# Norm Bounds and Underestimators for Unconstrained Polynomial Integer Minimization 

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#### Abstract

We consider the problem of minimizing a polynomial function over the integer lattice. Though impossible in general, we use a known sufficient condition for the existence of continuous minimizers to guarantee the existence of integer minimizers as well. In case this condition holds, we use sos programming to compute the radius of a $p$-norm ball which contains all integer minimizers. We prove that this radius is smaller than the radius known from the literature. Furthermore, we derive a new class of underestimators of the polynomial function. Using a Stellensatz from real algebraic geometry and again sos programming, we optimize over this class to get a strong lower bound on the integer minimum.

Our radius and lower bounds are evaluated experimentally. They show a good performance, in particular within a branch and bound framework.


Keywords integer optimization; polynomials; lower bounds; branch and bound

## 1. Introduction

Given a multivariate polynomial $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$, we consider its minimization over the integer lattice, i.e., the problem

$$
\begin{align*}
& \min f(x) \\
& \text { s.t. } x \in \mathbb{Z}^{n} . \tag{IP}
\end{align*}
$$

This is a special type of a nonlinear integer optimization problem and is incomputable in general: Hilbert's tenth problem asks if there exists an algorithm that decides whether for a given polynomial $f$ with integer coefficients the equation $f(x)=0$ has a solution

[^0]$x \in \mathbb{Z}^{n}$. Seventy years later it was proved by Matiyasevich Mat70 that no such algorithm can exist. So if there was an algorithm to solve IP, we would also get an algorithm to decide whether $f(x)=0$ has an integer solution by minimizing $f^{2}$ over $\mathbb{Z}^{n}$. Consequently, IP cannot be solved for general polynomials $f$. In this paper we consider a subclass that leads to solvable problems.

### 1.1. Outline

Once the notation, a little background on sos (sum of squares) programming and a Stellensatz from algebraic geometry are introduced (Section 2), we review, in order to make the problem tractable, a sufficient criterion from the literature for the existence of continuous minimizers (Section 3). This criterion actually holds for integer minimzers, too: Integer minimizers exist if the highest order terms of $f$ attain positive values on $\mathbb{R}^{n} \backslash\{0\}$, we say that the leading form of $f$ is positive definite. But deciding positive definiteness is NP hard, hence we approximate this problem by sos programming. However, this only tells us that minimizers exists, but not where they are located. We locate the minimizers by computing - again using sos programming - the radius of a $p$-norm ball that contains all integer minimizers (Section 4), or simply norm bounds on the minimizers. In principle, once a norm bound is known, IP is solvable by enumeration. We proceed by deriving a class of polynomials with obvious integer minimizer (Section 5) that serve as underestimators to $f$. Using sos programming, we may choose the underestimator $g$ with the strongest lower bound. Firstly, we search for a global underestimator which is later refined to underestimation on sublevel sets, yielding stronger bounds. This refinement further allows to prove that, provided $f$ has a positive definite leading form, there always are underestimators in our class that can be found by sos programming. To find the optimal solution to IP, instead of enumeration, we use an underestimator $g$ from our class to obtain lower bounds within a branch and bound approach (Section 6). We continue with an experimental evaluation of the norm bounds, of the lower bounds and of the performance of the underestimators within branch and bound on random instances. The paper ends with a conclusion and ideas for future research (Section 7 ).

### 1.2. Literature review

The literature on nonlinear integer programming is vast. For an overview, a presentation of key techniques and complexity results as well as numerous references for further reading, see the article HKLW10, which comes as chapter of [JLN ${ }^{+}$10]. For a recent survey on nonlinear mixed-integer programming (a subset of the variables may be continuous), see LL12.
Throughout our work we rely heavily on methods from constrained continuous polynomial optimization. Based on work of Shor Sho87, SS97, Parrilo Par00 suggested a method now known as sos programming that makes continuous polynomial optimization accessible to semidefinite programming (see, e.g., WSV00 for the latter), whilst Lasserre [Las01] published the dual approach, based on moment sequences. Since the emergence of the two ground-breaking publications by Parrilo and Lasserre, many results
on continuous polynomial optimization via sos techniques and its theoretical background have been published: The expository paper [PS03] shows that existing algebraic techniques are outperformed by the sos method. As in-depth treatments, we refer to [AL12] for the interplay of semidefinite, conic and polynomial optimization, and [BPT13] for a focus on the geometry involved. For an algebraic treatment, we mention Marshall's book [Mar08]. We point out Laurent's elegant survey [Lau09], which treats, among other aspects, the duality of the sos and moment approach.

A special case of our problem, unconstrained quadratic integer minimization, is considered by [BHS14]. We did not find results in the literature that consider the unconstrained integer minimization problem for multivariate polynomials of arbitrary degree. Regarding nonlinear integer minimization with constraints or additional assumptions, integrality turns even seemingly simple problems incomputable: Using the aforementioned result of Matiyasevich, Jeroslow Jer73 proved that there cannot be an algorithm for integer minimization of a linear form subject to quadratic constraints.

But substantial special cases are solvable, for example, every integer problem with a bounded feasibile set is solvable. More specifically, an important case is boolean programming, see BH 02 for a survey. A classic approach is linearization by introducing new variables and constraints (for early results see, e.g., [For60]). In theory, also a general bounded integer polynomial optimization problem can be reduced to the binary case Wat67, but this is not practicable since the number of variables grows too quickly. Another technique for boolean programming is the reduction to a quadratic problem which can be done with significantly fewer variables and constraints Ros75, BR07. Another substantial case that gained attention are (quasi-)convex problems, as the incomputability results do not hold for this case Kha83, KP00. HK13 present a Lenstra type algorithm for quasiconvex integer polynomial optimization.

For integer minimization of arbitrary polynomials, a common way of solving IP is branch and bound as proposed (originally only for convex functions) by [GR85]. A popular method is to calculate convex underestimators (see, e.g., [LT11) to obtain lower bounds. As a different approach, if the feasible set is a box, BD14 compute separable underestimators wich give lower bounds that are easy to obtain. In contrast, LHKW06 directly compute lower and upper bounds, i.e., no underestimators, for nonnegative polynomials on polytopes.

## 2. Preliminaries

In this section we collect some basic notation and facts as well as a few theorems from algebraic geometry that we use to derive our main results.

## Notation and basic properties of polynomials

We write a polynomial $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$ in $n$ unknowns $X_{1}, \ldots, X_{n}$ using multi-indices $\alpha=\left(\alpha_{1}, \ldots, \alpha_{n}\right) \in \mathbb{N}_{0}^{n}$ via

$$
f=\sum_{\alpha \in \mathbb{N}_{0}^{n}} a_{\alpha} X^{\alpha}=\sum_{\alpha \in \mathbb{N}_{0}^{n}} a_{\alpha} X_{1}^{\alpha_{1}} \cdots X_{n}^{\alpha_{n}},
$$

for some unique coefficients $a_{\alpha} \in \mathbb{R}$, only finitely many nonzero, and monomials $X^{\alpha}:=$ $X^{\alpha_{1}} \cdots X^{\alpha_{n}}$. The modulus of $\alpha \in \mathbb{N}_{0}^{n}$ is $|\alpha|=\alpha_{1}+\ldots+\alpha_{n}$. With these conventions, the degree of $f$ is given by

$$
\operatorname{deg} f:=\max \left\{|\alpha| \mid a_{\alpha} \neq 0\right\} .
$$

The ring of polynomials in the unknowns $X_{1}, \ldots, X_{n}$ is denoted by $\mathbb{R}\left[X_{1}, \ldots, X_{n}\right]$, which we abbreviate to $\mathbb{R}[\underline{X}]$. We use $\underline{X}$ here in order to distinguish the multivariate from the univariate case.
A polynomial $f$ is homogeneous if all monomials in $f$ have the same degree, say $d$. That is, $f$ is homogeneous if $f=\sum_{|\alpha|=d} a_{\alpha} X^{\alpha}$. In this case one has

$$
f(\lambda x)=\lambda^{d} f(x), \quad x \in \mathbb{R}^{n}, \lambda \in \mathbb{R}
$$

This implies that a homogeneous polynomial is uniquely determined by its values on any of the $p$-norm unit spheres

$$
\mathbb{S}_{p}^{n-1}:=\left\{x \in \mathbb{R}^{n} \mid\|x\|_{p}=1\right\}, \quad p \in[1, \infty] .
$$

A homogeneous polynomial $f$ is positive definite if $f(x)>0$ for $x \neq 0$. Similarly, a (possibly nonhomogeneous) polynomial $f$ is positive semidefinite if $f(x) \geq 0$ for all $x \in \mathbb{R}^{n}$, for short $f>0$ and $f \geq 0$. For a homogeneous polynomial $f$ and some $p \in[1, \infty]$, we often use the following equivalent characterization:

$$
\begin{align*}
& f \geq 0 \Longleftrightarrow \exists c \geq 0: f(x) \geq c \text { for all } x \in \mathbb{S}_{p}^{n-1}, \\
& f>0 \Longleftrightarrow \exists c>0: f(x) \geq c \text { for all } x \in \mathbb{S}_{p}^{n-1} \tag{1}
\end{align*}
$$

A homogeneous polynomial is also called a form. Any polynomial $f \in \mathbb{R}[\underline{X}]$ can be uniquely decomposed as

$$
f=\sum_{j=0}^{d} f_{j}
$$

where $d:=\operatorname{deg} f$ and the $f_{j}$ are homogeneous polynomials of degree $j$, called the homogeneous components of $f$. The highest degree component, $f_{d}$, is called the leading form of $f$.
Given a vector $h \in \mathbb{R}^{n}$, we denote by $\lfloor h\rceil$ the vector resulting of rounding each component of $h$ to its nearest integer. Finally, we need the notion of a sublevel set: For a function $f: U \rightarrow \mathbb{R}$ from some set $U$, the sublevel set of level $z \in \mathbb{R}$ is defined by

$$
\mathcal{L}_{\leq}^{f}(z)=\{x \in U \mid f(x) \leq z\} .
$$

## Nonnegativity and sums of squares

Continuous minimization of a polynomial as well as deciding non-negativity of a polynomial are well known to be NP-hard problems, even if one fixes the degree to $d=4$ [Nes00. Deciding if $g$ is an underestimator of $f$ means to decide if $f-g$ is nonnegative. As this is NP-hard we use a tractable sufficient criterion for nonnegativity in the following: We search for a decomposition into a sum of squares, or sos for short, which is a sufficient, but not necessary condition for nonnegativity Mar08. Formally, a polynomial $f \in \mathbb{R}[\underline{X}]$ is a sum of squares if there are $u_{1}, \ldots, u_{l} \in \mathbb{R}[\underline{X}]$ such that $f=\sum_{i=1}^{l} u_{i}^{2}$. We sometimes use the following property:

Lemma 1. Suppose $v=u_{1}^{2}+\cdots+u_{k}^{2}$ for some given $u_{1}, \ldots, u_{k} \in \mathbb{R}[\underline{X}]$ and $u_{1} \neq 0$. Then $v \neq 0$, and

$$
\operatorname{deg} v=2 \max _{1 \leq i \leq k} \operatorname{deg} u_{i} .
$$

Proof. See, e.g., Mar08, Cor. 1.1.3].
The convex cone

$$
\Sigma:=\left\{f \in \mathbb{R}[\underline{X}] \mid \exists u_{1}, \ldots, u_{l} \in \mathbb{R}[\underline{X}] \text { s.t. } f=\sum_{i=1}^{l} u_{i}^{2}\right\}
$$

in $\mathbb{R}[\underline{X}]$ contains all polynomials $f$ which are sos in $\mathbb{R}[\underline{X}]$. It is possible to optimize a linear form such that affine combinations of the decision variables and given polynomials lie in this cone: Such an sos optimization problem or sos program is tractable, as it is equivalent to a semidefinite program. For details, see e.g. [AL12, BPT13] on sos programming and WSV00 for semidefinite programming. Formally, an sos program has the form

$$
\begin{array}{rll}
\max & b_{1} y_{1}+\cdots+b_{m} y_{m} & \\
\text { s.t. } & a_{i 0}+y_{1} a_{i 1}+\cdots+y_{m} a_{i m} \in \Sigma, & i=1, \ldots, k,  \tag{2}\\
& y_{i} \in \mathbb{R}, & i=1, \ldots, m,
\end{array}
$$

where $y_{i} \in \mathbb{R}$ are the decision variables, and $b_{i} \in \mathbb{R}$ as well as $a_{i j} \in \mathbb{R}\left[X_{1}, \ldots, X_{n}\right]$ are fixed. In our paper we use sos programming for two purposes: To find an optimal underestimator, see Section 5 , and for constrained continuous minimization of polynomials as done at the end of Section 2. For both, we use a result from real algebraic geometry, known as Putinar's Stellensatz, outlined next.

