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Convex underestimators of polynomials

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***Abstract*— Convex underestimators of a polynomial on a box. Given a non convex polynomial $f \in \mathbb{R}[\mathbf{x}]$ and a box $\mathbf{B} \subset \mathbb{R}^n$, we construct a sequence of convex polynomials $(f_{dk}) \subset \mathbb{R}[\mathbf{x}]$, which converges in a strong sense to the "best" (convex and degree-d) polynomial underestimator f_d^* of f. Indeed, f_d^* minimizes the L_1-norm $\|f - g\|_1$ on $\mathbf{B}$, over all convex degree-d polynomial underestimators g of f. On a sample of problems with non convex f, we then compare the lower bounds obtained by minimizing the convex underestimator of f computed as above and computed via the popular αBB method. In all examples we obtain significantly better results.**

I. Introduction

Consider the general polynomial optimization problem $\mathbf{P}$:

$$\begin{aligned} \mathbf{P}: \quad f^* = \min_{\mathbf{x}} \quad & f(\mathbf{x}) \\ \text{s.t} \quad & g_i(\mathbf{x}) \geq 0, \quad i = 1, ..., m \\ & \mathbf{x} \in [\mathbf{x}^L, \mathbf{x}^U] \subset \mathbb{R}^n, \end{aligned}$$

where f, g_i are polynomials and $\mathbf{x}^l, \mathbf{x}^U \in \mathbb{R}^n$ define the box $[\mathbf{x}^L, \mathbf{x}^U] \subset \mathbb{R}^n$. To approximate f^* and global minimizers of $\mathbf{P}$, one popular method (especially for large scale optimization problems) is the deterministic global optimization algorithm $\alpha\mathbf{BB}$. It uses a branch and bound scheme where the lower bounds computed at nodes of the tree search are obtained by solving a *convex* problem where f is replaced with some convex underestimators on a box $\mathbf{B} \subset \mathbb{R}^n$; see e.g. Floudas [2], Androulakis I.P et al. [5]. Of course, the overall efficiency of the $\alpha\mathbf{BB}$ algorithm depends heavily on the quality of the lower bounds computed in the branch and bound tree search, and so, ultimately, on the quality of the underestimators of f that are used. Therefore, the development of tight convex underestimators for non convex polynomials on the feasible region (compact or non compact) is of crucial importance.

Many results are available in the literature for computing convex envelopes of simple functions in *explicit* form, on a box $\mathbf{B} \subset \mathbb{R}^n$. See for instance Floudas [2] for convex envelopes of bilinear, trilinear, and multilinear monomials. For a general non convex function f, a convex underestimator can be obtained from the original function f by adding a negative part. For instance, this part could be a negative quadratic polynomial of the form

$$\mathbf{x} \mapsto \mathcal{L}(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^n \alpha_i (x_i - x_i^L)(x_i - x_i^U),$$

e.g., as in Androulakis et al. [5], or an exponential term from the original function of the form

$$\mathbf{x} \mapsto \mathcal{L}(\mathbf{x}) = f(\mathbf{x}) - \sum_{i=1}^n (1 - \mathrm{e}^{\alpha_i (x_i - x_i^L)})(1 - \mathrm{e}^{\alpha_i (x_i^U - x_i)}),$$

e.g., as in Akrotirianakis and Floudas [6]).

Several heuristics have been proposed for choosing appropriate nonnegative coefficients $\alpha \in \mathbb{R}^n$ in a tradeoff between two conflicting criteria. On the one hand, the additional term must be *negative enough* to overpower all the non convexities, which requires positive semidefiniteness of the Hessian matrix $\nabla^2 \mathcal{L}$ of the twice-differentiable function $\mathcal{L}$. But on the other hand, this additional part should also be as small as possible to obtain good lower bounds when using $\mathcal{L}$ as a substitute for f in the Branch and Bound tree search. Indeed, bad lower bounds would slow down convergence of the $\alpha\mathbf{BB}$ method. The so-called scaled Gershgorin method is among the most efficient.

Contribution. We present a new class of convex underestimators for a non convex polynomial on a box $\mathbf{B} \subset \mathbb{R}^n$. We use two certificates for (a) $\mathcal{L} \leq f$ and (b), convexity of $\mathcal{L}$ on the box $\mathbf{B}$. More precisely, we are looking for a convex polynomial $f_d \in \mathbb{R}[\mathbf{x}]_d$ (with degree d fixed) which approximates f from below on a given box $\mathbf{B} \subset \mathbb{R}^n$. Hence a polynomial candidate f_d must satisfy two major conditions:

- $f \geq f_d$ on $\mathbf{B}$,
- The Hessian matrix $\nabla^2 f_d$ must be positive semidefinite (i.e., $\nabla^2 f_d \succeq 0$) on $\mathbf{B}$.

But of course, there are many potential polynomial candidates $f_d \in \mathbb{R}[\mathbf{x}]_d$ and therefore, a meaningful criterion to select the "best" among them is essential. A natural candidate criterion to evaluate how good is f_d, is the integral $J(f_d) := \int_{\mathbf{B}} |f - f_d| d\mathbf{x}$, which evaluates the L_1-norm of $f - f_d$ on $\mathbf{B}$. Indeed, minimizing J tends to minimize the discrepancy (or "error") between f and f_d, uniformly on $\mathbf{B}$. If desired, some flexibility is permitted by allowing any weight function $W : \mathbf{B} \to \mathbb{R}$, positive on $\mathbf{B}$, so as to minimize $J_W = \int_{\mathbf{B}} |f - f_d| \, W d\mathbf{x}$.

Fortunately, to certify $f - f_d \geq 0$ and $\nabla^2 f_d \succeq 0$ on $\mathbf{B}$, a powerful tool is available, namely Putinar's Positivstellensatz (or algebraic positivity certificate) [9], already extensively used in many other contexts, and notably in global polynomial optimization; see e.g. [8] and the many references therein. Moreover, since $f \geq f_d$, the criterion $J(f_d)$ to minimize becomes $\int_{\mathbf{B}} (f - f_d) d\mathbf{x}$ and is *linear* in the coefficients of f_d! Therefore, we end up with a hierarchy of semidefinite programs, parametrized by some integer $k \in \mathbb{N}$. This parameter k reflects the size (or complexity) of

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Putinar's positivity certificate. Any optimal solution of a semidefinite program in this hierarchy provides a convex degree-d polynomial underestimator $f_{dk} \in \mathbb{R}[\mathbf{x}]$.

