Math. Program., Ser. A
DOI 10.1007/s10107-016-1043-1

FULL LENGTH PAPER

Convergence analysis for Lasserre's measure-based hierarchy of upper bounds for polynomial optimization

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Received: 25 November 2014 / Accepted: 16 June 2016

Abstract We consider the problem of minimizing a continuous function f over a compact set $\mathbf{K}$. We analyze a hierarchy of upper bounds proposed by Lasserre (SIAM J Optim 21(3):864–885, 2011), obtained by searching for an optimal probability density function h on $\mathbf{K}$ which is a sum of squares of polynomials, so that the expectation $\int_{\mathbf{K}} f(x)h(x)dx$ is minimized. We show that the rate of convergence is no worse than $O(1/\sqrt{r})$, where $2r$ is the degree bound on the density function. This analysis applies to the case when f is Lipschitz continuous and $\mathbf{K}$ is a full-dimensional compact set satisfying some boundary condition (which is satisfied, e.g., for convex bodies). The rth upper bound in the hierarchy may be computed using semidefinite programming if f is a polynomial of degree d, and if all moments of order up to $2r+d$ of the Lebesgue measure on $\mathbf{K}$ are known, which holds, for example, if $\mathbf{K}$ is a simplex, hypercube, or a Euclidean ball.

Keywords Polynomial optimization · Semidefinite optimization · Lasserre hierarchy

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Published online: 12 July 2016

Mathematics Subject Classification 90C22 · 90C26 · 90C30

1 Introduction and preliminaries

1.1 Background

We consider the problem of minimizing a continuous function $f : \mathbb{R}^n \to \mathbb{R}$ over a compact set $\mathbf{K} \subseteq \mathbb{R}^n$. That is, we consider the problem of computing the parameter:

$$f_{\min,\mathbf{K}} := \min_{x\in\mathbf{K}} f(x).$$

Our main interest will be in the case where f is a polynomial, and $\mathbf{K}$ is defined by polynomial inequalities and equations. For such problems, active research has been done in recent years to construct tractable hierarchies of (upper and lower) bounds for $f_{\min,\mathbf{K}}$, based on using sums of squares of polynomials and semidefinite programming (SDP). The starting point is to reformulate $f_{\min,\mathbf{K}}$ as the problem of finding the largest scalar λ for which the polynomial $f-\lambda$ is nonnegative over $\mathbf{K}$ and then to replace the hard positivity condition by a suitable sum of squares decomposition. Alternatively, one may reformulate $f_{\min,\mathbf{K}}$ as the problem of finding a probability measure μ on K minimizing the integral $\int_{\mathbf{K}} f d\mu$. These two dual points of view form the basis of the approach developed by Lasserre [16] for building hierarchies of semidefinite programming based lower bounds for $f_{\min,\mathbf{K}}$ (see also [17,20] for an overview). Asymptotic convergence to $f_{\min,\mathbf{K}}$ holds (under some mild conditions on the set $\mathbf{K}$). Moreover, error estimates have been shown in [25,27] when $\mathbf{K}$ is a general basic closed semi-algebraic set, and in [5–8,10,12,28] for simpler sets like the standard simplex, the hypercube and the unit sphere. In particular, [27] shows that the rate of convergence of the hierarchy of lower bounds based on Schmüdgen's Positivstellensatz is in the order $O(1/\sqrt[c]{2r})$, while [25] shows a convergence rate in $O(1/\sqrt[c']{\log(2r/c')})$ for the (weaker) hierarchy of bounds based on Putinar's Positivstellensatz. Here, c, c' are constants (not explicitly known) depending only on $\mathbf{K}$, and $2r$ is the selected degree bound. For the case of the hypercube, [5] shows (using Bernstein approximations) a convergence rate in $O(1/r)$ for the lower bounds based on Schmüdgen's Positivstellensatz.

On the other hand, by selecting suitable probability measures on $\mathbf{K}$, one obtains upper bounds for $f_{\min,\mathbf{K}}$. This approach has been investigated, in particular, for minimization over the standard simplex and when selecting some discrete distributions over the grid points in the simplex. The multinomial distribution is used in [7,24] to show convergence in $O(1/r)$ and the multivariate hypergeometric distribution is used in [8] to show convergence in $O(1/r^2)$ for quadratic minimization over the simplex (and in the general case assuming a rational minimizer exists).

Additionnally, Lasserre [18] shows that, if we fix any measure μ on $\mathbf{K}$, then it suffices to search for a polynomial density function h which is a sum of squares and minimizes the integral $\int_{\mathbf{K}} fh d\mu$ in order to compute the minimum $f_{\min,\mathbf{K}}$ over $\mathbf{K}$ (see Theorem 1 below). By adding degree constraints on the polynomial density h we get a hierarchy of upper bounds for $f_{\min,\mathbf{K}}$ and our main objective in this paper is to analyze the quality of this hierarchy of upper bounds for $f_{\min,\mathbf{K}}$. Next we will recall this result of Lasserre [18] and then we describe our main results.

1.2 Lasserre's hierarchy of upper bounds

Throughout, $\mathbb{R}[x] = \mathbb{R}[x_1, \ldots, x_n]$ is the set of polynomials in n variables with real coefficients, and $\mathbb{R}[x]_r$ is the set of polynomials with degree at most r. $\Sigma[x]$ is the set of sums of squares of polynomials, and $\Sigma[x]_r = \Sigma[x] \cap \mathbb{R}[x]_{2r}$ consists of all sums of squares of polynomials with degree at most $2r$. We now recall the result of Lasserre [18], which is based on the following characterization for nonnegative continuous functions on a compact set $\mathbf{K}$.

Theorem 1 [18, Theorem 3.2] *Let $\mathbf{K} \subseteq \mathbb{R}^n$ be compact, let μ be an arbitrary finite Borel measure supported by $\mathbf{K}$, and let f be a continuous function on $\mathbb{R}^n$. Then, f is nonnegative on $\mathbf{K}$ if and only if*

$$\int_{\mathbf{K}} g^2 f d\mu \geq 0 \ \ \forall g \in \mathbb{R}[x].$$

Therefore, the minimum of f over $\mathbf{K}$ can be expressed as

$$f_{\min,\mathbf{K}} = \inf_{h \in \Sigma[x]} \int_{\mathbf{K}} hf d\mu \ \ \text{s.t.} \ \int_{\mathbf{K}} h d\mu = 1. \tag{1}$$

Note that formula (1) does not appear explicitly in [18, Theorem 3.2], but one can derive it easily from it. Indeed, one can write $f_{\min,\mathbf{K}} = \sup \{\lambda : f(x) - \lambda \geq 0 \text{ over } \mathbf{K}\}$. Then, by the first part of Theorem 1, we have $f_{\min,\mathbf{K}} = \sup \left\{\lambda : \int_{\mathbf{K}} h(f - \lambda)d\mu \geq 0 \ \forall h \in \Sigma[x]\right\}$. As $\int_{\mathbf{K}} h(f - \lambda)d\mu = \int_{\mathbf{K}} hf d\mu - \lambda \int_{\mathbf{K}} h d\mu$, after normalizing $\int_{\mathbf{K}} h d\mu = 1$, we can conclude (1).

If we select the measure μ to be the Lebesgue measure in Theorem 1, then we obtain the following reformulation for $f_{\min,\mathbf{K}}$, which we will consider in this paper:

$$f_{\min,\mathbf{K}} = \inf_{h \in \Sigma[x]} \int_{\mathbf{K}} h(x)f(x)dx \ \ \text{s.t.} \ \int_{\mathbf{K}} h(x)dx = 1.$$

By bounding the degree of the polynomial $h \in \Sigma[x]$ by $2r$, we can define the parameter:

$$\underline{f}_{\mathbf{K}}^{(r)} := \inf_{h \in \Sigma[x]_r} \int_{\mathbf{K}} h(x)f(x)dx \ \ \text{s.t.} \ \int_{\mathbf{K}} h(x)dx = 1. \tag{2}$$

Clearly, the inequality $f_{\min,\mathbf{K}} \leq \underline{f}_{\mathbf{K}}^{(r)}$ holds for all $r \in \mathbb{N}$. Lasserre [18] gives conditions under which the infimum is attained in the program (2).

Theorem 2 [18, Theorems 4.1 and 4.2] *Assume $\mathbf{K} \subseteq \mathbb{R}^n$ is compact and has non-empty interior and let f be a polynomial. Then, the program (2) has an optimal solution for every $r \in \mathbb{N}$ and*

$$\lim_{r\to\infty} \underline{f}_{\mathbf{K}}^{(r)} = f_{\min,\mathbf{K}}.$$

We now recall how to compute the parameter $\underline{f}_{\mathbf{K}}^{(r)}$ in terms of the moments $m_\alpha(\mathbf{K})$ of the Lebesgue measure on $\mathbf{K}$, where

$$m_\alpha(\mathbf{K}) := \int_{\mathbf{K}} x^\alpha dx \quad \text{for } \alpha \in \mathbb{N}^n,$$

and $x^\alpha := \prod_{i=1}^n x_i^{\alpha_i}$.

Let $N(n,r) := \{\alpha \in \mathbb{N}^n : \sum_{i=1}^n \alpha_i \le r\}$, and suppose $f(x) = \sum_{\beta\in N(n,d)} f_\beta x^\beta$ has degree d. If we write $h \in \Sigma[x]_r$ as $h(x) = \sum_{\alpha\in N(n,2r)} h_\alpha x^\alpha$, then the parameter $\underline{f}_{\mathbf{K}}^{(r)}$ from (2) can be reformulated as follows:

$$\begin{aligned} \underline{f}_{\mathbf{K}}^{(r)} = \min \; & \sum_{\beta\in N(n,d)} f_\beta \sum_{\alpha\in N(n,2r)} h_\alpha m_{\alpha+\beta}(\mathbf{K}) \\ \text{s.t.} \; & \sum_{\alpha\in N(n,2r)} h_\alpha m_\alpha(\mathbf{K}) = 1, \\ & \sum_{\alpha\in N(n,2r)} h_\alpha x^\alpha \in \Sigma[x]_r. \end{aligned} \tag{3}$$

Hence, if we know the moments $m_\alpha(\mathbf{K})$ for all $\alpha \in \mathbb{N}^n$ with $|\alpha| := \sum_{i=1}^n \alpha_i \le d + 2r$, then we can compute the parameter $\underline{f}_{\mathbf{K}}^{(r)}$ by solving the semidefinite program (3) which involves a LMI of size $\binom{n+2r}{2r}$. So the bound $\underline{f}_{\mathbf{K}}^{(r)}$ can be computed in polynomial time for fixed d and r (to any fixed precision).

