New Applications of Moment-SOS Hierarchies

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Imagination Technologies Seminar
London
2008 – 2010: Master at Tokyo University
**Hierarchical Domain Decomposition Methods**
(S. Yoshimura)

2010 – 2013: PhD at Inria Saclay LIX/CMAP
**Formal Proofs for Nonlinear Optimization**
(S. Gaubert and B. Werner)

2014 Jan-Sept: Postdoc at LAAS-CNRS
**Moment-SOS Applications**
(D. Henrion and J.B. Lasserre)
Mathematicians want to eliminate all the uncertainties on their results. Why?

M. Lecat, Erreurs des Mathématiciens des origines à nos jours, 1935.

130 pages of errors! (Euler, Fermat, Sylvester, …)
Errors and Proofs

Possible workaround: proof assistants

COQ (Coquand, Huet 1984)

HOL-LIGHT (Harrison, Gordon 1980)

Built in top of OCAML
Computer Science and Mathematics

- Tool: Formal Bounds for Global Optimization

- Collaboration with:
  - Benjamin Werner (LIX Polytechnique)
  - Stéphane Gaubert (Maxplus Team CMAP/INRIA Polytechnique)
  - Xavier Allamigeon (Maxplus Team)
Complex Proofs

- Complex mathematical proofs / mandatory computation

K. Appel and W. Haken, Every Planar Map is Four-Colorable, 1989.

From Oranges Stack...

Kepler Conjecture (1611):

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

Face-centered cubic Packing

Hexagonal Compact Packing
...to Flyspeck Nonlinear Inequalities

- The proof of T. Hales (1998) contains mathematical and computational parts

- Computation: check thousands of nonlinear inequalities

- Robert MacPherson, editor of The Annals of Mathematics: “[...] the mathematical community will have to get used to this state of affairs.”

- Flyspeck [Hales 06]: Formal Proof of Kepler Conjecture
...to Flyspeck Nonlinear Inequalities

- The proof of T. Hales (1998) contains mathematical and computational parts

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- Flyspeck [Hales 06]: Formal Proof of Kepler Conjecture

- Project Completion on 10 August by the Flyspeck team!!
Nonlinear inequalities: quantified reasoning with “∀”

\[ \forall x \in K, f(x) \geq 0 \]

NP-hard optimization problem
A “Simple” Example

In the computational part:

- Multivariate Polynomials:

\[
\Delta x := x_1 x_4 (-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) + x_2 x_5 (x_1 - x_2 + x_3 + x_4 - x_5 + x_6) + x_3 x_6 (x_1 + x_2 - x_3 + x_4 + x_5 - x_6) - x_2 (x_3 x_4 + x_1 x_6) - x_5 (x_1 x_3 + x_4 x_6)
\]
A “Simple” Example

In the computational part:

- **Semialgebraic** functions: composition of polynomials with $|·|, \sqrt{}, +, -, \times, /, \sup, \inf, \ldots$

$p(x) := \partial_4 \Delta x$
$q(x) := 4x_1 \Delta x$
$r(x) := p(x) / \sqrt{q(x)}$

$l(x) := -\frac{\pi}{2} + 1.6294 - 0.2213 (\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0) + 0.913 (\sqrt{x_4} - 2.52) + 0.728 (\sqrt{x_1} - 2.0)$
A “Simple” Example

In the computational part:

- Transcendental functions $\mathcal{T}$: composition of semialgebraic functions with $\arctan$, $\exp$, $\sin$, $+$, $-$, $\times$, $\ldots$
A “Simple” Example

In the computational part:

- Feasible set $K := [4, 6.3504]^3 \times [6.3504, 8] \times [4, 6.3504]^2$

Lemma_9922699028 from Flyspeck:

$$\forall x \in K, \arctan\left(\frac{p(x)}{\sqrt{q(x)}}\right) + l(x) \geq 0$$
Existing Formal Frameworks

Formal proofs for Global Optimization:

- Bernstein polynomial methods [Zumkeller’s PhD 08]
- SMT methods [Gao et al. 12]
- Interval analysis and Sums of squares
Existing Formal Frameworks

