int_{x_{2i-1}}^{x_{2i+1}} \left[\int_{x_{2i-1}}^{x_{2i+1}} \frac{(x-t)_+^r}{r!}\, dx - S_i\left(\frac{(\cdot - t)_+^r}{r!} \right) \right]^2 dt$$
$$= c_{r1} h_i^{2r+3},$$

where

$$c_{r1} = 2^{2r+3} \int_0^1 \left[\int_0^1 \frac{(z-u)_+^r}{r!}\, dz - \frac{1}{6}\left\{ \frac{(0-u)_+^r}{r!} + \frac{4(\frac{1}{2}-u)_+^r}{r!} + \frac{(1-u)_+^r}{r!} \right\} \right]^2 du,$$

the last equality due to a simple change of variables $z = (x - x_{2i-1})/2h_i$ and $u = (t - x_{2i-1})/2h_i$. Similarly, $M_{\omega_r}(Z_{i2}^2) = c_{r2} h_i^{2r+3}$, where

$$c_{r2} = 2^{2r+3} \int_0^1 \left[\int_0^1 \frac{(u-z)_+^r}{r!}\, dz - \frac{1}{6}\left\{ \frac{(u-0)_+^r}{r!} + \frac{4(u-\frac{1}{2})_+^r}{r!} + \frac{(u-1)_+^r}{r!} \right\} \right]^2 du.$$

Note that $c_r = c_{r1} + c_{r2}$. Since the specific values of c_r can easily be obtained, we omit this part. This completes the proof for $r \leq 3$.

Next consider $r \geq 4$. Divide the integral in $M_{\omega_r}(Z_{i1} Z_{j1})$ into two parts, i.e.,

$$M_{\omega_r}(Z_{i1} Z_{j1})$$
$$= \int_0^{x_{2i+1}} L_{i1}(t) \cdot L_{j1}(t)\, dt$$
$$= \left(\int_0^{x_{2i-1}} + \int_{x_{2i-1}}^{x_{2i+1}} \right) L_{i1}(t) \cdot L_{j1}(t)\, dt.$$

Then, for $t \in [0, x_{2i-1}]$,

$$\int_0^{x_{2i-1}} L_{i1}(t) \cdot L_{j1}(t)\, dt = \frac{h_i^5 h_j^5}{90^2} \int_0^{x_{2i-1}} \frac{(\xi_t - t)^{r-4}}{(r-4)!} \frac{(\eta_t - t)^{r-4}}{(r-4)!}\, dt$$
$$= A_{ijr} h_i^5 h_j^5.$$

where $\xi_t \in (x_{2i-1}, x_{2i+1})$ and $\eta_t \in (x_{2j-1}, x_{2j+1})$. A_{ijr} is bounded from below by $a_1 g(x_{2i-1})$, where $a_1 = 1/(90^2(r-4)!)$ and

$$g(t) = \sum_{p=0}^{r-4} \frac{(x_{2j-1} - x_{2i-1})^p}{p!} \frac{t^{2r-7-p}}{(r-4-p)!} \frac{1}{2r-7-p}.$$

Since $g(0) = 0$,

$$\begin{aligned} g(x_{2i-1}) &= \int_0^{x_{2i-1}} g'(t)\,dt \\ &= \int_0^{x_{2i-1}} t^{r-4} \sum_{p=0}^{r-4} \frac{(x_{2j-1} - x_{2i-1})^p}{p!} \frac{t^{r-4-p}}{(r-4-p)!}\,dt \\ &= \int_0^{x_{2i-1}} t^{r-4} \frac{(x_{2j-1} - x_{2i-1} + t)^{r-4}}{(r-4)!}\,dt \\ &= \left(\int_0^z + \int_z^{x_{2i-1}}\right) t^{r-4} \frac{(x_{2j-1} - x_{2i-1} + t)^{r-4}}{(r-4)!}\,dt, \end{aligned}$$

