INTRACTABILITY RESULTS FOR POSITIVE QUADRATURE FORMULAS AND EXTREMAL PROBLEMS FOR TRIGONOMETRIC POLYNOMIALS

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ABSTRACT. Lower bounds for the error of quadrature formulas with positive weights are proved. We get intractability results for quasi-Monte Carlo methods and, more generally, for positive formulas. We consider general classes of functions but concentrate on lower bounds for relatively small classes of trigonometric polynomials. We also conjecture that similar lower bounds hold for arbitrary quadrature formulas and state different equivalent conjectures concerning positive definiteness of certain matrices and certain extremal problems for trigonometric polynomials. We also study classes of functions with weighted norms where some variables are "more important" than others. Positive quadrature formulas are then tractable iff the sum of the weights is bounded.

1. INTRODUCTION

Consider quadrature formulas of the form

$$Q_n(f) = \sum_{i=1}^{n} c_i f(x_i) \tag{1}$$

with $c_i \in \mathbb{R}$ and $x_i \in [0, 1]^d$ for the approximation of the integral

$$I_d(f) = \int_{[0,1]^d} f(x)\, dx.$$

Let F be a class of integrable functions on $[0, 1]^d$. In this paper F always will be the unit ball in a suitable (finite or infinite dimensional) Hilbert space.

We define the (worst case) error of Q_n on F by

$$e(Q_n, F) = \sup\{|I_d(f) - Q_n(f)| \,:\, f \in F\}$$

and the nth minimal error by

$$e_n(F) = \inf_{Q_n} e(Q_n, F). \tag{2}$$

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The number $e_n(F)$ is the (worst case) error of the optimal quadrature formula (for the class F), using at most n knots. Obviously, the sequence $e_n(F)$ is nonincreasing. For all the F's in this paper we have

$$e(Q_0, F) = e_0(F) = 1,$$

where $Q_0(f) = 0$ is the trivial quadrature formula. Hence the problems are properly scaled for all d. We say that Q_n is positive if $c_i \geq 0$ for all $i = 1, \ldots, n$. Positive formulas are preferred due to their strong stability properties. Therefore we also define

$$e_n^+(F) = \inf_{Q_n} e(Q_n, F),$$

where the infimum only runs through the set of positive quadrature formulas (1).

The order of convergence of $e_n(F)$ is known for many function classes F. It is often of the form

$$e_n(F) \asymp n^{-k} \cdot (\log n)^\gamma. \tag{3}$$

We also often have

$$e_n(F) \asymp e_n^+(F),$$

but we usually do not know whether $e_n(F)$ and $e_n^+(F)$ are equal. Many results and references can be found in Niederreiter (1992), Novak (1988), Temlyakov (1991, 1994), Traub, Wasilkowski, Woźniakowski (1988), and Traub, Werschulz (1998). We mention two specific results. Let $W_2^k([0,1]^d)$ be the classical Sobolev space with the norm

$$\|f\|^2_{W_2^k} = \sum_{|\alpha| \leq k} \|D^\alpha f\|^2_{L_2}, \tag{4}$$

where $\alpha \in \mathbb{N}_0^d$ and $|\alpha| = \sum_{l=1}^d \alpha_l$, and let $\widetilde{W}_2^k([0,1]^d)$ be the unit ball of $W_2^k([0,1]^d)$. We assume the imbedding condition $2k > d$. It is well known from the work of Bakhvalov (1959) and Sobolev (1965) that

$$e_n(\widetilde{W}_2^k([0,1]^d) \asymp e_n^+(\widetilde{W}_2^k([0,1]^d) \asymp n^{-k/d}.$$

Instead of the norm (4) we can define a tensor product norm by

$$\|f\|^2_{H_2^k} = \sum_{\alpha_l \leq k} \|D^\alpha f\|^2_{L_2},$$

where the sum is over all $\alpha \in \mathbb{N}_0$ with $\alpha_l \leq k$ for all l. We obtain a space $H_2^k([0,1]^d)$ of functions with bounded mixed derivatives and denote its unit ball by $\widetilde{H}_2^k([0,1]^d)$. Observe that $f_1, \ldots, f_d \in H_2^k([0,1]) = W_2^k([0,1])$ implies $f_1 \otimes \cdots \otimes f_d \in H_2^k([0,1]^d)$ with

$$\|f_1 \otimes \cdots \otimes f_d\|_{H_2^k([0,1]^d)} = \prod_{l=1}^d \|f_l\|_{H_2^k([0,1])}. \tag{5}$$

The tensor product $f_1 \otimes \cdots \otimes f_d$ is defined by

$$(f_1 \otimes \cdots \otimes f_d)(x_1, \ldots, x_d) = \prod_{l=1}^{d} f_l(x_l).$$