## A result from algebraic geometry

In this section we introduce Putinar's Stellensatz. See [NS07] and the references therein for a discussion and the origins of the Stellensatz. For a finite collection of multivariate polynomials $S=\left\{g_{1}, \ldots, g_{s}\right\} \subset \mathbb{R}[\underline{X}]$, define the semi-algebraic set $K_{S}$ as

$$
\begin{equation*}
K_{S}:=\left\{x \in \mathbb{R}^{n} \mid g_{1}(x) \geq 0, \ldots, g_{s}(x) \geq 0\right\}, \tag{3}
\end{equation*}
$$

where our notation follows Mar08. The Stellensatz we consider gives a sufficient conditions which allows to construct every polynomial $f \in \mathbb{R}[\underline{X}]$ with $f>0$ on $K_{S}$ from the given inequalities $g_{i}(x) \geq 0$. To this end, for $S$ as above, the quadratic module generated by $S$ is given by

$$
\begin{equation*}
M_{S}:=\left\{\sum_{i=0}^{s} \sigma_{i} g_{i} \mid \sigma_{0}, \ldots, \sigma_{s} \in \Sigma\right\} \tag{4}
\end{equation*}
$$

where $g_{0}:=1$. For the Positivstellensatz to hold we need $M_{S}$ to be Archimedean. This is the case if there is a polynomial $q \in M_{S}$ such that the set $K_{\{q\}}=\left\{x \in \mathbb{R}^{n} \mid q(x) \geq 0\right\}$ is compact.
Theorem 2 (Putinar). Let $M_{S}$ be Archimedean and $f \in \mathbb{R}[\underline{X}]$. Then $f(x)>0$ for all $x \in K_{S}$ implies $f \in M_{S}$.

## Lower bounds for constrained continuous minimization

In Section 3 we will see that in order to decide existence of minimizers, we need to compute a lower bound on the minimum of the leading form on the sphere $\mathbb{S}_{p}^{n-1}$. As the sphere is semi-algebraic for even $p$, sos methods can be applied to find such a lower bound.
In the following we describe how lower bounds on

$$
\begin{align*}
\min & f(x) \\
\text { s.t. } & x \in K_{S} \tag{5}
\end{align*}
$$

where $K_{S}$ defined as in (3) can be derived by sos-programming. The method we outline follows Schweighofer [Sch05], based on Lasserre's [Las01] work. We consider a hierarchy $\mathrm{Q}_{k}, k=1,2, \ldots$, of sos programs

$$
\begin{array}{lll}
\max & y_{1} & \\
\text { s.t. } & f-y_{1}-\sum_{i=1}^{s} \sigma_{i} g_{i} \in \Sigma &  \tag{k}\\
& \operatorname{deg}\left(\sigma_{i} g_{i}\right) \leq k, & i=1, \ldots, s \\
& \sigma_{i} \in \Sigma, & i=1, \ldots, s \\
& y_{1} \in \mathbb{R} . &
\end{array}
$$

In $\mathrm{Q}_{k}$, the decision variables are $y_{1} \in \mathbb{R}$ and the real coefficients of $\sigma_{1}, \ldots, \sigma_{s} \in \mathbb{R}[\underline{X}]$. We then have that every feasible solution $y_{1}$ to $\mathrm{Q}_{k}$ gives a lower bound on (5), i.e., on $\min \left\{f(x) \mid x \in K_{S}\right\}$. Indeed, if $y_{1}$ is feasible, there are $\sigma_{0}, \ldots, \sigma_{s} \in \Sigma, \operatorname{deg}\left(\sigma_{i} g_{i}\right) \leq k$ for $i=1, \ldots, s$, such that

$$
\begin{gathered}
f=y_{1}+\sigma_{0}+\sum_{i=1}^{s} \sigma_{i} g_{i} \\
\Longrightarrow f(x)=y_{1}+\sigma_{0}(x)+\sum_{i=1}^{s} \sigma_{i}(x) g_{i}(x) \geq y_{1}, \quad x \in K_{S}
\end{gathered}
$$

as $\sigma_{i} \in \Sigma$, hence $\sigma_{i}$ are nonnegative, and $g_{i}(x) \geq 0$ on $K_{S}$ by definition of $K_{S}$. Hence $f$ is bounded from below by $y_{1}$ on $K_{S}$, i.e., every feasible solution to $\mathrm{Q}_{k}$ is a lower bound on (5). A justification for the ansatz $Q_{k}$ is the following well-known and easy consequence of Putinar's Positivstellensatz (Theorem 2):

Corollary 3. Let $M_{S}$ be Archimedean. Denote the minimum of (5) by $f^{*}$ and the minimum of $\mathrm{Q}_{k}$ by $y_{1}^{(k)}$. Then $y_{1}^{(k)} \nearrow f^{*}$ for $k \rightarrow \infty$.

Although finite convergence is not guaranteed [Las01], there are cases where an optimal solution $x \in K_{S}$ to (5) can be extracted from Q Q, see e.g. HL05. In the unconstrained case $\min \left\{f(x) \mid x \in \mathbb{R}^{n}\right\}$ given by $s=0$ (i.e. $K_{S}=\mathbb{R}^{n}$ ) in (5) even more is known: Instead of solving $\mathrm{Q}_{k}$ with respect to $K_{S}=\mathbb{R}^{n}$ which would be given as $\max \left\{y_{1} \mid f-y_{1} \in \Sigma\right\}$, one can consider the gradient variety ${ }^{11}$, resulting in $2 n$ constraints corresponding to the equations $\partial_{x_{1}} f=\ldots=\partial_{x_{n}} f=0$ and solve $\mathrm{Q}_{k}^{\prime}$ with respect to

$$
\begin{equation*}
S^{\prime}=\left\{\partial_{x_{1}} f, \ldots, \partial_{x_{n}} f,-\partial_{x_{1}} f, \ldots,-\partial_{x_{n}} f\right\} \tag{6}
\end{equation*}
$$

Then we have:
Theorem 4 ([NDS06]). Consider the set of polynomials of degree at most $d \in \mathbb{N}_{0}$ that possess a global continuous minimizer:

$$
\mathcal{F}_{d}:=\left\{f \in \mathbb{R}[\underline{X}] \mid \operatorname{deg}(f) \leq d \text { and } \exists x^{*} \in \mathbb{R}^{n} \text { s.t. } f\left(x^{*}\right)=f^{*}=\inf _{x \in \mathbb{R}^{n}} f(x)\right\} .
$$

Then, for the sos-programs $Q_{k}^{\prime}$ with gradient variety constraints $S^{\prime}$ from (6), finite convergence holds for almost all polynomials $f \in \mathcal{F}_{d}$. More precisely, there is a $k_{0} \in \mathbb{N}_{0}$ s.t. for the optimal solutions $y_{1}^{(k)}$ of $\mathrm{Q}_{k}^{\prime}$ one has $y_{1}^{(k)}=y_{1}^{\left(k_{0}\right)}=f^{*}$ for $k \geq k_{0}$. Moreover, a minimizer $x^{*}$ of (5) can then be extracted.

## 3. Existence of minimizers: sufficient and necessary conditions

Before we search for integer minimizers of a polynomial $f \in \mathbb{R}[\underline{X}]$, we review sufficient and necessary conditions to decide whether integer or continuous minimizers exist at all. For nonconstant univariate polynomials, this is equivalent to an even degree and a positive leading coefficient, which is in turn closely related to the behavior of $f(x)$ as $|x| \rightarrow \infty$. For multivariate $f$, the situation is similar once we decompose $f$ into its homogeneous components (see Section 2 for the definition). A positive definite leading form is a sufficient condition for the existence of continuous minimizers whilst positive semidefiniteness is a necessary condition Mar03, Mar09]. In our next result we show that this holds for integer minimizers as well. Together with some observations that will be of use later on, these results are reorganized in the following proposition.

[^1]Proposition 5. Let $f \in \mathbb{R}[X]$ with $\operatorname{deg} f=d>0$. The following implications hold:

$$
\begin{aligned}
f_{d}>0 \Rightarrow & \text { all } \mathcal{L}_{\leq}^{f}(z) \text { compact } \Rightarrow f \text { has } \text { i.m. } \Rightarrow \\
\Uparrow & \inf _{x \in \mathbb{Z}^{n}} f(x)>-\infty \Rightarrow f_{d} \geq 0 \Rightarrow d \text { even } \\
& \liminf _{|x| \rightarrow+\infty} f(x)=+\infty \Rightarrow f \text { has c.m. } \Rightarrow \inf _{x \in \mathbb{R}^{n}} f(x)>-\infty
\end{aligned}
$$

where i.m. abbreviates integer and c.m. continuous minimizers. In addition, none of the implications above can be strengthened.

Proof. Let $f_{d}>0$, and $c_{j}^{*}:=\min _{x \in S_{p}^{n-1}} f_{j}(x), j=0, \ldots, d$, where $c_{j}^{*}>-\infty$ for $j=0, \ldots, d-1$ by compactness of the sphere and $c_{d}^{*}>0$ since $f_{d}$ is positive definite. For $0 \neq x \in \mathbb{R}^{n}$ and $p \in[1, \infty]$ this means

$$
f(x)=\sum_{j=0}^{d} f_{j}(x)=\sum_{j=0}^{d} f_{j}\left(\frac{x}{\|x\|_{p}}\right)\|x\|_{p}^{j} \geq \sum_{j=0}^{d} c_{j}^{*}\|x\|_{p}^{j} .
$$

The expression on the right can be considered as a univariate polynomial in $\|x\|_{p}$ with positive leading coefficient, so $\liminf |x| \rightarrow+\infty) ~ f(x)=+\infty$ follows. If the latter holds, the sublevel sets $\mathcal{L}_{\leq}^{f}(z)$ must be bounded for all $z \in \mathbb{R}$. As $f$ is continuous, the sublevel sets are moreover closed, and compactness follows. In case the limit inferior is $s \in[-\infty,+\infty)$, pick $z \in(s,+\infty)$. There must be a sequence $x_{k} \in \mathbb{R}^{n},\left\|x_{k}\right\|_{p} \rightarrow \infty$ as $k \rightarrow \infty$, such that $f\left(x_{k}\right) \leq z$ for all $k$. Put differently, $x_{k} \in \mathcal{L}_{\leq}^{f}(z)$ for all $k$, hence the level set is unbounded, and the only equivalence in the diagram is proven. We show the two rightmost implications in the first row next, the remaining ones are straightforward. So suppose there is $x \in \mathbb{R}^{n}$ such that $f_{d}(x)<0$. By homogeneity, we may assume $x \in \mathbb{S}_{\infty}^{n-1}$. By continuity, there is a whole neighborhood $W$ of $x$ s.t. $f_{d}(y)<0$ for all $y \in W$. As $W \cap \mathbb{S}_{\infty}^{n-1} \neq \emptyset$, there is a point $r \in W \cap \mathbb{S}_{\infty}^{n-1}$ with rational coordinates $r_{i}=\frac{z_{i}}{n_{i}}, z_{i} \in \mathbb{Z}$, $n_{i} \in \mathbb{N}, i=1, \ldots, n$. Now for all $\lambda \in \mathbb{R}$,

$$
f(\lambda r)=\sum_{j=0}^{d} f_{j}(r) \lambda^{j},
$$

and since $f_{d}(r)<0$, we have $f(\lambda r) \rightarrow-\infty$ as $\lambda \rightarrow \infty$. Since $r_{i}=\frac{z_{i}}{n_{i}}, i=1, \ldots, n$, there is a lowest common denominator $l \in \mathbb{N}$ of the $r_{i}$. For $k \in \mathbb{N}$, we have especially $f(k l r) \rightarrow-\infty$ as $k \rightarrow \infty$. But since $k l r \in \mathbb{Z}^{n}, f$ is unbounded from below on $\mathbb{Z}^{n}$. For the last implication, let $d$ be odd. As $f_{d}$ is a nonzero polynomial, there is $x \in \mathbb{R}^{n}$ s.t. $f_{d}(x) \neq 0$. Homogeneity of (odd) order $d$ implies either $f_{d}(x)<0$ or $f_{d}(-x)<0$, therefore $f_{d}$ is not positive semidefinite.