Interval analysis

- Certified interval arithmetic in COQ [Melquiond 12]

- Taylor methods in HOL Light [Solovyev thesis 13]
  - Formal verification of floating-point operations

- robust but subject to the *Curse of Dimensionality*
Existing Formal Frameworks

Lemma from Flyspeck:

\[ \forall x \in K, \arctan\left(\frac{\partial_4 \Delta x}{\sqrt{4x_1 \Delta x}}\right) + l(x) \geq 0 \]

- Dependency issue using Interval Calculus:
  - One can bound \( \partial_4 \Delta x / \sqrt{4x_1 \Delta x} \) and \( l(x) \) separately
  - Too coarse lower bound: \(-0.87\)

- Subdivide \( K \) to prove the inequality

\[ K = \Rightarrow K_0 \quad K_1 \quad K_2 \quad K_3 \quad K_4 \]
Existing Formal Frameworks

Sums of squares techniques

- Formalized in HOL-LIGHT [Harrison 07] COQ [Besson 07]
- Precise methods but scalability and robustness issues (numerical)
- powerful: global optimality certificates without branching
- not so robust: handles moderate size problems
- Restricted to polynomials
Existing Formal Frameworks

Approximation theory: Chebyshev/Taylor models
- mandatory for non-polynomial problems
- hard to combine with SOS techniques (degree of approximation)
Existing Formal Frameworks

Can we develop a new approach with both keeping the respective strength of interval and precision of SOS?

Proving Flyspeck Inequalities is challenging: medium-size and tight
New Framework (in my PhD thesis)

- Certificates for lower bounds of Nonlinear optimization using:
  - Moment-SOS hierarchies
  - Maxplus approximation (Optimal Control)
- Verification of these certificates inside COQ
New Framework (in my PhD thesis)

Software Implementation NLCertify:

- https://forge.ocamlcore.org/projects/nl-certify/

- 15 000 lines of OCAML code

- 4000 lines of COQ code
Introduction

**Moment-SOS relaxations**

Semialgebraic Maxplus Optimization

Formal Nonlinear Optimization

Approximating Pareto curves

Polynomial image of semialgebraic sets

Program Analysis with Polynomial Templates

Conclusion
Polynomial Optimization Problems

- Semialgebraic set $K := \{ x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_m(x) \geq 0 \}$

- $p^* := \min_{x \in K} p(x)$: NP hard

- Sums of squares $\Sigma[x]$  
  e.g. $x_1^2 - 2x_1x_2 + x_2^2 = (x_1 - x_2)^2$

- $Q(K) := \left\{ \sigma_0(x) + \sum_{j=1}^m \sigma_j(x)g_j(x), \text{ with } \sigma_j \in \Sigma[x] \right\}$
The set $K$ is compact and the polynomial $N - \|x\|_2^2$ belongs to $Q(K)$ for some $N > 0$.

- Assume that $K$ is a box: product of closed intervals

- Normalize the feasibility set to get $K' := [-1, 1]^n$
  
  $K' := \{x \in \mathbb{R}^n : g_1 := 1 - x_1^2 \geq 0, \ldots, g_n := 1 - x_n^2 \geq 0\}$

- $n - \|x\|_2^2$ belongs to $Q(K')$
Convexification and the K Moment Problem

- Borel $\sigma$-algebra $\mathcal{B}$ (generated by the open sets of $\mathbb{R}^n$)

- $\mathcal{M}_+(K)$: set of probability measures supported on $K$. If $\mu \in \mathcal{M}_+(K)$ then
  1. $\mu : \mathcal{B} \to [0, 1], \mu(\emptyset) = 0, \mu(\mathbb{R}^n) < \infty$
  2. $\mu(\bigcup_i B_i) = \sum_i \mu(B_i)$, for any countable $(B_i) \subset \mathcal{B}$
  3. $\int_K \mu(dx) = 1$