It is known through the work of Frolov (1976) and Bykovskii (1985) that

$$e_n(\widetilde{H}_2^k([0,\,1]^d) \asymp e_n^+(\widetilde{H}_2^k([0,\,1]^d) \asymp n^{-k} \cdot (\log n)^{(d-1)/2}. \tag{6}$$

A result such as (3) of course implies (by definition of $\asymp$) a lower bound

$$e_n(F) \geq c_F \cdot n^{-k} \cdot (\log n)^{\gamma}$$

and also a similar upper bound

$$e_n(F) \leq \tilde{c}_F \cdot n^{-k} \cdot (\log n)^{\gamma}, \tag{7}$$

for all $n > 1$. Usually, however, the constants c_F and $\tilde{c}_F$ are not known, or if known they differ very much and they are not useful for, say, $d \geq 10$. Observe also that the sequence $n^{-k} \cdot (\log n)^{\gamma}$ is not always monotonically decreasing. If γ is large then (7) is useless even if we know the optimal $\tilde{c}_F$. It may happen that the sequence $n^{-k} \cdot (\log n)^{\gamma}$ is *increasing* for all reasonable n, say $n \leq 10^{10}$.

It is not our aim to discuss asymptotic results for $n \to \infty$, but lower bounds for "small" n or "relatively large" ε. We are interested in the case $n < 2^d$ and this also means that d should not be "too" small.[1]

The optimal order of $e_n(\widetilde{H}_2^k([0,\,1]^d)$ is between n^{-k} and $n^{-k+\delta}$, for any $\delta > 0$, independently of d. Hence we may say that the order of convergence does *not* depend on d.

We are interested, for example, in the following problem. Assume that $k \in \mathbb{N}$ and $\varepsilon < 1$ are fixed and define

$$n(d) = \inf\{n \,:\, e_n(\widetilde{H}_2^k([0,\,1]^d) \leq \varepsilon\}$$

and

$$n^+(d) = \inf\{n \,:\, e_n^+(\widetilde{H}_2^k([0,\,1]^d) \leq \varepsilon\}.$$

The problem is to verify whether $n(d)$ and $n^+(d)$ depend polynomially on d. If so integration is *tractable*, if not integration is *intractable*.

Observe that the known order (6), with unknown constants that depend on d, does not say anything about tractability. We will prove an *intractability* result for the $n^+(d)$, i.e., for positive quadrature formulas. For $n(d)$, intractability is still open, however, we conjecture that it holds.

[1] Our results and conjectures concerning lower bounds are formally for arbitrary $n, d \in \mathbb{N}$ but they are trivial for $n \geq C^d$. The constant $C > 1$ depends on the considered norm but is always at most 2.

Actually we prove lower bounds for certain classes F_d^β which are even smaller than the classes $\widetilde{H}_2^k([0,\,1]^d)$, hence the lower bounds are stronger. The elements of F_d^β are trigonometric polynomials of degree (less or equal) one in each variable, and the norm depends on the positive parameter β, see Section 2. In particular, F_d^β only contains periodic functions.

We also discuss related problems: extremal problems for trigonometric polynomials and problems with positive semidefinite matrices. Our results concern lower bounds on the numbers $e_n^+(\widetilde{H}_2^k([0,\,1]^d)$ and $e_n^+(F_d^\beta)$, we only conjecture that similar lower bounds also hold for quadrature formulas with arbitrary weights.

Explicit error bounds (without unknown constants) were recently obtained by Wasilkowski, Woźniakowski (1995, 1998) and Sloan, Woźniakowski (1997, 1998). The paper of Sloan and Woźniakowski (1998) contains upper and lower bounds for certain tensor product Hilbert spaces[2] and for quasi-Monte Carlo methods, i.e., only formulas with equal weights $c_i = 1/n$ are discussed. Some lower bounds can be generalized, however, to the class of positive quadrature formulas.

Weighted tensor product norms were studied in Sloan, Woźniakowski (1998) and in Wasilkowski, Woźniakowski (1998). We also discuss weighted norms, see Section 5. We prove that positive quadrature formulas are tractable iff the sum of the weights is bounded, see Theorem 5 and Remark 4.

The following result of Novak, Sloan, Woźniakowski (1997) was the starting point of this paper. Assume that H_1 is a Hilbert space of univariate functions and that H_d is the respective tensor product space, together with the cross-norm, as in (5). Let F_d be the unit ball of H_d and assume, to avoid trivial cases, that $e_1(F_1) > 0$. The last assumption means that the integration problem cannot be solved exactly for $d = 1$ with only one function value. Then it is always true that $e_d(F_d) > 0$ but it may happen that

$$e_{d+1}(F_d) = 0,$$

for all $d \in \mathbb{N}$. This means that a lower bound such as

$$e_n(F_d)^2 \geq 1 - n\,C^{-d} \tag{8}$$

with $C > 1$ independent on d is *not* true for arbitrary tensor product problems.

