Optimal approximative integration of Lipschitz functions

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ABSTRACT. Let ϕ be a strictly positive continuous weight function on $[0,1]$, and $n \in \mathbb{N}$. We indicate – for certain classes of functions ϕ – how to find $(x_0 =)0 < x_1 < \cdots < x_n < 1(= x_{n+1})$ and real numbers $c_0, c_1, \ldots, c_{n+1}$ such that $\sum_{k=0}^{n+1} c_k f(x_k)$ approximates as well as possible the weighted integral $\int_0^1 f(x)\phi(x)dx$ for Lipschitz functions $f : [0,1] \longrightarrow \mathbb{R}$.

In particular, an optimal solution can easily be found if ϕ is twice differentiable such that $-(\log\phi)''$ is nonnegative.

1. THE PROBLEM

Let ϕ and n be as in the abstract. In order to measure the strength of a quadrature formula $\sum_{k=0}^{n+1} c_k f(x_k) \approx \int_0^1 f(x)\phi(x)dx$ for Lipschitz functions f we introduce the following definition: For $(x_0 =)0 < x_1 < \cdots < x_n < 1$ $(= x_{n+1})$ and real $c_0, c_1, \ldots, c_{n+1}$ we denote by $M(x_1, \ldots, x_n; c_0, \ldots, c_{n+1})$ the number $\sup |\sum_{k=0}^{n+1} c_k f(x_k) - \int_0^1 f(x)\phi(x)dx|$, where the sup runs over all Lipschitz functions f with Lipschitz constant one. By M_n we mean the minimum of this function, and we want to determine the x_k, c_k such that M_n is attained there.

The problem of evaluating the weighted integral of Lipschitz functions by using a quadrature formula occurred in a number of papers which were concerned with the optimal reconstruction of stochastic processes ([2],[3],[4]). In these publications optimal *asymptotic* solutions are obtained, the main results read as follows:

- $\lim nM_n = (1/4)(\int_0^1 \sqrt{\phi(x)}dx)^2$.
- Let $x_1^n, \ldots, x_n^n$ be determined such that $\int\limits_{x_i^n}^{x_{i+1}^n} \sqrt{\phi(x)}dx =$ $\frac{1}{n+1}\int_0^1 \sqrt{\phi(x)}dx$ (the superscript "n" is an index here and not a power);

then, for certain $c_0^n, \ldots, c_{n+1}^n$ which can easily be determined one has $nM(x_1^n, \ldots, x_n^n; c_0^n, \ldots, c_{n+1}^n) \longrightarrow (1/4)(\int_0^1 \sqrt{\phi(x)}dx)^2$.

Here, however, we have in mind to find – for n given – the x_k, c_k such that they *exactly* provide the best possible approximation. Our techniques are different from those of the asymptotic approach, they are more in the spirit of Curbera's paper [1], where a slightly different question is considered: Whereas we investigate a general density ϕ on $[0,1]$, there the density of the normal distribution on the real line is discussed.

We begin with some simple observations. First we note that only such c_k have to be treated where $\sum_0^{n+1} c_k = \int_0^1 \phi(x)dx$ since otherwise $M(x_1, \ldots, x_n; c_0, \ldots, c_{n+1}) = \infty$; let's assume from now on that $\sum_0^{n+1} c_k = \int_0^1 \phi(x)dx = 1$. Secondly, we will reformulate our problem slightly. This is folklore, for the sake of completeness we indicate the simple proof.

Lemma 1.1 *With x_k, c_k as above the following holds:*

(i) *For $f \in C^1[0,1]$ and $\tau := \sum_0^n c_k \chi_{[x_k,1]}$ one has $\int_0^1 f'(x)\tau(x)dx = f(1) - \sum_0^{n+1} c_k f(x_k)$. Consequently, if we put $g(x) := \int_0^x \phi(t)dt$, then $|\sum_0^{n+1} c_k f(x_k) - \int_0^1 f(x)\phi(x)dx| = |\int_0^1 f'(x)(\tau(x) - g(x))dx|$.*

(ii) *$M(x_1, \ldots, x_n; c_0, \ldots, c_{n+1}) = \int_0^1 |g(x) - \tau(x)|dx$.*

Proof. (i) follows immediately from elementary calculus. The inequality "$\leq$" of (ii) is due to the fact that Lipschitz functions with Lipschitz constant one can be uniformly approximated by $f \in C^1[0,1]$ with $||f'||_\infty \leq 1$. And for the proof of "$\geq$" one only has to note that the right hand side is arbitrarly close to $\int_0^1 f'(x)(\tau(x) - g(x))dx$, where $||f'||_\infty \leq 1$. □