When $\mathbf{K}$ is the standard simplex $\Delta_n = \{x \in \mathbb{R}^n_+ : \sum_{i=1}^n x_i \le 1\}$, the unit hypercube $\mathbf{Q}_n = [0,1]^n$, or the unit ball $B_1(0) = \{x \in \mathbb{R}^n : \|x\| \le 1\}$, there exist explicit formulas for the moments $m_\alpha(\mathbf{K})$. Namely, for the standard simplex, we have

$$m_\alpha(\Delta_n) = \frac{\prod_{i=1}^n \alpha_i!}{(|\alpha|+n)!}, \tag{4}$$

see e.g., [15, Eq. (2.4)] or [13, Eq. (2.2)]. From this one can easily calculate the moments for the hypercube $\mathbf{Q}_n$:

$$m_\alpha(\mathbf{Q}_n) = \int_{\mathbf{Q}_n} x^\alpha dx = \prod_{i=1}^n \int_0^1 x_i^{\alpha_i} dx_i = \prod_{i=1}^n \frac{1}{\alpha_i+1}.$$

To state the moments for the unit Euclidean ball,

use the notation $[n] := \{1,\ldots,n\}$, the Euler gamma function $\Gamma(\cdot)$, and the notation for the double factorial of an integer k:

$$k!! = \begin{cases} k\cdot(k-2)\cdots 3\cdot 1, & \text{if } k>0 \text{ is odd,} \\ k\cdot(k-2)\cdots 4\cdot 2, & \text{if } k>0 \text{ is even,} \\ 1 & \text{if } k=0 \text{ or } k=-1. \end{cases}$$

In terms of this notation, the moments for the unit Euclidean ball are given by:

$$m_\alpha(B_1(0)) = \begin{cases} \frac{\pi^{n/2}\prod_{i=1}^n(\alpha_i-1)!!}{\Gamma\left(1+\frac{n+|\alpha|}{2}\right)2^{|\alpha|/2}} = \frac{\pi^{(n-1)/2}2^{(n+1)/2}\prod_{i=1}^n(\alpha_i-1)!!}{(n+|\alpha|)!!} & \text{if } \alpha_i \text{ is even for all } i\in[n], \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

One may prove relation (5) using

$$\int_{B_1(0)} x^\alpha dx = \frac{1}{\Gamma(1+(n+|\alpha|)/2)}\int_{\mathbb{R}^n} x^\alpha \exp\left(-\|x\|^2\right) dx$$

(see, e.g., [19, Theorem 2.1]), together with the fact (see, e.g., page 872 in [18]) that

$$\int_{-\infty}^{+\infty} t^p \exp\left(-t^2/2\right) dt = \begin{cases} \sqrt{2\pi}(p-1)!! & \text{if } p \text{ is even,} \\ 0 & \text{if } p \text{ is odd,} \end{cases}$$

and the identity $\Gamma(1+\frac{k}{2}) = \frac{k!!}{2^{(k+1)/2}}\sqrt{\pi}$ for all integers $k \in \mathbb{N}$ (see e.g., [1, Sect. 6.1.12]).

For a general polytope $\mathbf{K} \subseteq \mathbb{R}^n$, it is a hard problem to compute the moments $m_\alpha(\mathbf{K})$. In fact, the problem of computing the volume of polytopes of varying dimensions is already #P-hard [11]. On the other hand, any polytope $\mathbf{K} \subseteq \mathbb{R}^n$ can be triangulated into finitely many simplices (see e.g., [9]) so that one could use (4) to obtain the moments $m_\alpha(\mathbf{K})$ of $\mathbf{K}$. The complexity of this method depends on the number of simplices in the triangulation. However, this number can be exponentially large (e.g., for the hypercube) and the problem of finding the smallest possible triangulation of a polytope is NP-hard, even in fixed dimension $n = 3$ (see e.g., [9]).

Example

Consider the minimization of the Motzkin polynomial $f(x_1, x_2) = x_1^4x_2^2 + x_1^2x_2^4 - 3x_1^2x_2^2 + 1$ over the hypercube $\mathbf{K} = [-2, 2]^2$, which has four global minimizers at the points $(\pm 1, \pm 1)$, and $f_{\min,\mathbf{K}} = 0$. Figure 1 shows the computed optimal sum of squares density function h^*, for $r = 12$, corresponding to $\underline{f}_{\mathbf{K}}^{(12)} = 0.406076$. We observe that the optimal density h^* shows four peaks at the four global minimizers and thus, it appears to approximate the density of a convex combination of the Dirac measures at the four minimizers.

We will present several additional numerical examples in Sect. 4.

1.3 Our main results

In this paper we analyze the quality of the upper bounds $\underline{f}_{\mathbf{K}}^{(r)}$ from (2) for the minimum $f_{\min,\mathbf{K}}$ of f over K. Our main result is an upper bound for the range $\underline{f}_{\mathbf{K}}^{(r)} - f_{\min,\mathbf{K}}$, which applies to the case when f is Lipschitz continuous on $\mathbf{K}$ and when $\mathbf{K}$ is a

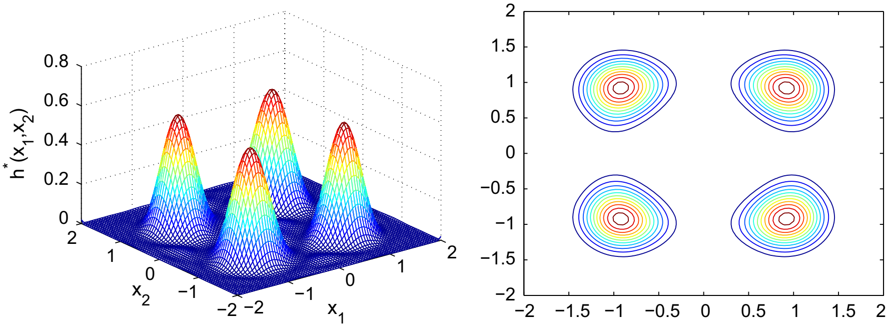

Fig. 1 Graph and *contour plot* of $h^*(x)$ on $[-2, 2]^2$ ($r = 12$ and $\deg(h^*) = 24$) for the Motzkin polynomial

full-dimensional compact set satisfying the additional condition from Assumption 1, see Theorem 3 below. We will use throughout the following notation about the set $\mathbf{K}$.

We let $D(\mathbf{K}) = \max_{x,y\in\mathbf{K}} \|x - y\|^2$ denote the (squared) diameter of the set $\mathbf{K}$, where $\|x\| = \sqrt{\sum_{i=1}^n x_i{}^2}$ is the ℓ_2-norm. Moreover, $w_{\min}(\mathbf{K})$ is the minimal width of $\mathbf{K}$, which is the minimum distance between two distinct parallel supporting hyperplanes of $\mathbf{K}$. Throughout, $B_\epsilon(a) := \{x \in \mathbb{R}^n : \|x - a\| \le \epsilon\}$ denotes the Euclidean ball centered at $a \in \mathbb{R}^n$ and with radius $\epsilon > 0$. With γ_n denoting the volume of the n-dimensional unit ball, the volume of the ball $B_\epsilon(a)$ is given by $\mathrm{vol}B_\epsilon(a) = \epsilon^n\gamma_n$.

We now formulate our geometric assumption about the set $\mathbf{K}$ which says (roughly) that around any point $a \in \mathbf{K}$ there is a ball intersecting a constant fraction of the unit ball.

Assumption 1 For all points $a \in \mathbf{K}$ there exist constants $\eta_\mathbf{K} > 0$ and $\epsilon_\mathbf{K} > 0$ such that

$$\mathrm{vol}(B_\epsilon(a) \cap \mathbf{K}) \ge \eta_\mathbf{K}\mathrm{vol}B_\epsilon(a) = \eta_\mathbf{K}\epsilon^n\gamma_n \quad \text{for all } 0 < \epsilon \le \epsilon_\mathbf{K}. \tag{6}$$

Note that Assumption 1 implies that the set $\mathbf{K}$ has positive Lebesgue density at all points $a \in \mathbf{K}$. For all sets $\mathbf{K}$ satisfying Assumption 1, we also define the parameter

$$r_\mathbf{K} := \max\left\{\frac{D(\mathbf{K})e}{2\epsilon_\mathbf{K}^3}, n\right\} \text{ if } \epsilon_\mathbf{K} \le 1, \quad \text{and } r_\mathbf{K} := \frac{D(\mathbf{K})e}{2} \text{ if } \epsilon_\mathbf{K} \ge 1. \tag{7}$$

Here, $e = 2.71828...$ denotes the base of the natural logarithm. Note that the parameters $\eta_\mathbf{K}$, $\epsilon_\mathbf{K}$ and $r_\mathbf{K}$ depend not only on the set $\mathbf{K}$ but also on the point $a \in \mathbf{K}$; we omit the dependance on a to simplify notation. Assumption 1 will be used in the case when the point a is a global minimizer in $\mathbf{K}$ of the polynomial to be analyzed.

For instance, convex bodies and, more generally, compact star-shaped sets satisfy Assumption 1 (see Sect. 5.1). We now give an example of a set $\mathbf{K}$ that does not satisfy Assumption 1 and refer to Sect. 5.1 for more discussion about Assumption 1.

Example 1 Consider the following set $\mathbf{K} \subseteq \mathbb{R}^2$, displayed in Fig. 2:

$$\mathbf{K} = \{x \in \mathbb{R}^2 : x \ge 0, (x_1 - 1)^2 + (x_2 - 1)^2 \ge 1\}.$$

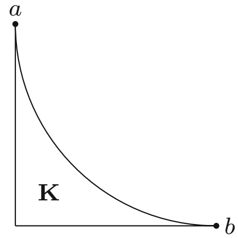

Fig. 2 This set $\mathbf{K}$ does not satisfy Assumption 1 at the points a and b

One can easily check that Assumption 1 is not satisfied, since the condition (6) does not hold for the two points a and b.

We now present our main result.

Theorem 3 *Assume that* $\mathbf{K} \subseteq \mathbb{R}^n$ *is compact and satisfies Assumption 1. Then there exists a constant* $\zeta(\mathbf{K})$ *(depending only on* $\mathbf{K}$*) such that, for all Lipschitz continuous functions* f *with Lipschitz constant* M_f *on* $\mathbf{K}$*, the following inequality holds:*

$$\underline{f}_{\mathbf{K}}^{(r)} - f_{\min,\mathbf{K}} \leq \frac{\zeta(\mathbf{K})M_f}{\sqrt{r}} \quad \text{for all } r \geq r_{\mathbf{K}} + 1. \tag{8}$$

Moreover, if f *is a polynomial of degree* d *and* $\mathbf{K}$ *is a convex body, then*

$$\underline{f}_{\mathbf{K}}^{(r)} - f_{\min,\mathbf{K}} \leq \frac{2d^2\zeta(\mathbf{K}) \sup_{x\in\mathbf{K}} |f(x)|}{w_{\min}(\mathbf{K})} \frac{1}{\sqrt{r}} \quad \text{for all } r \geq r_{\mathbf{K}} + 1. \tag{9}$$

The key idea to show this result is to select suitable sums of squares densities which we are able to analyse. For this, we will select a global minimizer a of f over $\mathbf{K}$ and consider the Gaussian distribution with mean a and, as sums of squares densities, we will select the polynomials $H_{r,a}$ obtained by truncating the Taylor series expansion of the Gaussian distribution, see relation (14).