We believe, however, that (8) is true for many *typical* tensor product problems. Observe that (8) implies *intractability.* Indeed, any quadrature formula with error less than ε, $0 < \varepsilon < 1$, needs at least exponentially many (in d) function evaluations. This holds even if ε is close to 1.

[2]The authors mainly study the spaces $H_2^1([0,\,1]^d)$ with a norm that fits to the L_2-version of the Koksma-Hlawka inequality. Different similar norms belong, in the case $k = 1$, to different discrepancies, see Hickernell (1998).

In this paper we prove lower bounds of the form

$$e_n^+(F_d)^2 \geq 1 - n\, C^{-d}$$

for all the classes F_d^β and hence for the larger classes $\widetilde{H}_2^k([0,\,1]^d)$. The constant $C > 1$ depends on $\beta > 0$ or $k \in \mathbb{N}$, respectively, but of course does not depend on d or n. It easily follows from Theorem 4 that

$$e_n^+(F_d^\beta)^2 \geq 1 - n\,(1 + \min(1, \beta))^{-d}.$$

Therefore we prove intractability results for positive quadrature formulas. In Section 4 we discuss the conjectured lower bound (8) for arbitrary quadrature formulas.

2. Optimal Error Bounds and Other Extremal Problems

We begin with a definition of the classes F_d^β. Define $V_d^{\mathbb{C}}$ as the space of all complex trigonometric polynomials of degree at most 1 in each variable. Hence $V_d^{\mathbb{C}}$ is the set of all f of the form

$$f(x) = \sum_{h \in \{-1,0,1\}^d} a_h\, e^{2\pi i h \cdot x}.$$

We have $\dim(V_d^{\mathbb{C}}) = 3^d$, as a vector space over the complex numbers. For our problem it is enough to consider real valued polynomials. These are characterized by $a_h = \overline{a}_{-h}$ for all h. The real-valued elements of $V_d^{\mathbb{C}}$ form a vector space V_d with $\dim(V_d) = 3^d$, over $\mathbb{R}$. The space V_1 is generated by $e_1 = 1$, $e_2(x) = \cos(2\pi x)$, and $e_3(x) = \sin(2\pi x)$. For $\beta > 0$, we define a scalar product $(\,\cdot\,,\,\cdot\,)_\beta$ on V_1 by

$$(e_i, e_j)_\beta = 0 \quad \text{for } i \neq j, \qquad (e_1, e_1)_\beta = 1, \qquad (e_2, e_2)_\beta = (e_3, e_3)_\beta = \beta^{-1}.$$

The functions e_1, e_2 and e_3 are orthogonal for all $\beta > 0$ but orthonormal only for $\beta = 1$. For $\beta = 2$ we get the L_2-norm on V_1. The usual Sobolev-Hilbert norms (4) are obtained for special values of β. Indeed, we have

$$\|e_2\|^2_{W_2^k} = \|e_3\|^2_{W_2^k} = \frac{1}{2} \cdot \sum_{j=0}^{k} (2\pi)^j;$$

hence the W_2^k-norm is a β-norm with

$$\beta = 2 \cdot \left(\sum_{j=0}^{k} (2\pi)^j \right)^{-1}. \tag{9}$$

On the space V_d we define the tensor product (cross-) norm by

$$(f_1 \otimes \cdots \otimes f_d,\, g_1 \otimes \cdots \otimes g_d)_\beta := \prod_{l=1}^{d} (f_l, g_l)_\beta.$$

Observe that

$$I_d(f) = (f, 1)_\beta \qquad \text{and} \qquad \|1\|_\beta = 1,$$

for all $d \in \mathbb{N}$ and $\beta > 0$. Let F_d^β denote the unit ball of V_d with respect to the β-norm. We have $e(Q_0, F_d^\beta) = e_0(F_d^\beta) = 1$. It is clear that

$$F_d^{\beta_1} \subset F_d^{\beta_2} \qquad \text{if} \qquad \beta_1 \leq \beta_2.$$

If β and k are related as in (9) then F_d^β is a subset of $\widetilde{H}_2^k([0,\, 1]^d)$ and the norms $\|\cdot\|_\beta$ and $\|\cdot\|_{H_2^k}$ coincide.

We discuss optimal quadrature formulas for F_d^β and their connection to best n-term approximation. The number $e_n(F_d^\beta)$ is defined as the error of an optimal quadrature formula (1) for the unit ball in V_d. A Dirac functional $f \mapsto f(x_i)$ can be written in the form

$$f(x_i) = (\delta_{x_i}^\beta, f)_\beta$$

for all $f \in V_d$, where

$$\delta_{x_i}^\beta(x) = \prod_{l=1}^d (1 + \beta\, \cos(2\pi(x_i^l - x^l)))$$

with x_i^l and x^l being the lth component of the vector x_i and x. The function

$$(x, t) \mapsto (\delta_x^\beta, \delta_t^\beta)_\beta = \prod_{l=1}^d (1 + \beta\, \cos(2\pi(x^l - t^l))),$$

where $x, t \in [0,\, 1]^d$, is called the (reproducing) kernel of V_d with respect to the β-norm. Observe that the kernel is nonnegative iff $\beta \leq 1$. It is easy to check that

$$e(Q_n, F_d^\beta) = \left\| 1 - \sum_{i=1}^n c_i \delta_{x_i}^\beta \right\|_\beta \tag{10}$$

for Q_n of the form (1).