We then provide a sequence of convex degree-d polynomial underestimators $(f_{dk}) \subset \mathbb{R}[\mathbf{x}]_d$, $k \in \mathbb{N}$, such that $\|f - f_{dk}\|_1 \to \|f - f_d^*\|_1$ for the L_1-norm on $\mathbf{B}$, where f_d^* minimizes $J(h)$ over all convex degree-d polynomial underestimators h of f on $\mathbf{B}$. In fact, any accumulation point φ^* of the sequence $(f_{dk}) \subset \mathbb{R}[\mathbf{x}]_d$ also minimizes $J(h)$ and $f_{dk_i} \to \varphi^*$ pointwise for some subsequence.

This convergence analysis which provides the theoretical justification of the above methodology is only theoretical, because in practice one let k fixed (and even to a small value). However, we also prove that if k is sufficiently large, then f_{dk} is necessarily better than the $\alpha\mathbf{BB}$ underestimator. Finally, a practical justification is also obtained from a comparison with the $\alpha\mathbf{BB}$ method carried out on a set of test examples taken from the literature. Recall that the main motivation for computing underestimators is to compute "good" lower bounds on a box $\mathbf{B}$ for non convex problems, and use these lower bounds in a Branch and Bound algorithm. Therefore, to compare the two underestimators, we have computed the lower bound obtained my minimizing each of them on the box $\mathbf{B}$. In all examples, the results obtained with the moment approach are significantly better. Finally, we also provide an alternative way to compute the coefficients α in the $\alpha\mathbf{BB}$ method. Namely, we propose to compute the coefficients α which minimize $\int_{\mathbf{B}} |f - \mathcal{L}| d\lambda$ (where $\mathcal{L}$ is the $\alpha\mathbf{BB}$-underestimator), which reduces to solving a single semidefinite program. A library of such α could be computed off-line for several important particular cases.

Typically in large scale problems (in particular, mixed integer nonlinear programs), the non convex objective function f is a sum of many functions f_i, each with a small number of variables. As convex underestimators of f would be too costly to compute one rather adds up convex underestimators of the f_i's, much easier to obtain and which can be computed separately. Hence the moment approach can be implemented. However, if some sparsity is present in the data then it may be worth trying the specific and efficient semidefinite relaxations of Waki et al. [10] that take sparsity into account, to compute a convex underestimator of f. (Such "sparse" semidefinite relaxations have been implemented in [10] for solving some non convex optimization problems with up to a thousand variables!)

II. Notation and definitions

Let $\mathbb{R}[\mathbf{x}]$ be the ring of real polynomials in the n variables $\mathbf{x} = (x_1, ...x_n)$, and for every $d \in N$, let $\mathbb{R}[\mathbf{x}]_d \subset \mathbb{R}[\mathbf{x}]$ be the vector space of polynomials of degree at most d whose dimensions is $s(d) := \binom{n+d}{n}$. Similary, let $\mathbb{R}[\mathbf{x}, \mathbf{y}]_d \subset \mathbb{R}[\mathbf{x}, \mathbf{y}]$ be the vector space of polynomials of degree at most d whose dimension is $v(d) := \binom{2n+d}{2n}$. Also, let $\Sigma[\mathbf{x}]_d \subset \mathbb{R}[\mathbf{x}]$ be the cone of sums of squares of degree at most $2d$. With $(\mathbf{x}^\alpha)$, $\alpha \in \mathbb{N}^n$, being the canonical (monomial) basis of $\mathbb{R}[\mathbf{x}]$, a polynomial $f \in \mathbb{R}[\mathbf{x}]_d$ is written

$$\mathbf{x} \mapsto f(\mathbf{x}) = \sum_{\alpha \in \mathbb{N}^n} f_\alpha \, \mathbf{x}^\alpha,$$

for some vector of coefficients $\mathbf{f} = (f_\alpha) \in \mathbb{R}^{s(d)}$.

Let $\mathbb{N}_d^n := \{\alpha \in \mathbb{N}^n : \Sigma_i \alpha_i \leq d\}$ and let the box $\mathbf{B} := [0,1]^n$ be described as the compact basic semi-algebraic set:

$$\mathbf{B} := \{\mathbf{x} \in \mathbb{R}^n : g_j(\mathbf{x}) (:= x_j(1 - x_j)) \geq 0, j = 1, \ldots, n\}.$$

Let g_o be the constant polynomial equal to 1, and let $Q_{\mathbf{B}} \subset \mathbb{R}[\mathbf{x}]$ be the quadratic module associated with the $g_j's$, i.e.,

$$Q_{\mathbf{B}} := \left\{ \sum_{j=0}^{n} \sigma_j g_j : \sigma_j \in \Sigma[\mathbf{x}], j = 1, ..., n \right\}.$$

The quadratic module $Q_{\mathbf{B}}$ is *Archimedean*, i.e., there exists some $M > 0$ such that the quadratic polynomial $\mathbf{x} \mapsto M - \|\mathbf{x}\|^2$ belongs to $Q_{\mathbf{B}}$. The following result is a direct consequence of Putinar's Positivstellensantz [9] for Archimedean quadratic modules.

Proposition 1 (Putinar [9]): Every polynomial strictly positive on $\mathbf{B}$ *belongs to* $Q_{\mathbf{B}}$.