Remark 1 When the polynomial f has a root in $\mathbf{K}$ (which can be assumed without loss of generality), the parameter $\sup_{x\in\mathbf{K}} |f(x)|$ involved in relation (9) can easily be upper bounded in terms of the range of values of f; namely,

$$\sup_{x\in\mathbf{K}} |f(x)| \leq f_{\max,\mathbf{K}} - f_{\min,\mathbf{K}},$$

where $f_{\max,\mathbf{K}}$ denotes the maximum value of f over $\mathbf{K}$. Hence relation (9) also implies an upper bound on $\underline{f}_{\mathbf{K}}^{(r)} - f_{\min,\mathbf{K}}$ in terms of the range $f_{\max,\mathbf{K}} - f_{\min,\mathbf{K}}$, as is commonly used in approximation analysis (see, e.g., [4,6]).

1.4 Contents of the paper

Our paper is organized as follows. In Sect. 2, we give a constructive proof for our main result in Theorem 3. In Sect. 3 we show how to obtain feasible points in $\mathbf{K}$ that correspond to the bounds $\underline{f}_{\mathbf{K}}^{(r)}$ through sampling. This is followed by a section with numerical examples (Sect. 4). Finally, in the concluding remarks (Sect. 5), we revisit Assumption 1, and discuss perspectives for future research.

2 Proof of our main result in Theorem 3

In this section we prove our main result in Theorem 3. Our analysis holds for Lipschitz continuous functions, so we start by reviewing some relevant properties in Sect. 2.1. In the next step we indicate in Sect. 2.2 how to select the polynomial density function h as a special sum of squares that we will be able to analyze. Namely, we let a denote a global minimizer of the function f over the set $\mathbf{K} \subseteq \mathbb{R}^n$. Then we consider the density function G_a in (12) of the Gaussian distribution with mean a (and suitable variance) and the polynomial $H_{r,a}$ in (14), which is obtained from the truncation at degree $2r$ of the Taylor series expansion of the Gaussian density function G_a. The final step will be to analyze the quality of the bound obtained by selecting the polynomial $H_{r,a}$ and this will be the most technical part of the proof, carried out in Sect. 2.3.

2.1 Lipschitz continuous functions

A function f is said to be Lipschitz continuous on $\mathbf{K}$, with Lipschitz constant M_f, if it satisfies:

$$|f(y) - f(x)| \leq M_f \|y - x\| \quad \text{for all } x, y \in \mathbf{K}.$$

If f is continuous and differentiable on $\mathbf{K}$, then f is Lipschitz continuous on $\mathbf{K}$ with respect to the constant

$$M_f = \max_{x \in \mathbf{K}} \|\nabla f(x)\|. \tag{10}$$

Furthermore, if f is an n-variate polynomial with degree d, then the Markov inequality for f on a convex body $\mathbf{K}$ reads as

$$\max_{x \in \mathbf{K}} \|\nabla f(x)\| \leq \frac{2d^2}{w_{\min}(\mathbf{K})} \sup_{x \in \mathbf{K}} |f(x)|,$$

see e.g., [4, relation (8)]. Thus, together with (10), we have that f is Lipschitz continuous on $\mathbf{K}$ with respect to the constant

$$M_f \leq \frac{2d^2}{w_{\min}(\mathbf{K})} \sup_{x \in \mathbf{K}} |f(x)|. \tag{11}$$

2.2 Choosing the polynomial density function $H_{r,a}$

Consider the function

$$G_a(x) := \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{\|x - a\|^2}{2\sigma^2}\right), \tag{12}$$

which is the probability density function of the Gaussian distribution with mean a and standard variance σ (whose value will be defined later). Let the constant $C_{\mathbf{K},a}$ be defined by

$$\int_{\mathbf{K}} C_{\mathbf{K},a} G_a(x) dx = 1. \tag{13}$$

Observe that $G_a(x)$ is equal to the function $\frac{1}{(2\pi\sigma^2)^{n/2}} e^{-t}$ evaluated at the point $t = \frac{\|x-a\|^2}{2\sigma^2}$.

Denote by $H_{r,a}$ the Taylor series expansion of G_a truncated at the order $2r$. That is,

$$H_{r,a}(x) = \frac{1}{(2\pi\sigma^2)^{n/2}} \sum_{k=0}^{2r} \frac{1}{k!} \left(-\frac{\|x-a\|^2}{2\sigma^2} \right)^k. \tag{14}$$

Moreover consider the constant $c^r_{\mathbf{K},a}$, defined by

$$\int_{\mathbf{K}} c^r_{\mathbf{K},a} H_{r,a}(x) dx = 1. \tag{15}$$

The next step is to show that $H_{r,a}$ is a sum of squares of polynomials and thus $H_{r,a} \in \Sigma[x]_{2r}$. This follows from the next lemma.

Lemma 1 *Let $\phi_{2r}(t)$ denote the (univariate) polynomial of degree $2r$ obtained by truncating the Taylor series expansion of e^{-t} at the order $2r$. That is,*

$$\phi_{2r}(t) := \sum_{k=0}^{2r} \frac{(-t)^k}{k!}.$$

Then ϕ_{2r} is a sum of squares of polynomials. Moreover, we have

$$0 \le \phi_{2r}(t) - e^{-t} \le \frac{t^{2r+1}}{(2r+1)!} \quad \text{for all } t \ge 0. \tag{16}$$

Proof First, we show that ϕ_{2r} is a sum of squares. As ϕ_{2r} is a univariate polynomial, by Hilbert's Theorem (see e.g., [20, Theorem 3.4]), it suffices to show that $\phi_{2r}(t) \ge 0$ for all $t \in \mathbb{R}$. As $\phi_{2r}(-\infty) = \phi_{2r}(+\infty) = +\infty$, it suffices to show that $\phi_{2r}(t) \ge 0$ at all the stationary points t where $\phi'_{2r}(t) = 0$. For this, observe that $\phi'_{2r}(t) = \sum_{k=1}^{2r} (-1)^k \frac{t^{k-1}}{(k-1)!}$, so that it can be written as $\phi'_{2r}(t) = -\phi_{2r}(t) + \frac{t^{2r}}{(2r)!}$. Hence, for all t with $\phi'_{2r}(t) = 0$, we have $\phi_{2r}(t) = \frac{t^{2r}}{(2r)!} \ge 0$.

Next, we show that $\phi_{2r}(t) \ge e^{-t}$ for all $t \ge 0$. Fix $t \ge 0$. Then, by Taylor Theorem (see e.g., [30]), one has $e^{-t} = \phi_{2r}(t) + \frac{\phi^{(2r+1)}(\xi) t^{2r+1}}{(2r+1)!}$ for some $\xi \in [0, t]$. As $\phi^{(2r+1)}(\xi) = -e^{-\xi}$, one can conclude that $e^{-t} - \phi_{2r}(t) = -\frac{e^{-\xi} t^{2r+1}}{(2r+1)!} \le 0$ and $e^{-t} - \phi_{2r}(t) \ge -\frac{t^{2r+1}}{(2r+1)!}$. □

We now consider the parameter $f^{(r)}_{\mathbf{K},a}$ defined as

$$f^{(r)}_{\mathbf{K},a} := \int_{\mathbf{K}} f(x) c^r_{\mathbf{K},a} H_{r,a}(x) dx. \tag{17}$$

Our main technical result is the following upper bound for the range $f^{(r)}_{\mathbf{K},a} - f_{\min,\mathbf{K}}$.

Theorem 4 *Assume $\mathbf{K} \subseteq \mathbb{R}^n$ is compact and satisfies Assumption 1, and consider the parameter $r_{\mathbf{K}}$ from (7). Then there exists a constant $\zeta(\mathbf{K})$ (depending only on $\mathbf{K}$) such that, for all Lipschitz continuous functions f with Lipschitz constant M_f on $\mathbf{K}$, the following inequality holds:*

$$f^{(r)}_{\mathbf{K},a} - f_{\min,\mathbf{K}} \leq \frac{\zeta(\mathbf{K}) M_f}{\sqrt{2r+1}}, \quad \textit{for all } r \geq \frac{r_{\mathbf{K}}}{2}. \tag{18}$$

Moreover, if f is a polynomial of degree d and $\mathbf{K}$ is a convex body, then

$$f^{(r)}_{\mathbf{K},a} - f_{\min,\mathbf{K}} \leq \frac{2d^2 \zeta(\mathbf{K}) \sup_{x \in \mathbf{K}} |f(x)|}{w_{\min}(\mathbf{K}) \sqrt{2r+1}}, \quad \textit{for all } r \geq \frac{r_{\mathbf{K}}}{2}. \tag{19}$$

We will give the proof of Theorem 4, which has lengthy technical details, in Sect. 2.3 below. We now show how to derive Theorem 3 as a direct application of Theorem 4.

Proof (of Theorem 3) Assume f is Lipschitz continuous with Lipschitz constant M_f on K and a is a minimizer of f over the set $\mathbf{K}$. Using the definitions (2) and (17) of the parameters and the fact that $H_{r,a}$ is a sum of squares with degree $4r$, it follows that

$$\underline{f}^{(2r+1)}_{\mathbf{K}} \leq \underline{f}^{(2r)}_{\mathbf{K}} \leq f^{(r)}_{\mathbf{K},a}, \quad \text{for all } r \in \mathbb{N}.$$

Then, from inequality (18) in Theorem 4, one obtains

$$\underline{f}^{(2r+1)}_{\mathbf{K}} - f_{\min,\mathbf{K}} \leq \underline{f}^{(2r)}_{\mathbf{K}} - f_{\min,\mathbf{K}} \leq f^{(r)}_{\mathbf{K},a} - f_{\min,\mathbf{K}} \leq \frac{\zeta(\mathbf{K}) M_f}{\sqrt{2r+1}} \quad \text{for all } r \geq \frac{r_{\mathbf{K}}}{2}.$$

Hence, for all $r \geq r_{\mathbf{K}} + 1$,

$$\underline{f}^{(r)}_{\mathbf{K}} - f_{\min,\mathbf{K}} \leq \frac{\zeta(\mathbf{K}) M_f}{\sqrt{r+1}} \leq \frac{\zeta(\mathbf{K}) M_f}{\sqrt{r}} \quad \text{for even } r,$$
$$\underline{f}^{(r)}_{\mathbf{K}} - f_{\min,\mathbf{K}} \leq \frac{\zeta(\mathbf{K}) M_f}{\sqrt{r}} \quad \text{for odd } r.$$

This concludes the proof for relation (8), and relation (9) follows from (19) in an analogous way. This finishes the proof of Theorem 3.

2.3 Analyzing the polynomial density function $H_{r,a}$

In this section we prove the result of Theorem 4. Recall that a is a global minimizer of f over $\mathbf{K}$. For the proof, we will need the following four technical lemmas.