Remark 1. For $n = 1$ we obtain

$$e(Q_n, F_d^\beta)^2 = 1 - 2c_1(\delta_{x_1}^\beta, 1)_\beta + c_1^2(\delta_{x_1}^\beta, \delta_{x_1}^\beta)_\beta = 1 - 2c_1 + c_1^2\,(1+\beta)^d. \tag{11}$$

A quasi-Monte Carlo method has (by definition) a weight $c_1 = 1$, its error is given by (11) and is huge for large β.

An optimal quadrature formula for $n = 1$ has a weight

$$c_1 = (1+\beta)^{-d}$$

and error

$$e_1(F_d^\beta)^2 = 1 - (1+\beta)^{-d}.$$

We obtain

$$\lim_{\beta\to\infty} e_1(F_d^\beta) = 1.$$

For $n = 2^d$, we have $e_n(F_d^\beta) = 0$ independently of β. Indeed, if $d = 1$ then $Q_2(f) = \frac{1}{2}(f(0) + f(\frac{1}{2}))$ is exact for V_1. The tensor product (and quasi-Monte Carlo) method Q_n uses $n = 2^d$ evaluations and is exact on V_d, hence $e(Q_n, F_d^\beta) = 0$ and $e_n(F_d^\beta) = 0$ for $n = 2^d$.

From Lemma 4 in Sloan and Woźniakowski (1998) it follows that

$$e(Q_n, F_d^\beta)^2 \geq 1 - n\,(1+\beta)^{-d} \tag{12}$$

for quasi-Monte Carlo methods if $\beta \leq 1$, i.e., if the kernel of the Hilbert space is positive. We will prove later a lower bound for $e_n^+(F_d^\beta)$ which implies (12), see Theorem 4. The lower bound (12) cannot be true for $\beta > 1$ since $e_n(Q_n, F_d^\beta) = 0$ for $n = 2^d$ and a quasi-Monte Carlo method Q_n. This answers a question from Sloan and Woźniakowski (1998). ■

In view of (10) we can also say that $e_n(F_d^\beta)$ is the error of the best approximation of the function $1 \in V_d$ by functions of the type $\sum_{i=1}^n c_i \delta_{x_i}^\beta$,

$$e_n(F_d^\beta) = \inf_{x_i,\, c_i} \left\| 1 - \sum_{i=1}^n c_i \delta_{x_i}^\beta \right\|_\beta. \tag{13}$$

As we shall see in a moment, the optimal error bounds $e_n(F_d^\beta)$ for quadrature formulas are related to the solution of the following extremal problem for trigonometric polynomials. For given points $x_i \in \mathbb{R}^d$ find

$$f \in V_d \quad \text{with} \quad f(x_1) = \cdots = f(x_n) = 1 \quad \text{and} \quad \|f\|_\beta \ \text{ minimized.}$$

We define the numbers

$$g(n,d,\beta) = \sup_{x_1,\ldots,x_n} \inf\{\|f\|_\beta^2 \,:\, f \in V_d,\ f(x_1) = \cdots = f(x_n) = 1\}. \tag{14}$$

Our first lemma is a simple geometrical statement which we do not prove. Just observe that $\dfrac{(x,e)x}{(x,x)}$ is the projection of a vector e along the direction x and $\dfrac{(x,e)^2}{(x,x)}$ is the square of the length of this projection.

Lemma 1. *Assume that H is a Hilbert space with $e \in H$ and $\|e\| = 1$. Let $X \subset H$ be a set which contains each αx if $x \in X$ and $\alpha \in \mathbb{R}$. Then*

$$\sup_{x\in X,\, x\neq 0} \frac{(x,e)^2}{(x,x)} + \inf_{x\in X} \|e - x\|^2 = 1. \qquad ■$$

Also the next lemma is simple and well known.

Lemma 2. *Assume that H is a Hilbert space with $g_1, \dots, g_n \in H$ such that the linear system*

$$(f, g_i) = \alpha_i, \qquad i = 1, \dots, n \tag{15}$$

has a solution in H. Then (15) has a unique solution f^* with minimal norm and f^* is of the form $f^* = \sum_{i=1}^n c_i g_i$. ■

We now apply Lemma 1 to $e = 1$ and $H = V_d$ with a β-norm. For X we take the set of all $\sum_{i=1}^n c_i \delta_{x_i}^\beta$, where $\delta_{x_i}^\beta \in B_d^\beta = \{\delta_x^\beta \,:\, x \in [0,\, 1]^d\}$. Note that $B_d^\beta = B_1^\beta \otimes \cdots \otimes B_1^\beta$.