- \text{supp}(\mu) is the smallest set $K$ such that $\mu(\mathbb{R}^n \setminus K) = 0$
Convexification and the K Moment Problem

\[ p^* = \inf_{x \in K} p(x) = \inf_{\mu \in \mathcal{M}_+(K)} \int_K p \, d\mu \]
Let \((x^\alpha)_{\alpha \in \mathbb{N}^n}\) be the monomial basis

**Definition**

A sequence \(y\) has a representing measure on \(K\) if there exists a finite measure \(\mu\) supported on \(K\) such that

\[
y_\alpha = \int_K x^\alpha \mu(dx), \quad \forall \alpha \in \mathbb{N}^n.
\]
Convexification and the K Moment Problem

$L_y(q) : q \in \mathbb{R}[x] \mapsto \sum_{\alpha} q_{\alpha} y_{\alpha}$

**Theorem [Putinar 93]**

Let $K$ be compact and $Q(K)$ be Archimedean. Then $y$ has a representing measure on $K$

iff

$L_y(\sigma) \geq 0$, $L_y(g_j \sigma) \geq 0$, $\forall \sigma \in \Sigma[x]$.
Lasserre’s Hierarchy of SDP relaxations

- Moment matrix
  \[ M(y)_{u,v} := L_y(u \cdot v), \ u, v \text{ monomials} \]

- Localizing matrix \( M(g_j y) \) associated with \( g_j \)
  \[ M(g_j y)_{u,v} := L_y(u \cdot v \cdot g_j), \ u, v \text{ monomials} \]
Lasserre’s Hierarchy of SDP relaxations

- $M_k(y)$ contains $\binom{n+2k}{n}$ variables, has size $\binom{n+k}{n}$

- Truncated matrix of order $k = 2$ with variables $x_1, x_2$:

$$
M_2(y) = \begin{pmatrix}
1 & x_1 & x_2 & x_1^2 & x_1x_2 & x_2^2 \\
1 & y_{1,0} & y_{0,1} & y_{2,0} & y_{1,1} & y_{0,2} \\
x_1 & y_{1,0} & y_{2,0} & y_{1,1} & y_{3,0} & y_{2,1} & y_{1,2} \\
x_2 & y_{0,1} & y_{1,1} & y_{0,2} & y_{2,1} & y_{1,2} & y_{0,3} \\
x_1^2 & y_{2,0} & y_{3,0} & y_{2,1} & y_{4,0} & y_{3,1} & y_{2,2} \\
x_1x_2 & y_{1,1} & y_{2,1} & y_{1,2} & y_{3,1} & y_{2,2} & y_{1,3} \\
x_2^2 & y_{0,2} & y_{1,2} & y_{0,3} & y_{2,2} & y_{1,3} & y_{0,4}
\end{pmatrix}
$$
Consider $g_1(x) := 2 - x_1^2 - x_2^2$. Then $v_1 = \lceil \deg g_1 / 2 \rceil = 1$.

$$
M_1(g_1 y) = x_1 \begin{pmatrix} 1 \\ 2 - y_{2,0} - y_{0,2} \\ 2y_{1,0} - y_{3,0} - y_{1,2} \\ 2y_{0,1} - y_{2,1} - y_{0,3} \end{pmatrix} x_1 \begin{pmatrix} x_1 \\ 2y_{1,0} - y_{3,0} - y_{1,2} \\ 2y_{2,0} - y_{4,0} - y_{2,2} \\ 2y_{1,1} - y_{3,1} - y_{1,3} \end{pmatrix} x_2 \begin{pmatrix} x_2 \\ 2y_{0,1} - y_{2,1} - y_{0,3} \\ 2y_{1,1} - y_{3,1} - y_{1,3} \\ 2y_{0,2} - y_{2,2} - y_{0,4} \end{pmatrix} x_2
$$

$$
M_1(g_1 y)(3, 3) = L(g_1(x) \cdot x_2 \cdot x_2) = L(2x_2^2 - x_1^2 x_2^2 - x_2^4)
$$