Lemma 2 *Assume* $\mathbf{K} \subseteq \mathbb{R}^n$ *is compact and satisfies Assumption 1. Then, for all* $0 < \epsilon \leq \epsilon_{\mathbf{K}}$ *and* $r \in \mathbb{N}$*, we have:*

$$c^r_{\mathbf{K},a} \leq C_{\mathbf{K},a} \leq \frac{(2\pi\sigma^2)^{n/2}\exp\left(\frac{\epsilon^2}{2\sigma^2}\right)}{\eta_{\mathbf{K}}\epsilon^n\gamma_n}. \tag{20}$$

Proof By Lemma 1, $\phi_{2r}(t) \geq e^{-t}$ for all $t \geq 0$, which implies $H_{r,a}(x) \geq G_a(x)$ for all $x \in \mathbb{R}^n$. Together with the relations (13) and (15) defining the constants $C_{\mathbf{K},a}$ and $c^r_{\mathbf{K},a}$, we deduce that $c^r_{\mathbf{K},a} \leq C_{\mathbf{K},a}$. Moreover, by the definition (13) of the constant $C_{K,a}$, one has

$$\begin{aligned}
\frac{1}{C_{\mathbf{K},a}} &= \int_{\mathbf{K}} G_a(x)dx = \int_{\mathbf{K}} \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{\|x-a\|^2}{2\sigma^2}\right)dx \\
&\geq \int_{\mathbf{K}\cap B_\epsilon(a)} \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{\|x-a\|^2}{2\sigma^2}\right)dx \\
&\geq \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{\epsilon^2}{2\sigma^2}\right) \mathrm{vol}(\mathbf{K}\cap B_\epsilon(a)).
\end{aligned}$$

We now use relation (6) from Assumption 1 in order to conclude that $\mathrm{vol}(\mathbf{K} \cap B_\epsilon(a)) \geq \eta_{\mathbf{K}}\epsilon^n\gamma_n$, which gives the desired upper bound on $C_{K,a}$. □

Lemma 3 *Given* $\tilde{x} \in \mathbb{R}^n$ *and a function* $F : \mathbb{R}_+ \to \mathbb{R}$*, define the function* $f : \mathbb{R}^n \to \mathbb{R}$ *by* $f(x) = F(\|x - \tilde{x}\|)$ *for all* $x \in \mathbb{R}^n$*. Then, for all* $\rho_2 \geq \rho_1 \geq 0$*, one has*

$$\int_{B_{\rho_2}(\tilde{x})\setminus B_{\rho_1}(\tilde{x})} f(x)dx = n\gamma_n \int_{\rho_1}^{\rho_2} z^{n-1}F(z)dz,$$

where $\gamma_n = \frac{\pi^{(n-1)/2}2^{(n+1)/2}}{n!!}$ *is the volume of the unit Euclidean ball in* $\mathbb{R}^n$*.*

Proof Apply a change of variables using spherical coordinates as explained, e.g., in [3].

Lemma 4 *For all positive integers* r *and* n*, one has* $\left(\frac{1}{2r+1}\right)^{-\frac{n}{4(2r+1)+2n}} < 6n$*.*

Proof Let $n \in \mathbb{N}$ be given. Denote

$$g(r) := \left(\frac{1}{2r+1}\right)^{-\frac{n}{4(2r+1)+2n}} = (2r+1)^{\frac{n}{4(2r+1)+2n}} \quad (r \geq 0).$$

Observe that, $g(0) = 1$, $g(r) > 0$ for all $r \geq 0$, $\ln(g(r)) = \frac{n}{8r+4+2n}\ln(2r+1)$, and thus $\lim_{r\to\infty} g(r) = 1$. It suffices to show $g(r^*) < 6n$ for all stationary points r^*. Since

$$\frac{d\ln(g(r))}{dr} = \frac{-8n\ln(2r+1)}{(8r+4+2n)^2} + \frac{2n}{(2r+1)(8r+4+2n)},$$

and $g'(r) = \frac{1}{g(r)}\frac{d\ln(g(r))}{dr}$, any stationary point r^* satisfies

$$\frac{d\ln(g(r^*))}{dr} = 0 \Longleftrightarrow (2r^*+1)\left[\ln(2r^*+1) - 1\right] = \frac{n}{2}.$$

Since

$$(2r^*+1)(\ln(3)-1) \leq (2r^*+1)\left[\ln(2r^*+1) - 1\right] = \frac{n}{2},$$

one has $2r^*+1 \leq \frac{n}{2(\ln(3)-1)} < 6n$. Since $g(r) \leq 2r+1$ for all $r \geq 0$, one has $g(r^*) \leq 2r^*+1 < 6n$. □

Lemma 5 *Assume* $\mathbf{K} \subseteq \mathbb{R}^n$ *is compact and satisfies Assumption 1. Then, for all* $0 < \epsilon \leq \epsilon_{\mathbf{K}}$*, one has*

$$\int_{\mathbf{K}} C_{\mathbf{K},a}\|x-a\|G_a(x)dx \leq \epsilon + \frac{n\sigma^{n+1}p(n)}{\epsilon^n \eta_{\mathbf{K}}} e^{\frac{\epsilon^2}{2\sigma^2}},$$

where $p(n) := \int_0^{+\infty} t^n e^{-t^2/2}dt$ *is a constant depending on n, given by*

$$p(n) = \begin{cases} 1 & \text{if } n = 1, \\ \sqrt{\frac{\pi}{2}}\prod_{j=1}^{k}(2j-1) & \text{if } n = 2k \text{ and } k \geq 1, \\ \prod_{j=1}^{k}(2j) & \text{if } n = 2k+1 \text{ and } k \geq 1. \end{cases} \quad (21)$$

Proof Let $\varphi := \int_{\mathbf{K}} C_{\mathbf{K},a}\|x-a\|G_a(x)dx$ denote the integral that we need to upper bound. We split the integral φ as $\varphi = \varphi_1 + \varphi_2$, depending on whether x lies in the ball $B_\epsilon(a)$ or not.

First, we upper bound the term φ_1 as

$$\varphi_1 := \int_{\mathbf{K}\cap B_\epsilon(a)} \|x-a\|C_{\mathbf{K},a}G_a(x)dx \leq \epsilon\int_{\mathbf{K}\cap B_\epsilon(a)} C_{\mathbf{K},a}G_a(x)dx \leq \epsilon\int_{\mathbf{K}} C_{\mathbf{K},a}G_a(x)dx = \epsilon.$$

Second, we bound the integral

$$\varphi_2 := C_{\mathbf{K},a}\int_{\mathbf{K}\setminus B_\epsilon(a)} \|x-a\|G_a(x)dx.$$

Since $\mathbf{K} \subseteq B_{\sqrt{D(\mathbf{K})}}(a)$, one has

$$\varphi_2 \leq C_{\mathbf{K},a}\int_{B_{\sqrt{D(\mathbf{K})}}(a)\setminus B_\epsilon(a)} \|x-a\|G_a(x)dx,$$

where the right hand side, by Lemma 3, is equal to

$$\frac{C_{\mathbf{K},a} n \gamma_n}{(2\pi\sigma^2)^{n/2}} \int_{\epsilon}^{\sqrt{D(\mathbf{K})}} z^n \exp\left(-\frac{z^2}{2\sigma^2}\right) dz.$$

By a change of variable $t = \frac{z}{\sigma}$, one obtains

$$\varphi_2 \leq \frac{C_{\mathbf{K},a} n \gamma_n \sigma}{(2\pi)^{n/2}} \int_{\epsilon/\sigma}^{\sqrt{D(\mathbf{K})}/\sigma} t^n \exp\left(-\frac{t^2}{2}\right) dt,$$

and thus

$$\varphi_2 \leq \frac{C_{\mathbf{K},a} n \gamma_n \sigma}{(2\pi)^{n/2}} \int_{0}^{+\infty} t^n \exp\left(-\frac{t^2}{2}\right) dt = \frac{C_{\mathbf{K},a} n \gamma_n \sigma}{(2\pi)^{n/2}} p(n).$$

Here we have set $p(n) := \int_0^{+\infty} t^n e^{-\frac{t^2}{2}} dt$ which can be checked to be given by (21) (e.g., using induction on n).

Now, combining with the upper bound for $C_{\mathbf{K},a}$ from (20), we obtain

$$\varphi_2 \leq \frac{n \sigma^{n+1} p(n)}{\epsilon^n \eta_{\mathbf{K}}} e^{\frac{\epsilon^2}{2\sigma^2}}.$$

Therefore, we have shown:

$$\varphi = \varphi_1 + \varphi_2 \leq \epsilon + \frac{n \sigma^{n+1} p(n)}{\epsilon^n \eta_{\mathbf{K}}} e^{\frac{\epsilon^2}{2\sigma^2}},$$

which shows the lemma. □

We are now ready to prove Theorem 4.

Proof (of Theorem 4) Observe that, if f is a polynomial, then we can use the upper bound (11) for its Lipschitz constant and thus the inequality (19) follows as a direct consequence of the inequality (18). Therefore, it suffices to show the relation (18).

Recall that a is a minimizer of f over $\mathbf{K}$. As f is Lipschitz continuous with Lipschitz constant M_f on K, we have

$$f(x) - f(a) \leq M_f \|x - a\| \quad \forall x \in \mathbf{K}.$$

This implies

$$f^{(r)}_{\mathbf{K},a} - f_{\min,\mathbf{K}} = \int_{\mathbf{K}} c^r_{\mathbf{K},a} H_{r,a}(x)(f(x) - f(a)) dx \leq M_f \int_{\mathbf{K}} \|x - a\| c^r_{\mathbf{K},a} H_{r,a}(x) dx.$$

Our objective is now to show the existence of a constant $\zeta(\mathbf{K})$ such that

$$\psi := \int_{\mathbf{K}} c^r_{\mathbf{K},a} \|x - a\| H_{r,a}(x) dx \leq \frac{\zeta(\mathbf{K})}{\sqrt{2r+1}}, \quad \text{for all } r \geq r_{\mathbf{K}}, (see (7))$$

by which we can then conclude the proof for (18).

