Lower bounds certification for multivariate real functions using SDP

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Two Problems

$K \subset \mathbb{R}^n$: a compact set
$f : K \to \mathbb{R}$: a real multivariate function

Two challenging problems:

1. $\inf_{x \in K} f(x)$ when f is a multivariate polynomial of degree d
   Number of variables n is large, no sparsity $\Longrightarrow$ very hard to solve using Interval Arithmetic

Example:

$K := [0, 1]^n$, random numbers $(r_i)_{1 \leq i \leq n}$:

$f_d := \left(\frac{1}{n} \sum_{i=1}^{n} \frac{4}{r_i^2} x_i (r_i - x_i)\right)^{\lceil d/2 \rceil}$, the range of f_d is $[0, 1]$

2. $\inf_{x \in K} f(x)$ when f is a multivariate real function involving transcendental univariate functions

Contents

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1. Lower bounds of multivariate polynomial with large number of variables
2. Lower bounds of transcendental multivariate functions

SOS and SDP Relaxations

Polynomial Optimization Problem (POP):

Let $f, g_1, \cdots, g_m \in \mathbb{R}[X_1, \cdots, X_n]$
$K_{pop} := \{x \in \mathbb{R}^n : g_1(x) \geq 0, \cdots, g_m(x) \geq 0\}$ is the feasible set
General POP: compute $f^*_{pop} = \inf_{x \in K_{pop}} f(x)$

Example:

$f := 10 - x_1^2 - x_2^2$, $g_1 := 1 - x_1^2 - x_2^2$
$K_{pop} := \{x \in \mathbb{R}^2 : g_1(x) \geq 0\}$ is the feasible set

SOS and SDP Relaxations

Convexify the problem:

$f^*_{pop} = \inf_{x \in K_{pop}} f_{pop}(x) = \inf_{\mu \in \mathcal{P}(K_{pop})} \int f_{pop} \, d\mu$, where $\mathcal{P}(K_{pop})$ is the set of all probability measures μ supported on the set K_{pop}.

Equivalent formulation:

$f^*_{pop} = \min \{ L(f) : L : \mathbb{R}[X] \to \mathbb{R}$ linear, $L(1) = 1$ and each $\mathcal{L}_{g_j}$ is SDP $\}$, with $g_0 = 1$, $\mathcal{L}_{g_0}, \cdots, \mathcal{L}_{g_m}$ defined by:

$$\begin{array}{rcccl} \mathcal{L}_{g_j} & : & \mathbb{R}[X] \times \mathbb{R}[X] & \to & \mathbb{R} \\ & & (p, q) & \mapsto & L(p \cdot q \cdot g_j) \end{array}$$

SOS and SDP Relaxations: Lasserre Hierarchy

- $\mathcal{B} := (X^\alpha)_{\alpha \in \mathbb{N}^n}$: the monomial basis and $y_\alpha = L(X^\alpha)$, this identifies L with the infinite series $y = (y_\alpha)_{\alpha \in \mathbb{N}^n}$
- Infinite moment matrix M:
  $M(y)_{u,v} := L(u \cdot v), \; u, \, v \in \mathcal{B}$
- Localizing matrix $M(g_j y)$:
  $M(g_j y)_{u,v} := L(u \cdot v \cdot g_j), \; u, \, v \in \mathcal{B}$
- $k \geq k_0 := \max\{\lceil \deg f_{pop} \rceil / 2, \lceil \deg g_0 / 2 \rceil, \cdots, \lceil \deg g_m / 2 \rceil\}$
  Index $M(y)$ and $M(g_j y)$ with elements in $\mathcal{B}$ of degree at most k, it gives the semidefinite relaxations hierarchy:

$$Q_k : \begin{cases} \inf_y L(f) & = \int f_\alpha \, x^\alpha \, d\mu(x) = \sum_\alpha f_\alpha \, y_\alpha \\ M_{k - \lceil \deg g_j / 2 \rceil}(g_j y) & \succcurlyeq 0, \qquad 0 \leq j \leq m, \\ y_1 & = 1 \end{cases}$$

SOS and SDP Relaxations

Convergence Theorem [Lasserre]:

The sequence $\inf(Q_k)_{k \geq k_0}$ is non-decreasing and under the SOS assumption converges to f^*_{pop}.