where $z = x_{2i-1}/2$. Then,

$$\begin{aligned} &g(x_{2i-1}) \\ &\geq \int_0^z t^{r-4} \frac{(x_{2j-1} - x_{2i-1})^{r-4}}{(r-4)!}\,dt + \int_z^{x_{2i-1}} z^{r-4} \frac{(x_{2j-1} - x_{2i-1} + t)^{r-4}}{(r-4)!}\,dt \\ &= \frac{z^{r-3}}{r-3} \frac{(x_{2j-1} - x_{2i-1})^{r-4}}{(r-4)!} + z^{r-4} \frac{x_{2j-1}^{r-3} - (x_{2j-1} - x_{2i-1} + z)^{r-3}}{(r-3)!} \\ &\geq \frac{z^{r-3}}{(r-3)!}(x_{2j-1} - x_{2i-1})^{r-4} + z^{r-4} \frac{(x_{2i-1} - z)x_{2j-1}^{r-4}}{(r-3)!} \\ &\geq \frac{x_{2i-1}^{r-3}}{(r-3)!2^{r-3}}(x_{2j-1} - x_{2i-1})^{r-4} + \frac{x_{2i-1}^{r-3}}{(r-3)!2^{r-3}} x_{2j-1}^{r-4}. \end{aligned}$$

Thus,

$$\begin{aligned} A_{ijr} \geq\ & \frac{a_1}{(r-3)!2^{r-3}} x_{2i-1}^{r-3} (x_{2j-1} - x_{2i-1})^{r-4} \\ &+ \frac{a_1}{(r-3)!2^{r-3}} x_{2i-1}^{r-3} x_{2j-1}^{r-4}. \end{aligned}$$

A_{ijr} is also bounded from above by

$$A_{ijr} \le a_1 \frac{x_{2i+1}^{r-3}}{(r-4)!} \sum_{p=0}^{r-4} \binom{r-4}{p} (x_{2j+1} - x_{2i+1})^p \frac{x_{2i+1}^{r-4-p}}{(2r-7-p)}$$
$$\le \frac{a_1}{(r-3)!} x_{2i+1}^{r-3} x_{2j+1}^{r-4}.$$

For $t \in [x_{2i-1}, x_{2i+1}]$, we have

$$\int_{x_{2i-1}}^{x_{2i+1}} L_{i1}(t) \cdot L_{j1}(t)\, dt = -\frac{h_j^5}{90} \int_{x_{2i-1}}^{x_{2i+1}} L_{i1}(t) \cdot \frac{(\eta_t - t)^{r-4}}{(r-4)!}\, dt$$
$$= B_{ijr} \cdot h_i^{r+2} h_j^5.$$

The bounds on B_{ijr} can also be computed as

$$a_2(x_{2j-1} - x_{2i+1})^{r-4} \le B_{ijr} \le a_2(x_{2j+1} - x_{2i-1})^{r-4},$$

where $a_2 = \frac{2(r+2)+(r-4)2^r}{135(r-4)!(r+2)!}$. Similarly,

$$M_{\omega_r}(Z_{i2}Z_{j2}) = \int_{x_{2j-1}}^{1} L_{i2}(t) \cdot L_{j2}(t)\, dt$$
$$= \left(\int_{x_{2j-1}}^{x_{2j+1}} + \int_{x_{2j+1}}^{1} \right) L_{i2}(t) \cdot L_{j2}(t)\, dt,$$

with

$$\int_{x_{2j+1}}^{1} L_{i2}(t) \cdot L_{j2}(t)\, dt = \frac{h_i^5 h_j^5}{90^2} \int_{x_{2j+1}}^{1} \frac{(\xi_t - t)^{r-4}}{(r-4)!} \frac{(\eta_t - t)^{r-4}}{(r-4)!}\, dt$$
$$= A'_{ijr} \cdot h_i^5 h_j^5,$$

and

$$\int_{x_{2j-1}}^{x_{2j+1}} L_{i2}(t) \cdot L_{j2}(t)\, dt = -\frac{h_i^5}{90} \int_{x_{2j-1}}^{x_{2j+1}} \frac{(\xi_t - t)^{r-4}}{(r-4)!} \cdot L_{j2}(t)\, dt$$
$$= B'_{ijr} \cdot h_i^5 h_j^{r+2},$$

where $\xi_t \in (x_{2i-1}, x_{2i+1})$, $\eta_t \in (x_{2j-1}, x_{2j+1})$, A'_{ijr} and B'_{ijr} are independent of h_i and h_j. Note that $a_r = \min\{a_2, a_1/((r-3)!2^{r-3})\}$, $a'_r = \max\{a_2, a_1/(r-3)!\}$, A_{ijr}, B_{ijr}, A'_{ijr}, and B'_{ijr}, which, after some straightforward calculation, provides the bounds on c_{ijr}. This completes the proof. ■

In the next theorem that is the main theorem of this paper, we show that the *Simpson's quadrature* with equally spaced points is optimal in the average case setting when $r \leq 3$.