For this, we split the integral ψ as the sum of two terms:

$$\psi = \underbrace{\int_{\mathbf{K}} c^r_{\mathbf{K},a} \|x-a\| G_a(x) dx}_{=:\psi_1} + \underbrace{\int_{\mathbf{K}} c^r_{\mathbf{K},a} \|x-a\| (H_{r,a}(x) - G_a(x)) dx}_{=:\psi_2}.$$

First, we upper bound the term ψ_1. As $c^r_{\mathbf{K},a} \le C_{\mathbf{K},a}$ (by (20)), we can use Lemma 5 to conclude that, for all $0 < \epsilon \le \epsilon_{\mathbf{K}}$,

$$\psi_1 \le \int_{\mathbf{K}} C_{\mathbf{K},a} \|x-a\| G_a(x) dx \le \epsilon + \frac{n\sigma^{n+1} p(n)}{\epsilon^n \eta_{\mathbf{K}}} e^{\frac{\epsilon^2}{2\sigma^2}} = \epsilon \underbrace{\left[1 + \frac{n\sigma^{n+1} p(n)}{\epsilon^{n+1} \eta_{\mathbf{K}}} e^{\frac{\epsilon^2}{2\sigma^2}} \right]}_{=:\mu_1} = \epsilon \mu_1. \tag{22}$$

Second we bound the integral

$$\psi_2 = \int_{\mathbf{K}} c^r_{\mathbf{K},a} \|x-a\| (H_{r,a}(x) - G_a(x)) dx.$$

We can upper bound the function $H_{r,a}(x) - G_a(x)$ using the estimate from (16) and we get

$$H_{r,a}(x) - G_a(x) \le \frac{1}{(2\pi\sigma^2)^{n/2}} \frac{\|x-a\|^{4r+2}}{(2\sigma^2)^{2r+1}(2r+1)!}.$$

Then we have

$$\begin{aligned} \psi_2 &\le \frac{1}{(2\pi\sigma^2)^{n/2}} \int_{\mathbf{K}} c^r_{\mathbf{K},a} \frac{\|x-a\|^{4r+3}}{(2\sigma^2)^{2r+1}(2r+1)!} dx \\ &= \frac{1}{(2\pi\sigma^2)^{n/2}} \frac{c^r_{\mathbf{K},a}}{(2\sigma^2)^{2r+1}(2r+1)!} \int_{\mathbf{K}} \|x-a\|^{4r+3} dx. \end{aligned}$$

Now we upper bound the integral $\int_{\mathbf{K}} \|x-a\|^{4r+3} dx$. Since $\mathbf{K} \subseteq B_{\sqrt{D(\mathbf{K})}}(a)$, one has

$$\int_{\mathbf{K}} \|x-a\|^{4r+3} dx \le \int_{B_{\sqrt{D(\mathbf{K})}}(a)} \|x-a\|^{4r+3} dx,$$

where the right hand side, by Lemma 3, is equal to

$$n\gamma_n \int_0^{\sqrt{D(\mathbf{K})}} z^{4r+n+2} dz = \frac{n\gamma_n D(\mathbf{K})^{\frac{4r+n+3}{2}}}{4r+n+3} \le n\gamma_n D(\mathbf{K})^{\frac{4r+n+3}{2}}.$$

Thus, we obtain

$$\psi_2 \le \frac{1}{(2\pi\sigma^2)^{n/2}} \frac{c^r_{\mathbf{K},a}}{(2\sigma^2)^{2r+1}(2r+1)!} n\gamma_n D(\mathbf{K})^{\frac{4r+n+3}{2}}.$$

We now use the upper bound for $c^r_{\mathbf{K},a}$ from (20):

$$c^r_{\mathbf{K},a} \leq \frac{(2\pi\sigma^2)^{n/2} \exp\left(\frac{\epsilon^2}{2\sigma^2}\right)}{\eta_{\mathbf{K}} \epsilon^n \gamma_n}$$

and we obtain

$$\psi_2 \leq \frac{n \exp\left(\frac{\epsilon^2}{2\sigma^2}\right) D(\mathbf{K})^{\frac{4r+n+3}{2}}}{\eta_{\mathbf{K}} \epsilon^n (2r+1)!(2\sigma^2)^{2r+1}}.$$

Finally we use the Stirling's inequality:

$$(2r+1)! \geq \sqrt{2\pi(2r+1)} \left(\frac{2r+1}{e}\right)^{2r+1},$$

and obtain

$$\begin{aligned} \psi_2 &\leq \underbrace{\frac{n \exp\left(\frac{\epsilon^2}{2\sigma^2}\right) D(\mathbf{K})^{\frac{n+1}{2}}}{\eta_{\mathbf{K}}}}_{=:\mu_2} \left(\frac{D(\mathbf{K})e}{2\sigma^2 \epsilon^{n/(2r+1)}(2r+1)}\right)^{2r+1} \frac{1}{\sqrt{2\pi(2r+1)}} \\ &= \frac{\mu_2}{\sqrt{2\pi(2r+1)}} \left(\frac{D(\mathbf{K})e}{2\sigma^2 \epsilon^{n/(2r+1)}(2r+1)}\right)^{2r+1}. \end{aligned} \tag{23}$$

We can now upper bound the quantity $\psi = \psi_1 + \psi_2$, by combining the upper bound for ψ_1 in (22) with the above upper bound (23) for ψ_2. That is,

$$\psi \leq \epsilon\mu_1 + \frac{\mu_2}{\sqrt{2\pi(2r+1)}} \left(\frac{D(\mathbf{K})e}{2\sigma^2 \epsilon^{n/(2r+1)}(2r+1)}\right)^{2r+1}.$$

We now indicate how to select the parameters ϵ and σ.

First we select $\sigma = \epsilon$, so that both parameters μ_1 and μ_2 appearing in (22) and (23) are constants depending on n and $\mathbf{K}$, namely

$$\mu_1 = 1 + \frac{np(n)e^{1/2}}{\eta_{\mathbf{K}}} \quad \text{and} \quad \mu_2 = \frac{ne^{1/2} D(\mathbf{K})^{\frac{n+1}{2}}}{\eta_{\mathbf{K}}}.$$

Next we select ϵ so that $\frac{D(\mathbf{K})e}{2\epsilon^{2+n/(2r+1)}(2r+1)} = 1$, i.e.,

$$\epsilon = \left(\frac{D(\mathbf{K})e}{2(2r+1)}\right)^{\frac{2r+1}{2(2r+1)+n}} = \left(\frac{D(\mathbf{K})e}{2}\right)^{\frac{2r+1}{2(2r+1)+n}} \left(\frac{1}{2r+1}\right)^{\frac{1}{2} - \frac{n}{4(2r+1)+2n}}.$$

Summarizing, we have shown that

$$\psi \le \left(\frac{1}{2r+1}\right)^{\frac{1}{2}-\frac{n}{4(2r+1)+2n}} \left[\left(\frac{D(\mathbf{K})e}{2}\right)^{\frac{2r+1}{2(2r+1)+n}} \mu_1 + \frac{\mu_2}{\sqrt{2\pi}}\left(\frac{1}{2r+1}\right)^{\frac{n}{4(2r+1)+2n}}\right]$$
$$\le \left(\frac{1}{2r+1}\right)^{\frac{1}{2}} 6n\left(\mu_1 \max\left\{1, \sqrt{\frac{D(\mathbf{K})e}{2}}\right\} + \frac{\mu_2}{\sqrt{2\pi}}\right). \tag{24}$$

To obtain the last inequality (24), we use the inequality $\left(\frac{1}{2r+1}\right)^{-\frac{n}{4(2r+1)+2n}} < 6n$ (recall Lemma 4), together with the two inequalities $\left(\frac{D(\mathbf{K})e}{2}\right)^{\frac{2r+1}{2(2r+1)+n}} \le \max\left\{1, \sqrt{\frac{D(\mathbf{K})e}{2}}\right\}$ and $\left(\frac{1}{2r+1}\right)^{\frac{n}{4(2r+1)+2n}} \le 1$.

Since we have assumed $\epsilon \le \epsilon_{\mathbf{K}}$ (recall Lemma 2), this implies the condition $r \ge \frac{D(\mathbf{K})e}{4}\epsilon_{\mathbf{K}}^{-\left(2+\frac{n}{2r+1}\right)} - \frac{1}{2}$, i.e., the inequality (24) holds for all $r \ge \frac{D(\mathbf{K})e}{4}\epsilon_{\mathbf{K}}^{-\left(2+\frac{n}{2r+1}\right)} - \frac{1}{2}$. If $\epsilon_{\mathbf{K}} \le 1$ and $r \ge n/2$, then we have $\epsilon_{\mathbf{K}}^{-(2+\frac{n}{2r+1})} \le \epsilon_{\mathbf{K}}^{-3}$ and thus the inequality (24) holds for all $r \ge \max\left\{\frac{D(\mathbf{K})e}{4\epsilon_{\mathbf{K}}^3}, \frac{n}{2}\right\}$. If $\epsilon_{\mathbf{K}} \ge 1$ then $\epsilon_{\mathbf{K}}^{-(2+\frac{n}{2r+1})} \le 1$ and thus (24) holds for all integers $r \ge \frac{D(\mathbf{K})e}{4}$. Hence, the inequality (24) holds for all $r \ge r_{\mathbf{K}}/2$, where $r_{\mathbf{K}}$ is as defined in (7).

Finally, by defining the constant

$$\zeta(\mathbf{K}) := 6n\left(\mu_1 \max\left\{1, \sqrt{\frac{D(\mathbf{K})e}{2}}\right\} + \frac{\mu_2}{\sqrt{2\pi}}\right),$$

which indeed depends only on $\mathbf{K}$ and its dimension n, we can conclude the proof for (18).

Remark 2 Note that in the proof of Theorem 4, we use Assumption 1 only for the selected minimizer $a \in \mathbf{K}$ (and we use it only in the proof of Lemma 2). Hence, if the selected point a lies in the interior of $\mathbf{K}$, i.e., if there exists $\delta > 0$ such that $B_\delta(a) \subseteq \mathbf{K}$, then the result of Theorem 4 (and thus Theorem 3) holds when selecting $\eta_{\mathbf{K}} = 1$ and $\epsilon_{\mathbf{K}} = \delta$.

Our results extend also to unconstrained global minimization:

$$f^* := \min_{x\in\mathbb{R}^n} f(x),$$

if we know that f has a global minimizer a and we know a ball $B_\delta(0)$ containing a. We can then indeed minimize f over a compact set K, which can be chosen to be the ball $B_\delta(0)$ or a suitable hypercube containing a.

3 Obtaining feasible solutions through sampling

In this section we indicate how to sample feasible points in the set $\mathbf{K}$ from the optimal density function obtained by solving the semidefinite program (2).

Let $f \in \mathbb{R}[x]$ be a polynomial. Suppose $h^*(x) \in \Sigma[x]_r$ is an optimal solution of the program (2), i.e., $\underline{f}_{\mathbf{K}}^{(r)} = \int_{\mathbf{K}} f(x)h^*(x)dx$ and $\int_{\mathbf{K}} h^*(x)dx = 1$.

Then h^* can be seen as the probability density function of a probability distribution on $\mathbf{K}$, denoted as $\mathcal{T}_{\mathbf{K}}$ and, for all random vector $X = (X_1, \dots, X_n) \sim \mathcal{T}_{\mathbf{K}}$, the expectation of $f(X)$ is given by:

$$\mathbb{E}\left[f(X)\right] = \int_{\mathbf{K}} f(x)h^*(x)dx = \underline{f}_{\mathbf{K}}^{(r)}. \tag{25}$$

As we now recall one can generate random samples $x \in \mathbf{K}$ from the distribution $\mathcal{T}_{\mathbf{K}}$ using the well known *method of conditional distributions* (see e.g., [21, Sect. 8.5.1]). Then we will observe that with high probability one of these sample points satisfies (roughly) the inequality $f(x) \le \underline{f}_{\mathbf{K}}^{(r)}$ (see Theorem 5 for details).