SDP relaxations:

Many solvers (e.g. Sedumi, SDPA) solve the pair of (standard form) semidefinite programs:

$$(SDP) \left\{ \begin{array}{lll} \mathcal{P}: & \min\limits_{y} & \sum\limits_{\alpha} c_\alpha y_\alpha \\ & \text{subject to} & \sum\limits_{\alpha} F_\alpha \, y_\alpha - F_0 \succcurlyeq 0 \\ \mathcal{D}: & \max\limits_{Y} & \text{Trace}\,(F_0 \, Y) \\ & \text{subject to} & \text{Trace}\,(F_\alpha \, Y) = c_\alpha \end{array} \right.$$

SDP relaxation Q_k at order $k \geq \max_j \{\lceil \deg f_{pop}/2 \rceil, \lceil \deg g_j/2 \rceil\}$:

- $\mathcal{O}(n^{2k})$ moment variables
- linear matrix inequalities (LMIs) of size $\mathcal{O}(n^k)$

polynomial in n, exponential in k

On our example:

$K := [0,1]^n$, random numbers $(r_i)_{1 \leq i \leq n}$:

$$f_d := \Big(\frac{1}{n} \sum_{i=1}^{n} \frac{4}{r_i^2} x_i (r_i - x_i)\Big)^{\lceil d/2 \rceil}$$

$\deg g_j = 1$, $k \geq d \implies$ at least $\mathcal{O}(n^{2d})$ moment variables with LMIs of size $\mathcal{O}(n^d)$!!

Large-scale POP

Multivariate Taylor-Models Underestimators:

- $f : K \to \mathbb{R}$ is a multivariate polynomial
- Consider a minimizer guess x_c obtained by heuristics
- Let q_{x_c} be the quadratic form defined by:

$$\begin{aligned} q_{x_c} : K &\longrightarrow \mathbb{R} \\ x &\longmapsto f(x_c) + \mathcal{D}_f(x_c)\,(x - x_c) \\ &\quad + \frac{1}{2}(x - x_c)^T \mathcal{D}_f^2(x_c)\,(x - x_c) + \lambda(x - x_c)^2 \end{aligned}$$

with $\lambda := \min_{x \in K} \{\lambda_{\min}(\mathcal{D}_f^2(x) - \mathcal{D}_f^2(x_c))\}$

Theorem:

$\forall x \in K, f(x) \geq q_{x_c}$, that is q_{x_c} understimates f on K.
q_{x_c} is called a quadratic cut.

How to compute λ? How to compute a lower bound of f?

- $\lambda := \min_{x \in K} \{\lambda_{\min}(\mathcal{D}_f^2(x) - \mathcal{D}_f^2(x_c))\}$
- Bound the Hessian difference on K by POP (using SDP relaxations) to get $\bar{\mathcal{D}}_f^2$:
- Define the symmetric matrix B containing the bounds on the entries of $\bar{\mathcal{D}}_f^2$.
- Let $\mathcal{S}^n$ be the set of diagonal matrices of sign.
  $\mathcal{S}^n := \{\text{diag}\,(s_1, \cdots, s_n),\ s_1 = \pm 1, \cdots\ s_n = \pm 1\}$
  $\lambda := \lambda_{\min}(\bar{\mathcal{D}}_f^2 - \mathcal{D}_f^2(x_c)\bar{I})$: minimal eigenvalue of an interval matrix

Robut Optimization with Reduced Vertex Set [Calafiore, Dabbene]

The robust interval SDP problem $\lambda_{\min}(\bar{\mathcal{D}}_f^2 - \mathcal{D}_f^2(x_c)\bar{I})$ is equivalent to the following SDP in the single variable $t \in \mathbb{R}$:

$$\begin{cases} \min & -t \\ \text{s.t.} & -t\, I - \mathcal{D}_f^2(x_c) - S\, B\, S \succeq 0,\ S = \text{diag}\,(1,\ \tilde{S}),\ \forall \tilde{S} \in \mathcal{S}^{n-1} \end{cases}$$