$$
= 2y_{0,2} - y_{2,2} - y_{0,4}
$$
Lasserre’s Hierarchy of SDP relaxations

- Truncation with moments of order at most $2k$

- $v_j := \lceil \deg g_j / 2 \rceil$

Hierarchy of semidefinite relaxations:

\[
\begin{align*}
\inf_y L_y(p) &= \sum_{\alpha} \int_K p_\alpha x^\alpha \, \mu(dx) = \sum_{\alpha} p_\alpha y_\alpha \\
M_k(y) &\succeq 0, \\
M_{k-v_j}(g_j y) &\succeq 0, \quad 1 \leq j \leq m, \\
y_1 &= 1.
\end{align*}
\]
Semidefinite Optimization

- $F_0, F_\alpha$ symmetric real matrices, cost vector $c$

Primal-dual pair of semidefinite programs:

\[
\begin{align*}
\mathcal{P} : & \quad \inf_y \sum_\alpha c_\alpha y_\alpha \\
& \quad \text{s.t.} \quad \sum_\alpha F_\alpha y_\alpha - F_0 \succeq 0
\end{align*}
\]

\[
\begin{align*}
\mathcal{D} : & \quad \sup_Y \text{Trace } (F_0 Y) \\
& \quad \text{s.t.} \quad \text{Trace } (F_\alpha Y) = c_\alpha, \quad Y \succeq 0.
\end{align*}
\]

- Freely available SDP solvers (CSDP, SDPA, SEDUMI)
\( \mathcal{M}_+(K) \): space of probability measures supported on \( K \)

**Polynomial Optimization Problems (POP)**

\[
\begin{align*}
\text{(Primal)} & \quad \inf \int_K p \, d\mu \\
\text{s.t.} & \quad \mu \in \mathcal{M}_+(K)
\end{align*}
\]

\[
\begin{align*}
\text{(Dual)} & \quad \sup \lambda \\
\text{s.t.} & \quad \lambda \in \mathbb{R}, \\
& \quad p - \lambda \in Q(K)
\end{align*}
\]
Truncated quadratic module $Q_k(K) := Q(K) \cap \mathbb{R}_{2k}[x]$

For large enough $k$, zero duality gap [Lasserre 01]:

Polynomial Optimization Problems (POP)

\[
\begin{align*}
\inf_{\alpha} \sum_{\alpha} p_{\alpha} y_\alpha &= \sup \lambda \\
\text{s.t.} \quad M_{k-v_j}(g_j y) \succeq 0, \quad 0 \leq j \leq m, &\quad \text{s.t.} \quad \lambda \in \mathbb{R}, \\
y_1 &= 1 &\quad p - \lambda \in Q_k(K)
\end{align*}
\]
Practical Computation

- Hierarchy of SOS relaxations:
  \[ \lambda_k := \sup_{\lambda} \left\{ \lambda : p - \lambda \in Q_k(K) \right\} \]

- Convergence guarantees \( \lambda_k \uparrow p^* \) [Lasserre 01]

- If \( p - p^* \in Q_k(K) \) for some \( k \) then:
  \[ y^* := (1, x_1^*, x_2^*, (x_1^*)^2, x_1^*x_2^*, \ldots, (x_1^*)^{2k}, \ldots, (x_n^*)^{2k}) \]
  is a global minimizer of the primal SDP [Lasserre 01].
Caprasse Problem

\[ \forall x \in [-0.5, 0.5]^4, \quad -x_1 x_3^3 + 4x_2 x_3^2 x_4 + 4x_1 x_3 x_4^2 + 2x_2 x_4^3 + 4x_1 x_3 + 4x_2^2 - 10x_2 x_4 - 10x_4^2 + 5.1801 \geq 0. \]

scale_pol = true: scaled on \([0, 1]^4\)

relax_order = 2: SOS of degree at most 4

bound_squares_variables = true:
redundant constraints \(x_1^2 \leq 1, \ldots, x_4^2 \leq 1\)
The “No Free Lunch” Rule

- Exponential dependency in
  1. Relaxation order $k$ (SOS degree)
  2. number of variables $n$