In order to sample a random vector $X = (X_1, \dots, X_n) \sim \mathcal{T}_{\mathbf{K}}$, we assume that, for each $i = 2, \dots, n$, we know the cumulative conditional distribution of X_i given that $X_j = x_j$ for $j = 1, \dots, i-1$, defined in terms of probabilities as

$$F_i(x_i \mid x_1, \dots, x_{i-1}) := \mathbf{Pr}\left[X_i \le x_i \;\mid\; X_1 = x_1, \dots, X_{i-1} = x_{i-1}\right].$$

Additionally, we assume that we know the cumulative marginal distribution function of X_i, defined as:

$$F_i(x_i) := \mathbf{Pr}\left[X_i \le x_i\right].$$

Then one can generate a random sample $x = (x_1, \dots, x_n) \in \mathbf{K}$ from the distribution $\mathcal{T}_{\mathbf{K}}$ by the following algorithm:

- Generate x_1 with cumulative distribution function $F_1(\cdot)$.
- Generate x_2 with cumulative distribution function $F_2\left(\cdot|x_1\right)$.

  $\vdots$
- Generate x_n with cumulative distribution function $F_n\left(\cdot|x_1, \dots, x_{n-1}\right)$.

Then return $x = (x_1, x_2, \dots, x_n)^T$.

There remains to explain how to generate a (univariate) sample point x with a given cumulative distribution function $F(\cdot)$, since this operation is carried out at each of the n steps of the above algorithm. For this one can use the classical *inverse-transform method* (see e.g., [21, Sect. 8.2.1]), which reduces to sampling from the uniform distribution on [0, 1] and can be described as follows:

- Generate a sample u from the uniform distribution over [0, 1].
- Return $x = F^{-1}(u)$ (if F is strictly monotone increasing, or $x = \min\{y : F(y) \ge u\}$ otherwise).

Hence, in order to be able to apply the method of conditional distributions for sampling from $\mathbf{K}$ we need to solve the equation $x = F^{-1}(u)$. For instance, when $F(\cdot)$ is a univariate polynomial, solving the equation $x = F^{-1}(u)$ reduces to computing the eigenvalues of the corresponding companion matrix (see, e.g., [20, Sect. 2.4.1]). This applies, e.g., when $\mathbf{K}$ is the hypercube or the simplex, as we see below.

As an illustration, we first indicate how to compute the cumulative marginal and conditional distributions $F_i(\cdot)$ and $F_i(\cdot \mid x_1 \dots x_{i-1})$ for the case of the hypercube $\mathbf{K} = \mathbf{Q}_n = [0, 1]^n$. As before we are given a sum of squares density function $h^*(x)$ on $[0, 1]^n$. For $i = 1, \dots, n$, define the polynomial function $f_{1\dots i} \in \mathbb{R}[x_1, \dots, x_i]$ by

$$f_{1\dots i}(x_1, \dots, x_i) = \int_0^1 \cdots \int_0^1 h^*(x_1, \dots, x_n) dx_{i+1} \cdots dx_n. \tag{26}$$

Then the cumulative marginal distribution function $F_1(\cdot)$ is given by

$$F_1(x_1) = \int_0^{x_1} f_1(y) dy$$

and, for $i = 2, \dots, n$, the cumulative conditional distribution function $F_i(\cdot \mid x_1 \dots x_{i-1})$ is given by

$$F_i(x_i \mid x_1 \dots x_{i-1}) = \frac{\int_0^{x_i} f_{1\dots i}(x_1, \dots, x_{i-1}, y) dy}{f_{1\dots(i-1)}(x_1, \dots, x_{i-1})}.$$

The computation of the cumulative marginal and conditional distributions can be carried out in the same way for the simplex $\mathbf{K} = \Delta_n$, after replacing the function $f_{1\dots i} \in \mathbb{R}[x_1, \dots, x_i]$ in (26) by

$$f_{1\dots i}(x_1, \dots, x_i) = \int_0^{1-x_i-x_{i+1}-\cdots-x_{n-1}} \int_0^{1-x_i-\cdots-x_{n-2}} \cdots \int_0^{1-x_i} h^*(x_1, \dots, x_n) dx_{i+1} \cdots dx_n.$$

Note that in both cases the functions $F_i(x_i \mid x_1 \dots x_{i-1})$ are indeed univariate polynomials. We will apply this sampling method to several examples of polynomial minimization over the hypercube and the simplex in the next section.

We now observe that if we generate sufficiently many samples from the distribution $\mathcal{T}_{\mathbf{K}}$ then, with high probability, one of these samples is a point $x \in \mathbf{K}$ satisfying (roughly) $f(x) \le \underline{f}_{\mathbf{K}}^{(r)}$.

Theorem 5 *Let $X \sim \mathcal{T}_{\mathbf{K}}$. For all $\epsilon > 0$,*

$$\mathbf{Pr}\left[f(X) \ge \underline{f}_{\mathbf{K}}^{(r)} + \epsilon \left(\underline{f}_{\mathbf{K}}^{(r)} - f_{\min,\mathbf{K}}\right)\right] \le \frac{1}{1+\epsilon}.$$

Proof Let $X \sim \mathcal{T}_{\mathbf{K}}$ so that $\mathbb{E}[f(X)] = \underline{f}_{\mathbf{K}}^{(r)}$. Define the nonnegative random variable

$$Y := f(X) - f_{\min,\mathbf{K}}.$$

Then, one has $\mathbb{E}[Y] = \underline{f}_{\mathbf{K}}^{(r)} - f_{\min,\mathbf{K}}$. Given $\epsilon > 0$, the Markov Inequality (see e.g., [23, Theorem 3.2]) implies

$$\mathbf{Pr}[Y \geq (1+\epsilon)\mathbb{E}[Y]] \leq \frac{1}{1+\epsilon}.$$

This completes the proof. □

For given $\epsilon > 0$, if one samples N times independently from $\mathcal{T}_{\mathbf{K}}$, one therefore obtains an $x \in \mathbf{K}$ such that

$$f(x) < \underline{f}_{\mathbf{K}}^{(r)} + \epsilon \left(\underline{f}_{\mathbf{K}}^{(r)} - f_{\min,\mathbf{K}} \right)$$

with probability at least $1 - \left(\frac{1}{1+\epsilon}\right)^N$. For example, if $N \geq 1 + \frac{1}{\epsilon}$ then this probability is at least $1 - 1/e$.

4 Numerical examples

In this section, we consider several well-known polynomial test functions from global optimization that are listed in Table 1.

For these functions, we calculate the parameter $\underline{f}_{\mathbf{K}}^{(r)}$ by solving the SDP (3) for increasing values of the order r. As already mentioned by Lasserre [18, Sect. 4], this computation may be done as a generalised eigenvalue problem—one does not actually have to use an SDP solver. This follows from the fact that the SDP (3) only has one constraint. In particular, $\underline{f}_{\mathbf{K}}^{(r)}$ is equal to the largest scalar λ for which $A - \lambda B \succeq 0$, i.e., the smallest generalized eigenvalue of the system:

$$Ax = \lambda Bx \qquad (x \neq 0),$$

where the symmetric matrices A and B are of order $\binom{n+r}{r}$ with rows and columns indexed by $N(n,r)$, and

$$A_{\alpha,\beta} = \sum_{\delta \in N(n,d)} f_\delta \int_{\mathbf{K}} x^{\alpha+\beta+\delta} dx, \quad B_{\alpha,\beta} = \int_{\mathbf{K}} x^{\alpha+\beta} dx \quad \alpha, \beta \in N(n,r). \tag{27}$$

We performed the computation on a PC with AMD Phenom(tm) 9600B Quad-Core CPU (2.30 GHz) and with 4 GB RAM. The generalized eigenvalue computation was done in Matlab using the `eig` function.

We record the values $\underline{f}_{\mathbf{K}}^{(r)}$ as well as the CPU times (needed to solve the SDP) in Tables 2, 3, 4, 5, and 6 for minimization over the hypercube, the simplex and the ball. Note that we only list the time for solving the generalised eigenvalue problem, and not for constructing the matrices A and B in (27). In other words, we assume the necessary moments are computed beforehand, and that the time needed to construct the matrices A and B in (27) is negligible if the relevant moments are known.

Table 1 Test functions

Name	Formula	Minimum ($f_{\min,\mathbf{K}}$)	Search domain ($\mathbf{K}$)
Booth function	$f = (x_1+2x_2-7)^2+(2x_1+x_2-5)^2$	$f(1,3) = 0$	$[-10, 10]^2$
Matyas function	$f = 0.26(x_1^2+x_2^2) - 0.48x_1x_2$	$f(0,0) = 0$	$[-10, 10]^2$
Three-Hump Camel function	$f = 2x_1^2 - 1.05x_1^4 + \frac{1}{6}x_1^6 + x_1x_2 + x_2^2$	$f(0,0) = 0$	$[-5, 5]^2$
Motzkin polynomial	$f = x_1^4x_2^2 + x_1^2x_2^4 - 3x_1^2x_2^2 + 1$	$f(\pm 1, \pm 1) = 0$	$[-2, 2]^2$
Styblinski–Tang function (n-variate)	$f = \sum_{i=1}^n \frac{1}{2}x_i^4 - 8x_i^2 + \frac{5}{2}x_i$	$f(-2.093534, \ldots, -2.093534) = -39.16599n$	$[-5, 5]^n$
Rosenbrock function (n-variate)	$f = \sum_{i=1}^{n-1} 100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2$	$f(1, \ldots, 1) = 0$	$[-2.048, 2.048]^n$
Matyas function (Modified-S)	$f = 0.26[(20x_1 - 10)^2 + (20x_2 - 10)^2] - 0.48(20x_1 - 10)(20x_2 - 10)$	$f(0.5, 0.5) = 0$	Δ_2
Three-Hump Camel function (Modified-S)	$f = 2(10x_1 - 5)^2 - 1.05(10x_1 - 5)^4 + \frac{1}{6}(10x_1 - 5)^6 + (10x_1 - 5)(10x_2 - 5) + (10x_2 - 5)^2$	$f(0.5, 0.5) = 0$	Δ_2
Matyas function (Modified-B)	$f = 0.26[(20x_1^2 - 10)^2 + (20x_2^2 - 10)^2] - 0.48(20x_1^2 - 10)(20x_2^2 - 10)$	$f(\pm\frac{\sqrt{2}}{2}, \pm\frac{\sqrt{2}}{2}) = 0$	$B_1(0)$
Three-Hump Camel function (Modified-B)	$f = 2(10x_1^2 - 5)^2 - 1.05(10x_1^2 - 5)^4 + \frac{1}{6}(10x_1^2 - 5)^6 + (10x_1^2 - 5)(10x_2^2 - 5) + (10x_2^2 - 5)^2$	$f(\pm\frac{\sqrt{2}}{2}, \pm\frac{\sqrt{2}}{2}) = 0$	$B_1(0)$