Theorem 1. *Let $d, n \in \mathbb{N}$ and $\beta > 0$. The numbers $g(n, d, \beta)$, see (14), and $e_n(F_d^\beta)$, see (2), are related by*

$$g(n, d, \beta) + e_n(F_d^\beta)^2 = 1. \qquad ■$$

Proof: Let $f^* \in V_d$ be the least square solution (with respect to the β-norm) of $f(x_i) = 1$, for $i = 1, \dots, n$. The abstract version is

$$(f, \delta_{x_i}^\beta) = 1, \qquad i = 1, \dots, n,$$

where $\delta_{x_i}^\beta \in B_d^\beta$. We know that $(1, \delta^\beta) = 1$ for all $\delta^\beta \in B_d^\beta$, hence f^* is the orthogonal projection of 1 on span $\{\delta_{x_1}^\beta, \dots, \delta_{x_n}^\beta\}$. Hence,

$$\|f^*\|_\beta^2 = 1 - \inf_{c_i} \|1 - \sum_{i=1}^n c_i \delta_{x_i}^\beta\|_\beta^2.$$

This is true for any given $x_1, \dots, x_n$. We take the supremum with respect to x_i and obtain

$$g(n, d, \beta) = 1 - \inf_{c_i, x_i} \|1 - \sum_{i=1}^n c_i \delta_{x_i}^\beta\|_\beta^2 = 1 - e_n(F_d^\beta)^2,$$

as claimed. ■

Theorem 2. *Let $d, n \in \mathbb{N}$ and $\beta > 0$ and $\Phi > 0$. Then the following statements are equivalent:*

(a) *$g(n, d, \beta) \le \Phi$;*
(b) *$e_n(F_d^\beta)^2 \ge 1 - \Phi$;*
(c) *any matrix $A \in \mathbb{R}^{n \times n}$ with entries a_{ij} defined by*

$$a_{ij} = \left(\prod_{l=1}^d 1 + \beta \cos(\alpha_i^l - \alpha_j^l) \right) - \frac{1}{\Phi} \quad \textit{with } \alpha_i^l \in \mathbb{R},$$

is positive semidefinite, i.e., the eigenvalues of A are nonnegative;

(d) *any linear system of the form*

$$\sum_{i=1}^{n} c_i \prod_{l=1}^{d} (1+\beta \cos(\alpha_i^l - \alpha_j^l)) = 1, \tag{16}$$

$j = 1, \ldots, n$, has a solution c with $\sum_{i=1}^{n} c_i \le \Phi$.

Proof: It is clear that (a) and (b) are equivalent by Theorem 1. By Lemma 1 and (13) we know that

$$e_n(F_d^\beta)^2 = 1 - \sup \left\{ \frac{(x,1)_\beta^2}{(x,x)_\beta} \ : \ x = \sum_{i=1}^{n} c_i \delta_{x_i}^\beta, \ \delta_{x_i}^\beta \in B_d^\beta, \ c_i \in \mathbb{R}, \ x \neq 0 \right\}. \tag{17}$$

We now modify this formula. We write vectors in V_1 with respect to the basis $(e_1,\, e_2,\, e_3)$, hence $1 = e_1 = (1, 0, 0)$ and

$$B_1^\beta = \{(1,\ \beta \cos \alpha,\ \beta \sin \alpha) \ : \ \alpha \in \mathbb{R}\}\,.$$

Each $\delta_{x_i}^\beta \in B_d^\beta$ is of the form

$$\delta_{x_i}^\beta = \delta_{x_i^1}^\beta \otimes \cdots \otimes \delta_{x_i^d}^\beta, \qquad \delta_{x_i^l}^\beta = (1,\ \beta \cos \alpha_i^l,\ \beta \sin \alpha_i^l)$$

with

$$(\delta_{x_i}^\beta, \delta_{x_j}^\beta)_\beta = \prod_{l=1}^{d} \left(1 + \beta\ \cos(\alpha_i^l - \alpha_j^l)\right).$$

In (17) we have $(x,1)_\beta = \sum_{i=1}^{n} c_i$ and we obtain

$$e_n(F_d^\beta)^2 = 1 - \sup \frac{\left(\sum_{i=1}^{n} c_i\right)^2}{\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j \prod_{l=1}^{d} \left(1 + \beta\ \cos(\alpha_i^l - \alpha_j^l)\right)}.$$

If we define $0/0 = 0$ then we can allow arbitrary c_i and α_i^l. Hence the second statement is equivalent to

$$\left(\sum_{i=1}^{n} c_i\right)^2 \le \Phi \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j \prod_{l=1}^{d} \left(1 + \beta\ \cos(\alpha_i^l - \alpha_j^l)\right).$$

The last inequality is equivalent to Statement (c).

