Quadrature Formulas for Multivariate Convex Functions

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Abstract. We study optimal quadrature formulas for convex functions in several variables. In particular, we answer the following two questions: Are adaptive methods better than nonadaptive ones? And: Are randomized (or Monte Carlo) methods better than deterministic methods?

1. Introduction and Results

We study optimal rates of convergence of quadrature formulas for convex functions in several variables. We mainly consider the classes

$$\mathcal{F}_d = \{f : [0,1]^d \to [-1,1] \mid f \text{ convex}\},$$

but we will see that the lower bounds also hold for smaller classes (where we have a bound for the gradient of f) and the upper bounds also hold for larger classes (where we replace "convex" by "convex in each x_i-direction"). We will prove that the error of optimal deterministic methods is of the order

$$n^{-2/d}. \tag{1}$$

This order can be obtained by nonadaptive methods, adaptive methods do not give a better order of convergence. If we allow randomized (or Monte Carlo) methods then the order of the optimal methods is

$$n^{-2/d-1/2}, \tag{2}$$

where we have to use a slightly different notion of the error than in the deterministic case. The upper bound is proved by an adaptive method and we believe that non-adaptive methods are worse. We construct nonadaptive Monte Carlo methods with an error of the order

$$n^{-3/(2d)-1/2} \tag{3}$$

and conjecture that this is optimal. We could not prove the respective lower bound, however.

The basic facts and, in particular, the statements (1–3) are known for the integration problem in one dimension, see Novak and Petras (1994). We give some comments and begin with deterministic quadrature formulas.

For each quadrature formula, the error in the class of convex functions on, e.g., $[0,1]$ is not uniformly bounded. For the study of optimal quadrature formulas we therefore have to restrict the class of convex functions. The classes

$$F_{uv} = \{f : [0,1] \to \mathbf{R} \mid f \text{ convex},\ f'_+(0) \geq u,\ f'_-(1) \leq v\},$$

where $v > u$, were studied by Glinkin (1984), Zwick (1988), and Novak (1993). The following is known for these classes. Let $n \in \mathbf{N}$ and $t_i = (2i-1)/(2n)$. Then the affine and nonadaptive formula

$$Q_n^*(f) = \frac{1}{16n^2} \cdot (v-u) + \frac{1}{n} \sum_{i=1}^{n} f(t_i) \tag{4}$$

is optimal even in the class of adaptive formulas of the form

$$Q_n(f) = \phi(f(t_1), \ldots, f(t_n)),$$

where the knot t_i may depend on the 'already known' function values, i.e., $t_i = t_i(f(t_1), \ldots, f(t_{i-1}))$, and ϕ is an arbitrary mapping. Defining the maximal error of Q_n on a class F by

$$\Delta_{\max}(Q_n, F) = \sup_{f \in F} \{ | \int_0^1 f(x)\, dx - Q_n(f) | \},$$

we have

$$\Delta_{\max}(Q_n^*, F_{uv}) = \frac{v-u}{16n^2}.$$

We prefer, however, the more general classes $\mathcal{F}_d$ without the smoothness assumptions, because for each convex function on $[0,1]^d$, an appropriate nontrivial multiple is in $\mathcal{F}_d$. The class $\mathcal{F}_1$ was studied by Braß (1982) who proved the following. Let c_n be defined by

$$c_n = \begin{cases} 2(n^2+2n+1)^{-1} & \text{if } n \text{ is odd and} \\ 2(n^2+2n+2)^{-1} & \text{if } n \text{ is even.} \end{cases}$$