Let $\mathbf{K} \in \mathbb{R}^n$ be the closure of some open bounded set, and let $\mathbf{U} := \{\mathbf{x} \in \mathbb{R}^n := \|\mathbf{x}\|^2 \leq 1\}$. Recall that $f \in \mathbb{R}[\mathbf{x}]_d$ is convex on $\mathbf{K}$ if and only if $\nabla^2 f(\mathbf{x})$ is positive semidefinite on $\mathbf{K}$. Equivalently, f is convex if and only if $\mathbf{T} f_d \geq 0$ on $\mathbf{K} \times \mathbf{U}$, where $\mathbf{T} : \mathbb{R}[\mathbf{x}] \to \mathbb{R}[\mathbf{x}, \mathbf{y}]$ is the mapping:

$$h \mapsto \mathbf{T}h(\mathbf{x}, \mathbf{y}) := \mathbf{y}' \nabla^2 h(\mathbf{x}) \mathbf{y}, \quad \forall h \in \mathbb{R}[\mathbf{x}]. \qquad (1)$$

The vector of coefficients $((\mathbf{T}h)_{\alpha\beta}), \alpha, \beta \in \mathbb{N}^n$, of the polynomial $\mathbf{T}h \in \mathbb{R}[\mathbf{x}, \mathbf{y}]$ is a vector with finitely many zeros and is obtained from the vector $\mathbf{h}$ of $h \in \mathbb{R}[\mathbf{x}]$ by a linear mapping with associated infinite matrix $\mathbf{T}$ whose rows (resp. columns) are indexed in the canonical basis of $\mathbb{R}[\mathbf{x}, \mathbf{y}]$ (resp. $\mathbb{R}[\mathbf{x}]$) and with entries:

$$\mathbf{T}((\alpha, \beta), \delta) = (\mathbf{T}\mathbf{x}^\delta)_{\alpha\beta}, \quad \alpha, \beta, \delta \in \mathbb{N}^n. \qquad (2)$$

Next let $\mathbf{f} = (f_\alpha)$ be the vector of coefficients of $f \in \mathbb{R}[\mathbf{x}]$. Expanding the polynomial $\mathbf{T}f = \mathbf{y}' \nabla^2 f(\mathbf{x}) \mathbf{y}$ in the canonical basis $(\mathbf{x}^\alpha \mathbf{y}^\beta)$ of $\mathbb{R}[\mathbf{x}, \mathbf{y}]_d$, yields

$$\mathbf{y}' \nabla^2 f(\mathbf{x}) \mathbf{y} = \sum_{(\alpha, \beta) \in \mathbb{N}_d^{2n}} (\mathbf{T}f)_{\alpha\beta} \mathbf{x}^\alpha \mathbf{y}^\beta = \sum_{\delta \in \mathbb{N}_d^n} f_\delta \mathbf{T} \mathbf{x}^\delta.$$

III. Main result

Let λ denote the Borel probability measure uniformly distributed on the unit ball $\mathbf{B} := [0,1]^n$ (i.e. a normalization of the Lebesgue measure on $\mathbb{R}^n$), and consider the associated optimization problem:

$$\min_{h \in \mathbb{R}[\mathbf{x}]_d} \left\{ \int_{\mathbf{B}} (f - h) d\lambda : \quad f - h \geq 0 \text{ on } \mathbf{B}; \; h \text{ convex on } \mathbf{B} \right\}, \qquad (3)$$

whose optimal value is denoted by ρ_d. Equivalently,

$$\rho_d = \min_{h\in\mathbb{R}[\mathbf{x}]_d} \Big\{ \int_{\mathbf{B}} (f-h)d\lambda : \quad f-h\geq 0 \text{ on } \mathbf{B}; \quad \mathbf{T}\, h \geq 0 \text{ on } \mathbf{S} \Big\}, \quad (4)$$

where $\mathbf{T}$ is defined in (1), and $\mathbf{S} = \mathbf{B}\times\mathbf{U}$.

Lemma 1: The optimization problem (4) has an optimal solution $f_d^*\in\mathbb{R}[\mathbf{x}]_d$.

Proof: Observe that for every feasible solution $f_d\in\mathbb{R}[\mathbf{x}]_d$, $f_d\leq f$ on $\mathbf{B}$ and so

$$\int_{\mathbf{B}} (f-f_f)\,d\lambda = \int_{\mathbf{B}} |f-f_d|\,d\lambda = \|f-f_d\|_1,$$

where $\|\cdot\|_1$ denotes the norm on $L_1([0,1]^n)$, and which also defines a norm on $\mathbb{R}[\mathbf{x}]_d$ (or, equivalently, on $\mathbb{R}^{s(d)}$). Indeed, if $f,g\in\mathbb{R}[\mathbf{x}]$ and $\|f-g\|_1 = 0$ then $f=g$, almost everywhere on $\mathbf{B}$, and so on all of $\mathbf{B}$ because both are polynomials and $\mathbf{B}$ has nonempty interior. So if $(f_{dk})\subset\mathbb{R}[\mathbf{x}]_d$, $k\in\mathbb{N}$, is a minimizing sequence then $f_{dk}\in\Delta_a := \{h : \|f-h\|_1\leq a\}$ for all k (where $a := \int_{\mathbf{B}}(f-f_{d0})\,d\lambda$), and $\int_{\mathbf{B}}(f-f_{dk})\,d\lambda \to \rho_d$ as $k\to\infty$. Notice that $\Delta_a\subset\mathbb{R}[\mathbf{x}]_d$ is a ball and a compact set. Therefore, there is a subsequence k_i and a element $f_d^*\in\Delta_a$ such that $f_{dk_i}\to f_d^*$ as $i\to\infty$. Therefore, $f_{dk_i}(\mathbf{x})\to f_d^*(\mathbf{x})$ for every $\mathbf{x}\in\mathbf{B}$. Next, since $f_{dk_i}\leq f$ on $\mathbf{B}$, by the Bounded Convergence Theorem,

$$\rho_d = \lim_{i\to\infty}\int_{\mathbf{B}}(f-f_{dk_i})\,d\lambda \to \int_{\mathbf{B}}(f-f_d^*)\,d\lambda.$$