- Computing $\lambda_k$ involves $\binom{n+2k}{n}$ variables

- At fixed $k$, $O(n^{2k})$ variables
Example from Flyspeck

\[ K := [4, 6.3504]^6 \]
\[
\Delta(x) = x_1 x_4 (-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) \\
+ x_2 x_5 (x_1 - x_2 + x_3 + x_4 - x_5 + x_6) \\
+ x_3 x_6 (x_1 + x_2 - x_3 + x_4 + x_5 - x_6) \\
- x_2 (x_3 x_4 + x_1 x_6) - x_5 (x_1 x_3 + x_4 x_6)
\]
\[
\partial_4 \Delta x = x_1 (-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) + x_2 x_5 + x_3 x_6 - x_2 x_3 - x_5 x_6
\]
\[
p(x) = \partial_4 \Delta x, \quad q(x) := 4 x_1 \Delta x
\]

\[
f^*_{sa} := \inf_{x \in K} \frac{p(x)}{\sqrt{q(x)}}
\]
Semialgebraic Extension [Lasserre-Putinar 10]

Example from Flyspeck:

\[ z_1 := \sqrt{q(x)}, \]
\[ m_1 \leq \inf_{x \in K} z_1(x), \quad M_1 \geq \sup_{x \in K} z_1(x), \]
\[ \hat{K} := \{(x, z) \in \mathbb{R}^8 : x \in K, h_1(x, z) \geq 0, \ldots, h_6(x, z) \geq 0\} \]
\[ h_1 := z_1 - m_1 \quad h_4 := -z_1^2 + q(x) \]
\[ h_2 := M_1 - z_1 \quad h_5 := z_2z_1 - p(x) \]
\[ h_3 := z_1^2 - q(x) \quad h_6 := -z_2z_1 + p(x) \]

\[ f_{sa}^* := \inf_{(x,z) \in \hat{K}} z_2 \text{ and SOS yields } \lambda_2 = -0.618 < \lambda_3 = -0.445. \]
Introduction

Moment-SOS relaxations

**Semialgebraic Maxplus Optimization**

Formal Nonlinear Optimization

Approximating Pareto curves

Polynomial image of semialgebraic sets

Program Analysis with Polynomial Templates

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

- $f$ is underestimated by a semialgebraic function $f_{sa}$

- Reduce the problem $f_{sa}^* := \inf_{x \in K} f_{sa}(x)$ to a polynomial optimization problem (POP)
Maxplus Approximation

- Initially introduced to solve Optimal Control Problems [Fleming-McEneaney 00]

- **Curse of dimensionality** reduction [McEaneney Kluberg, Gaubert-McEneaney-Qu 11, Qu 13]. Allowed to solve instances of dim up to 15 (inaccessible by grid methods)

- In our context: approximate **transcendental** functions
Maxplus Approximation

Definition

Let $\gamma \geq 0$. A function $\phi : \mathbb{R}^n \to \mathbb{R}$ is said to be $\gamma$-semiconvex if the function $x \mapsto \phi(x) + \frac{\gamma}{2} \|x\|_2^2$ is convex.
Nonlinear Function Representation

Exact parsimonious maxplus representations

\[ y \quad a \]
Nonlinear Function Representation

Exact parsimonious maxplus representations

\[ y \]

\[ a \]
Abstract syntax tree representations of multivariate transcendental functions:

- leaves are **semialgebraic** functions of $A$

- nodes are univariate functions of $D$ or binary operations
For the “Simple” Example from Flyspeck:
Maxplus Optimization Algorithm

First iteration:

1 control point \( \{a_1\} \): \( m_1 = -4.7 \times 10^{-3} < 0 \)
Second iteration:

\[ l(x) + \arctan r(x) \]

2 control points \( \{a_1, a_2\} \): \( m_2 = -6.1 \times 10^{-5} < 0 \)
Maxplus Optimization Algorithm

Third iteration:

3 control points \( \{a_1, a_2, a_3\} \): \( m_3 = 4.1 \times 10^{-6} > 0 \)