Then the linear formula

$$Q_n(f) = \begin{cases} c_n \cdot \left(\sum_{i=1}^{\frac{n-1}{2}} 2if(i^2 c_n) + 2if(1 - i^2 c_n) + nf(1/2) \right) & \text{if } n \text{ is odd and} \\ c_n \cdot \left(\sum_{i=1}^{\frac{n}{2}} 2if(i^2 c_n) + 2if(1 - i^2 c_n) \right) & \text{if } n \text{ is even} \end{cases} \tag{5}$$

is optimal for $\mathcal{F}_1$ in the class of all nonadaptive quadrature formulas. The maximal error of the optimal formula is given by

$$\Delta_{\max}(Q_n, \mathcal{F}_1) = c_n. \tag{6}$$

Though adaptive formulas might be slightly better than nonadaptive formulas for $\mathcal{F}_1$, it follows from the results for F_{uv} that n^{-2} is also the optimal order of convergence for adaptive formulas. The maximal error of the n-point Gaussian formula on the class $\mathcal{F}_1$ is less than $\frac{\pi^2}{3n^2}$, see Petras (1993b). Therefore the Gaussian formulas are "almost optimal" for $\mathcal{F}_1$. More of the known results concerning deterministic quadrature formulas in the one-dimensional case can be found in the survey of Petras (1993a).

Some results are even known for $d > 1$. See, in particular, Sonnevend (1983) and Gruber (1993). We want to point out, however, that we do not require smoothness, such as C^1 or even C^2, for our upper bounds. We also do not know any previous work concerning error bounds for stochastic methods.

In the randomized setting we consider general (adaptive) stochastic rules of the form

$$Q_n^\omega(f) = \phi^\omega(f(t_1^\omega), \ldots, f(t_n^\omega)),$$

i.e., the knots t_i^ω are random variables (which can be chosen nonadaptively or adaptively) and also the ϕ^ω is randomly chosen. Then, as usual, the error of Q_n^ω is defined in a 'worst case stochastic sense',

$$\Delta_{\max}(Q_n^\omega, \mathcal{F}_d) = \sup_{f \in F} E(|\int_{[0,1]^d} f(t)\,dt - Q_n^\omega(f)|).$$

It is known from Novak and Petras (1994) that in the case $d = 1$ nonadaptive stochastic methods are at most slightly better than (adaptive or nonadaptive) deterministic methods, the optimal order is n^{-2}. We also proved that adaptive Monte Carlo methods are better and here the optimal order is $n^{-5/2}$.

These results are quite different from known results for unit balls of Hölder or Sobolev spaces. It is known for all these classes that adaptive methods are not better than nonadaptive ones – for deterministic methods as well as for stochastic methods – while randomized methods are better than deterministic methods, see Novak (1988) and Traub, Wasilkowski, Woźniakowski (1988). Classes of monotone functions were studied by Novak (1992) for $d = 1$ and by Papageorgiou (1993) for $d > 1$. The results are similar to the results of the present paper.

2. Proofs

We have to prove five statements:

a) the lower bounds (1) for adaptive deterministic methods;
b) the upper bound (1) for nonadaptive deterministic methods;
c) the lower bounds (2) for adaptive Monte Carlo methods;
d) the upper bounds (3) for nonadaptive Monte Carlo methods.
e) the upper bounds (2) for adaptive Monte Carlo methods;

a) More precisely, we prove for deterministic methods Q_n involving $n = \frac{1}{2}k^d$ nodes, where $k/2 \in \mathbf{N}$, that

$$\Delta_{\max}(Q_n, \mathcal{F}_d) \geq \frac{b_d}{2^d d(d+2)} \cdot (2n)^{-2/d}.$$