Finally, we prove that (a) and (d) are equivalent. Using Lemma 2 and the definition of $g(n, d, \beta)$ we see that (a) is equivalent to the following. Each linear system $\sum_{i=1}^{n} c_i (\delta_{x_i}^\beta, \delta_{x_j}^\beta)_\beta = 1$ for $j = 1, \ldots, n$ has a solution and

$$\left\| \sum_{i=1}^{n} c_i \delta_{x_i}^\beta \right\|_\beta^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j\, (\delta_{x_i}^\beta, \delta_{x_j}^\beta)_\beta = \sum_{i=1}^{n} c_i \le \Phi. \qquad \blacksquare$$

3. Quadrature Formulas with Positive Weights

By definition of the $e_n^+(F_d^\beta)$ we have

$$e_n^+(F_d^\beta) = \inf\left\{ \left\| 1 - \sum_{i=1}^n c_i \delta_{x_i}^\beta \right\|_\beta \,:\, \delta_{x_i}^\beta \in B_d^\beta,\ c_i \ge 0 \right\}.$$

We say that the $(\delta_{x_1}^\beta, \dots, \delta_{x_m}^\beta)$ are admissible if

$$\left\| 1 - \sum_{i=1}^m c_i^* \delta_{x_i}^\beta \right\|_\beta = \inf_{c_i \in \mathbb{R}} \left\| 1 - \sum_{i=1}^m c_i \delta_{x_i}^\beta \right\|_\beta$$

implies $c_i^* \ge 0$ for $i = 1, \dots, m$. This means that an optimal quadrature formula Q_m with knots $x_1, \dots, x_m$ has nonnegative weights. If $m = 1$ then each $\delta_{x_1}^\beta$ is admissible. It can be checked that the same is true for $m = 2$, but already in the case $m = 3$ and $d = 2$ there are knots $x_1, \dots, x_m$ such that the $\delta_{x_i}^\beta$ are not admissible. The following lemma is known from optimization theory, see e.g. Luenberger (1969, p. 71), but also can be proved in a straightforward way.

Lemma 3.

$$e_n^+(F_d^\beta) = \inf\left\{ \left\| 1 - \sum_{i=1}^m c_i \delta_{x_i}^\beta \right\|_\beta \,:\, m \le n,\ c_i \in \mathbb{R},\ (\delta_{x_1}^\beta, \dots, \delta_{x_m}^\beta) \textit{ are admissible} \right\}. \qquad \blacksquare$$

Using this we obtain two equivalent statements which can be proved similarly as in Theorem 2.

Theorem 3. *Let $d, n \in \mathbb{N}$ and $\beta > 0$ and $\Phi > 0$. Then the following statements are equivalent:*

(a) $e_n^+(F_d^\beta)^2 \ge 1 - \Phi$;

(b) *Any linear system of the form*

$$\sum_{i=1}^m c_i \prod_{l=1}^d (1 + \beta \cos(\alpha_i^l - \alpha_j^l)) = 1, \tag{18}$$

$j = 1, \dots, m$, with $m \le n$ and a solution that satisfies $c_i \ge 0$ for all i fulfills $\sum_{i=1}^m c_i \le \Phi$. $\blacksquare$

Consider the linear system (18) for $\beta \le 1$ and $c_i \ge 0$. Let $a_{ij} = \prod_{l=1}^d (1 + \beta \cos(\alpha_i^l - \alpha_j^l))$. The diagonal elements are $a_{ii} = (1 + \beta)^d$ and the off-diagonal elements a_{ij} are at least $(1-\beta)^d$. Summing up all the equations we get

$$\begin{aligned} m = \sum_{i,j=1}^m c_i a_{ij} &= \sum_{i=1}^m c_i \Big(\sum_{j=1}^m a_{ij} \Big) \\ &\geq \sum_{i=1}^m c_i \Big((1+\beta)^d + (m-1)(1-\beta)^d \Big) . \end{aligned}$$

This yields

$$\sum_{i=1}^n c_i \leq \frac{m}{(1+\beta)^d + (m-1)(1-\beta)^d} \leq \frac{n}{(1+\beta)^d + (n-1)(1-\beta)^d} .$$

Using Theorem 3 and the fact that $F_d^{\beta_1} \subset F_d^{\beta_2}$ for $\beta_1 \leq \beta_2$ we obtain the following lower bound.