It remains to prove that f_d^* is a feasible solution of (4). So, let $\mathbf{x}\in\mathbf{B}$ be fixed, arbitrary. Then since $f-f_{dk}\geq 0$ on $\mathbf{B}$, the pointwise convergence $f_{dk_i}\to f_d^*$ yields $f(\mathbf{x})-f_d^*(\mathbf{x})\geq 0$. Hence $f-f_d^*\geq 0$ on $\mathbf{B}$. Similarly, let $(\mathbf{x},\mathbf{y})\in\mathbf{S}$ be fixed, arbitrary. Again, from $f_{dk}(\mathbf{x},\mathbf{y})\geq 0$, the convergence $f_{dk_i}\to f_d^*$, and the definition of $\mathbf{T}$ in (1), it immediately follows that $\mathbf{T}f_d^*(\mathbf{x},\mathbf{y})\geq 0$. Therefore, $\mathbf{T}f_d^*\geq 0$ on $\mathbf{S}$, and so $\mathbf{f}_d^*$ is feasible for (4). ∎

With $\mathbf{U} := \{\mathbf{y}\in\mathbb{R}^n : \|\mathbf{y}\|^2\leq 1\}$, the set $\mathbf{S}=\mathbf{B}\times\mathbf{U}\subset\mathbb{R}^{2n}$ is a compact basic semi-algebraic set. Note that in (4) one has replaced the constraint "h is convex on $\mathbf{B}$" with $\mathbf{T}h\geq 0$ on $\mathbf{S}$. So, let $Q_{\mathbf{S}}\subset\mathbb{R}[\mathbf{x},\mathbf{y}]$ be the quadratic module associated with $\mathbf{S}$, i.e.,

$$Q_{\mathbf{S}} = \{\sum_{j=0}^{n+1}\theta_j\, g_j \;:\; \theta_j\in\Sigma[\mathbf{x},\mathbf{y}], j=0,...,n+1\},$$

where $(\mathbf{x},\mathbf{y})\mapsto g_{n+1}(\mathbf{x},\mathbf{y}) := 1-||\mathbf{y}||^2$; it is straightforward to show that $Q_{\mathbf{S}}$ is Archimedean.

By Proposition 1, $\rho = \int_{\mathbf{B}} fd\lambda - \rho_d$, and the optimal solution f_d^* of (3) is an optimal solution of the problem $\mathbf{P}_d$ defined by:

$$\rho_d = \max_{f_d\in\mathbb{R}[\mathbf{x}]_d}\Big\{\int_{\mathbf{B}} f_d d\lambda : f-f_d\in Q_{\mathbf{B}}; \mathbf{T}f_d\in Q_{\mathbf{S}}\Big\}, \quad (5)$$

So with $\mathbf{T}$ being the mapping defined in (1), introduce the following semidefinite relaxation $\mathbf{P}_{dk}$ of $\mathbf{P}_d$, defined by:

$$\begin{cases} \max_{h\in\mathbb{R}[x]_d} & \int_{\mathbf{B}} h\, d\lambda \\ & f(\mathbf{x}) = h(\mathbf{x}) + \sum_{j=0}^n \sigma_j(\mathbf{x})g_j(\mathbf{x}) \quad \forall\mathbf{x} \\ \text{s.t.} & \mathbf{T}h(\mathbf{x},\mathbf{y}) = \sum_{j=0}^n \theta_j(\mathbf{x},\mathbf{y})g_j(\mathbf{x}) \\ & \qquad +\theta_{n+1}(\mathbf{x},\mathbf{y})g_{n+1}(\mathbf{x},\mathbf{y}) \quad \forall\mathbf{x},\mathbf{y} \\ & \sigma_0\in\Sigma[\mathbf{x}]_k,\ \sigma_j\in\Sigma[\mathbf{x}]_{k-1},\ j\geq 1 \\ & \theta_0\in\Sigma[\mathbf{x},\mathbf{y}]_k, \theta_j\in\Sigma[\mathbf{x},\mathbf{y}]_{k-1},\ j\geq 1 \end{cases} \quad (6)$$

with $k\geq\max[\lceil d/2\rceil, \lceil(\deg f)/2\rceil]$ and optimal value ρ_{dk}.

Theorem 1: Let ρ_d be the optimal value of (4) and consider the hierarchy of semidefinite relaxations (6) with associated sequence of optimal values (ρ_{dk}), $k\in\mathbb{N}$. Then $\int_{\mathbf{B}} fd\lambda - \rho_{dk}\downarrow\rho_d$ as $k\to\infty$, so that $\|f-f_{dk}\|_1\downarrow\rho_d$ if $f_{dk}\in\mathbb{R}[\mathbf{x}]_d$ is any optimal solution of (6). Moreover, any accumulation point $\varphi^*\in\mathbb{R}[\mathbf{x}]_d$ of the sequence $(f_{dk})\subset\mathbb{R}[\mathbf{x}]_d$, is an optimal solution of (4), and $f_{dk_i}\to\varphi^*$ pointwise for some subsequence (k_i), $i\in\mathbb{N}$.

Proof: Let $f_d^*\in\mathbb{R}[\mathbf{x}]_d$ be an optimal solution of (4), which by Lemma 1, is guaranteed to exist. As f_d^* is convex on $\mathbf{B}$, $\nabla^2 f_d^*\succeq 0$ on $\mathbf{B}$. Let $\epsilon>0$ be fixed and such that $\epsilon\|\mathbf{x}\|^2 < 1$ on $\mathbf{B}$. Let $g_\epsilon := f_d^* - \epsilon + \epsilon^2\|\mathbf{x}\|^2)$, so that $\nabla^2 g_\epsilon\succeq\epsilon^2\mathbf{I}$ on $\mathbf{B}$. Hence, by the matrix version of Putinar's Theorem (see [8, Theorem 2.22]), there exist SOS matrix polynomials $\mathbf{F}_j$, $j=0,\ldots,n$, such that

$$\nabla^2 g_\epsilon(\mathbf{x}) = \mathbf{F}_0(\mathbf{x}) + \sum_{j=1}^n \mathbf{F}_j(\mathbf{x})\, g_j(\mathbf{x}).$$