Here, $b_d \geq \big(\pi(d+1)\big)^{-1/2}(2e\pi/d)^{d/2}$ denotes the volume of the d-dimensional unit ball. Let $x = (x_1, \ldots, x_d)$, and define $f \in \mathcal{F}_d$ by

$$f(x) = -1 + \frac{8}{d}\sum_{i=1}^{d}\left(x_i - \frac{1}{2}\right)^2.$$

We divide $[0,1]^d$ into the d-cubes $G_1, \ldots, G_{2n}$, whose edges have the lengths k^{-1}. Assume that they are ordered in such a way that all nodes of Q_n for the function f are in $G_{n+1} \cup \ldots \cup G_{2n}$. Let y_i be the center of G_i, let $\tilde{h}_i : \mathbf{R}^d \to \mathbf{R}$ represent the hyperplane which is tangent to f at the point y_i, and let $h_i(x) = \tilde{h}_i(x) + 2/(dk^2)$. Note that $h_i(x) \geq f(x)$ if and only if x is in the largest d-dimensional ball, which is contained in G_i. Define

$$g = \max\big\{f, h_1, \ldots, h_n\big\} \in \mathcal{F}_d.$$

Using that $h_i(x) - f(x) = 2/(dk^2) - h$ if and only if $\|x - y_i\|_2 = \sqrt{\frac{hd}{8}}$, we obtain

$$\delta_n := \int_{G_i} g(x) - f(x)\, dx = \int_0^{\frac{2}{dk^2}} b_d \left(\frac{hd}{8}\right)^{d/2} dh = \frac{1}{n} \cdot \frac{2^{1-d} b_d}{d(d+2)} \cdot (2n)^{-2/d}.$$

From $Q_n(g) = Q_n(f)$, we obtain the stated lower bound.

b) Let Q_n be a given quadrature formula and let Q_n^d be the corresponding product formula on $C\big([0,1]^d\big)$ involving n^d nodes (cf. Davis and Rabinowitz (1984)). Note that the function $\int_{[0,1]^{d-1}} f(x_1, \ldots, x_{d-1}, \cdot)\, dx_1 \ldots dx_{d-1}$ is convex on $[0,1]$ and that $f(\cdot, \ldots, \cdot, x_d)$ is convex on $[0,1]^{d-1}$. Therefore, we may apply the technique of Haber (1970) and obtain that

$$\Delta_{\max}(Q_n^d, \mathcal{F}_d) \leq \Delta_{\max}(Q_n, \mathcal{F}_1) \cdot \sum_{k=0}^{d-1} \|Q_n\|^k.$$

If we choose Q_n as in equation (5), we have

$$\Delta_{\max}(Q_n^d, \mathcal{F}_d) \leq \frac{2d}{(n+1)^2}.$$

c) Consider the equidistribution μ on the following set of 2^{2n} functions,

$$\mathcal{F}_d^* := \big\{ \max\{f, h_{i_1}, \ldots, h_{i_k}\} \mid \{i_1, \ldots, i_k\} \subset \{1, 2, \ldots, 2n\} \big\} \subset \mathcal{F}_d,$$

where we adopt here and in the following the notation of part a). We first want to estimate the expectation of the error of a deterministic (adaptive) method for the class $\mathcal{F}_d^*$. It is obvious that an additional function value at $t_i \in G_j$ only gives additional information if $f(t_i) < h_j(t_i)$ and if no further node is in G_j. Therefore, we have 2^n distinct combinations of function values depending on whether the function value at t_i is $f(t_i)$ or $h_j(t_i)$, where $i = 1, \ldots, n$. For each of these combinations, the sum of all occurring errors is at least

$$\delta_n \cdot \sum_{k=0}^{n} \binom{n}{k} \left| k - \frac{n}{2} \right| \geq \delta_n \cdot 2^{n-2} \sqrt{2n}$$

(for the last inequality, cf. Novak (1992)). We obtain

$$E_\mu \left(\Big| \int_{[0,1]^d} f(x)\, dx - Q_n(f) \Big| \right) \geq \frac{2^n \cdot \delta_n 2^{n-2} \sqrt{2n}}{2^{2n}}.$$

Fubini's theorem shows that this is also a lower bound for the worst-case expectation for the error of any adaptive stochastic formula.