Finally, a collection of counterexamples proving that none of the implications of the proposition can be strengthened can be found in Beh13].

In the following, we rely on the sufficient condition $f_{d}>0$ to ensure the existence of integer minimizers. As deciding nonnegativity of $f_{d}$ is NP hard, we compute a lower bound $c_{d}$ on the leading form $f_{d}$ restricted to the sphere, i.e.,

$$
\begin{equation*}
c_{d} \leq c_{d}^{*}=\min _{x \in \mathbb{S}_{p}^{n-1}} f_{d}(x) \tag{7}
\end{equation*}
$$

If $c_{d}>0$ we know from (1) that $f_{d}>0$, so integer minimizers exist by Proposition 5 , Our approach fails if $c_{d} \leq 0$ unless we find a point $x \in \mathbb{S}_{p}^{n-1}$ s.t. $f_{d}(x)<0$ which certifies that $f_{d}$ is not positive semidefinite, and hence $f$ cannot have minimizers.

## 4. Norm bounds on the minimizers

### 4.1. A new bound on the norm of integer minimizers

If $f=\sum_{\alpha} a_{\alpha} X^{\alpha}$ satisfies $c_{d}^{*}=\min _{x \in \mathbb{S}_{p}^{n-1}} f_{d}(x)>0$, i.e., $f_{d}$ is positive definite and a lower bound $c_{d}$ on the minimum with $0<c_{d} \leq c_{d}^{*}$ is known, it is possible to give a bound $R \geq 0$ on the norm of the continuous minimizers. We only found one bound in the literature, which assumes $p=2$,

$$
\begin{equation*}
R_{\text {lit }}:=\max \left(1, \frac{1}{c_{d}} \sum_{j=1}^{d-1}\left\|f_{j}\right\|_{1}\right)=\max \left(1, \frac{1}{c_{d}} \sum_{0<|\alpha|<d}\left|a_{\alpha}\right|\right) \tag{8}
\end{equation*}
$$

from Marshall where $\|f\|_{1}:=\sum_{\alpha}\left|a_{\alpha}\right|$ for $f=\sum_{\alpha} a_{\alpha} X^{\alpha}$; it is a special case (empty constraint set) of a more general result Mar03]. Laurent Lau09] gives a more elementary proof for Marshall's bound (8) by showing $f(x)>f(0)$ for $\|x\|_{2}>R_{\text {lit }}$. Hence $R_{\text {lit }}$ gives a valid bound on integer minimizers as well. However, for non-sparse polynomials, this bound may get quite large. Within branch and bound approaches it is crucial to find a small bound $R$ to reduce the number of feasible solutions - scaling $R$ by a constant $C>0$, the number of integer points that satisfy the norm bound scales with a factor of (roughly) $C^{n}$. We hence suggest a different approach: In the following theorem, we still compute $R \geq 0$ with $f(x)>f(0)$ for $\|x\|_{p}>R$, but instead of bounding all homogeneous components simultaneously, we compute constants $c_{j}$ such that $c_{j} \leq c_{j}^{*}=\min _{x \in \mathbb{S}_{p}^{n-1}} f_{j}(x)$ on a suitable sphere $\mathbb{S}_{p}^{n-1}$.

Theorem 6. Let $f \in \mathbb{R}[\underline{X}]$ with $\operatorname{deg} f=d>0$. For a fixed $p \in[1, \infty]$, let $c_{j} \in \mathbb{R}$ s.t. $f_{j}(x) \geq c_{j}$ for all $x \in \mathbb{S}_{p}^{n-1}, j=1, \ldots, n$. Suppose $c_{d}>0$. Let $R$ denote the largest nonnegative real root of the univariate polynomial $q: \mathbb{R} \rightarrow \mathbb{R}$,

$$
q(\lambda):=\sum_{j=1}^{d} c_{j} \lambda^{j}
$$

1. Then, integer as well as continuous minimizers $x^{\prime}$ of $f$ (do exist and) satisfy $\left\|x^{\prime}\right\|_{p} \leq R$.

Let $x^{*}$ be any of the integer minimizers.
2. We have $\left|x_{i}^{*}\right| \leq\lfloor R\rfloor$, for $i=1, \ldots, n$.

Proof. We prove 1, the other assertion follows directly from integrality of $x^{*}$. By compactness of the sphere, every $f_{j}$ is bounded below by some $c_{j} \in \mathbb{R}$. We observed in (1) that $c_{d}>0$ implies positive definiteness of $f_{d}$, hence integer and continuous minimizers exist and $d$ is even (Proposition 5). Using homogeneity,

$$
\begin{equation*}
f(x)-f(0)=\sum_{j=1}^{d} f_{j}(x)=\sum_{j=1}^{d} f_{j}\left(\frac{x}{\|x\|_{p}}\right)\|x\|_{p}^{j} \geq \sum_{j=1}^{d} c_{j}\|x\|_{p}^{j}=q\left(\|x\|_{p}\right) \tag{9}
\end{equation*}
$$

for $x \neq 0$. Since $q$ is univariate and of degree $d>0$, it has at most $d$ real roots. As $q(0)=0, q$ has roots in $[0, \infty)$, and we denote the largest of them by $R$. As before, $c_{d}>0$ yields $\lim _{\lambda \rightarrow+\infty} q(\lambda)=+\infty$. This together with the intermediate value theorem implies $q(\lambda)>0$ for $\lambda>R$. Thus, eq. (9) forces $f(x)>f(0)$ for $\|x\|_{p}>R$.
Remark 7. The larger the $c_{j}$ the smaller the resulting norm bound $R$. Formally, let $q=\sum_{j=1}^{n} c_{j} \lambda^{j}, \tilde{q}=\sum_{j=1}^{n} \tilde{c}_{j} \lambda^{j}$, such that $c_{j} \geq \tilde{c}_{j}$, and call the largest nonnegative roots $R$ and $\tilde{R}$, respectively. Wlog, it suffices to consider the case that $c_{j}=\tilde{c}_{j}$ for $j \neq k$ and $c_{k}>\tilde{c}_{k}$ for some $k \in\{1, \ldots, n\}$. Now $q(\lambda)-\tilde{q}(\lambda)=\left(c_{k}-\tilde{c}_{k}\right) \lambda^{k}>0$ for $\lambda>0$ and by assumption on $c_{k}, \tilde{c}_{k}$. Thus, $q(\lambda)>\tilde{q}(\lambda)$ for $\lambda>0$, hence $R<\tilde{R}-$ unless $\tilde{R}=0$. In this case $R=\tilde{R}=0$.

Before we present different methods of computing valid $c_{j}$, we compare $R$ and $R_{\text {lit }}$. In the experiments in Section 6, we show that our norm bound $R$ is drastically smaller than $R_{\text {lit }}$. Also, it can be proven that our norm bounds are never larger and, except for special cases, are actually strictly smaller than the bound from the literature.

Proposition 8. Let $f$ with $\operatorname{deg} f=d>0$ and $c_{d}>0$ such that $f_{d}(x) \geq c_{d}$ for all $x \in \mathbb{S}_{2}^{n-1}, j=1, \ldots, n$. Compute $R \in[0, \infty)$ as in Theorem 6 for

$$
\begin{equation*}
c_{j}:=-\left\|f_{j}\right\|_{1}, \quad j=1, \ldots, d-1 \tag{10}
\end{equation*}
$$

and compute $R_{\text {lit }} \in[1, \infty)$ as in (8). Then $R \leq R_{\text {lit }}$. If moreover $d>2$ and there is a coefficient $a_{\alpha} \neq 0$ of $f$ with $|\alpha|<d-1$, then $R<R_{\text {lit }}$ for $R \neq 1$ and $R=R_{\text {lit }}$ for $R=1$.

Proof. At first we observe that the numbers $c_{j}=-\left\|f_{j}\right\|_{1}$ in 10 are indeed valid lower bounds, for general $p \in[1, \infty]$ : As $\|x\|_{p} \leq 1$ implies $\|x\|_{\infty} \leq 1$ and hence $\left|x^{\alpha}\right| \leq 1$, one has

$$
f_{j}(x)=\sum_{|\alpha|=j} a_{\alpha} x^{\alpha} \geq \sum_{|\alpha|=j}-\left|a_{\alpha}\right|\left|x^{\alpha}\right| \geq \sum_{|\alpha|=j}-\left|a_{\alpha}\right|=-\left\|f_{j}\right\|_{1}=c_{j}, x \in \mathbb{S}_{p}^{n-1}
$$

We prove the case $d>2$ and $a_{\alpha} \neq 0$ for some $\alpha$ with $|\alpha|<d-1$. The claim obviously holds in case $R<1$. For the cases $R=1$ and $R>1$, define $q(\lambda)=\sum_{j=1}^{d} c_{j} \lambda^{j}$ as before and let $\tilde{q}(\lambda)=c_{d} \lambda^{d}+\left(\sum_{j=1}^{d-1} c_{j}\right) \lambda^{d-1}$. Then we have

$$
\begin{equation*}
q(\lambda)>\tilde{q}(\lambda) \text { for } \lambda>1, \quad q(\lambda)=\tilde{q}(\lambda) \text { for } \lambda=1 \tag{11}
\end{equation*}
$$

as $c_{j} \leq 0$ for $j=1, \ldots, d-1$ and one $c_{k}<0$ for some $k \in\{1, \ldots, d-2\}$ by the assumption on $a_{\alpha}$. By definition, the largest nonnegative real root of $q$ is $R$, and the largest nonnegative real root $\tilde{R}$ of $\tilde{q}$ is

$$
\tilde{R}=-\frac{1}{c_{d}} \sum_{j=1}^{d-1} c_{j}=\frac{1}{c_{d}} \sum_{0<|\alpha|<d}\left|a_{\alpha}\right|
$$

and, by definition, $R_{\mathrm{lit}}=\max (1, \tilde{R})$. If $R=1$, we infer from (11) that $0=q(1)=\tilde{q}(1)$, so $R_{\mathrm{lit}}=1$. In case $R>1$, we infer from (11) that $0=q(R)>\tilde{q}(R)$, so $R<R_{\mathrm{lit}}$ as $\tilde{q}(\lambda) \rightarrow+\infty$ for $\lambda \rightarrow+\infty$. The proof for the two remaining cases, $d=2$ or all $a_{\alpha}=0$ for $|\alpha|<d-1$, is similar as $q=\tilde{q}$ in these cases.

We now present different ways of computing bounds $c_{j}$ on $c_{j}^{*}=\min _{x \in \mathbb{S}_{p}^{n-1}} f_{j}(x)$.