Table 2 $\underline{f}_{\mathbf{K}}^{(r)}$ for Booth, Matyas, Three–Hump Camel and Motzkin functions over the hypercube

r	Booth function		Matyas function		Three–Hump Camel function		Motzkin polynomial	
	Value	Time (s)	Value	Time (s)	Value	Time (s)	Value	Time (s)
1	244.680	0.000666	8.26667	0.000739	265.774	0.000742	4.2	0.000719
2	162.486	0.000061	5.32223	0.000072	29.0005	0.000062	1.06147	0.000088
3	118.383	0.000083	4.28172	0.000072	29.0005	0.000066	1.06147	0.000080
4	97.6473	0.000079	3.89427	0.000119	9.58064	0.000117	0.829415	0.000118
5	69.8174	0.000171	3.68942	0.000208	9.58064	0.000177	0.801069	0.000189
6	63.5454	0.000277	2.99563	0.000263	4.43983	0.000263	0.801069	0.000208
7	47.0467	0.000423	2.54698	0.000343	4.43983	0.001146	0.708889	0.000395
8	41.6727	0.000587	2.04307	0.000417	2.55032	0.000647	0.565553	0.000584
9	34.2140	0.000657	1.83356	0.000655	2.55032	0.000586	0.565553	0.000766
10	28.7248	0.000997	1.47840	0.000780	1.71275	0.000782	0.507829	0.001210
11	25.6050	0.001181	1.37644	0.009241	1.71275	0.001026	0.406076	0.001261
12	21.1869	0.001942	1.11785	0.001753	1.2775	0.001693	0.406076	0.001712
13	19.5588	0.002352	1.0686	0.001857	1.2775	0.002031	0.3759	0.003427
14	16.5854	0.002829	0.8742	0.002253	1.0185	0.002629	0.3004	0.003711
15	15.2815	0.003618	0.8524	0.002270	1.0185	0.002936	0.3004	0.002351
16	13.4626	0.003452	0.7020	0.003580	0.8434	0.003452	0.2819	0.003672
17	12.2075	0.004248	0.6952	0.004662	0.8434	0.004652	0.2300	0.004349
18	11.0959	0.005217	0.5760	0.005510	0.7113	0.004882	0.2300	0.006060
19	9.9938	0.007200	0.5760	0.005610	0.7113	0.006752	0.2185	0.007641
20	9.2373	0.009707	0.4815	0.006975	0.6064	0.007031	0.1817	0.007686

Table 3 $\underline{f}_{\mathbf{K}}^{(r)}$ for Styblinski–Tang and Rosenbrock functions (with $n = 10$) over the hypercube

r	Sty.–Tang ($n = 10$)		Rosenb. ($n = 10$)	
	Value	Time (s)	Value	Time (s)
1	−57.1688	0.098	3649.85	0.0005
2	−94.5572	0.001	2813.66	0.0009
3	−108.873	0.011	2393.63	0.0156
4	−132.8810	0.349	1956.81	0.4004
5	−146.7906	9.245	1701.85	12.997

Table 4 $\underline{f}_{\mathbf{K}}^{(r)}$ for Styblinski–Tang and Rosenbrock functions (with $n = 15$) over the hypercube

r	Sty.–Tang ($n = 15$)		Rosenb. ($n = 15$)	
	Value	Time (s)	Value	Time (s)
1	−82.8311	0.001071	5887.5	0.094693
2	−130.464	0.001707	4770.71	0.002282
3	−148.5594	0.170907	4160.78	0.157897
4	−180.9728	16.796383	3552.04	24.696591

Table 5 $\underline{f}_{\mathbf{K}}^{(r)}$ for Styblinski–Tang and Rosenbrock functions (with $n = 20$) over the hypercube

r	Sty.–Tang ($n = 20$)		Rosenb. ($n = 20$)	
	Value	Time (s)	Value	Time (s)
1	−107.875	0.972741	8158.36	0.000949
2	−164.11	0.344403	6806.74	0.011370
3	−185.6488	2.655447	6029.02	2.955319

For instance, in Table 2, we have $n = 2$ and we can compute the parameter $\underline{f}_{\mathbf{K}}^{(r)}$ up to order $r = 20$ for four test functions. Moreover, in Tables 3, 4 and 5, we have $n = 10, 15, 20$, respectively, and the parameter $\underline{f}_{\mathbf{K}}^{(r)}$ can be computed up to order $r = 5$, $r = 4$ and $r = 3$, respectively. Note that in all cases the computation is very fast (at most a few seconds). However, for larger values of n or r we sometimes encountered numerical instability. This may be due to inaccurate calculation of the moments, or to inherent ill-conditioning of the matrices A and B in (27). Indeed the matrix B has a Hankel-type structure and it is a known fact that Hankel matrices are ill-conditioned (see [2]). These issues are of practical importance, but beyond the scope of the present study. Also, one must bear in mind that the order of the matrices A and B grows as $\binom{n+r}{r}$, and this imposes a practical limit on how large the values of n and r may be when computing $\underline{f}_{\mathbf{K}}^{(r)}$.

Furthermore, we use the method described in Sect. 3 to generate samples that are feasible solutions of (2). We report results for the bivariate Rosenbrock and the Three–Hump Camel functions over the hypercube, and for the Matyas and Three-Hump Camel functions (Modified-S) over the simplex. For each order $r \geq 1$, the

Table 6 $\underline{f}_{\mathbf{K}}^{(r)}$ for Matyas and Three-Hump Camel functions (modified) over the simplex and the Euclidean ball

r	Matyas (Modified-S)		Th.-H. C. (Modified-S)		Matyas (Modified-B)		Th.-H. C. (Modified-B)	
	Value	Time (s)	Value	Time (s)	Value	Time (s)	Value	Time (s)
1	7.2243	0.222604	84.354	0.000457	18.000	0.000379	146.41	0.000454
2	4.6536	0.000085	22.398	0.000081	6.3995	0.000049	138.91	0.000052
3	3.9404	0.000124	12.353	0.000115	6.3995	0.000054	48.508	0.000069
4	3.7067	0.000176	3.9153	0.000112	4.4091	0.000133	39.673	0.000111
5	3.2317	0.000696	2.9782	0.000489	4.4091	0.000187	18.045	0.000264
6	2.7328	0.000275	1.3303	0.000255	3.9652	0.000292	13.881	0.000309
7	2.2985	0.000511	1.1773	0.000334	3.9652	0.000323	7.7876	0.000300
8	1.9536	0.001432	0.77992	0.000560	3.8536	0.000395	5.7685	0.000608
9	1.6639	0.000709	0.73202	0.000666	3.8536	0.000517	3.8699	0.000636
10	1.4293	0.003370	0.60846	0.001034	3.4943	0.000687	2.8359	0.000704

Table 7 Sampling results for the Rosenbrock function ($n = 2$) over the hypercube

r	$\underline{f}_{\mathbf{K}}^{(r)}$	Mean	Variance	Minimum	Sample size
1	214.648	121.125	14005.5	0.00451826	20
		209.9	80699.0	0.0008754	1000
2	152.310	184.496	58423.9	4.94265	20
		149.6	54455.0	0.02805	1000
3	104.889	146.618	64611.2	0.0113339	20
		110.1	26022.0	0.0665	1000
4	75.6010	62.4961	5803.21	0.0542813	20
		75.65	45777.0	0.007285	1000
5	51.5037	58.4032	4397.0	0.668679	20
		50.64	6285.0	0.01382	1000
6	41.7878	35.4183	2936.24	1.16154	20
		37.64	3097.0	0.06188	1000
7	30.1392	29.6545	1022.2	1.05813	20
		27.11	1332.0	0.02044	1000
8	25.8329	19.5392	301.334	0.505628	20
		34.32	4106.0	0.074	1000
9	19.4972	20.8982	328.475	0.564992	20
		18.65	593.6	0.07951	1000
10	17.3999	9.37959	146.496	0.562473	20
		15.33	685.7	0.1448	1000
11	13.6289	8.74923	52.1436	0.75774	20
		15.7	7498.0	0.1719	1000
12	12.5024	5.43151	66.561	0.438172	20
		12.7	764.7	0.0945	1000
Uniform Sample		489.722	433549.0	9.0754	20
		465.729	361150.0	0.0771463	1000

sample sizes 20 and 1000 are used. We also generate samples uniformly from the feasible set, for comparison. We give the results in Tables 7, 8, 9 and 10, where we record the mean, variance and the minimum value of these samples together with $\underline{f}_{\mathbf{K}}^{(r)}$ (which equals the sample mean by (25)).

Note that the average of the sample function values approximate $\underline{f}_{\mathbf{K}}^{(r)}$ reasonably well for sample size 1000, but poorly for sample size 20. Moreover, the average sample function value for uniform sampling from $\mathbf{K}$ is much higher than $\underline{f}_{\mathbf{K}}^{(r)}$. Also, the minimum function value for sampling from $\mathcal{T}_{\mathbf{K}}$ is significantly lower than the minimum function value obtained by uniform sampling for most values of r. In terms of generating "good" feasible solutions, sampling from $\mathcal{T}_{\mathbf{K}}$ therefore outperforms uniform sampling from $\mathbf{K}$ for these examples, as one would expect.

Table 8 Sampling results for the Three–Hump Camel function over the hypercube

r	$\underline{f}_{\mathbf{K}}^{(r)}$	Mean	Variance	Minimum	Sample size
1	265.774	216.773	177142.0	0.106854	20
		261.23	193466.0	0.11705	1000
2	29.0005	28.0344	2964.85	1.1718	20
		27.712	6712.8	0.014255	1000
3	29.0005	14.9951	523.904	0.452655	20
		32.363	16681.0	0.0088426	1000
4	9.58064	2.99756	14.1201	0.175016	20
		10.364	1944.0	0.010013	1000
5	9.58064	4.41907	14.1358	0.419394	20
		9.1658	643.88	0.0015924	1000
6	4.43983	7.98481	245.089	0.126147	20
		4.5791	493.12	0.0035581	1000
7	4.43983	3.96711	20.3193	0.260331	20
		3.7911	57.847	0.0076111	1000
8	2.55032	2.18925	3.87943	0.0310113	20
		2.2302	8.3767	0.0028817	1000
9	2.55032	1.38102	2.27433	0.138641	20
		3.2217	812.18	0.00014805	1000
10	1.71275	1.03179	0.992636	0.0645815	20
		1.5069	3.9581	0.0014225	1000
11	1.71275	1.30757	1.90985	0.0320489	20
		1.6379	7.2518	0.0021144	1000
12	1.27749	0.841194	0.914514	0.0369565	20
		1.2105	2.3	0.0005154	1000
Uniform sample		304.032	163021.0	1.65885	20
		243.216	183724.0	0.00975034	1000

5 Concluding remarks

We conclude with some additional remarks on Assumption 1, and some discussion on perspectives for future work.

5.1 Revisiting Assumption 1

In this section we consider in more detail Assumption 1, the geometric assumption which we made about the set **K**. First we recall another condition, known as the *interior cone condition*, which is classically used in approximation theory (see, e.g., Wendland [29]).