OK!
Maxplus Optimization Algorithm

Input: tree $t$, box $K$, SOS relaxation order $k$, precision $p$
Output: bounds $m$ and $M$, approximations $t_2^-$ and $t_2^+$

1. if $t \in \mathcal{A}$ then $t^- := t$, $t^+ := t$
2. else if $u := \text{root}(t) \in D$ with child $c$ then
3. \hspace{1em} $m_c, M_c, c^-, c^+ := \text{samp}_\text{approx}(c, K, k, p)$
4. \hspace{1em} $I := [m_c, M_c]$
5. \hspace{1em} $u^-, u^+ := \text{unary}_\text{approx}(u, I, c, p)$
6. \hspace{1em} $t^-, t^+ := \text{compose}_\text{approx}(u, u^-, u^+, I, c^-, c^+)$
7. else if $bop := \text{root}(t)$ with children $c_1$ and $c_2$ then
8. \hspace{1em} $m_i, M_i, c_i^-, c_i^+ := \text{samp}_\text{approx}(c_i, K, k, p)$ for $i \in \{1, 2\}$
9. \hspace{1em} $t^-, t^+ := \text{compose}_\text{bop}(c_1^-, c_1^+, c_2^-, c_2^+, bop, [m_2, M_2])$
10. end
11. return $\text{min}_\text{sa}(t^-, K, k), \text{max}_\text{sa}(t^+, K, k), t^-, t^+$
The precision is an integer $d$

The best-uniform degree-$d$ polynomial approximation of $u$:

$$\min_{h \in \mathbb{R}_d[x]} \|u - h\|_{\infty} = \min_{h \in \mathbb{R}_d[x]} \left( \sup_{x \in I} |u(x) - h(x)| \right)$$

Implementation in Sollya [Chevillard-Joldes-Lauter 10]

Interface of NLCertify with Sollya
SWF: $\min_{x \in [1,500]^n} f(x) = - \sum_{i=1}^{n} x_i \sin(\sqrt{x_i})$

- replace $\sin(\sqrt{\cdot})$ by a degree-$d$ Chebyshev polynomial
- Hard to combine with SOS
High-degree Polynomial Approximation + SOS

Indeed:

- Small $d$: lack of accuracy $\implies$ expensive Branch and Bound

- Large $d$: “No free lunch” rule with $\binom{n+d}{n}$ SDP variables
SWF with $n = 10, d = 4$:

- 38 min to compute a lower bound of $-430n$
Comparison on Global Optimization Problems

\[
\min_{x \in [1,500]^n} f(x) = - \sum_{i=1}^{n} x_i \sin(\sqrt{x_i}) \quad \text{Interval Arithmetic for sin + SOS}
\]

\[
f^* \lesssim -418.9n
\]

<table>
<thead>
<tr>
<th>( n )</th>
<th>lower bound</th>
<th>( n_{\text{lifting}} )</th>
<th>#boxes</th>
<th>time</th>
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<tbody>
<tr>
<td>10</td>
<td>(-430n)</td>
<td>0</td>
<td>3830</td>
<td>129 s</td>
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<td>&gt; 10 h</td>
</tr>
<tr>
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<td>2n</td>
<td>274</td>
<td>1.9 h</td>
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Comparison on Global Optimization Problems

\[ \min_{x \in [1,500]^n} f(x) = -\sum_{i=1}^{n} x_i \sin(\sqrt{x_i}) \]

\[ f^* \lesssim -418.9n \]

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Comparison on Global Optimization Problems

\[
\min_{x \in [1,500]^n} f(x) = - \sum_{i=1}^{n-1} (x_i + x_{i+1}) \sin(\sqrt{x_i})
\]

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<td>1000</td>
<td>(-967n)</td>
<td>2( n )</td>
<td>1</td>
<td>543 s</td>
</tr>
<tr>
<td>1000</td>
<td>(-968n)</td>
<td>( n )</td>
<td>1</td>
<td>272 s</td>
</tr>
</tbody>
</table>
Comparison on Global Optimization Problems

\[
\min_{x \in [1,500]^n} f(x) = -\sum_{i=1}^{n-1} (x_i + x_{i+1}) \sin(\sqrt{x_i})
\]