(Recall that a SOS matrix polynomial $\mathbf{F}\in\mathbb{R}[\mathbf{x}]^{q\times q}$ is a matrix polynomial of the form $\mathbf{x}\mapsto\mathbf{L}(\mathbf{x})'\mathbf{L}(\mathbf{x})$ for some matrix polynomial $\mathbf{L}\in\mathbb{R}[\mathbf{x}]^{p\times q}$ for some $p\in\mathbb{N}$). And so, for every $j=0,\ldots,n$, the polynomial $(\mathbf{x},\mathbf{y})\mapsto\theta_j^\epsilon(\mathbf{x},\mathbf{y}) := \mathbf{y}'\mathbf{F}_j\mathbf{y}$ is SOS for every $j=0,\ldots,n$, and

$$\mathbf{T}g_\epsilon = \sum_{j=0}^n \theta_j^\epsilon(\mathbf{x},\mathbf{y})\, g_j(\mathbf{x}) + \theta_{n+1}^\epsilon(\mathbf{x},\mathbf{y})(1-\|\mathbf{y}\|^2).$$

Moreover, observe that $f-g_\epsilon = f-f_d^* + \epsilon(1-\epsilon\|\mathbf{x}\|^2)$ is strictly positive on $\mathbf{B}$. Hence by Putinar's Theorem,

$$f-g_\epsilon = \sum_{j=0}^n \sigma_j^\epsilon g_j,$$

for some SOS polynomials $\sigma_j\in\mathbb{R}[\mathbf{x}]$, $j=1,\ldots,n$. Let $2t\geq\max\{[\max_j\deg\sigma_j + 2, \max_j[\deg\mathbf{F}_j+4]\}$. Then the polynomial g_ϵ is a feasible solution of (6) whenever $k\geq t$. Its value satisfies

$$\int_{\mathbf{B}} g_\epsilon d\lambda = \int_{\mathbf{B}}(f_d^* - \epsilon + \epsilon^2\|\mathbf{x}\|^2)d\lambda \geq \int_{\mathbf{B}} f_d^* d\lambda - \epsilon,$$

and so $\rho_{dt}\geq\rho_d-\epsilon$. As $\epsilon>0$ was arbitrary and the sequence (ρ_{dk}) is monotone non decreasing, the first result follows. Next, any optimal solution $f_{dk}\in\mathbb{R}[\mathbf{x}]_d$ of (6) satisfies $\|f - f_{dk}\|_1 \leq \int_{\mathbf{B}} f d\lambda - \rho_{d1} =: a$ and so belongs to the ball $\Delta_a := \{h : \|f - h\|_1 \leq a\}$. Let $\varphi^* \in \Delta_a$ be an arbitrary accumulation point of the sequence (f_{dk}) for some subsequence (k_i), $i \in \mathbb{N}$. Proceeding as in the proof of Lemma 1, $f_{dk_i} \to \varphi^*$ pointwise, $f - \varphi^* \geq 0$ and $\nabla^2 \varphi^* \succeq 0$ on $\mathbf{B}$. Moreover, by the Bounded Convergence Theorem

$$\rho_d = \lim_{i\to\infty} \rho_{dk_i} = \lim_{i\to\infty} \int_{\mathbf{B}} (f - f_{dk_i}) d\lambda = \int_{\mathbf{B}} (f - \varphi^*) d\lambda,$$

which proves that φ^* is an optimal solution of (4). ∎

Theorem 1 states that the optimal value of the semidefinite relaxation (6) can become as close as desired to that of problem (4), and accumulation points of solutions of (6) are also optimal solutions of (4). The price to pay is the size of the semidefinite program (6) which becomes larger and larger as k increases. In practice, on let k fixed at a small value and the computational experiments presented below indicate that even with k small ($k = \lceil(\deg f)/2\rceil$), the polynomial f_{dk} does not change much with k, and provides better lower bounds than the $\alpha\mathbf{BB}$-underestimator.

IV. Comparing the moment and $\alpha\mathbf{BB}$ methods

A. *Convex underestimators from the $\alpha\mathbf{BB}$ method*

To obtain a convex underestimator of a non convex polynomial, the $\alpha\mathbf{BB}$ method is based on a decomposition of f into a sum of non convex terms of special type (e.g., linear, bilinear, tri-linear, fractional, fractional tri- and quadrilinear) and non convex terms of arbitrary type. The terms of special type are replaced with their convex envelopes which are already known (see Floudas [2]).

For an arbitrary type f, the underestimator $\mathcal{L}$ is obtained by adding a separable negative quadratic polynomial, i.e.,

$$\mathcal{L}(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{n} \alpha_i (x_i - x_i^L)(x_i - x_i^U), \qquad (7)$$

where the positive coefficients α_i's are determined so as to make the polynomial underestimator $\mathcal{L}$ convex. As $\mathcal{L}$ is convex on $\mathbf{B}$ if and only if its Hessian $\nabla^2\mathcal{L}$ is positive semidefinite on $\mathbf{B}$, the coefficients α_i, $, i = 1, \ldots, n$ must satisfy

$$\nabla^2\mathcal{L}(\mathbf{x}) = \nabla^2 f(\mathbf{x}) + 2\Delta \succeq 0, \quad \forall \mathbf{x} \in \mathbf{B}, \qquad (8)$$

where $\Delta = \mathrm{diag}\{\alpha_1, \alpha_2, ..., \alpha_n\}$ is referred to as the *diagonal shift matrix*. The *separation distance* between the original polynomial f and its convex underestimator $\mathcal{L}$ is

$$d_{\alpha\mathbf{BB}} = f(\mathbf{x}) - \mathcal{L}(\mathbf{x}) = -\sum_{i=1}^{n} \alpha_i (x_i - x_i^L)(x_i - x_i^U) \geq 0,$$

which achieves its maximum at the middle point of the interval $[\mathbf{x}^L, \mathbf{x}^U]$. Therefore,

$$d_{\alpha\mathbf{BB}}^{max} = -\frac{1}{4}\sum_{i=1}^{n} \alpha_i (x_i^U - x_i^L)^2.$$

hence, the value of $d_{\alpha\mathbf{BB}}$ is proportional to the $\alpha_i's$ and the size of the domains $[\mathbf{x}^L, \mathbf{x}^U]$. A number of methods to calculate the parameters diagonal Δ have been developed using interval analysis (see e.g. Floudas [2]), and are based on the following result:

Theorem 2: Let $[\mathcal{H}_f]$ be a real symmetric interval matrix such that $\nabla^2 f(\mathbf{x}) \in [\mathcal{H}_f], \forall \mathbf{x} \in [\mathbf{x}^L, \mathbf{x}^U]$. If $[\nabla^2_{\mathcal{L}}] := [\mathcal{H}_f] + 2\Delta \succeq 0$ then $\mathcal{L}$ is convex on $[\mathbf{x}^L, \mathbf{x}^U]$.