Table 9 Sampling results for the Matyas function (Modified-S) over the simplex

r	$\underline{f}_{\mathbf{K}}^{(r)}$	Mean	Variance	Minimum	Sample size
1	7.2243	6.3018	37.373	1.2448	20
		7.0542	64.863	0.31812	1000
2	4.6536	5.7252	34.964	1.8924	20
		4.5932	8.293	0.91671	1000
3	3.9404	3.5187	0.31411	2.4465	20
		3.7544	1.3576	0.071075	1000
4	3.7067	3.4279	1.7187	0.92913	20
		3.8679	6.5113	0.027508	1000
5	3.2317	3.8273	10.173	0.40131	20
		3.1485	6.1263	0.035796	1000
6	2.7328	2.2606	3.3343	0.2595	20
		2.5997	10.8	0.0016761	1000
7	2.2985	2.4568	4.1652	0.18947	20
		2.1541	12.868	0.002669	1000
8	1.9536	0.9223	0.94139	0.064404	20
		1.9418	9.5627	0.0000037429	1000
9	1.6639	1.4446	1.9372	0.048915	20
		1.7266	16.738	0.0019792	1000
10	1.4293	2.0005	2.0226	0.016453	20
		1.4917	16.035	0.00015252	1000
Uniform sample		26.428	641.59	0.085716	20
		11.905	256.0	0.010946	1000

Definition 1 [29, Definition 3.1] A set $\mathbf{K} \subseteq \mathbb{R}^n$ is said to satisfy an interior cone condition if there exist an angle $\theta \in (0, \pi/2)$ and a radius $\rho > 0$ such that, for every $x \in \mathbf{K}$, a unit vector $\xi(x)$ exists such that the set

$$C(x, \xi(x), \theta, \rho) := \{x + \lambda y : y \in \mathbb{R}^n, \|y\| = 1, y^T \xi(x) \geq \cos\theta, \lambda \in [0, \rho]\} \quad (28)$$

is contained in $\mathbf{K}$.

For instance, as we now recall, Euclidean balls and star-shaped sets satisfy the interior cone condition.

Lemma 6 *[29, Lemma 3.10] Every Euclidean ball with radius $r > 0$ satisfies an interior cone condition with radius $\rho = r$ and angle $\theta = \pi/3$.*

Definition 2 [29, Definition 11.25] A set $\mathbf{K}$ is said to be *star-shaped* with respect to a ball $B_r(x_c)$ if, for every $x \in \mathbf{K}$, the closed convex hull of $\{x\} \cup B_r(x_c)$ is contained in $\mathbf{K}$.

Table 10 Sampling results for the Three-Hump Camel function (Modified-S) over the simplex

r	$\underline{f}_{\mathbf{K}}^{(r)}$	Mean	Variance	Minimum	Sample size
1	84.354	104.93	122488.0	0.33441	20
		89.732	48238.0	0.0011036	1000
2	22.398	37.036	9864.0	0.57012	20
		22.292	10102.0	0.0022204	1000
3	12.353	3.4161	49.898	0.28108	20
		11.707	1515.9	0.00065454	1000
4	3.9153	2.4193	9.0182	0.16865	20
		3.6768	592.96	0.0016775	1000
5	2.9782	1.8336	6.3414	0.11311	20
		2.5237	47.619	0.00097905	1000
6	1.3303	2.355	26.176	0.0092016	20
		1.2134	8.7253	0.00040725	1000
7	1.1773	1.0385	1.0569	0.053695	20
		1.092	6.718	0.00050329	1000
8	0.77992	0.9737	0.73522	0.10604	20
		0.72927	0.73641	0.00048517	1000
9	0.73202	0.69755	0.19107	0.051634	20
		0.65302	0.28537	0.00024601	1000
10	0.60846	0.67575	0.17453	0.010351	20
		0.5616	0.17821	0.00044175	1000
Uniform sample		518.48	354855.0	0.9165	20
		485.77	391577.0	0.32713	1000

Proposition 1 *[29, Proposition 11.26] If* $\mathbf{K}$ *is bounded, star-shaped with respect to a ball* $B_r(x_c)$*, then* $\mathbf{K}$ *satisfies an interior cone condition with radius* $\rho = r$ *and angle* $\theta = 2\arcsin\left[\frac{r}{2\sqrt{D(\mathbf{K})}}\right]$.

In fact, any set satisfying the interior cone condition also satisfies the following stronger version of Assumption 1.

Assumption 2 There exist constants $\eta_{\mathbf{K}} > 0$ and $\epsilon_{\mathbf{K}} > 0$ such that, for all points $a \in \mathbf{K}$,

$$\mathrm{vol}(B_\epsilon(a) \cap \mathbf{K}) \geq \eta_{\mathbf{K}} \mathrm{vol} B_\epsilon(a) = \eta_{\mathbf{K}} \epsilon^n \gamma_n \quad \text{for all } 0 < \epsilon \leq \epsilon_{\mathbf{K}}. \tag{29}$$

Hence the only difference with Assumption 1 is that the constants $\eta_{\mathbf{K}}$ and $\epsilon_{\mathbf{K}}$ now depend only on the set $\mathbf{K}$ and not on the choice of $a \in \mathbf{K}$. Clearly, Assumption 2 implies Assumption 1. Moreover, any set satisfying the interior cone condition satisfies Assumption 2.

Lemma 7 *If a set* $\mathbf{K} \subseteq \mathbb{R}^n$ *satisfies the interior cone condition (28) then* $\mathbf{K}$ *also satisfies Assumption 2 (and thus Assumption 1), where we set*

$$\eta_{\mathbf{K}} = \left[\frac{\sin\theta}{1+\sin\theta}\right]^n \quad \textit{and} \quad \epsilon_{\mathbf{K}} = \rho.$$

Proof Assume that $\mathbf{K}$ satisfies the interior cone condition (28). Then, using [29, Lemma 3.7], we know that, for every $x \in \mathbf{K}$ and $h \le \rho/(1+\sin\theta)$, the closed ball $B_{h\sin\theta}(x + h\xi(x))$ is contained in $C(x, \xi(x), \theta, \rho)$ and thus in $\mathbf{K}$. Then, for all $x_0 \in \mathbf{K}$ and $\epsilon \in (0, \rho]$, after setting $h = \epsilon/(1+\sin\theta)$, one can obtain

$$\begin{aligned}\frac{\mathrm{vol}(B_\epsilon(x_0)\cap\mathbf{K})}{\mathrm{vol}B_\epsilon(x_0)} &\ge \frac{\mathrm{vol}C(x_0, \xi(x_0), \theta, \epsilon)}{\mathrm{vol}B_\epsilon(x_0)} \ge \frac{\mathrm{vol}B_{h\sin\theta}(x_0 + h\xi(x_0))}{\mathrm{vol}B_\epsilon(x_0)} \\ &= \left[\frac{\sin\theta}{1+\sin\theta}\right]^n.\end{aligned}$$

Thus, Assumption 2 holds after setting $\eta_{\mathbf{K}} = \left[\frac{\sin\theta}{1+\sin\theta}\right]^n$ and $\epsilon_{\mathbf{K}} = \rho$. □

As any convex body (i.e., full-dimensional convex and compact) is star-shaped with respect to any ball it contains, the next result follows as a direct application of Proposition 1 and Lemma 7.

Corollary 1 *Any convex body satisfies the interior cone condition and thus Assumptions 1 and 2.*

As an illustration we now consider the parameters $\eta_{\mathbf{K}}$, $\epsilon_{\mathbf{K}}$, and $r_{\mathbf{K}}$ (from relation (7)) when $\mathbf{K}$ is the hypercube, the simplex and the Euclidean ball.

Remark 3 Consider first the case when $\mathbf{K}$ is the hypercube $\mathbf{Q}_n = [0, 1]^n$. By Proposition 1, it satisfies the interior cone condition with radius $\rho = 1/2$ and angle $\theta = 2\arcsin\left[\frac{1}{4\sqrt{n}}\right]$. Hence, Assumption 2 holds with $\epsilon_{\mathbf{K}} = 1/2$ and $\eta_{\mathbf{K}} = \left(\frac{\sqrt{16n-1}}{8n+\sqrt{16n-1}}\right)^n$ (which is $\sim \left(\frac{1}{2\sqrt{n}}\right)^n$ for n large). Moreover, as $D(\mathbf{K}) = n$, it follows that $r_{\mathbf{K}} = 4ne$.

Consider now the case when $\mathbf{K}$ is the full-dimensional simplex Δ_n. By Proposition 1, it satisfies the interior cone condition with radius $\rho = \frac{1}{n+\sqrt{n}}$ and angle $\theta = 2\arcsin\left[\frac{1}{2\sqrt{2}(n+\sqrt{n})}\right]$ (since the ball with center $\rho(1,\ldots,1)^T$ and radius ρ is contained in $\widehat{\Delta}_n$). Hence Assumption 2 holds with $\epsilon_{\mathbf{K}} = \frac{1}{n+\sqrt{n}}$ and $\eta_{\mathbf{K}} = \left(\frac{\sqrt{8(n+\sqrt{n})^2-1}}{4(n+\sqrt{n})^2+\sqrt{8(n+\sqrt{n})^2-1}}\right)^n$ (which is $\sim \left(\frac{1}{\sqrt{2}n}\right)^n$ for n large). As $D(\mathbf{K}) = 2$, it follows that $r_{\mathbf{K}} = e(n+\sqrt{n})^3$.

Finally, for the Euclidean ball $\mathbf{K} = B_1(0)$, we have $\epsilon_{\mathbf{K}} = 1$, $\eta_{\mathbf{K}} = \left(\frac{\sqrt{3}}{2+\sqrt{3}}\right)^n$ and $r_{\mathbf{K}} = \max\{2e, n\}$.

Table 11 Computation times (in sec) for Lasserre's lower bounds of the first order

n	Styblinski–Tang function	Rosenbrock function
10	9.1	0.2
15	251.2	0.4
20	11125.4	0.5

5.2 Perspectives

In this paper we have analyzed the measure-based hierarchy of upper bounds $\underline{f}_{\mathbf{K}}^{(r)}$ and shown that their rate of convergence is in $O(1/\sqrt{r})$. We do not know whether $1/\sqrt{r}$ is the right estimate and understanding the exact rate of convergence is still an open problem.

We have carried out some computational experiments which indicate that in practice the convergence of the upper bounds is rather slow. On the other hand the sampling approach of Sect. 3 often provides good feasible solutions for the examples in Sect. 4, even for small values of r. One may therefore explore using the sampling technique (for small r) as a way of generating starting points for multi-start global optimization algorithms.

In comparison, the hierarchy of moment-based lower bounds introduced by Lasserre [16] performs well in practice, with moreover the attractive feature of admitting optimality certificates (see, e.g., [16,17,20,26]). As an illustration we considered the minimization over the hypercube $[-1, 1]^n$ of the (scaled) Styblinski-Tang and Rosenbrock functions with $n = 10, 15, 20$ variables and in all cases the global minimum was found using Gloptipoly at the relaxation of smallest order; see Table 11 for the computation times.

However, as already mentioned in the introduction, the known estimates about the rate of convergence of Lasserre's lower bounds are quite weak. Hence there is a discrepancy between the theoretical and practical performance, which raises the problem of finding sharper estimates on the convergence rate that better match the practical performance.

Acknowledgments We thank Jean Bernard Lasserre for bringing our attention to his work [18] and for several valuable suggestions, and Dorota Kurowicka for valuable discussions on multivariate sampling techniques.

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