<table>
<thead>
<tr>
<th>( n )</th>
<th>lower bound</th>
<th>( n_{\text{lifting}} )</th>
<th>#boxes</th>
<th>time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>(-967n)</td>
<td>(2n)</td>
<td>1</td>
<td>543 s</td>
</tr>
<tr>
<td>1000</td>
<td>(-968n)</td>
<td>(n)</td>
<td>1</td>
<td>272 s</td>
</tr>
</tbody>
</table>
Convergence of the Optimization Algorithm

- Let $f$ be a multivariate transcendental function
- Let $t_p^-$ be the underestimator of $f$, obtained at precision $p$
- Let $x_{opt}^p$ be a minimizer of $t_p^-$ over $K$

Theorem [X. Allamigeon S. Gaubert VM B. Werner 13]

Every accumulation point of the sequence $(x_{opt}^p)$ is a global minimizer of $f$ on $K$.

Ingredients of the proof:
- Convergence of Lasserre SOS hierarchy
- Uniform approximation schemes (Maxplus/Minimax)
Polynomial Approximations for Semialgebraic Functions

- Inspired from [Lasserre - Thanh 13]
- Let $f_{sa} \in \mathcal{A}$ defined on a box $K \subset \mathbb{R}^n$
- Let $\mu_n$ be the standard Lebesgue measure on $\mathbb{R}^n$
- Best polynomial underestimator $h \in \mathbb{R}_d[x]$ of $f_{sa}$ for the $L_1$ norm:

$$\left( P^{sa} \right) \left\{ \begin{array}{l}
\min_{h \in \mathbb{R}_d[x]} \int_K (f_{sa} - h) d\mu_n \\
\text{s.t. } f_{sa} - h \geq 0 \text{ on } K.
\end{array} \right.$$ 

**Lemma**

Problem $(P^{sa})$ has a degree-$d$ polynomial minimizer $h_d$. 

---

V. Magron

New Applications of Moment-SOS Hierarchies

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Polynomial Approximations for Semialgebraic Functions

- b.s.a.l. $\hat{K} := \{(x, z) \in \mathbb{R}^{n+p} : g_1(x, z) \geq 0, \ldots, g_m(x, z) \geq 0\}$
- The quadratic module $\mathcal{M}(\hat{K})$ is Archimedean
- The optimal solution $h_d$ of $(P_{sa})$ is a maximizer of:

\[
(P_d) \begin{cases} 
\max_{h \in \mathbb{R}_d[x]} & \int_{[0,1]^n} h \, d\mu_n \\
\text{s.t.} & (z_p - h) \in \mathcal{M}(\hat{K}) 
\end{cases}
\]
Polynomial Approximations for Semialgebraic Functions

- Let $m_d$ be the optimal value of Problem $(P^{sa})$
- Let $h_{dk}$ be a maximizer of the SOS relaxation of $(P_d)$

**Convergence of the SOS Hierarchy**

The sequence $\left( \|f_{sa} - h_{dk}\|_1 \right)_{k \geq k_0}$ is non-increasing and converges to $m_d$. Each accumulation point of the sequence $(h_{dk})_{k \geq k_0}$ is an optimal solution of Problem $(P^{sa})$. 
Polynomial Approximations for Semialgebraic Functions

\[ f_{sa}(x) := \frac{\partial_4 \Delta x}{\sqrt{4x_1 \Delta x}} \]

<table>
<thead>
<tr>
<th>(d)</th>
<th>(k)</th>
<th>Upper bound of (|f_{sa} - h_{dk}|_1)</th>
<th>Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>0.8024</td>
<td>-1.171</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.3709</td>
<td>-0.4479</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>1.617</td>
<td>-1.056</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.1766</td>
<td>-0.4493</td>
</tr>
</tbody>
</table>
Polynomial Approximations for Semialgebraic Functions

\[ \text{rad}^2 : (x_1, x_2) \mapsto \frac{-64x_1^2 + 128x_1x_2 + 1024x_1 - 64x_2^2 + 1024x_2 - 4096}{-8x_1^2 + 8x_1x_2 + 128x_1 - 8x_2^2 + 128x_2 - 512} \]