Among the most efficient methods is the scaled Gershgorin method where $(\alpha_i) \in \mathbb{R}^n$ is determined by

$$\alpha_i = \max\Big\{0, -\frac{1}{2}(\underline{f}_{ii} - \sum_{j\neq i} \max\{|\underline{f}_{ii}|, |\overline{f}_{ij}|\})\frac{d_j}{d_i}\Big\} \qquad (9)$$

where $\underline{f}_{ii}$ and $\overline{f}_{ij}$ are the lower and upper bounds of $\partial^2 f/\partial x_i \partial x_j$ in the interval $[\mathbf{x}^L, \mathbf{x}^U]$ and $d_i, i = 1, 2, ..., n$ are some chosen positive parameters. Notice that computing good upper and lower bounds may be time consuming.

B. *Comparison with the moment method*

Given an arbitrary polynomial $f \in \mathbb{R}[\mathbf{x}]$ and $d \in \mathbb{N}$, one searches for an *ideal* polynomial $f_d^* \in \mathbb{R}[\mathbf{x}]_d$ convex on $\mathbf{B}$, that is an optimal solution of $\mathbf{P}_d$, i.e., f_d^* solves:

$$\rho_d = \max_{h\in\mathbb{R}[\mathbf{x}]_d} \left\{ \int_{\mathbf{B}} h\, d\lambda : f - h \in Q_{\mathbf{B}};\ \mathbf{T}\, h \in Q_{\mathbf{S}} \right\} \qquad (10)$$

(See Lemma 1.) In practice, one obtains a convex underestimator $f_{dk} \in \mathbb{R}[\mathbf{x}]_d$ by solving the semidefinite relaxation (6) of $\mathbf{P}_d$ for a small value of k, typically $k = \lceil d/2\rceil$.

We can now compare f_{dk} with the $\alpha\mathbf{BB}$ underestimator $\mathcal{L}$ in (7), with $x_i^L = 0$ and $x_i^U = 1$ (possibly after scaling).

Lemma 2: With f being a non convex polynomial, let $f_{dk} \in \mathbb{R}[\mathbf{x}]_d$ be an optimal solution of (6) and let $\mathcal{L}$ be as in (7). If $\nabla^2\mathcal{L}(\mathbf{x}) \succ 0$ for all $\mathbf{x} \in \mathbf{B}$ then

$$\|f - f_{dk}\|_1 \leq \|f - \mathcal{L}\|_1, \qquad (11)$$

whenever k is sufficiently large, i.e., the convex underestimator f_{dk} is better than $\mathcal{L}$ for the L_1-norm $\int_{\mathbf{B}} |f - g| d\lambda$.

Proof: Observe that

$$f(\mathbf{x}) - \mathcal{L}(\mathbf{x}) = \sum_{i=1}^{n} \underbrace{\alpha_i}_{\sigma_i \in \Sigma[\mathbf{x}]_0} x_i(1 - x_i),$$

that is, the separation distance $d_{\alpha\mathbf{BB}}$ is a very specific element of $Q_{\mathbf{B}}$, where the SOS weights σ_j are the constant polynomials α_j, $j = 1, \ldots, n$.

Moreover, if $\mathbf{T}\mathcal{L} \succ 0$ on $\mathbf{B}$ then by [8, Theorem 2.22]

$$\nabla^2\mathcal{L}(\mathbf{x}) = \sum_{j=0}^{n} \mathbf{F}_j(\mathbf{x})\, g_j(\mathbf{x}),$$

for some SOS polynomial matrices $\mathbf{x} \mapsto \mathbf{F}_j(\mathbf{x})$ (i.e., of the form $\mathbf{L}_j(\mathbf{x})\mathbf{L}_j(\mathbf{x})'$ for some matrix polynomials $\mathbf{L}_j$) and so

$$\mathbf{T}\mathcal{L}(\mathbf{x}, \mathbf{y}) = \mathbf{y}'\nabla^2\mathcal{L}(\mathbf{x})\mathbf{y} = \sum_{j=0}^{n} \underbrace{(\mathbf{L}_j(\mathbf{x})\mathbf{y})^2}_{\theta_j \in \Sigma[\mathbf{x}, \mathbf{y}]} g_j(\mathbf{x}).$$

Hence $\mathbf{T}\mathcal{L} \in Q_{\mathbf{S}}$ and $\mathcal{L}$ is a feasible solution of (6) as soon as $2k \geq \max_j \deg \mathbf{F}_j + 4$. Therefore, at least for k sufficiently large k,

$$\int_{\mathbf{B}} f_{dk} d\lambda \geq \int_{\mathbf{B}} \mathcal{L}\, d\lambda,$$

and so as $f \geq f_{dk}$ and $f \geq \mathcal{L}$ on $\mathbf{B}$, (11) holds. ∎

C. Computational results

We consider the two natural choices, $d = \deg f$ and $d = 2$ (and $k = \max[\lceil d/2 \rceil, \lceil (\deg f)/2 \rceil]$). With the former one searches for the best convex underestimator of same degree as f, while with the latter one searches for the best quadratic underestimator of f. Recall that the main motivation for computing underestimators is to compute "good" lower bounds on a box $\mathbf{B}$ for non convex problems, and use these lower bounds in a Branch and Bound algorithm. Therefore, to compare the moment and $\alpha\mathbf{BB}$ underestimators, we have chosen non convex optimization problems in the literature, and replaced the original non convex objective function by its moment and $\alpha\mathbf{BB}$ underestimator, respectively f_d and $\mathcal{L}$. We then compare the minimum f^*_{mom} (resp. $f^*_{\alpha\mathbf{BB}}$) obtained by minimizing[1] f_d (resp. $\mathcal{L}$) on the box $\mathbf{B}$. We also provide the respective values of the L_1-norm $\int_{\mathbf{B}} |f - f_d| d\lambda$ and $\int_{\mathbf{B}} |f - \mathcal{L}| d\lambda$. In view of (7), the latter is easy to compute.