d) Let $k \geq 3$ be an odd number and

$$x_i = \begin{cases} 2 \frac{(i-1)^2}{(k-1)^2} & \text{if } i \leq \frac{k+1}{2} \\ 1 - x_{k+1-i} & \text{else.} \end{cases}$$

We also put $l_i = (x_{i+1} - x_i)$ and $t_i = \frac{1}{2}(x_i + x_{i+1})$, where $i = 1, \ldots, k-1$. We divide $[0,1]^d$ into $(k-1)^d$ little boxes of the form

$$G_i = [x_{i_1}, x_{i_1+1}] \times \ldots \times [x_{i_d}, x_{i_d+1}],$$

where $(i_1, \ldots, i_d) \in \{1, \ldots, k-1\}^d$. The volume of G_i is

$$|G_i| = \prod_{r=1}^{d} l_{i_r},$$

the midpoint is $(t_{i_1}, \ldots, t_{i_d})$. Let

$$I_i^u(f) = |G_i|\, 2^{-d} \sum_{\tilde{y}} f(\tilde{y}),$$

where $\tilde{y}$ runs through all 2^d corners of G_i and let

$$I_i^l(f) = |G_i|\, f(t_{i_1}, \ldots, t_{i_d}).$$

We also put

$$S^u_{k^d,d}(f) = \sum_{i=1}^{(k-1)^d} I_i^u(f) \quad \text{and} \quad S^l_{(k-1)^d,d}(f) = \sum_{i=1}^{(k-1)^d} I_i^l(f).$$

It is clear that

$$S^l_{(k-1)^d,d}(f) \le \int_{[0,1]^d} f(x)\,dx \le S^u_{k^d,d}(f).$$

By a computation that is similar to that in part b) one obtains

$$S^u_{k^d,d}(f) - S^l_{(k-1)^d,d}(f) := F(f) \le \frac{8d}{(k-1)^2}. \tag{7}$$

For the following we need a bound for each single

$$F_i(f) := I_i^u(f) - I_i^l(f),$$

where $f \in \mathcal{F}_d$. We therefore estimate $f(\tilde{y}) - f(t_{i_1}, \ldots, t_{i_d})$ for each corner $\tilde{y} = (y_{i_1}, \ldots, y_{i_d})$ of G_i. Choose without restriction $G_i \subset [0, \frac{1}{2}]^d$ and consider the representation

$$\begin{aligned} f(\tilde{y}) - f(t_{i_1}, \ldots, t_{i_d}) &= f(y_{i_1}, \ldots, y_{i_d}) - f(t_{i_1}, y_{i_2}, \ldots, y_{i_d}) \\ &\quad + f(t_{i_1}, y_{i_2}, \ldots, y_{i_d}) - f(t_{i_1}, t_{i_2}, y_{i_3}, \ldots, y_{i_d}) \\ &\quad + \ldots \\ &\quad + f(t_{i_1}, \ldots, t_{i_{d-1}}, y_{i_d}) - f(t_{i_1}, \ldots, t_{i_d}). \end{aligned}$$

Since $g := f(t_{i_1}, \ldots, t_{i_{r-1}}, \cdot, y_{i_{r+1}}, \ldots, y_{i_d})$ is convex and $\|g\| \le 1$, we have for $y_{i_r} < t_{i_r}$ that

$$g(y_{i_r}) \le \frac{y_{i_r} g(t_{i_r}) + (t_{i_r} - y_{i_r}) g(0)}{t_{i_r} - 0},$$

i.e.,

$$g(y_{i_r}) - g(t_{i_r}) \le (t_{i_r} - y_{i_r}) \frac{g(0) - g(t_{i_r})}{t_{i_r}} \le \frac{l_{i_r}}{t_{i_r}} = \frac{4i_r - 2}{2i_r^2 - 2i_r + 1} \le \frac{8}{l_{i_r}(k-1)^2}.$$