Solving the previous SDP is expensive because the dimension of $\mathcal{S}^n$ grows exponentially. Instead, we can underestimate λ:

- Write $\bar{\mathcal{D}_f^2} - \mathcal{D}_f^2(x_c)\bar{I} := \bar{X} + \bar{Y}$ with
  $\bar{X}_{ij} := [\frac{a_{ij} + b_{ij}}{2}, \frac{a_{ij} + b_{ij}}{2}]$ and $\bar{Y}_{ij} := [-\frac{b_{ij} - a_{ij}}{2}, \frac{b_{ij} - a_{ij}}{2}]$
- $\lambda_{\min}(\bar{X} + \bar{Y}) \geq \lambda_{\min}(\bar{X}) + \lambda_{\min}(\bar{Y}) = \lambda_{\min}(\bar{X}) - \lambda_{\max}(-\bar{Y})$
- $\lambda_{\max}(\bar{Y}) \leq \max_i \sum_j \frac{b_{ij} - a_{ij}}{2}$

Computing a lower bound of $\lambda_{\min}(\bar{X})$ is easier because $\bar{X}$ is a real matrix. We can do it again by SDP: $\begin{cases} \min & -t \\ \text{s.t.} & -t\, I - \bar{X} \succeq 0 \end{cases}$

... and how to compute a lower bound of the polynomial f?

Large-scale POP
Computing lower bounds

Input: f, box K, SDP relaxation order k, control points sequence $s = (x_1) \in K$, n_{cuts} (final number of quadratic cuts)

Output: lower bound m of f

$cuts := 1$

while $cuts \leq n_{cuts}$ **do**

  For $c \in \{1, \dots, \#s\}$: compute λ using robust SDP or $\lambda_{\min}$ approximation and compute q_{x_c}

  $f_p := \max_{1 \leq c \leq p} q_{x_c}$, $K_{pop} := \{x \in K : z \geq q_{x_1}(x), \cdots, z \geq q_{x_p}(x)\}$

  Compute a lower bound m of f_p by POP at the SDP relaxation order k: $m \leq \inf_{x \in K_{pop}} z$

  $x_{opt} :=$ `guess_argmin` (f_p): a minimizer candidate for f_p

  $s := s \cup \{x_{opt}\}$

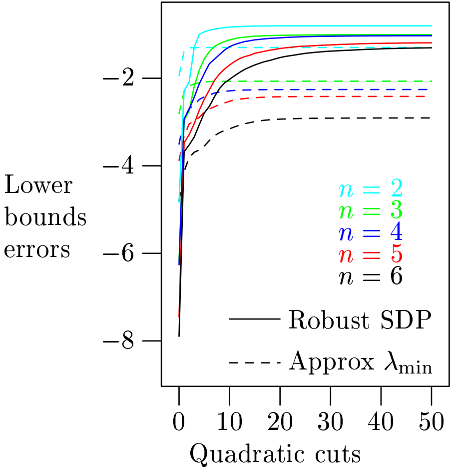
  $cuts := cuts + 1$

done

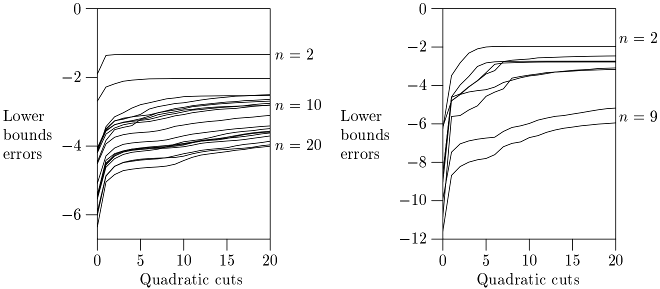
$$K := [0,1]^n$$

$$f_6 := \Big(\frac{1}{n}\sum_{i=1}^{n}\frac{4}{r_i^2}x_i(r_i - x_i)\Big)^3$$

- We compare the quality of the successive lower bounds (previous algorithm) with different λ underestimators
- $\lambda_{\text{robust}} \geq \lambda_{\text{approx}} \implies$ Better quadratic approximations when using the Robust SDP approach



- When n is large, Robust SDP approach is too expensive. It becomes impossible to compute λ and the quadratic cuts q_{x_c}.