Theorem 4. *Let $d, n \in \mathbb{N}$ and $\beta > 0$. Define $\tilde\beta = \min(\beta, 1)$. Then*

$$e_n^+(F_d^\beta)^2 \geq 1 - n \cdot \Big((1+\tilde\beta)^d + (n-1)(1-\tilde\beta)^d \Big)^{-1} . \qquad \blacksquare \tag{19}$$

Remark 2. Theorem 3 looks like a lower bound for $e_n^+(F_d^\beta)$ due to statement (a). The complete statement is the equivalence of (a) and (b), however, and hence Theorem 3 can also be used to prove upper bounds. For $\beta = 1$ we obtain

$$e_n^+(F_d^1)^2 = 1 - n\, 2^{-d}, \qquad n = 1, \ldots, 2^d.$$

The lower bound follows from (19), the upper bound follows from Theorem 3. Assume that $n \leq 2^d$. Then we can choose the $\alpha_i^l \in \{0, \pi\}$ in such a way that for each pair (i, j) with $i \neq j$ there is an l such that $a_i^l \neq a_j^l$ and hence

$$\prod_{l=1}^d (1 + \beta \cos(\alpha_i^l - \alpha_j^l)) = 0.$$

Hence the linear system (18) is the trivial system $c_i \cdot 2^d = 1$, for all i, and we obtain $\sum_{i=1}^n c_i = n\, 2^{-d}$. Therefore the equivalent conditions of Theorem 3 cannot be true for a $\Phi < n\, 2^{-d}$.

4. Conjectures

We do not know whether arbitrary quadrature formulas are better than positive quadrature formulas. We tried to prove that

$$e_n^+(F_d^\beta) = e_n(F_d^\beta) \tag{20}$$

but did not succeed. For $\beta = 1$ we conjecture that

$$e_n^+(F_d^\beta)^2 = e_n(F_d^\beta)^2 = 1 - n\,2^{-d}.$$

Due to Theorem 2 we get equivalent conjectures about an extremal problem for trigonometric polynomials and about positive semidefinite matrices:

1. For any given points $x_1, \ldots, x_n \in [0, 1]^d$ there is a trigonometric polynomial of degree one in each variable such that $f(x_1) = \cdots = f(x_n) = 1$ and $\|f\|_\beta \leq 2^{-d/2} \cdot n^{1/2}$, where $\beta \geq 1$. In particular, we conjecure this for the L_2-norm, where $\beta = 2$.
2. Any matrix $A \in \mathbb{R}^{n \times n}$ with entries a_{ij} defined by

$$a_{ij} = \left(\prod_{l=1}^{d} \frac{1 + \cos(\alpha_i^l - \alpha_j^l)}{2} \right) - \frac{1}{n}$$

   is positive semidefinite.[3]

Remark 3. It seems that these conjectures are related to the Hadamard product of matrices, see Horn (1990), and also to positive definite functions, see Stewart (1976). We performed some numerical experiments and obviously did not find a counterexample to the above conjectures. It would be very interesting to have general results for which classes F we have $e_n^+(F) = e_n(F)$.

5. Weighted Norms

If d is large then often some variables are "more important" than others. To model such a situation we consider weighted tensor product norms, where different norms are taken for the different variables. Weighted tensor product norms were recently studied in Sloan, Woźniakowski (1998). The authors concentrate on quasi-Monte Carlo formulas (with equal weights $c_i = 1/n$) and prove upper as well as lower bounds with respect to weighted discrepancies. In the paper of Wasilkowski, Woźniakowski (1998) the authors study general weighted tensor product problems. For the problem of numerical integration they prove upper bounds by means of a weighted tensor product algorithm.

First we generalize the spaces $H_2^k([0, 1]^d)$ and F_d^β. We now assume that $k \in \mathbb{N}^d$ or $\beta \in \mathbb{R}_+^d$ and define a normed space $H_2^k([0, 1]^d)$ by

$$\|f_1 \otimes \cdots \otimes f_d\|_{H_2^k} = \prod_{l=1}^{d} \|f_l\|_{H_2^{k_l}}.$$

[3] This conjecture was stated as an open problem in the NA Digest in November 1997. So far, no solution seems to be known.

Similarly, we define a class F_d^β by the norm

$$\|f_1 \otimes \cdots \otimes f_d\|_\beta = \prod_{l=1}^{d} \|f_l\|_{\beta_l}$$

on V_d. All the previous results can be modified to this more general situation. We obtain

$$\delta_{x_i}^\beta(x) = \prod_{l=1}^{d} (1 + \beta_l \, \cos(2\pi(x_i^l - x^l)))$$

and

$$B_d^\beta = B_1^{\beta_1} \otimes \cdots \otimes B_1^{\beta_d}.$$

We only state the lower bound for positive formulas, analogously to Theorem 3 and Theorem 4.

Theorem 5. *Let $d, n \in \mathbb{N}$ and $\beta \in \mathbb{R}_+^d$ and $\Phi > 0$. Then the following statements are equivalent:*

(a) $e_n^+(F_d^\beta)^2 \geq 1 - \Phi$*;*

(b) *Any linear system of the form*

$$\sum_{i=1}^{m} c_i \prod_{l=1}^{d} (1 + \beta_l \cos(\alpha_i^l - \alpha_j^l)) = 1,$$

$j = 1, \ldots, m$, *with* $m \leq n$ *and a solution that satisfies* $c_i \geq 0$ *for all* i *fulfills* $\sum_{i=1}^m c_i \leq \Phi$.