1. We saw in the proof of Proposition 8 that $c_{j}=-\left\|f_{j}\right\|_{1}$ gives valid lower bounds for any $p \in[1, \infty]$. However, this bound is rather rough and only useful for the lower order forms, that is those $f_{j}$ with $j<d$.
2. The arguably easiest way to find such $c_{j}$ by sos programming is to minimize $f_{j}$ on the sphere $\mathbb{S}_{p}^{n-1}$ : More specifically, for $p \in 2 \mathbb{N}$, the constraint $\|x\|_{p}=1$ is equivalent to the constraint $\sum_{i=1}^{n} x_{i}^{p}=1$, which is semi-algebraic for even $p>0$. The hierarchy $\mathrm{Q}_{k}$ with $g_{1}=1-\sum_{i=1}^{n} X_{i}^{p}$ and $g_{2}=\sum_{i=1}^{n} X_{i}^{p}-1$ can be rewritten as

$$
\begin{array}{ll}
\max & y_{1} \\
\text { s.t. } & f_{j}-y_{1}-q \cdot\left(1-\sum_{i=1}^{n} X_{i}^{p}\right) \in \Sigma  \tag{12}\\
& q \in \mathbb{R}[\underline{X}], \operatorname{deg} q \leq k \\
& y_{1} \in \mathbb{R}
\end{array}
$$

where we used $\sigma_{1} g_{1}+\sigma_{2} g_{2}=\left(\sigma_{1}-\sigma_{2}\right) g_{1}=q g_{1}$, some $q \in \mathbb{R}[\underline{X}]$, as any polynomial can be written as the difference of sums of squares, e.g. using $4 q=(q+1)^{2}-(q-1)^{2}$.
3. A different lower bound on the leading form can be computed via the program

$$
\begin{equation*}
\max \gamma \text { s.t. } \quad f_{d}-\gamma \cdot \sum_{i=1}^{n} X_{i}^{d} \in \Sigma, \tag{13}
\end{equation*}
$$

from Nie12] choosing $p=d$.
4. We present two refined approaches of item 1 in the Appendix: As a first step, we replace the underlying estimate $\left\|x^{\alpha}\right\| \leq 1$ by $\left\|x^{\alpha}\right\| \leq\left\|\hat{x}^{\alpha}\right\|$, where $\hat{x}$ is a maximizer of $x^{\alpha}$ on the sphere. In a second step, considering all orthants separately allows then to furthermore get rid of approximately half of the terms.
Remark 9. If $p \in 2 \mathbb{N}$, the set $M_{S}$ with $S=\left\{1-\sum_{i=1}^{n} X_{i}^{p}, \sum_{i=1}^{n} X_{i}^{p}-1\right\}$ is Archimedean. Hence, from Corollary 3, the optimal objective values of (12) converge, for $k \rightarrow \infty$, to $c_{j}^{*}=\min _{x \in \mathbb{S}_{p}^{n-1}} f_{j}(x)-$ which are, by Remark 7 , the best possible bounds $c_{j}$.

### 4.2. Application to systems of polynomial equations

In this section, we consider an application to systems of polynomial equations; we test our approach on random instances of polynomials in the next section. It is a common approach to solve a system of equations $g_{i}(x)=0, i=1, \ldots, s$, with solutions restricted to, say, $x \in \mathbb{Z}^{n}, \mathbb{Q}^{n}$ or $\mathbb{R}^{n}$, by minimizing $f=g_{1}^{2}+\ldots g_{s}^{2}$ over the integers, rationals or reals, respectively. If the minimum is 0 at some $x$, the equations have a solution at $x$; if the minimum is nonzero, there cannot be any solution.

### 4.2.1. Diophantine equations

As an example, does the system

$$
\begin{aligned}
-3 x_{1}^{3}+x_{1}^{2} x_{2}-x_{1}^{2}+2 x_{1} x_{2}+x_{1}-2 x_{2}^{2}-2 x_{2}+4 & =0 \\
2 x_{2}^{3}+x_{1} x_{2}^{2}+4 x_{2}-5 & =0
\end{aligned}
$$

possess an integer solution? Denote the polynomials in $\mathbb{Z}\left[X_{1}, X_{2}\right]$ on the left hand side in the first and second equation by $g_{1}$ and $g_{2}$, respectively, and consider $f:=g_{1}^{2}+g_{2}^{2}$. The homogeneous components of $f$ are bounded from below on $\mathbb{S}_{6}^{1}$ by

$$
\left(c_{1}, \ldots, c_{6}\right)=(-60.49,-13.03,-41.76,-7.85,-24.45,2.59),
$$

we found the values by solving (12) numerically. The univariate polynomial $q(\lambda)=$ $\sum_{j=1}^{6} c_{j} \lambda^{j}$ has only two real roots: 0 and $R \approx 9.90$. Thus, by Theorem 6 , integer minimizers exist and must be in the box $[-9,9]^{2}$. Iterating over all integer points in the box one finds $f\left(x_{1}, x_{2}\right)=0$ at $\left(x_{1}, x_{2}\right)=(-1,1)$. From the perspective of number theory, our method provides search bounds on solutions of a system of Diophantine equations if the leading form of $f=\sum_{j=1}^{s} g_{j}^{2}$ is positive definite.

### 4.2.2. Bounds on algebraic varieties

Similarly to the systems of Diophantine equations, our bounds apply to real algebraic varieties: Given $g_{1}, \ldots, g_{s} \in \mathbb{R}[\underline{X}]$, the variety of the $g_{i}$ is $V\left(g_{1}, \ldots, g_{s}\right)=\left\{x \in \mathbb{R}^{n} \mid g_{1}(x)=\right.$ $\left.0, \ldots, g_{s}(x)=0\right\}$. If the leading form of $f=\sum_{j=1}^{s} g_{j}^{2}$ is positive definite, we may give a norm bound on all points of the variety. As an example, let us consider the system from [CLO07, Example 2, Sec. 2 § 8]:

$$
\begin{align*}
x^{2}+y^{2}+z^{2} & =1  \tag{14}\\
x^{2}+z^{2} & =y \\
x & =z \\
x, y, z & \in \mathbb{C}
\end{align*}
$$

Computing the $c_{j}$ by solving (12) for $p=2$ yields $\left(c_{1}, \ldots, c_{4}\right)=(0,-2.0,-0.77,1.0)$ and gives us $R \approx 1.86$ as a 2 -norm bound on all points in the variety. It is known that the variety consists of exactly four points: The system has two real and two complex solutions $\left(x, y, z_{i}\right)$ with $z_{i} \in\left\{ \pm \frac{1}{2} \sqrt{ \pm \sqrt{5}-1}\right\}$, where the real solutions suffice $\|(x, y, z)\|_{2}=1$ by (14). We conclude that in this case our bound is not far off.

## 5. A class of underestimators

### 5.1. Global underestimation

Now let $f, g: \mathbb{R}^{n} \rightarrow \mathbb{R}$. We then have

$$
\begin{equation*}
\left(\forall x \in \mathbb{R}^{n}: g(x) \leq f(x)\right) \Longrightarrow \inf _{x \in \mathbb{Z}^{n}} g(x) \leq \inf _{x \in \mathbb{Z}^{n}} f(x) \tag{15}
\end{equation*}
$$

where $^{\inf }{ }_{x \in \mathbb{Z}^{n}} g(x)$ gives a stronger bound on the integer minimum of $f$ than $\inf _{x \in \mathbb{R}^{n}} g(x)$. Using the integer minimum of $g$ to derive a lower bound on the integer minimum of $f$ makes only sense if integer minimization of $g$ is easy compared to integer minimization of $f$. We motivate our class of easy-to-minimize underestimators $g$ with an observation on monomials with a shift in the argument which shall serve as the building blocks to the more general underestimators.

Observation 10. For some $h \in \mathbb{R}^{n}$ and $\alpha \in \mathbb{N}_{0}^{n}$, let

$$
g=(X-h)^{\alpha}=\prod_{j=1}^{n}\left(X_{j}-h_{j}\right)^{\alpha_{j}}
$$

be a shifted monomial. If all $\alpha_{i}$ are even, $g$ has a continuous minimizer at $h$ and an integer minimizer at $\lfloor h\rceil$. If one $\alpha_{i}$ is odd, $g$ is not bounded from below and does not have continuous or integer minimizers.

Our underestimators are conic combination of shifted monomials with even $\alpha_{j}, j=$ $1, \ldots, n$, as the combinations inherit the integer minimizer $\lfloor h\rceil$. More precisely:

Proposition 11. Let a polynomial $g \in \mathbb{R}[\underline{X}]$ be given as $g=\sum_{\alpha} b_{\alpha}(X-h)^{2 \alpha}$ with $b_{\alpha} \geq 0$ for $\alpha \neq 0$, and $h \in \mathbb{R}^{n}$.

1. The restriction of $g$ to $\prod_{i=1}^{k-1}\left\{x_{i}\right\} \times \mathbb{R} \times \prod_{i=k+1}^{n}\left\{x_{i}\right\}$ that is, the univariate function $y \mapsto g\left(x_{1}, \ldots, x_{k-1}, y, x_{k+1}, \ldots, x_{n}\right)$ for fixed $x \in \mathbb{R}^{n}$ is nonincreasing for $y \leq h_{k}$ and nondecreasing for $y \geq h_{k}, k \in\{1, \ldots, n\}$.
2. We have $g\left(x_{1}, \ldots, x_{n}\right) \geq g\left(x_{1}, \ldots, x_{k-1},\left\lfloor h_{k}\right\rceil, x_{k+1}, \ldots, x_{n}\right)$ for every $x \in \mathbb{Z}^{n}$.
3. $h$ is a continuous and $\lfloor h\rceil$ an integer minimizer of $g$.

Proof. The claimed properties hold for every term $(X-h)^{2 \alpha}$. Thus they hold for conic combinations of such terms.

Three properties make these polynomials $g$ useful underestimators: integer minimization is trivial, and all nonlinearity is confined to the parameter $h$. Also, the fact that the expression is linear in the $b_{\alpha}$ makes them accessible to optimization. Proposition 11 motivates

Notation 12. We denote the set of conic combinations of monomials with a shift of $h$ by

$$
\mathscr{C}(h):=\left\{g \in \mathbb{R}[\underline{X}] \mid g=\sum_{\alpha \in J} b_{\alpha}(X-h)^{2 \alpha}, b_{\alpha} \in \mathbb{R}_{\geq 0} \text { for all } \alpha \neq 0, J \subset \mathbb{N}_{0}^{n} \text { finite }\right\}
$$

As an example, the polynomial

$$
g=\left(X_{1}-1.5\right)^{4}\left(X_{2}-2\right)^{6}+0.3\left(X_{1}-1.5\right)^{2}\left(X_{3}-3.2\right)^{8}-1 \in \mathscr{C}(1.5,2,3.2)
$$

with $J=\{(4,6,0),(2,0,8),(0,0,0)\}$ has an integer minimizer at $(1,2,3)$.
Proposition 13. Let $g \in \mathscr{C}(h)$ satisfy $g(x) \leq f(x)$ for all $x \in \mathbb{R}^{n}$. Then

$$
g(\lfloor h\rceil) \leq \inf _{x \in \mathbb{Z}^{n}} f(x)
$$

Proof. This follows from (15) and Proposition 11.
For determining an underestimator $g$ we still have to choose $h$ and the coefficients $b_{\alpha}$. This is described next.

Choice of $h$ : In principle, every $h \in \mathbb{R}^{n}$ may be chosen. Heuristically, we chose an (approximate) continuous minimizer of $f$ since $g$ has its continuous minimizer at $h$. In fact, every nontrivial $g$ looks like an elliptic paraboloid or a parabolic cylinder near $h$, as does $f$ near every local minimum. For almost all $f$, the continuous minimizer of $f$ can be found using sos methods (Theorem 4).