Now consider any $h \in C^1[0,1]$ such that $h'(x) > 0$ for every x. Then $x \mapsto \int_0^1 |h(x) - h(t)|dt$ has a unique minimum at $x = 1/2$. Consequently, in order to minimize $\int_0^1 |g(x) - \sum_0^n c_k \chi_{[x_k,1]}(x)|dx$, one has to take into account only such c_k which satisfy $c_0 + \cdots + c_k = g(\frac{x_k + x_{k+1}}{2})$. To phrase it otherwise: With $D_n := \{(x_1, \ldots, x_n) \mid 0 \leq x_1 \leq \cdots \leq x_n \leq 1\}$ define Φ_n on D_n by $\int_0^1 |g(x) - \sum_0^n c_k \chi_{[x_k,1]}(x)|dx$, where the c_k are calculated recursively by $c_0 + \cdots + c_k = g(\frac{x_k + x_{k+1}}{2})$; then $M_n = \min \Phi_n$. It is easy to see that $\Phi_n(x_1, \cdots, x_n) = M_n$ implies that $(x_1, \cdots, x_n)$ lies in the interior of D_n (if e. g. $x_1 < x_2 = x_3 < x_4 \cdots$, then $\Phi_n(x_1, (x_1 + x_2)/2, x_3, x_4, \cdots) < \Phi_n(x_1, x_2, x_3, x_4, \cdots)$). Hence the gradient of Φ_n vanishes at the $(x_1, \ldots, x_n)$ we are looking for, which just means that the following system of equations is satisfied:

$$\begin{aligned} g(x_k) &= \frac{1}{2}[g(\frac{x_k + x_{k-1}}{2}) + g(\frac{x_k + x_{k+1}}{2})], \\ & k = 0, \dots, n, \text{with } x_0 := 0, x_{n+1} := 1. \end{aligned} \tag{1.1}$$

In general there can be (even infinitely) many solutions of (1.1). Of course one could try to find all of them and to calculate which one leads to the minimal $\Phi_n(x_1, \dots, x_n)$. This, however, will usually not be tractable. On the other hand, if one would know in advance that (1.1) has a unique solution $(x_1, \dots, x_n)$, then one only had to construct *any* $(x_1, \dots, x_n)$ which satisfies (1.1), and Φ_n would be minimal there.

But finding a solution of (1.1) is simple, it can for example be done rather effectively by the following *shooting method*: Start with a "small" x_1 and determine x_2 from the equation $g(x_1) = \frac{1}{2}[g(\frac{x_1+x_0}{2}) + g(\frac{x_1+x_2}{2})]$. Similarly one calculates $x_3, \dots, x_{n+1}$. This will usually provide an x_{n+1} which is smaller than one, or the procedure stops since some x_k is too big to calculate x_{k+1}. In this case, start again with a larger or smaller x_1 and repeat this procedure until $x_{n+1} = 1$ within the desired accuracy. (This necessitates the calculation of g^{-1}. In some cases it might be better to solve (1.1) by Newton methods, where, however, inverses of large matrices have to be calculated.)

Summing up, we arrive at the following

> *Problem:* Let $g : [0, 1] \longrightarrow \mathbb{R}$ be a strictly monotone continuous function, and $n \in \mathbb{N}$. Under what conditions is it true that (1.1) has only one solution?

We will investigate this problem independently of our approach concerning the approximative calculation of weighted integrals of Lipschitz functions (in this case we know in addition that $g(0) = 0, g(1) = 1$, but this will not be of any importance). *Section 2* contains some preparations, our main results can be found in *section 3.*

2. The z-function

From now on g will be a fixed function as in the preceding problem. In order to prove positive results we will have to assume that g satisfies some additional smoothness conditions.

Definition 2.1 *For $v \in [0,1]$ and $u \geq 0$ we want to define $z = z(v,u)$ implicitly by the equation*

$$g(v) = \frac{g(v-u) + g(v+z)}{2}; \tag{2.1}$$

note that this can be done whenever v, u satisfy $0 \leq u \leq v \leq 1$ and $g(v) + (g(v) - g(v-u)) \leq g(1)$.

The importance of the z-function stems from the following fact. Define functions $X_k(x), t_k(x)$ for "sufficiently small" $x \in [0,1]$ by

- $X_0(x) := 0, t_0(x) := x$ for $0 \leq x \leq 1$;
- $X_{k+1}(x) := X_k(x) + 2t_k(x)$ whenever $X_k(x), t_k(x)$ are defined;
- $t_{k+1}(x) := z(X_{k+1}(x), t_k(x))$ provided that $(X_{k+1}(x), t_k(x))$ lies in the domain of z.