Computational results: Figure 1 and Figure 2 illustrate an example with the bivariate polynomial $f(\mathbf{x}) = -3x_1 - 4x_2 + 10x_1^2 + 9x_2^2 + 6x_1^3 + 7x_2^3$ in the box $\mathbf{B} = [-1.5, 1]^2$. The global minimum is $f^* = -0.5957$ to be compared with $f_{mom} = -7.7149$ and $f_{\alpha\mathbf{BB}} = -68.4650$.

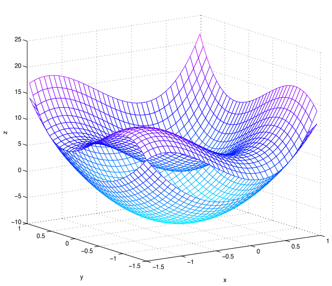

Fig. 1. $f^* = -0.5957$; $f_{mom} = -7.7149$

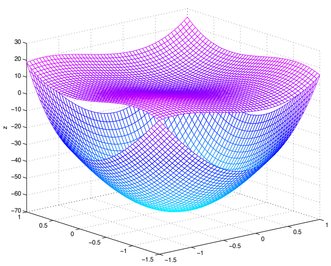

Fig. 2. $f^* = -0.5957$; $f_{\alpha\mathbf{BB}} = -68.4650$

1) Choice 1: $d = \deg f$: Table I displays results for several nonconvex polynomials f with $n > 2$ variables and various degrees. The examples are test functions f taken from Gounaris and Floudas [3]. One may see that the lower bound f_{mom} obtained from the moment method is significantly better (and even much better) than the lower bound $f_{\alpha\mathbf{BB}}$ obtained from the $\alpha\mathbf{BB}$ method.

Prob	n	deg f	$[\mathbf{x}^L, \mathbf{x}^U]$	$f_{\alpha\mathbf{BB}}$	f_{mom}	f^*
Test2	4	3	[0,1]	-1.54	-1.225	-1
Test3	5	4	[-1,1]	-15	-14	-6
——	5	4	[1,3]	-73.45	-73.05	-66
Test4	6	6	[-1,1]	-60.15	-10.06	-3
Test5	3	6	[-2,2]	-411.2	-12.66	-1
Test10	4	4	[0,1]	-197.54	-54.28	0
Test11	4	4	[0,1]	-33.02	-0.85	0
Test14	3	4	[-5,1]	-2409	-1020	-300
——	4	4	[-5,1]	-3212	-1360	-400
——	5	4	[-5,1]	-4015	-1700	-500

TABLE I
COMPARING f_{mom} AND $f_{\alpha\mathbf{BB}}$; $d = \deg f$

2) Choice 2: $d = 2$ (quadratic underestimator): Given $f \in \mathbb{R}[\mathbf{x}]$, one searches for a convex polynomial $f_d \in \mathbb{R}[\mathbf{x}]_2$ of the form $\mathbf{x} \mapsto f_d(\mathbf{x}) = \mathbf{x}'\mathbf{A}\mathbf{x} + \mathbf{a}'\mathbf{x} + b$ for some real positive semidefinite symmetric matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, vector $\mathbf{a} \in \mathbb{R}^n$ and scalar b. Let $\mathbf{M}_\lambda$ be the moment matrix of order 1 of the (normalized) Lebesgue measure λ, i.e.,

$$\mathbf{M}_\lambda = \begin{bmatrix} 1 & \gamma' \\ \gamma & \Lambda \end{bmatrix}$$

with $\gamma_i = \int_{\mathbf{B}} x_i d\lambda$ for all $i = 1, \ldots, n$, and $\Lambda_{ij} = \int_{\mathbf{B}} x_i x_j d\lambda$ for all $1 \leq i, j \leq n$. The semidefinite relaxation $\mathbf{P}_{dk}$ in (6) reads:

$$\begin{cases} \max\limits_{b,\mathbf{a},\mathbf{A}} & b + \mathbf{a}'\gamma + \langle \mathbf{A}, \Lambda \rangle \\ \text{s.t.} & f(\mathbf{x}) = f_d(\mathbf{x}) + \sum_{j=0}^{n} \sigma_j(\mathbf{x}) g_j(\mathbf{x}) \quad \forall \mathbf{x} \\ & \mathbf{A} \succeq 0;\ \sigma_0 \in \Sigma[\mathbf{x}]_d,\ \sigma_j \in \Sigma[\mathbf{x}]_{d-1},\ j \geq 1. \end{cases} \tag{12}$$

Table II displays results for a number of optimization polynomial problems taken from Floudas [2]. On a box $\mathbf{B}$ that contains the feasible set, we compute the convex $\alpha\mathbf{BB}$ underestimator $\mathcal{L}$ and the (only degree-2) moment underestimator f_d of the initial objective function f. We then compute their respective minimum $f_{\alpha\mathbf{BB}}$ and f_{mom} on $\mathbf{B}$. As can be seen from Table I and Table II, the lower bound f_{mom} is significantly better (and sometimes much better) than $f_{\alpha\mathbf{BB}}$, even with only a convex quadratic underestimator, and in most examples, the lower bound f_{mom} is very close to the global minimum f^*. Finally, Table III displays the respective values of $\int_{\mathbf{B}} |f - \mathcal{L}| d\lambda$ and $\int_{\mathbf{B}} |f - f_d| d\lambda$. Once again, the score of the moment underestimator f_d is significantly better than that of the $\alpha\mathbf{BB}$ underestimator $\mathcal{L}$.

D. Computing α in the $\alpha\mathbf{BB}$ method

The above approach can also be used to provide a new and systematic way to compute the coefficients $\alpha \in \mathbb{R}^n_+$ of the $\alpha\mathbf{BB}$ method. Indeed it suffices to impose the additional requirement that the underestimator has the $\alpha\mathbf{BB}$ form (7).