(a) $d = 4$

(b) $d = 6$

- Bottleneck: computation of the $n(n+1)$ bounds of the Hessian entries $\bar{\mathcal{D}}_f^2 - \mathcal{D}_f^2(x_c)\bar{I}$ (multivariate polynomial of degree $d-2$)

Bounding multivariate transcendental functions

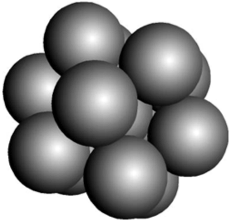
- Now, consider a semialgebraic compact set $K \subset \mathbb{R}^n$ and $f : K \to \mathbb{R}$ a multivariate transcendental function
- We want to compute a precise lower bound of f. The previous approach only gives a hierarchy of coarse bounds

Motivations?
How to approach the univariate transcendental functions involved in f?

Kepler Conjecture (1611):

The maximal density of sphere packings in 3-space is $\frac{\pi}{\sqrt{18}}$

- It corresponds to the way people would intuitively stack oranges, as a pyramid shape
- The proof of T. Hales (1998) consists of thousands of non-linear inequalities
- Many recent efforts have been done to give a formal proof of these inequalities: Flyspeck Project
- Motivation: get positivity certificates and check them with Proof assistants like COQ



Inequalities issued from Flyspeck non-linear part involve:

1. Semi-Algebraic functions algebra $\mathcal{A}$: composition of polynomials with $|\cdot|$, $(\cdot)^{\frac{1}{p}} (p \in \mathbb{N}_0), +, -, \times, /, \sup, \inf$
2. Transcendental functions $\mathcal{T}$: composition of semi-algebraic functions with arctan, arcos, arcsin, exp, log, $|\cdot|$, $(\cdot)^{\frac{1}{p}} (p \in \mathbb{N}_0), +, -, \times, /, \sup, \inf$

Lemma$_{9922699028}$ from Flyspeck

$K := [4, 6.3504]^3 \times [6.3504, 8] \times [4, 6.3504]^2 \qquad P, Q \in \mathbb{R}[X]$

$$\forall x \in K, -\frac{\pi}{2} + \mathit{arctan} \frac{P(x)}{\sqrt{Q(x)}} + 1.6294 - 0.2213 (\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0) + 0.913 (\sqrt{x_4} - 2.52) + 0.728 (\sqrt{x_1} - 2.0) \geq 0.$$

Tight inequality: global optimum $\simeq 1.7 \times 10^{-4}$

Given K a compact set, and f a transcendental function, bound from below $f^* = \inf_{x \in K} f(x)$ and prove $f^* \geq 0$

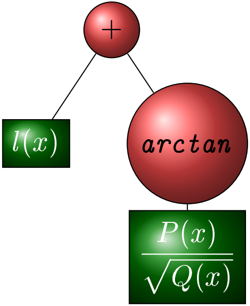
1. f is approximated by a semi-algebraic function f_{sa}
2. Reduce the problem $\inf_{x \in K} f_{sa}(x)$ to a polynomial optimization problem (POP) in a lifted space K_{pop}
3. Solve classically the POP problem $\inf_{x \in K_{pop}} f_{pop}(x)$ using a sparse variant hierarchy of SDP relaxations by Lasserre

$$f^* \geq f^*_{sa} \geq f^*_{pop} \underbrace{\geq 0}_{\text{If the relaxations are accurate enough}}$$

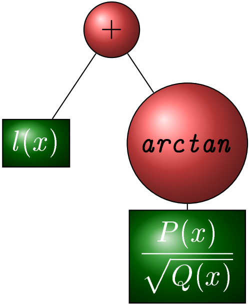
Bounding multivariate transcendental functions