With this notation at hand we can translate the problem of finding a solution of (1.1) by

- Let $(x_1, \ldots, x_n)$ be a solution of (1.1). Then $X_{n+1}(x_1/2) = 1$.
- Conversely, if $X_{n+1}(x) = 1$ for some $0 < x < 1$, then $x_k := X_k(x)$ $(k = 1, \ldots, n)$ provides a solution of (1.1).

This gives rise to a natural sufficient condition: (1.1) will have a unique solution as soon as one knows that all X_k are differentiable, and

$$X'_{n+1}(x) > 0 \text{ whenever } X_{n+1}(x) = 1. \tag{2.2}$$

Our positive results all rely on this simple observation. X_{n+1} is differentiable provided that $g \in C^1[0,1]$, but usually we will need higher smoothness properties; we will assume from now on that $g \in C^3[0,1]$.

Lemma 2.2

(i) $(\partial z/\partial u)(v,u) = g'(v-u)/g'(v+z)$. *In particular it follows that* $(\partial z/\partial u)(v,0) = 1$ *and that* $z \le u$ *(resp.* $z \ge u$*) if* g' *is increasing (resp. decreasing). Similarly, if we consider* u *as a function of* v *and* z*, one has* $(\partial u/\partial z)(v,z) = g'(v+z)/g'(v-u)$.

(ii) $(\partial z/\partial v)(v,u) = (2g'(v) - g'(v-u))/g'(v+z) - 1$. *Consequently* $\partial z/\partial v \ge 0$ *iff* $g'(v) \ge (g'(v-u) + g'(v+z))/2$*; it also follows that* $(\partial z/\partial v)(v,0) = 0$.

(iii) $(\partial^2 z/\partial u^2)(v,u) =$
$-(g''(v-u)g'^2(v+z) + g''(v+z)g'^2(v-u))/g'^3(v+z)$.
Similar expressions hold for $\partial^2 u/\partial z^2$ *and* $\partial^2 z/\partial v^2$*, and one can conclude that* $(\partial^2 z/\partial u^2)(v,0) = -2g''(v)/g'(v), (\partial^2 z/\partial v^2)(v,0) = 0$.

Proof. All these formulas follow easily by differentiating the equation by which z is defined. □

3. FUNCTIONS g WITH A UNIQUE SOLUTION OF (1.1)

Proposition 3.1 *Let* g *be three times differentiable.*

(i) *Suppose that* $\partial z/\partial v \ge 0$*. Then there is a unique solution of (1.1) and thus a unique best quadrature formule to approximate the integrals with weight* g' *of Lipschitz functions.*

(ii) *The preceding condition is fulfilled if* $\log g'$ *is a concave function, i. e. if* $(\log g')'' \le 0$.

Proof. (i) We have $\partial z/\partial u > 0$ by the preceding lemma and $\partial z/\partial v \ge 0$ by assumption. It follows inductively that $t'_k > 0, X'_k \ge 0$ for $k = 1, \ldots, n$. Hence $X'_{n+1} > 0$ wherever it is defined.

(ii) It suffices by lemma 2.2(ii) to show that $w(v,u) := 2g'(v) - (g'(v-u) + g'(v+z)) \ge 0$ on the domain of z. We fix v and consider w as a function of u. Clearly $w(v,0) = 0$, and$(\partial w/\partial u)(v,u) = g''(v-u) - g''(v+z)(\partial z/\partial u(v,u) = g''(v-u) - g''(v+z)g'(v-u)/g'(v+z)$.. This expression is nonnegative iff $g''(v-u)/g'(v-u) \ge g''(v+z)/g'(v+z)$, and the last inequality holds since by assumption g''/g' is a decreasing function: $(g''/g')' = (\log g')'' \le 0$.

□

We present some *examples*:

- $g(x) = e^{ax}, a > 0$.

- $g(x) = 1 - e^{-ax}, a > 0$.
- $g(x) = x^r, r \geq 1$.
- $g'(x) = e^{-ax^2}, a > 0$ (this is Curbera's example [1]).
- $g''' \leq 0$ on $]0, 1]$.