We easily see that the same inequality holds for $y_{i_r} > t_{i_r}$. Finally, we obtain

$$\begin{aligned} F_i(f) &\le \left(\prod_{r=1}^d l_{i_r}\right) 2^{-d} \sum_{\tilde{y}} \sum_{r=1}^d \frac{8}{l_{i_r}(k-1)^2} = \frac{2^{3-d}}{(k-1)^2} \sum_{\tilde{y}} \sum_{r=1}^d \prod_{\substack{j=1 \\ j \ne r}}^d l_{i_j} \\ &\le \frac{2^{3-d}}{(k-1)^2} \sum_{\tilde{y}} d \cdot \left(\frac{2k-4}{(k-1)^2}\right)^{d-1} \le 2d \left(\frac{2}{k-1}\right)^{d+1}. \end{aligned} \tag{8}$$

Now we are ready to define a nonadaptive Monte Carlo method with an order $n^{-3/(2d)-1/2}$. For $i = 1, \ldots, (k-1)^d$ we independently and randomly choose a

$$\omega \in \prod_{j=1}^{d} [-l_{i_j}/2, l_{i_j}/2]$$

according to the normed Lebesgue measure and put

$$\Phi_i(\omega)(f) = |G_i|\, 2^{-d} \sum_{(\alpha_1,\ldots,\alpha_d)\in\{-1,1\}^d} f(t_{i_1} + \alpha_1\omega_1, \ldots, t_{i_d} + \alpha_d\omega_d).$$

It is easy to see that

$$E(\Phi_i(f)) = \int_{G_i} f(x)\, dx$$

and hence the Monte Carlo method

$$Q(f) = \sum_{i=1}^{(k-1)^d} \Phi_i(f)$$

has expectation $E(Q(f)) = \int_{[0,1]^d} f(x)\, dx$. By induction one can prove

$$I_i^l(f) \le \int_{G_i} f(x)\, dx \le I_i^u(f)$$

and

$$I_i^l(f) \le \Phi_i(\omega)(f) \le I_i^u(f)$$

and so obtains

$$|\int_{G_i} f(x)\, dx - \Phi_i(\omega)(f)| \le I_i^u(f) - I_i^l(f) = F_i(f)$$

for each ω and $f \in F_d$. For the stochastic error of $Q(f)$ we obtain by (7) and (8)

$$E(|\int_{[0,1]^d} f(x)\, dx - Q(f)|) \le (\sum_{i=1}^{(k-1)^d} F_i(f)^2)^{1/2} \le$$
$$(\max_i F_i(f) \cdot \sum_{i=1}^{(k-1)^d} F_i(f))^{1/2} < \left(2d \left(\frac{2}{k-1}\right)^{d+1} \cdot \frac{8d}{(k-1)^2}\right)^{1/2} =$$
$$2d \left(\frac{2}{k-1}\right)^{(d+3)/2}$$

Since we need $2^d(k-1)^d$ function values to compute $Q(f)$ we obtain the claimed order of convergence.

e) The basic idea is the same as in Novak and Petras (1994) for the case $d=1$. We define an adaptive Monte Carlo method in three steps.

i) The first step is deterministic and nonadaptive. For a given $k \geq 2$ we compute $S^u_{k^d,d}(f)$ and $S^l_{(k-1)^d,d}(f)$, as defined in part d). We need $k^d+(k-1)^d$ function values to do this.

ii) The second step is still deterministic, but depends on f. We do not compute new function values but define an adaptive partition of $[0,1]^d$ into boxes $G_{i,j}$. For $i=1,\dots,(k-1)^d$ we define

$$\lambda_i = \lceil \frac{F_i(f)}{F(f)}(k-1)^d \rceil.$$

We divide each box G_i into λ_i subsets $G_{i,j}$ For the total number λ of sets $G_{i,j}$ we obtain by $\lambda_i < \frac{F_i(f)}{F(f)}(k-1)^d+1$ that $\lambda < 2(k-1)^2$. The definition of $G_{i,j}$ is as follows. We set

$$H_j := [t_{i_1} - j\frac{l_{i_1}}{2\lambda_i}, t_{i_1} + j\frac{l_{i_1}}{2\lambda_i}] \times \prod_{r=2}^{d} [x_{i_r}, x_{i_r+1}], \qquad j=1,\dots,\lambda_i$$

and

$$G_{i,1} = H_1, \qquad G_{i,j} = H_j \setminus H_{j-1}, \qquad j=2,\dots,\lambda_i.$$