General Framework

- The first step is to build the abstract syntax tree from an inequality, where leaves are semi-algebraic functions and nodes are univariate transcendental functions (arctan, exp, ...) or basic operations ($+$, $\times$, $-$, $/$).
- With $l := -\frac{\pi}{2} + 1.6294 - 0.2213\,(\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0) + 0.913\,(\sqrt{x_4} - 2.52) + 0.728\,(\sqrt{x_1} - 2.0)$, the tree of the example is:



- Let $t \in \mathcal{T}$ be a transcendental univariate elementary function such as $\mathtt{arctan}$, $\mathtt{exp}$, ..., defined on a real interval I. Let $d \in \mathbb{N}$ given.
- Minimax: Best uniform degree d polynomial approximation $\hat{t}$: solution of $||\epsilon||_\infty := \min_{p \in \mathbb{R}_d[X]} ||t - p||_\infty$
- Existence and uniqueness of $\hat{t}$
- Remez algorithm implementation in Sollya: computes $\hat{t}$ for each univariate transcendental function involved in the Flyspeck inequalities with given $I := [a, b]$ and $d \in \mathbb{N}$
- Also computes a certified upper bound of $||\epsilon||_\infty$ related to the minimax polynomial



Two kinds of semialgebraic leaves:

- multivariate functions: $\frac{P(x)}{\sqrt{Q(x)}}$: we can get the bounds by POP using lifting variables
- sum of univariate functions: $l := -\frac{\pi}{2} + 1.6294 - 0.2213\,(\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0) + 0.913\,(\sqrt{x_4} - 2.52) + 0.728\,(\sqrt{x_1} - 2.0)$: we can approximate $\sqrt{\cdot}$ by a minimax polynomial with Sollya

$$\frac{P(x)}{\sqrt{Q(x)}} \text{ on } K := [4, 6.3504]^3 \times [6.3504, 8] \times [4, 6.3504]^2 ?$$

Lifting procedure by POP:

1. Get bounds of $P(x)$ by POP
2. Get bounds of $Q(x)$ by POP and $\sqrt{Q(x)}$ by interval arithmetic
3. Lifting variable representing $\sqrt{Q(x)}$: $q \in I_q$
4. Coarse bounds of $\dfrac{P(x)}{\sqrt{Q(x)}}$ by interval arithmetic: interval I_z
5. Lifting variable representing $\dfrac{P(x)}{\sqrt{Q(x)}}$: $z \in I_z$
6. Lifting space:
   $K_{\text{pop}} := \{(x, q, z) \in K \times I_q \times I_z \, : \, q^2 = Q(x), zq = P(x)\}$
7. Solving $\inf_{(x,q,z) \in K_{\text{pop}}} z$ by POP gives a lower bound of $\dfrac{P(x)}{\sqrt{Q(x)}}$

8. We get an interval I enclosing $\dfrac{P(x)}{\sqrt{Q(x)}}$ from POP.
9. Minimax polynomials for the univariate real functions of f:

t	d	Upper bound of $\|\|\epsilon\|\|_\infty$
$\arctan$ on I	5	2.01×10^{-4}
$\sqrt{}$ on $[4, 6.3504]$	4	2.50×10^{-5}
$\sqrt{}$ on $[6.3504, 8]$	2	9.34×10^{-8}

10. We obtain a minimax polynomial for $\arctan$. With the minimax polynomial for $\sqrt{}$: we can approach l by $\hat{l}$.

Again by using POP:

- Lifting variable representing $\sqrt{Q(x)}$: $q \in I_q$
- Lifting variable representing $\dfrac{P(x)}{\sqrt{Q(x)}}$: $z \in I_z$
- Lifting space:
  $K_{\text{pop}} := \{(x, q, z) \in K \times I_q \times I_z \ : \ q^2 = Q(x), zq = P(x), \}$
- Solving $\inf_{(x,q,z) \in K_{\text{pop}}} \hat{l}(x) + \widehat{\arctan}(z)$ by POP gives a lower bound of $\hat{f} := \hat{l}(x) + \widehat{\arctan}(z)$
- Finally, Subtract the minimax errors $||\epsilon||_\infty$ to $\hat{f}$ gives a lower bound of f

End

Thanks for your attention! Questions?