Define $\tilde{\beta}_l = \min(\beta_l, 1)$. *Then*

$$e_n^+(F_d^\beta)^2 \geq 1 - n \cdot \left(\prod_{l=1}^{d} (1 + \tilde{\beta}_l) + (n-1) \prod_{l=1}^{d} (1 - \tilde{\beta}_l) \right)^{-1}$$

and, in particular,

$$e_n^+(F_d^\beta)^2 \geq 1 - n \cdot \prod_{l=1}^{d} (1 + \tilde{\beta}_l)^{-1}. \tag{21}$$

Remark 4. Assume that a sequence $\{\beta_l\}_{l=1}^\infty$ is given. Then we obtain a sequence of classes F_d^β, where $d \in \mathbb{N}$. The lower bound in (21) does not converge (for fixed n and $d \to \infty$) to 1 iff $\lim_{d\to\infty} \prod_{l=1}^d (1 + \beta_l) < \infty$ or, equivalently, iff

$$\sum_{l=1}^{\infty} \beta_l < \infty. \tag{22}$$

This lower bound is optimal, i.e., the numbers

$$n^+(d, \varepsilon) = \min\{n \, : \, e_n^+(F_d^\beta) \leq \varepsilon\}$$

are bounded from above by $n^+(\varepsilon) < \infty$ if and only if (22) holds. This can be proved in a nonconstructive way, along the lines of Sloan, Woźniakowski (1988). The proof goes as follows. Let $Q_{n,d}(x_1, \dots, x_n)$ denote the quasi-Monte Carlo method

$$Q_{n,d}(f) = \frac{1}{n} \sum_{i=1}^{n} f(x_i) \tag{23}$$

and let

$$e^{\beta}(Q_{n,d}(x_1, \dots, x_n)) = \left(-1 + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} (\delta_{x_i}^{\beta}, \delta_{x_j}^{\beta})_{\beta} \right)^{1/2} \tag{24}$$

be its error for the class F_d^{β}, see (10). One can compute the average

$$e_n^{\mathrm{avg}}(F_d^{\beta}) = \left(\int_{[0,1]^{nd}} e^{\beta}(Q_{n,d}(x_1, \dots, x_n))^2 \; dx_1 \dots dx_n \right)^{1/2}$$

over all sample points x_i. Define

$$\varrho_d^{\beta} = \frac{\int_{[0,1]^d} (\delta_x^{\beta}, \delta_x^{\beta}) \, dx}{\int_{[0,1]^{2d}} (\delta_x^{\beta}, \delta_t^{\beta}) \, dx \, dt}.$$

Then it follows from Sloan, Woźniakowski (1998) that

$$e_n^{\mathrm{avg}}(F_d^{\beta}) = \frac{\sqrt{\varrho_d^{\beta} - 1}}{\sqrt{n}}.$$

In our case we easily obtain

$$e_n^{\mathrm{avg}}(F_d^{\beta})^2 = \frac{\left(\prod_{l=1}^{d} (1 + \beta_l) \right) - 1}{n}. \tag{25}$$

The mean value theorem implies

$$e_n^{+}(F_d^{\beta})^2 \le \frac{\left(\prod_{l=1}^{d} (1 + \beta_l) \right) - 1}{n}.$$

Hence, $e_n^{+}(F_d^{\beta}) \le C \, n^{-1/2}$ with C independent of d holds iff $\sum_{i=1}^{\infty} \beta_i < \infty$.

A disadvantage of quasi-Monte Carlo methods (23) with the average worst case error (25) is the following: For small n the error can be much larger than 1 which is the error of the trivial formula $Q_0(f) = 0$. Therefore we modify (23) and consider formulas

$$Q_{n,d}(f) = c \sum_{i=1}^{n} f(x_i),$$

where $c > 0$. For its error we obtain

$$e^{\beta}(Q_{n,d}(x_1, \dots, x_n))^2 = 1 - 2nc + c^2 \sum_{i=1}^{n} \sum_{j=1}^{n} (\delta_{x_i}^{\beta}, \delta_{x_j}^{\beta})_{\beta}$$

and one can again compute the average over all sets of knots. The optimal c is given by

$$c^* = \frac{1}{n - 1 + \prod_{l=1}^{d}(1+\beta_l)} \tag{26}$$

and with this c^* we obtain an average error

$$e_n^{\mathrm{avg}}(F_d^\beta)^2 = \frac{\left(\prod_{l=1}^{d}(1+\beta_l)\right) - 1}{n - 1 + \prod_{l=1}^{d}(1+\beta_l)}, \tag{27}$$

which is always smaller than 1. Comparing (25) with (27) we note that the modified weights (26) give better bounds for all n. For large n, however, the improvement is negligible.

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