Choice of $b_{\alpha}$ : We choose the $b_{\alpha}$ so that the lower bound $g(\lfloor h\rceil)$ is maximized. In other words, we wish to maximize the expression

$$
g(\lfloor h\rceil)=\sum_{\alpha \in J} b_{\alpha}(\lfloor h\rceil-h)^{2 \alpha}
$$

subject to $g \leq f$. The higher order terms in $g$ ensure a certain aggressiveness in the growth behavior away from $h$, even for small coefficients $b_{\alpha}$, which leads to strong bounds. Using the notation $w_{\alpha}:=(\lfloor h\rceil-h)^{2 \alpha}$, we get the following optimization problem:

$$
\begin{aligned}
\max _{J, b_{\alpha}} & \sum_{\alpha \in J} w_{\alpha} b_{\alpha} \\
\text { s.t. } & f(x)-\sum_{\alpha \in J} b_{\alpha}(x-h)^{2 \alpha} \geq 0 \quad \forall x \in \mathbb{R}^{n} \\
& b_{\alpha} \geq 0 \quad \text { for } \alpha \neq 0
\end{aligned}
$$

with decision variables $b_{\alpha} \in \mathbb{R}, \alpha \in J$ and $J \subset \mathbb{N}_{0}^{n}$ finite. Since this program is not tractable in general, we consider the following sos version instead:

$$
\begin{array}{rll}
y=\max & \sum_{\alpha \in J} w_{\alpha} b_{\alpha} &  \tag{GLOB}\\
\text { s.t. } & f-\sum_{\alpha \in J} b_{\alpha}(X-h)^{2 \alpha} & \text { is } \operatorname{sos} \text { in } \mathbb{R}\left[X_{1}, \ldots, X_{n}\right], \\
& b_{\alpha} & \text { is sos in } \mathbb{R}\left[X_{1}, \ldots, X_{n}\right] \text { for } \alpha \neq 0 .
\end{array}
$$

The decision variables are the real $b_{\alpha}, \alpha \in J$. Note that $b_{\alpha} \in \Sigma$ is equivalent to $b_{\alpha} \geq 0$. Once $J$ is fixed, GLOB is a valid sos program. We show in Corollary 17 that it is sufficient to choose $J=\left\{\alpha \in \mathbb{N}_{0}^{n}| | \alpha \mid \leq \operatorname{deg}(f) / 2\right\}$.
In the following we identify a solution $b_{\alpha}, \alpha \in J$, with the polynomial $g$ it defines, that is with $g=\sum_{\alpha \in J} b_{\alpha}(X-h)^{2 \alpha}$, and hence may say that a polynomial is a feasible or optimal solution to GLOB We note that every feasible solution to GLOB (for any choice of $h$ ) gives valid lower bounds on IP;
Theorem 14. Let $f \in \mathbb{R}[\underline{X}], h \in \mathbb{R}^{n}$ and $g=\sum_{\alpha \in J} b_{\alpha}(X-h)^{2 \alpha} \in \mathscr{C}(h)$ be a feasible solution to GLOB for some $J$. Then

1. $g(\lfloor h\rceil) \leq \inf _{x \in \mathbb{Z}^{n}} f(x)$.

If moreover $f-f(h) \in \Sigma$ holds and $g$ is an optimal solution to GLOB, then
2. $g(\lfloor h\rceil) \geq f(h)$.

Proof. Claim 1 holds as $g$ being feasible to GLOB implies $f-g \in \Sigma$, hence $f-g \geq 0$, and the claim follows by Proposition 13. Concerning Claim 2, observe that $f-f(h) \in \Sigma$ implies that $h$ is a continuous minimizer of $f$ and that the constant polynomial $\tilde{g}=f(h)$ is a feasible solution to GLOB, hence $g(\lfloor h\rceil) \geq \tilde{g}(\lfloor h\rceil)=f(h)$ for every optimal solution $g \in \mathscr{C}(h)$.

### 5.2. Improving the underestimators

## Motivation

A quite restrictive condition in GLOB is that it requires $g(x) \leq f(x)$ globally, i.e., for all $x \in \mathbb{R}^{n}$. Actually, this is not necessary for our purposes. It is enough to require $g(x) \leq f(x)$ only for those $x \in \mathbb{R}^{n}$ that satisfy $f(x) \leq f(q)$ for some $q \in \mathbb{Z}^{n}$. That is, for all $q \in \mathbb{Z}^{n}$, we have

$$
\begin{equation*}
\left(\forall x \in \mathcal{L}_{\leq}^{f}(f(q)): g(x) \leq f(x)\right) \Longrightarrow \inf _{x \in \mathbb{Z}^{n}} g(x) \leq \inf _{x \in \mathbb{Z}^{n}} f(x) \tag{16}
\end{equation*}
$$

in other words, the integer minimum of $g$ is a lower bound on the integer minimum of $f$ even if $g$ is an underestimator of $f$ only on a sublevel set $\mathcal{L}_{\leq}^{f}(f(q))$. If we make use of this in our sos program, the lower bound can only improve.

But before we delve into the details, let us consider the potential payoff by taking a look at the example in Figure 1a. The plot depicts the univariate polynomial

$$
f=0.2 \cdot(X-0.3)^{6}-5 \cdot(X-0.3)^{4}+32 \cdot(X-0.3)^{2} .
$$

along with two underestimators $g_{\mathrm{GLOB}}, g_{\mathrm{SLS}}$. A short calculation shows that $f$ has five local extrema at 0.3 and $0.3 \pm \sqrt{\frac{25 \pm \sqrt{145}}{3}}$, and that the local minimizers are at $x=0.3$ and at $x_{ \pm}=0.3 \pm \sqrt{\frac{25+\sqrt{145}}{3}} \approx 0.3 \pm 3.51$. Considering that $f$ has a positive definite leading form, one of the local minimizers must be a global one, and comparing the function values shows that $x=0.3$ is the continuous minimum. Moreover, $f$ must have its integer minimizer in $[-3,3]$ as $\min \left\{f\left(x_{+}\right), f\left(x_{-}\right)\right\}>f(0)$; comparing the function values shows that $f$ has a single integer minimizer at $x=0$ with value $f(0) \approx 2.84$. The underestimator $g_{\mathrm{GLOB}} \in \mathscr{C}(h)$, computed as optimal solution to GLOB is given by ${ }^{2}$
$g_{\mathrm{GLOB}} \approx 8.71 \cdot 10^{-11} \cdot(X-0.3)^{6}+1.09 \cdot 10^{-09} \cdot(X-0.3)^{4}+0.75 \cdot(X-0.3)^{2}-1.22 \cdot 10^{-09}$,
is globally below $f$. To find an underestimator on a sublevel set, we first fix the level $z=f(q)$ heuristically. Note that any $q \in \mathbb{Z}$ is a feasible solution to IP and hence an upper bound; any integer minimum must be contained in $\mathcal{L}_{\leq}^{f}(f(q))$. As $h=0.3$ is the global minimizer, we choose $q=\lfloor h\rceil=0$ here. The polynomial $g_{\text {SLS }}$, given by

$$
g_{\mathrm{SLS}} \approx 9.09 \cdot(X-0.3)^{6}+11.80 \cdot(X-0.3)^{4}+39.36 \cdot(X-0.3)^{2}-0.81
$$

is an underestimator on the sublevel set $\mathcal{L}_{\leq}^{f}(f(0))=[0,0.6]$, as can be seen in Figure 1b. It will be shown in the next section how this function can be found. The plot reveals the shortcomings of global underestimation: Any global underestimator in $\mathscr{C}(0.3)$ cannot go above the local minimizers of $f$. This "barrier" from above turns $g_{\text {GLOB }}$ in this example essentially into a quadratic underestimator for small $x$ as the ratio of the higher order coefficients and the one in front of the quadratic term is of order $10^{-10}$. The underestimator $g_{\text {SLS }}$ however is a degree 6 polynomial whose higher order coefficients are not small at all. Note that $g_{\mathrm{GLOB}}$ is much closer to $f$ near 0.3 compared to the new underestimator $g_{\text {SLS }}$. However, the quality of the resulting lower bound depends on the function values at 0 and there $g_{\mathrm{SLS}}$ is closer to $f$ than $g_{\mathrm{GLOB}}$. The lower bounds the two underestimators provide are $g_{\mathrm{GLOB}}(0) \approx 0.07$ and $g_{\mathrm{SLS}}(0) \approx 2.84$. In this case, we are lucky as the lower bound on the integer minimum and $f(0)$ coincide, showing once more that $f$ has its integer minimizer at 0 .

## The sos program for computing the improved underestimator

How do we compute the improved underestimator? At first, we observe that every sublevel set $\mathcal{L}_{\leq}^{f}(z), z \in \mathbb{R}$, of $f$ is semi-algebraic. Indeed, with the notation from (3) and $\tilde{S}:=\{z-f\}$, we have

$$
\mathcal{L}_{\leq}^{f}(z)=\left\{x \in \mathbb{R}^{n} \mid z-f(x) \geq 0\right\}=K_{\tilde{S}}
$$

[^2]

Figure 1: Global underestimator $g_{\text {GLOB }}$ and an underestimator $g_{\mathrm{SLS}}$ on a sublevel set.

Moreover, $\mathcal{L}_{\leq}^{f}(z)$ is compact if the leading form of $f$ is positive definite (see Proposition 5. Compactness of $\mathcal{L}_{\leq}^{f}(z)$ in turn implies that the quadratic module $M_{S} \subset$ $\mathbb{R}\left[X_{1}, \ldots, X_{n}\right]$ generated by $S^{-}:=\{f-g, z-f\}$, for any $g \in \mathbb{R}\left[X_{1}, \ldots, X_{n}\right]$, is thus by definition Archimedean. Hence, for every feasible underestimator $g \in \mathscr{C}(h)$ the existence of a representation for $f-g$ as in Putinar's Positivstellensatz (Theorem 2) is guaranteed. This motivates the following program:

$$
\begin{array}{rll}
y^{(k)}=\max & \sum_{\alpha \in J} w_{\alpha} b_{\alpha} &  \tag{SLS}\\
\text { s.t. } & f-\sum_{\alpha \in J} b_{\alpha}(X-h)^{2 \alpha}-\sigma(z-f) & \text { is sos in } \mathbb{R}\left[X_{1}, \ldots, X_{n}\right], \\
& b_{\alpha} \text { for } \alpha \neq 0, \sigma & \text { are sos in } \mathbb{R}\left[X_{1}, \ldots, X_{n}\right],
\end{array}
$$

The decision variables are the real $b_{\alpha}$ as for GLOB and, additionally, the real coefficients of the polynomial $\sigma$. As before, we use the notation $w_{\alpha}:=(\lfloor h\rceil-h)^{2 \alpha}$. SLS is a valid sos program once $J$ and the degree of $\sigma$ are fixed.

Theorem 15. Let $f \in \mathbb{R}[\underline{X}], h \in \mathbb{R}^{n}$ and $g \in \mathscr{C}(h)$ be a feasible solution to SLS with $z \geq f(q)$ for some $q \in \mathbb{Z}^{n}$.

1. Then $g(\lfloor h\rceil) \leq \inf _{x \in \mathbb{Z}^{n}} f(x)$.
2. If $J$ is fixed, $y^{(-\infty)} \leq y^{(0)} \leq y^{(2)} \leq y^{(4)} \leq$.. 3
3. If $f_{d}$ is positive definite, there is $k_{0} \in \mathbb{N}_{0}$ such that SLS is feasible for all $k \geq k_{0}$.
4. SLS with $k=-\infty$ is GLOB.
5. If $f-f(h) \in \Sigma$ and $g$ is optimal, then $g(\lfloor h\rceil) \geq f(h)$.