[1] All computations were made by running the Gloptipoly software described in Henrion et al. [4], for solving the Generalized Problem of Moments whose global optimization is only a special case. The $\alpha\mathbf{BB}$ underestimator was computed via the scaled Gershgorin method.

Prob	n	m	$f_{\alpha\mathbf{BB}}$	f_{mom}	f^*
Fl.2.2	5	11	-18.9	-18.9	-17
Fl.2.3	6	8	-5270.9	-361.50	-361
Fl.2.4	13	21	-592	-195	-195
Fl.2.6	10	21	-269.833	-269.45	-268.01
Fl.2.8C1	20	30	-560	-560	-394.75
Fl.2.8C2	20	30	-1050	-1050	-884
Fl.2.8C3	20	30	-13600	-12000	-8695
Fl.2.8C4	20	30	-920	-920	-754.75
Fl.2.8C5	20	30	-16645	-10010	-4150.41

TABLE II
COMPARING f_{mom} AND $f_{\alpha\mathbf{BB}}$; $d = 2$

Prob	$\int_{\mathbf{B}} \lvert f - \mathcal{L} \rvert d\lambda$	$\int_{\mathbf{B}} \lvert f - f_d \rvert d\lambda$
Test2	1	0.625
Test3(1)	373.33	192.44
Test3(2)	1653.3	1529.6
Test4	3840	467.04
Test5	6336.5	1485.3
Test10	133.33	57.00
Test11	46.33	1
Test14(1)	5.63e+05	1.18e+05
Test14(2)	5.25e+06	1.10e+06
Test14(3)	4.59e+07	9.67e+06
Fl.2.2	41.66	41.66
Fl.2.3	67500	833.33
Fl.2.4	8122.5	900
Fl.2.6	8.33	5.83
Fl.2.8C1	1.22e+24	1.22e+24
Fl.2.8C2	1.22e+24	1.22e+24
Fl.2.8C3	2.44e+25	2.44e+25
Fl.2.8C4	1.22e+24	1.22e+24
Fl.2.8C5	3.35e+15	3.35e+15

TABLE III
COMPARING $\int_{\mathbf{B}} |f - \mathcal{L}|)d\lambda$ AND $\int_{\mathbf{B}} |f - f_d|d\lambda$

And so, possibly after a rescaling of the box $\prod_{i=1}^n [x_i^L, x_i^U]$ to $[0,1]^n$, one wishes to minimize

$$\int_{\mathbf{B}} (f - \mathcal{L}) d\lambda = \underbrace{\int_{\mathbf{B}} f d\lambda}_{\text{constant}} + \sum_{i=1}^n \alpha_i \int_{\mathbf{B}} x_i(1 - x_i) d\lambda, \quad (13)$$

$= \int_{\mathbf{B}} f d\lambda + \frac{1}{6} \sum_{i=1}^n \alpha_i$, under the convexity constraint:

$$\mathbf{y}'\nabla^2\mathcal{L}(\mathbf{x})\mathbf{y} \;=\; \sum_{j=1}^{n+1} \theta_j\, g_j\,;\; \theta_j \in \Sigma[\mathbf{x},\mathbf{y}]_{d-v_j},\; \forall j,$$

where $d \geq 1 + \deg f$. The parameter $d \in \mathbb{N}$ is now the maximum degree allowed in the Putinar certificate of convexity. Therefore computing the best α_i's reduce to solving

$$\begin{array}{ll} \min & \{\sum_{i=1}^n \alpha_i \;:\; \mathbf{y}'\nabla^2 f(\mathbf{x})\mathbf{y} = -2\sum_{i=1}^n \alpha_i y_i^2 + \sum_{j=0}^{n+1} \theta_j g_j \\ & \alpha \geq 0;\; \theta_{n+1} \in \mathbb{R}[\mathbf{x},\mathbf{y}]_{df+1};\; \theta_j \in \Sigma[\mathbf{x},\mathbf{y}]_{df-v_j}\}, \end{array}$$

a semidefinite program! Results for various box sizes in Table IV show that this strategy can yield significantly better lower bounds than with the scaled Gershgorin method, at least on the examples with highly nonconvex functions. Indeed, for various box sizes, the resulting lower bound f_{mom} is always much better than the $f_{\alpha\mathbf{BB}}$ bound.

Prob	$[x^L, x^U]$	$f_{\alpha\mathbf{BB}}$	f_{mom}	f^*
Fl 8.2.7	$[0,1]^5$	-899.5	-2.76	-0.5
Fl 8.2.7	$[-1,1]^5$	-2999	-23	-0.6
Fl 8.2.7	$[-5,5]^5$	-63000	-2987	-982
Test 10	$[0,1]^4$	-197.5	-61.9	0
Test 10	$[-1,1]^4$	-870.2	-323.8	0
Test 10	$[-5,5]^4$	-137e+05	-4.73e+04	-19

TABLE IV
COMPARING f_{mom} AND $f_{\alpha\mathbf{BB}}$; $d = 2$

V. CONCLUSION

By solving a hierarchy of semidefinite programs one may approximate, as closely as desired on a box $\mathbf{B} \subset \mathbb{R}^n$, the best degree-$d$ convex polynomial underestimator g of a nonconvex polynomial f, i.e. the one which minimizes the L_1-norm $\int_{\mathbf{B}} |f - g| d\lambda$. On a sample of non convex problems from the literature, the resulting lower bounds computed by minimizing this convex underestimator (even obtained at the first semidefinite program in the hierarchy), are significantly better than those obtained by minimizing the popular $\alpha\mathbf{BB}$ underestimator. The $\alpha\mathbf{BB}$ estimator may be cheaper to compute, but in fact this depends on how much effort is spent to get "good" upper and lower bounds in (9), since the latter bounds directly affect its quality. But remember that for large scale discrete optimization problems, one typically considers *sums* of convex underestimators involving few variables rather than a single underestimator involving all variables! And so in this situation, our underestimator is also cheap to compute.

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