THEOREM 3.1. *For any information N_n of cardinality n,*

$$e^{avg}(S, N_n; \mu_r) = \Omega\left(n^{-\min\{r+1,4\}}\right).$$

For the information N_n^* that uses n equally spaced points,

$$e^{avg}(S, N_n^*; \mu_r) = \Theta\left(n^{-\min\{r+1,4\}}\right).$$

Thus, the error of Simpson's quadrature is minimal (modulo a multiplicative constant) when equally spaced points are used. Furthermore, for $r \leq 3$, Simpson's quadrature at equally spaced points is almost optimal among all algorithms that use n functions values at arbitrary points.

Proof. Assume $r \leq 3$. Since Z_i's are independent,

$$e^{avg}(S, N_n; \mu_r)^2 = \sum_{i=1}^{k} M_{\mu_r}(Z_i^2) = c_r \cdot \sum_{i=1}^{k} h_i^{2r+3}$$

with c_r given in Lemma 3.1. To minimize the above expression, we need to solve

$$\frac{\partial}{\partial h_j} \sum_{i=1}^{k} h_i^{2r+3} = 0, \text{ for } j = 1, 2, \ldots, k,$$

subject to $\sum_{i=1}^{k} h_i = 1/2$. Then, since $h_k = \frac{1}{2} - \sum_{i=1}^{k-1} h_i$,

$$\begin{aligned}
&\frac{\partial}{\partial h_j}\left(\sum_{i=1}^{k-1} h_i^{2r+3} + \left(\frac{1}{2} - \sum_{i=1}^{k-1} h_i\right)^{2r+3}\right) \\
=&(2r+3)h_j^{2r+2} - (2r+3)\left(\frac{1}{2} - \sum_{i=1}^{k-1} h_i\right)^{2r+2} \\
=&0, \text{ for } j = 1, \dots, k-1.
\end{aligned}$$

Thus, we have

$$h_j = \frac{1}{2} - \sum_{i=1}^{k-1} h_i = h_k \text{ for } j = 1, \dots, k-1.$$

Hence, $\sum h_i^{2r+3}$ is minimized when all h_i's are equal. Let $h = h_i$ for all i. Then, we have

$$\begin{aligned}
e^{avg}(S, N_n; \mu_r)^2 &= c_r \sum_{i=1}^{k} h_i^{2r+3} \\
&\geq c_r \sum_{i=1}^{k} h^{2r+3} \\
&= \frac{c_r}{2} h^{2r+2} \\
&= e^{avg}(S, N_n^*; \mu_r)^2.
\end{aligned}$$

This completes the case of $r \leq 3$.

Consider $r \geq 4$. Then, according to Lemma 3.1, we have

$$\begin{aligned}
e^{avg}(S, N_n; \mu_r)^2 &= M_{\mu_r}\left(\left(\sum_i Z_i\right)^2\right) \\
&= \sum_i \sum_j M_{\mu_r}(Z_i Z_j) = \sum_i \sum_j c_{ijr} h_i^5 h_j^5,
\end{aligned}$$

Since $c_{ijr} \geq a_r \left(\frac{1}{3}\right)^{2r-7}$ if $x_{2i-1} \geq \frac{1}{3}$ or $x_{2j+1} \leq \frac{2}{3}$, we have

$$e^{avg}(S, N_n; \mu_r)^2 \geq a_r(\frac{1}{3})^{2r-7}(\sum_{x_{2i-1} \geq \frac{1}{3}} \sum_{j \geq i} h_i^5 h_j^5 + \sum_{x_{2j+1} < \frac{2}{3}} \sum_{i < j} h_i^5 h_j^5)$$
$$= \Omega(n^{-8}).$$

Finally, for equally spaced points, $e^{avg}(S, N_n^*; \mu_r)^2 \leq a'_r \sum_i \sum_j h^{10} = O(h^8)$. This completes the proof. ■

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Sung Hee Choi
Department of Computer Science
Sun Moon University, Asan
Choongnam 336-840, Korea

Bum Il Hong
Department of Mathematics
Kyung Hee University
Yongin, Kyunggi 449-701, Korea