The $G_{i,j}$ are sets with symmetry center in $(t_{i_1},\dots,t_{i_d})$. We define

$$I^u_{i,j}(f) = |G_{i,j}| 2^{-d} \sum_{\tilde{y}} f(\tilde{y}),$$

where $\tilde{y}$ runs through all corners of H_j, and

$$I^l_{i,j}(f) = |G_{i,j}| f(t_{i_1},\dots,t_{i_d}) = \frac{|G_i|}{\lambda_i} f(t_{i_1},\dots,t_{i_d}).$$

Again, we obtain

$$I^l_{i,j}(f) \leq \int_{G_{i,j}} f(x)\,dx \leq I^u_{i,j}(f).$$

Furthermore, the numbers $I^u_{i,j}(f) - I^l_{i,j}(f)$ are increasing for increasing j and $I^u_{i,\lambda_i}(f) - I^l_{i,\lambda_i}(f) = \frac{1}{\lambda_i}\left(I^u_i(f) - I^l_i(f)\right)$, such that

$$I^u_{i,j}(f) - I^l_{i,j}(f) \leq \frac{F_i(f)}{\lambda_i} \leq \frac{F(f)}{(k-1)^d}.$$

iii) The stochastic step is as in part d) with the nonadaptive boxes G_i replaced by the adaptive sets $G_{i,j}$. The only difference in the definition of the quadrature formula for $G_{i,j}$ is that ω is randomly chosen in

$$\Big([t_{i_1} - j\frac{l_{i_1}}{2\lambda_i}, t_{i_1} - (j-1)\frac{l_{i_1}}{2\lambda_i}] \cup [t_{i_1} + (j-1)\frac{l_{i_1}}{2\lambda_i}, t_{i_1} + j\frac{l_{i_1}}{2\lambda_i}]\Big) \times \prod_{r=2}^{d}[-\frac{l_{i_r}}{2}, \frac{l_{i_r}}{2}].$$

For the stochastic error of the resulting method we obtain

$$E(|\int_{[0,1]^d} f(x)\,dx - Q(f)|) \le (\sum_{i=1}^{\lambda} \frac{F(f)^2}{(k-1)^{2d}})^{1/2} < 8\sqrt{2}\,d(k-1)^{-2-d/2}.$$

In this step we compute $\lambda \cdot 2^d < 2(k-1)^d\,2^d$ function values, together certainly less than $2^{d+2}k^d$. Hence we obtain the claimed order of convergence.

Remarks. a) Again we stress that we cannot prove that the upper bound (3) is optimal. This open problem seems to be related with difficult discrepancy problems that are studied in the book of Beck and Chen (1987). A related open problem concerns the integration of multivariate monotone functions. Papageorgiou (1993) proved optimal rates for deterministic and for randomized methods but it is unclear whether (for $d > 1$) adaptive Monte Carlo methods are better than nonadaptive ones.

b) In all proofs of upper bounds we did not really use that the functions are convex. It is enough to demand that f is convex in each x_i-direction. So the upper bounds even hold for larger classes.

c) Similarly, the lower bounds even hold (with different constants) for smaller classes where we demand, in addition, that the functions are C^1 with a Lipschitz constant 1.

d) The ratios of our upper and lower bounds are increasing exponentially with increasing dimension. It might be interesting to study the exact behaviour of the distinct constants with respect to the dimension in the different settings.

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