Proof. Statement 1 holds as $g$ feasible implies $f-g-\sigma(z-f) \in \Sigma$. Hence $f(x)-g(x) \geq 0$ for those $x$ with $f(x) \leq z$, especially for those $x$ with $f(x) \leq f(q)$ as $f(q) \leq z$ by assumption. The claim follows by (16).
Statement 2 is clear as we only allow more coefficients for $\sigma$.
To see Statement 3. note that $\mathcal{L}_{\leq}^{f}(z)$ is nonempty as $z \geq f(q)$ and moreover compact (Theorem 5p, so $f(x)>c$ for some $c \in \mathbb{R}$ and all $x \in \mathcal{L}_{\leq}^{f}(z)$. Hence $f-c \in M_{\{z-f\}}$ by Putinar's Positivstellensatz (Theorem 22). This means $\bar{f}-c=\sigma_{0}+\sigma(z-f)$ for some $\operatorname{sos} \sigma_{0}, \sigma \in \mathbb{R}[\underline{X}]$. Thus $g:=c$ is a feasible solution, and $k_{0}:=\operatorname{deg} \sigma$.
To see Statement 4, we note that $k=-\infty$ corresponds to $\sigma=0$, in which case SLS is GLOB
Statement 5 is a consequence of Statements 2 and 4 and Theorem 14
We have not yet addressed the degree of $g$ in GLOB and SLS nor the degree of $\sigma$ in SLS The following proposition shows that once the degree of $\sigma$ in SLS is fixed, the degree of $g$ in any feasible solution is bounded from above in terms of $\operatorname{deg} f$ and $\operatorname{deg} \sigma$.
Proposition 16. Let $f \in \mathbb{R}[\underline{X}], g \in \mathscr{C}(h)$ with $\operatorname{deg} f>0, \operatorname{deg} g>0, z \in \mathbb{R}$ and $\sigma \in \Sigma$ such that

$$
\begin{equation*}
f-g-\sigma(z-f) \text { is sos. } \tag{17}
\end{equation*}
$$

Then

$$
\operatorname{deg}(g) \leq \operatorname{deg}(f)+\max \{\operatorname{deg}(\sigma), 0\}
$$

Proof. Eq. 17) is equivalent to $f-g-\sigma(z-f)=\sigma_{0}$ for some $\sigma_{0} \in \Sigma$, or

$$
\begin{equation*}
g+\sigma_{0}=f(1+\sigma)-z \sigma . \tag{18}
\end{equation*}
$$

Hence $\quad \operatorname{deg}(g) \leq \max \left\{\operatorname{deg}(g), \operatorname{deg}\left(\sigma_{0}\right)\right\} \stackrel{(\mathrm{I})}{=} \operatorname{deg}\left(g+\sigma_{0}\right) \stackrel{(\mathrm{II})}{=} \operatorname{deg}(f(1+\sigma)-z \sigma)$

$$
\begin{aligned}
& \stackrel{(\mathrm{III})}{=} \max \{\operatorname{deg}(f(1+\sigma)), \operatorname{deg}(z \sigma)\} \stackrel{(\mathrm{IV})}{=} \operatorname{deg}(f(1+\sigma)) \\
& \stackrel{(\mathrm{V})}{=} \operatorname{deg}(f)+\operatorname{deg}(1+\sigma) \stackrel{(\mathrm{VI})}{=} \operatorname{deg}(f)+\max \{\operatorname{deg}(\sigma), 0\} .
\end{aligned}
$$

As $g-g(h) \in \Sigma$ and $\operatorname{deg} g>0$, equality (I) follows from Lemma 1. Equality in (II) follows from eq. (18). Using $\operatorname{deg} f>0$, the equalities in (III) and (IV) follow from a typical degree argument: If $u, v \in \mathbb{R}[\underline{X}], \operatorname{deg} u \neq \operatorname{deg} v$, we have $u+v \neq 0$ and $\operatorname{deg}(u+v)=\max (\operatorname{deg} u, \operatorname{deg} v)$. Equality in (V) holds as the degree is multiplicative, (VI) follows easily if one distinguishes the cases $\sigma=0, \sigma \in \mathbb{R}_{\geq 0}$ and $\operatorname{deg} \sigma>0$.

[^3]Corollary 17. Let $g \in \mathscr{C}(h)$ be a feasible solution for GLOB. Then $\operatorname{deg} g \leq \operatorname{deg} f$.
Proof. Use Proposition 16 with $\sigma=0$ and the result follows from Statement 4 of Theorem 15.

## 6. Implementation and results on random instances

### 6.1. Experimental setup

To evaluate our results, we ran computer experiments: For a fixed number of variables $n$ and an even degree $d$, we created instances of random polynomials

$$
\begin{equation*}
f=\sum_{|\alpha| \leq d} a_{\alpha} X^{\alpha}=\sum_{|\alpha| \leq d} a_{\alpha} X_{1}^{\alpha_{1}} \cdots X_{n}^{\alpha_{n}}, \quad a_{\alpha} \sim \mathcal{U}(-1,1) \text { i.i.d.. } \tag{19}
\end{equation*}
$$

As we are only interested in polynomials with positive definite leading form, we restricted ourselves to those polynomials that satisfy

$$
\begin{equation*}
a_{(d, 0, \ldots, 0)}>0, a_{(0, d, 0, \ldots, 0)}>0, \ldots, a_{(0, \ldots, 0, d)}>0 \tag{A}
\end{equation*}
$$

since a polynomial with at least one of these coefficients nonpositive cannot be positive definite. Then, we solved program (12) with $k=d+2$ to compute a lower bound $c_{d}$ on $\min _{x \in \mathbb{S}_{2}^{n-1}} f_{d}(x)$ to determine whether $f$ indeed has a positive definite leading form. If $c_{d} \leq 0$, we discarded the instance, else we know that $f_{d}$ is positive definite. In the first part of the experiments, for every tuple $(n, d)$ with $n=2,3,4$ and $d=$ $2,4,6,8,10$, we created 1000 random instances of polynomials that satisfy condition (A). In Figure 2 we plot how many of these have been detected to satisfy $f_{d}>0$. As $d$ and $n$ increase, the probability of positive definiteness should decrease - as, loosely speaking, more (independent) random variables $a_{\alpha}$ simultaneously influence the result which is reflected in the plot. We then use these instances to evaluate the norm bounds (see Section 6.2). In the second part of the experiments, for four tuples $(n, d)$, we again generated polynomials according to (19) and took the first 50 of them that were detected to have a positive definite leading form as input for the optimization problem which is in turn solved by branch and bound (see Section 6.3).
We use MATLAB ${ }^{4}$ 2014b 64-bit, SOSTOOLS $3.00\left[\mathrm{PAV}^{+} 13\right]$ to translate the sos programs into semidefinite programs and CSDP 6.1.0 [Bor99] to solve the latter. The experiments were conducted on GNU/Linux (Ubuntu 12.04) running on 2 Intel ${ }^{\circledR}$ Xeon ${ }^{\circledR}$ X5650 CPUs (each 6 cores) with a total of 96 GB RAM.

[^4]

Figure 2: Instances with detected positive definite leading form.

### 6.2. Evaluating the norm bounds

Once positive definiteness is certificated by some $c_{d}>0$, the bounds on the norm of the minimizers can be computed. We summarize the steps to compute a norm bound on the minimizer $5^{5}$ in algorithmic form (Algorithm (1).
For $n$ and $d$ as described above, and each of the 1000 randomly created polynomials that has been detected to have a positive definite leading form, we computed the bound from the literature $R_{\text {lit }}$ from eq. (8) and our new bound $R$ (Theorem (6) such that $\left\|x^{\prime}\right\|_{2} \leq \min \left(R_{\mathrm{lit}}, R\right)$ holds for every continuous and integer minimizer of $f$. Figure 3 depicts a selection of $d$ and $n$ : Those with smallest degree, $d=2$, and the maximal degree $d \leq 10$ such that we still detected some instances with $f_{d}>0$. We conclude that for the quadratic case $d=2$, our approach does not yield significantly better results. However, for a higher number of variables and $d \geq 4$ we outperform the classic norm bound on all instances. Most prominently of this selection, for $(n, d)=(3,8)$, we are better by a factor $C=R_{\mathrm{lit}} / R$ of 50 throughout and in some instances we are better by a factor of $C \approx 100$. This means the number of feasible solutions decreases by a factor of up to $C^{n} \approx 100^{3}$ in this example.

### 6.3. Evaluating our underestimators within branch and bound

We evaluated the underestimators in a branch and bound framework. Firstly, we present an algorithm that shows how special properties of our underestimators can be exploited

[^5]```
Algorithm 1 Norm bound on minimizers
    input \(f \in \mathbb{R}\left[X_{1}, \ldots, X_{n}\right]\) with \(\operatorname{deg} f \in 2 \mathbb{N}\), parameters \(p \in 2 \mathbb{N}, k_{\max } \in \mathbb{N}_{0}\)
    \(k \leftarrow 0\)
    \(c_{d} \leftarrow-\infty\)
    \(x \leftarrow\) NULL
    while \(k \leq k_{\text {max }}\) and \(c_{d}<0\) and \(x=\) NULL do
        solve program (12) for \(j=d\) and parameter \(k\)
        \(c_{d} \leftarrow\) optimal value
        if optimal solution can be extracted then
            \(x \leftarrow\) optimal solution
        end if
        \(k \leftarrow k+1\)
    end while
    if \(c_{d}<0\) and \(x \neq\) NULL then
        output \(x\)
        print \(f_{d}(x)<0\) so \(f\) has neither i.m. nor c.m.. // Proposition 5
    else if \(c_{d} \leq 0\) then
        print Cannot decide \(f_{d}>0\) for \(k \leq k_{\text {max }}\).
    else \(\quad / / c_{d}>0\) in the following
        print \(f\) has integer and continuous minimizers. \(/ / f_{d}>0\) by (1)
        for \(j=1, \ldots, d-1\) do
            \(c_{j} \leftarrow \max\) of (10) and (12) // can be improved by also taking (22) into account
        end for
        define \(q: \mathbb{R} \rightarrow \mathbb{R}, q(\lambda)=\sum_{j=1}^{d} c_{j} \lambda^{j}\)
        \(R \leftarrow\) largest root of \(q\) in \(\mathbb{R}\)
        // \(R \geq 0\) by Theorem \(\sqrt{6}\)
        output \(R\)
        print The minimizers \(x^{\prime}\) suffice \(\left\|x^{\prime}\right\|_{p} \leq R\).
                            // Theorem 6
    end if
```



Figure 3: Bounds on the norm of minimizers for different dimensions $n$ and degrees $d$.
to speed up branching and pruning. In the actual experiments, we generated polynomials according to (19), where we restricted ourselves to the tuples $(n, d)=(2,4),(2,6),(3,4)$ and $(4,2)$ to keep the problem size tractable and to have an acceptably high ratio of positive definite polynomials (compare Figure 22). We generated random polynomials until we had 50 that were detected to have a positive definite leading form and which were then used as input to the optimization problem. In the following we present an evluation of the initial lower bound $g(L h\rceil)$ and a runtime comparison with other lower bounds from the literature.

### 6.3.1. Algorithm

Our branch and bound framework is depth first. This keeps memory usage small and allows us to quickly obtain good feasible solutions. We do not reorder the variables. Subproblems are collected in a list $\mathcal{L}$; every subproblem $\mathcal{P} \in \mathcal{L}$ is of the form $\mathcal{P}=\left(m, r_{1}, \ldots, r_{m}\right)$, where $m \in\{0, \ldots, n\}$ encodes the number of fixed variables

$$
\begin{aligned}
\left(r_{1}, \ldots, r_{m}\right) \in \mathbb{Z}^{m} \text {; i.e., } \\
\qquad \begin{aligned}
\min \quad & f\left(r_{1}, \ldots, r_{m}, x_{m+1}, \ldots, x_{n}\right) \\
& x_{m+1}, \ldots, x_{n} \in \mathbb{Z}
\end{aligned}
\end{aligned}
$$

$$
\left(\mathcal{P}=\left(m, r_{1}, \ldots, r_{m}\right)\right)
$$

and (0) encodes the initial problem. Algorithm 2 states the whole procedure.