The condition $(\log g')'' \leq 0$ seems to be rather restrictive. However, computer simulation indicates that even for rather simple g with positive $(\log g')''$ the function X_{n+1} can fail to be monotone. The reader is referred to the APPENDIX: Figure 1 provides a sketch of the $X_1, X_2, \ldots$ for the case $g(x) = e^x$; the X_k are monotone as it is guaranteed by 3.2(i). On the other hand, one can see in figure 2 how for $g(x) = 2x - 1 + 6(2x-1)^3, x \in [0, 1]$, none of the functions $X_2, X_3, \ldots$ is increasing. Hence, by a suitable scaling $x \mapsto ax$, for every $n > 1$ one can produce several solutions of $X_{n+1}(x) = 1$.

We close this paper with a general result concerning the structure of the solutions of (1.1): the $x_{k+1} - x_k$ necessarily are of the same order:

Proposition 3.2 *Suppose that $g \in C^2[0, 1]$.*

(i) *There exists $M > 0$ such that $z/u \leq 1 + Mu$ and $u/z \leq 1 + Mz$ whenever $z(u, v)$ is defined. M can be chosen as $2||g'||^2||g''||/(\min g')^3$.*

(ii) *With $K := e^M$ the following holds: Whenever $(x_1, \ldots, x_n)$ is a solution of (1.1), then $x_{k+1} - x_k \in [\frac{1}{(n+1)K}, \frac{K}{n+1}]$.*

Proof. (i) One only has to use a Taylor expansion of $z = z(v, u)$ (resp. $u = u(v, z)$) as a function of u (resp. z); the derivatives are calculated in lemma 2.2.

(ii) We adopt the notation preceding lemma 2.2, and we have to provide bounds for the $(x_{k+1} - x_k)/2 = t_k := t_k(x)$ if x is such that $X_{n+1}(x) = 1$. $\log t_k/t_0 = \sum_0^{k-1} \sum t_{j+1}/t_j = \sum \log z(X_{j+1}, t_j)/t_j \leq \sum \log(1 + Mt_j) \leq \sum Mt_j \leq M/2$, and $\log t_0/t_k = \sum \log t_j/t_{j+1} = \sum \log t_j/z(X_{j+1}, t_j) \leq \sum \log(1 + Mt_{j+1}) \leq M/2$, so that $e^{-M/2} \leq t_k/t_0 \leq e^{M/2}$ for every k (note only that $\log(1 + x) \leq x$ and that $\sum_0^{k-1} t_j \leq \sum_0^{n+1} t_j = 1/2$).

Thus $(n+1)t_0 e^{-M/2} \leq 1/2 = \sum t_j \leq (n+1)t_0 e^{M/2}$, which finally leads to $\frac{e^{-M}}{2}\frac{1}{n+1} \leq e^{-M/2}t_0 \leq t_k \leq e^{M/2}t_0 \leq \frac{e^M}{2}\frac{1}{n+1}$. □

Final remark: The author is aware of the fact that the preceding results are of limited practical interest. Consider e. g. the function $g(x) = x^2$ and n=6. By the asymptotic approach (cf. section 1) a reasonable choice of the $x_1, \ldots, x_6$ is to divide the area under $\sqrt{g'}$ into seven like pieces, and this gives the numbers $0.1952, 0.3628, 0.5119, 0.6475, 0.7728, 0.8898$. The best possible values (calculated by the shooting method) are $0.1950, 0.3625, 0.5116, 0.6473$, $0.7727, 0.8898$. It is plain that the differences are negligible so that there is hardly any gain when passing from the asymptotic approach to the exact solution (in particular since the error M_6 is ≈ 0.016). The situation is in favor for the exact $x's$ only for very small n (e. g. $g(x) = x^2$ as before, $n = 2$; a trisection of the area under $\sqrt{g'}$ gives $0.4807, 0.7631$, the best possible values, however, are $0.4578, 0.7535$, so that the differences are of the order of $M_2 \approx 0.04$). On the other hand, there are cases where the asymptotic solutions coincide with the exact ones, this holds e. g. when $g(x) = e^{ax}$.

Nevertheless it is in the author's opinion an interesting problem to derive conditions under which optimal quadrature formulas can explicitly and easily be found, that is under which (1.1) has a unique solution. As an example how uniqueness can help in investigating the structure of these solutions wo want to point out how *symmetry properties* can easily be derived. Suppose that g satisfies $1 - g(x) = g(1 - x)$ and that there is precisely one solution of (1.1). By our assumption on g it follows easily that $\Phi_n(x_1, \ldots, x_n) = \Phi_n(1 - x_n, \ldots, 1 - x_{1)}$, hence uniqueness gives $x_k = 1 - x_{n-k}$. (This occurs whenever the density ϕ we started with is symmetric with respect to the midpoint of the interval, e. g. when dealing with the density of the normal distribution.)

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