```
Algorithm 2 Branch and Bound
    input \(f \in \mathbb{R}\left[X_{1}, \ldots, X_{n}\right], h \in \mathbb{R}^{n}, p\)-norm bound \(R\) on minimizers, \(k \in 2 \mathbb{N}_{0}\)
    \(x^{*} \leftarrow\lfloor h\rceil \quad / /\) initial guess for integer minimizer
    \(u \leftarrow f\left(x^{*}\right) \quad / /\) upper bound on integer minimum
    \(\mathcal{L} \leftarrow\{(0)\} \quad / /\) initial list of subproblems
    find underestimator \(g\) : solve SLS with \(h, \operatorname{deg} g \leq \operatorname{deg} \sigma=k \quad / /\) or GLOB, resp.
    while \(\mathcal{L} \neq \emptyset\) do
        pick \(\mathcal{P}=\left(m, r_{1}, \ldots, r_{m}\right) \in \mathcal{L}\) with \(m\) maximal
    8: \(\quad \mathcal{L} \leftarrow \mathcal{L} \backslash\{\mathcal{P}\}\)
        if \(m<n\) then
            \(L \leftarrow\left\lfloor\sqrt[p]{R^{p}-\left|r_{1}\right|^{p}-\cdots-\left|r_{m}\right|^{p}}\right\rfloor\)
            let \(\tilde{g}: \mathbb{R} \rightarrow \mathbb{R}, \tilde{g}\left(x_{m+1}\right)=g\left(r_{1}, \ldots, r_{m}, x_{m+1},\left\lfloor h_{m+2}\right\rceil, \ldots,\left\lfloor h_{n}\right\rceil\right)\)
            if \(\tilde{g}\left(\left\lfloor h_{m+1}\right\rceil\right) \leq u\) then // otherwise prune
                find \(L_{1} \in[-L, L] \cap \mathbb{Z}\) minimal with \(\tilde{g}\left(L_{1}\right) \leq u\)
                if such an \(L_{1}\) exists then
                        find \(L_{2} \in[-L, L] \cap \mathbb{Z}\) maximal with \(\tilde{g}\left(L_{2}\right) \leq u\)
                else
                        \(L_{1} \leftarrow+\infty, L_{2} \leftarrow-\infty\).
                end if
                for all \(r_{m+1} \in\left[L_{1}, L_{2}\right] \cap \mathbb{Z}\) do \(\quad / /\left[L_{1}, L_{2}\right]=\emptyset\) if \(L_{1}=+\infty\)
                        \(\mathcal{L} \leftarrow \mathcal{L} \cup\left\{\left(m+1, r_{1}, \ldots, r_{m+1}\right)\right\} \quad / /\) actual branching
                end for
            end if
        else \(\quad / /\) all variables \(x_{i}\) were fixed to values \(r_{i}\)
            if \(f(r)<u\) then // update upper bound
                \(x^{*} \leftarrow r\)
                \(u \leftarrow f(r)\)
            end if
        end if
    end while
    output \(x^{*}, u\)
    print \(f\) attains its integer minimum \(u\) at \(x^{*}\).
```

Proposition 18. 1. Algorithm 2 is correct, that is, it always terminates after a finite number of steps with an optimal integer solution $x^{*}$ that satisfies $f\left(x^{*}\right)=u$.
2. The integers $L_{1}$ and $L_{2}$ (in lines 13 (8) 15) can be found with binary search in $\left\lceil\log _{2}(L)\right\rceil+2 \leq\left\lceil\log _{2}(R)\right\rceil+2$ evaluations of $\tilde{g}$ if $L>0$.

Proof. Let $x^{*}$ be any optimal solution. To prove1. it suffices to show that the algorithm terminates and no problem with $\left(n, x^{*}\right)$ as subproblem gets pruned in Step 12 or lost in Step 19. To see termination of the algorithm, we observe that the number of subproblems is finite as the sets $B_{m}=\left\{y \in \mathbb{Z}^{m} \mid\|y\|_{p} \leq R\right\}, m=1, \ldots, n$ are finite, every subproblem $\left(m, r_{1}, \ldots, r_{m}\right)$ suffices $\left(r_{1}, \ldots, r_{m}\right) \in B_{m}$ and no subproblem is inserted into the list $\mathcal{L}$ more than once. To see that $x^{*}$ does not get discarded in Step 12, define

$$
\begin{equation*}
\tilde{g}\left(x_{m+1}\right):=g\left(x_{1}^{*}, \ldots, x_{m}^{*}, x_{m+1},\left\lfloor h_{m+2}\right\rceil, \ldots,\left\lfloor h_{n}\right\rceil\right) \tag{20}
\end{equation*}
$$

and suppose $\tilde{g}\left(\left\lfloor h_{m+1}\right\rceil\right)>u$. Hence

$$
\tilde{g}\left(\left\lfloor h_{m+1}\right\rceil\right)>u \geq f\left(x^{*}\right) \geq g\left(x^{*}\right) \geq g\left(x_{1}^{*}, \ldots, x_{m}^{*},\left\lfloor h_{m+1}\right\rceil, \ldots,\left\lfloor h_{n}\right\rceil\right)=\tilde{g}\left(\left\lfloor h_{m+1}\right\rceil\right)
$$

a contradiction, where we used the monotonicity property of $g$ (Proposition 11) and that $g(x) \leq f(x)$ for $x \in \mathcal{L}_{\leq}^{f}(f(q))$, a fortiori for $x \in \mathcal{L}_{\leq}^{f}\left(f\left(x^{*}\right)\right)$. Suppose that $x^{*}$ gets lost in Step 19. Necessarily, $x_{m+1}^{*}<L_{1}$ or $x_{m+1}^{*}>L_{2}$. We derive a contradiction for $x_{m+1}^{*}<L_{1}$, the other case is identical. Observe that $x_{m+1}^{*} \in[-L, L]$ as every optimal integer solution satisfies $\sum_{j=1}^{n}\left|x_{j}^{*}\right|^{p} \leq R^{p}$, so we must have $\left|x_{m+1}^{*}\right|=\sqrt[p]{\left|x_{m+1}^{*}\right|^{p}} \leq$ $\sqrt[p]{R^{p}-\left|x_{1}^{*}\right|^{p}-\ldots-\left|x_{m}^{*}\right|^{p}}$. As $x_{m+1}^{*}$ is integer, we may round down - in other words, $x_{m+1}^{*} \in[-L, L]$. By definition of $L_{1}$ and Proposition 11, we have $\tilde{g}\left(x_{m+1}^{*}\right)>u$ with $\tilde{g}$ from (20), thus, using Proposition 11 again,

$$
\tilde{g}\left(x_{m+1}^{*}\right)>u \geq f\left(x^{*}\right) \geq g\left(x^{*}\right) \geq \tilde{g}\left(x_{m+1}^{*}\right)
$$

a contradiction.
We finally show that Claim 2 holds. We prove the claim for $h_{k+1} \geq 0$, the proof for $h_{k+1} \leq 0$ is similar. In case $h_{k+1}>L, L_{1}$ exists if and only if $\tilde{g}(L) \leq u$ as $\tilde{g}\left(x_{k+1}\right)$ is non-increasing for $x_{k+1} \leq h_{k+1}$ (by Proposition 11; necessarily, $L_{2}:=L$. Using binary search on $[-L, L], L_{1}$ can be found using at most $\left\lceil\log _{2}(2 L)\right\rceil=\left\lceil\log _{2}(L)\right\rceil+1$ further evaluations of $\tilde{g}$. In case $0 \leq h_{k+1} \leq L, L_{1}$ exists as $\tilde{g}\left(\left\lfloor h_{k+1}\right\rceil\right) \leq u$ in Step 12 , Again using binary search, $L_{1} \in\left[-L,\left\lfloor h_{k+1}\right\rceil\right]$ can be found in no more than $\left\lceil\log _{2}(2 L)\right\rceil$ evaluations. As $\tilde{g}\left(x_{k+1}\right)=\tilde{g}\left(h_{k+1}-x_{k+1}\right)$, it only needs at most one more evaluation of $\tilde{g}$ to find $L_{2}$, so we find both numbers in no more than $\left\lceil\log _{2}(L)\right\rceil+2$ evaluations of $\tilde{g}$.

Remark 19. Concerning our implemenation, we chose $\operatorname{deg} g=\operatorname{deg} f$ for GLOB and SLS and $\operatorname{deg} \sigma=2$ for SLS. For the parameter $h \in \mathbb{R}^{n}$ we chose an (approximate) continuous minimizer computed via the SOSTOOLS function findbound.m - however, the algorithm accepts arbitrary $h \in \mathbb{R}^{n}$. We determined $R$ using Algorithm 1 ,

### 6.3.2. The initial lower bound on the minimum

Before we compare our underestimators with lower bounds from the literature, we directly evaluate our initial lower bound $g(\lfloor h\rceil)$. To this end, we define a ratio $Q$ as follows: Let $h$ be a continuous minimizer of $f$ (if found by sos methods), $x^{*}$ an integer minimizer of $f$ found during $\mathrm{B} \& \mathrm{~B}$ and $g$ be a solution to GLOB or SLS. Then

$$
Q:=\frac{g(\lfloor h\rceil)-f(h)}{f\left(x^{*}\right)-f(h)}
$$

takes values in $[0,1]$, is invariant under scaling of $f$ by constants $\lambda>0$ and addition of constants $c \in \mathbb{R}$ to $f$ - and, needless to say, the larger $Q$, the tighter the lower bound. See Figure 4 for the results.


Figure 4: Lower bound comparison using the ratio $Q$.
By Theorem 15, SLS gives bounds that are at least as good as GLOB. The plots show that SLS often gives strictly tighter bounds.

### 6.3.3. Presentation of other bounds

It is not straightforward to compare the performance of our lower bounds with bounds from the literature. In our setting, we compute a single underestimator per instance which is then merely evaluated during the branch and bound process ${ }^{6}$. We could not find other underestimators with this property that give sensible results in branch and bound. However, there are lower bounds in the literature that are more general than ours since they consider restricted polynomial optimization problems and can hence be applied to any polynomial - not only to those with positive definite leading form and are suitable for branch and bound if computed anew at each node. In addition to Algorithm 2 (with GLOB and SLS) we implemented the following four algorithms in a

[^6]MATLAB framework for solving IP three of them are branch and bound approaches as Algorithm 2 which use other bounds (taken from [BD14], [LHKW06], and the continuous relaxation) while our last algorithm is a simple brute force approach.

- For arbitrary polynomials on boxes, Buchheim and D'Ambrosio BD14 suggested to compute, for every term of $f$, the $L^{1}$-best separable underestimator. The sum of the underestimators is again separable, so its integer minimization is a univariate problem. For degree $d \leq 4$ and arbitrary $n$, they provide explicit underestimators. We hardcoded the explicit underestimators, and used the MATLAB builtins polyval, polyder and roots to evaluate and differentiate the separable underestimators, and to compute their roots, respectively. As a suitable box at the subproblem $\mathcal{P}=\left(m, r_{1}, \ldots, r_{m}\right)$ we chose the box $[-L, L]^{n-m}$ where $L=\left\lfloor\sqrt[p]{R^{p}-\left|r_{1}\right|^{p}-\cdots-\left|r_{m}\right|^{p}}\right\rfloor$. The authors suggest to successively halve the box into subboxes which does not fit into our scheme. This approach is abbreviated SEP in the plots.
- For nonnegative polynomials on polytopes $P$, De Loera et al. LHKW06 approximate the maximum of $f$ on $P \cap \mathbb{Z}^{n}$ by the sequence $\sqrt[k]{\sum_{x \in P \cap \mathbb{Z}^{n}} f(x)^{k}}$. Each member of the sequence can be computed in polynomial time, using a reformulation as a limit of a rational function which in turn is based on the generating function of $P$. We did experiments with $k=2$ and $k=4$, the latter taking significantly longer, without giving much better results, so we restricted ourselves to $k=2$. Note that the suggested implementation uses residue techniques, while we just use symbolic limit computations. On the other hand, we improved the bounds as follows: To make their approach applicable to not necessarily nonnegative polynomials, the authors suggest to add the sufficiently large constant

$$
c:=\|f\|_{0}\|f\|_{\infty} M^{d}
$$

to obtain $\bar{f}=f+c$ nonnegative on $P$. Here, $M \geq 0$ is a bound on the polyhedron s.t. $\left|x_{i}\right| \leq M$ for all $x \in P$; for $f=\sum_{\alpha} a_{\alpha} X^{\alpha}$, we use the zero "norm" $\|f\|_{0}:=\#\left\{\alpha \mid a_{\alpha} \neq 0\right\}$ and the infinity norm $\|f\|_{\infty}:=\max _{\alpha}\left\{\left|a_{\alpha}\right|\right\}$. However, the constant $c^{\prime}:=\sum_{j=0}^{d}\left\|f_{j}\right\|_{1} M^{j}$ suffices to ensure that $f+c^{\prime}$ is nonnegative on $P$. A short calculation shows that $c^{\prime} \leq c$ if $M \geq 1$, and in dense instances one often has $c^{\prime} \ll c$. As polyhedron we again chose the box $[-L, L]^{n-m}$ from the previous bound. This bound is abbreviated to POLYFIX in the plots.

- We compute an sos approximation of the global continuous relaxation ( $\mathbf{C R}$ in the plots) at each subproblem $\mathcal{P}=\left(m, r_{1}, \ldots, r_{m}\right)$, that is

$$
\begin{aligned}
\max & \lambda \\
\text { s.t. } & f\left(r_{1}, \ldots, r_{m}, X_{m+1}, \ldots, X_{n}\right)-\lambda \text { is } \operatorname{sos} \text { in } \mathbb{R}\left[X_{m+1}, \ldots, X_{n}\right]
\end{aligned}
$$

- Brute force enumeration with no lower bounds, abbreviated BF. As $f$ has to be evaluated at each node, we use matlabFunction to convert the Symbolic Math

Toolbox object that encodes $f$ into a function handle that can be evaluated significantly faster.

- Algorithm 2 using GLOB with parameters as described in Remark 19 .
- Algorithm 2 using SLS with parameters as described in Remark 19 .


### 6.3.4. Runtime comparison

The implementation of the six different algorithms from Section 6.3.3 into our B\&Bframework gave the runtimes in Figure 5 (logarithmic scale). On every instance each of the lower bounds had a maximum of 5 minutes to complete; if this time constraint was violated, the process was interrupted and the lower bound considered as unsuccessful on this instance. If the parameter $h$ could not be found by SOSTOOLS' findbound.m function, GLOB and SLS were considered to have violated the time constraint.



Figure 5: Runtimes in [s].

We infer from the plots that for a small number of variables, the problem size (i.e., $R$ ), is mostly so small that brute force is often the fastest approach. However, if instances get larger, brute force fails necessarily as the processing time is linear in the number of nodes. SEP is quite fast in small instances, but for large instances the running time deteriorates as an underestimator is computed at each node. In our setting, POLYFIX takes too long to be competitive. The continuous relaxation is satisfactory for smaller instances but fails in some large instances. Concerning our bounds, in the two plots of Figure 5 with $n=2$, there is a surprisingly little variance in runtime for GLOB and SLS. This can be explained from a further plot, see Figure 6, in which we break down the preprocessing time, i.e., the time needed to compute a approximate continuous minimizer $h$ and the underestimator $g$, and the time needed for the actual branch and bound. It can be seen that the preprocessing time is more or less independent from the instance and takes in most instances significantly longer than the actual branch and bound. Also, it seems at first that SLS takes mostly longer than GLOB. However, this holds only true for the preprocessing phase: The corresponding sos program is larger, and so are preprocessing times. Indeed, Figure 6 reveals that GLOB has shorter preprocessing times throughout, but is inferior in $\mathrm{B} \& \mathrm{~B}$, as expected.


Figure 6: Preprocessing (P) and $\mathrm{B} \& \mathrm{~B}(\mathrm{~B})$ times -GLOB on the left, SLS on the right.

## 7. Conclusion and Outlook

In this paper we presented a new way of finding underestimators for integer polynomial optimization and improved the bounds on the norm of integer and continuous minimizers. We implemented both ideas within a branch \& bound approach showing how they improve its performance.

Currently we compute one underestimator at the beginning of the branch and bound process which is used for generating lower bounds throughout the whole algorithm. Instead, one could also compute a new underestimator at each node of the branch and bound tree. This would improve the bounds but due to the comparatively large compu-
tation time for solving an sos-program does not pay off in terms of overall efficiency. We currently analyze in which nodes the computation of a new underestimators improves the procedure. Along the lines of [BHS14] we plan to analyze how to find an underestimator which is likely to be a good one for all subnodes.
We also point out that our procedure can be extended to mixed-integer polynomial optimization: The norm bounds apply in the mixed-integer case as well, and we may use the proposed class of underestimators, but with their mixed-integer minima (which are also simple to obtain). Our underestimators can in principle also be used for constrained polynomial optimization; however, it is subject to further investigation if the bounds provided are sharp enough for this case. We hence work on sos-programs which provide underestimators which are able to take into account given constraints.

## A. Computing the norm bounds

In Remark 7 we saw that we get a tighter norm bound $R$ on the minimizers the closer the $c_{j}$ get to their optimal value $c_{j}^{*}$. In the following, we present two means that improve on the approach 1, in Section 4.1 that do not rely on sos programming. The second method we present is a refinement of the first. For both, we improve the norm bound $R$ by replacing the estimate $\left|x^{\alpha}\right| \leq 1$ on $\mathbb{S}_{p}^{n-1}$ with $\left|x^{\alpha}\right| \leq \hat{x}^{\alpha}$, where $\hat{x}$ is a continuous maximizer of the function $\mathbb{S}_{p}^{n-1} \rightarrow \mathbb{R}, x \mapsto x^{\alpha}$.

## A.1. A direct improvement

One has the following closed form for the continuous minimizer $\hat{x}$ with nonnegative coordinates:

Lemma 20. Let $0 \neq \alpha \in \mathbb{N}_{0}^{n}$ and $p \in[1, \infty)$. Then, the monomial $X^{\alpha}$ attains its maximum on $\mathbb{S}_{p}^{n-1}$ at $\hat{x}$ with coordinates

$$
\begin{equation*}
\hat{x}_{i}=\sqrt[p]{\frac{\alpha_{i}}{\sum_{i=1}^{n} \alpha_{i}}}, \quad i=1, \ldots, n \tag{21}
\end{equation*}
$$

Proof. By a simple analysis, the proof can be reduced to $\alpha_{i} \geq 1$ for $i=1, \ldots, n$ and then to maximization of $X^{\alpha}$ on $\left\{x \in \mathbb{S}_{p}^{n-1} \mid x_{1}>0, \ldots, x_{n}>0\right\}$. Using the method of Lagrange multipliers, the claim follows from a short calculation.

Observation 21. Denote by $\hat{x}_{(\alpha)}$ the maximizer of $X^{\alpha}$ on $\mathbb{S}_{p}^{n-1}$ as in 21). Hence for $x \in \mathbb{S}_{p}^{n-1}$ we have

$$
\begin{equation*}
f_{j}(x)=\sum_{|\alpha|=j} a_{\alpha} x^{\alpha} \geq \sum_{|\alpha|=j}-\left|a_{\alpha}\right| \cdot\left(\hat{x}_{(\alpha)}\right)^{\alpha}=: c_{j} . \tag{22}
\end{equation*}
$$

This $c_{j}$ is as least as large as approach 1. from Section 4.1 since, for $0 \neq \alpha,\left(\hat{x}_{(\alpha)}\right)^{\alpha}<1$ - unless $X^{\alpha} \in \mathbb{R}\left[X_{i}\right]$ for some $i$, in which case $\hat{x}_{(\alpha)}=e_{i}$, the $i$-th unit vector, and thus $\left(\hat{x}_{(\alpha)}\right)^{\alpha}=1$.

## A.2. A different approach

This last approach on computing bounds $c_{j}$ is different to the ones before, as we actually compute $2^{n}$ norm bounds: We restrict $f$ to each of the $2^{n}$ orthants

$$
H_{\tau}=\left\{x \in \mathbb{R}^{n} \mid \tau_{i} x_{i} \geq 0\right\} \text { for } \tau \in\{-1,1\}^{n}
$$

and compute norm bound on integer minimizers of every $\left.f\right|_{H_{\tau}}$. This has the advantage that, roughly speaking, we may neglect half of the terms of $f=\sum a_{\alpha} X^{\alpha}$. Also, minimization on $H_{\tau}$ can be reduced to minimization on $H_{(1, \ldots, 1)}$, i.e., the set of those $x \in \mathbb{R}^{n}$ with $x \geq 0$, as we shall see in a moment.
Introducing the notation $|a|^{-}=|\min (a, 0)|$ for $a \in \mathbb{R}$ and with $\hat{x}$ from (21), we have for every term $a_{\alpha} x^{\alpha} \geq-\left|a_{\alpha}\right|^{-} x^{\alpha} \geq-\left|a_{\alpha}\right|^{-} \hat{x}^{\alpha}$ as $x \geq 0$, thus

$$
f_{j}(x)=\sum_{|\alpha|=j} a_{\alpha} x^{\alpha} \geq \underbrace{\sum_{|\alpha|=j}-\left|a_{\alpha}\right|^{-} \hat{x}^{\alpha}}_{=: c_{j}^{(1, \ldots, 1)}}, \quad x \in \mathbb{S}_{p}^{n-1} \text { and } x \geq 0,
$$

which means about half of the coefficients are neglected in comparison to (22), if signs are distributed equally among the $a_{\alpha}$. Now let $R^{(1, \ldots, 1)}$ be the largest real root of

$$
q^{(1, \ldots, 1)}(\lambda):=c_{d} \lambda^{d}+\sum_{j=1}^{d-1} c_{j}^{(1, \ldots, 1)} \lambda^{j} .
$$

The verbatim argument of Theorem 6 shows that $f(x)>f(0)$ for $\|x\|_{p}>R^{(1, \ldots, 1)}$ and $x \geq 0$. This bounds integer and continuous minimizers on $H_{(1, \ldots, 1)}$. Bounding the norm of minimizers of $f$ on $H_{\tau}, \tau \in\{-1,1\}^{n}$, can be reduced to bounding the norm of minimizers on $H_{(1, \ldots, 1)}$ by a simple change of coordinates. To this end, let $\tau(x)=\left(\tau_{1} x_{1}, \ldots, \tau_{n} x_{n}\right)$, $x \in \mathbb{R}^{n}$, and $f^{\tau}$ be the polynomial

$$
f^{\tau}(x):=f(\tau(x))=\sum_{\alpha} a_{\alpha} \tau^{\alpha} x^{\alpha}, \quad \tau \in\{-1,1\}^{n} .
$$

As $\tau^{\alpha} \in\{-1,1\}, f$ and $f^{\tau}$ merely differ in the sign of their coefficients, and $f_{d}^{\tau}(x) \geq c_{d}$ still holds for $x \in \mathbb{S}_{p}^{n-1}$ as the sphere is $\tau$-invariant, that is $\tau\left(\mathbb{S}_{p}^{n-1}\right)=\mathbb{S}_{p}^{n-1}$. Similarly to before, denote by $R^{\tau}$ the largest real root of

$$
q^{\tau}(\lambda)=c_{d} \lambda^{d}+\sum_{j=1}^{d-1} c_{j}^{\tau} \lambda^{j},
$$

with $c_{j}^{\tau}=-\left|a_{\alpha} \tau^{\alpha}\right|^{-} \hat{x}^{\alpha}$. It is now clear that $f^{\tau}(x)>f(0)$ for $\|x\|_{p}>R^{\tau}$ and $x \geq 0$, equivalently, $f(x)>f(0)$ for $\|x\|_{p}>R^{\tau}$ and $x \in H_{\tau}$.
This results in more effort in the preprocessing, but reduces the number of feasible solutions.

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[^1]:    ${ }^{1}$ In case of unconstrained continuous minimization, provided minimizers exist, restricting minimization of $f$ to the subset of $\mathbb{R}^{n}$ where the gradient vanishes does not change the set of optimal solutions.

[^2]:    ${ }^{2}$ For this example we solved GLOB for $h=0.3$ and $\operatorname{deg} g=6$, using SOSTOOLS 3.00 and CSDP 6.1.0.

[^3]:    ${ }^{3}$ Note that every sos polynomial $\sigma \neq 0$ has even degree.

[^4]:    ${ }^{4}$ MATLAB is a registered trademark of The MathWorks Inc., Natick, Massachusetts

[^5]:    ${ }^{5}$ In the algorithm, we abbreviate integer minimizer(s) to i.m. and continuous minimizer(s) to c.m..

[^6]:    ${ }^{6}$ By fixing some variables at each node and then computing new underestimators, this could be improved but would need additional runtime for the computation of the new underestimator.