- Linear and quadratic underestimators for \( \text{rad}^2 \) \((k = 3)\):
Polynomial Approximations for Semialgebraic Functions

\[ \text{rad}_2 : (x_1, x_2) \mapsto \frac{-64x_1^2 + 128x_1x_2 + 1024x_1 - 64x_2^2 + 1024x_2 - 4096}{-8x_1^2 + 8x_1x_2 + 128x_1 - 8x_2^2 + 128x_2 - 512} \]

- Linear and quadratic underestimators for \( \text{rad}_2 \) \((k = 3)\):
Contributions

Published:


In revision:

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**Formal Nonlinear Optimization**

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The General “Formal Framework”

- We check the correctness of SOS certificates for POP.
- We build certificates to prove interval bounds for *semialgebraic* functions.
- We bound formally *transcendental* functions with *semialgebraic* approximations.
Formal SOS bounds

When $q \in \mathcal{Q}(K)$, $\sigma_0, \ldots, \sigma_m$ is a positivity certificate for $q$

Check symbolic polynomial equalities $q = q'$ in COQ

- Existing tactic `ring` [Grégoire-Mahboubi 05]

- Polynomials coefficients: arbitrary-size rationals `bigQ` [Grégoire-Théry 06]

- Much simpler to verify certificates using sceptical approach

- Extends also to semialgebraic functions
Checking Polynomial Equalities: \texttt{ring} tactic

- Sparse Horner normal form

\begin{verbatim}
Inductive PolC : Type :=
  | Pc : bigQ \to PolC
  | Pinj : positive \to PolC \to PolC
  | PX : PolC \to positive \to PolC \to PolC.
\end{verbatim}

- \((Pc \ c)\) for constant polynomials

- \((Pinj \ i \ p)\) shifts the index of \(i\) in the variables of \(p\)

- \((PX \ p \ j \ q)\) evaluates to \(p x_1^j + q(x_2, \ldots, x_n)\)

- Encoding SOS certificates with Sparse Horner polynomials
Bounding the Polynomial Remainder

- Normalized POP \( (x \in [0, 1]^n) \)

\[
\epsilon_{\text{pop}}(x) := p(x) - \lambda_k - \sum_{j=0}^{m} \sigma_j(x)g_j(x)
\]

- \( \forall x \in [0, 1]^n, \epsilon_{\text{pop}}(x) \geq \epsilon_{\text{pop}}^* := \sum_{\epsilon_\alpha \leq 0} \epsilon_\alpha \)
Formal SOS Results

- **POP1**: $\forall x \in K, \partial_4 \Delta x \geq -41$.

- **POP2**: $\forall x \in K, \Delta x \geq 0$.

<table>
<thead>
<tr>
<th>Problem</th>
<th>$n$</th>
<th>NLCertify</th>
<th>micromega [Besson 07]</th>
</tr>
</thead>
<tbody>
<tr>
<td>POP1</td>
<td>6</td>
<td>0.08 s</td>
<td>9.00 s</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.09 s</td>
<td>0.36 s</td>
</tr>
<tr>
<td>POP2</td>
<td>3</td>
<td>0.39 s</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>13.2 s</td>
<td>–</td>
</tr>
</tbody>
</table>

Sparse SOS relaxations $\implies$ Speedup
Benchmarks for Flyspeck Inequalities

<table>
<thead>
<tr>
<th>Inequality</th>
<th>#boxes</th>
<th>Time</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>9922699028</td>
<td>39</td>
<td>190 s</td>
<td>2218 s</td>
</tr>
<tr>
<td>3318775219</td>
<td>338</td>
<td>1560 s</td>
<td>19136 s</td>
</tr>
</tbody>
</table>

- Comparable with Taylor interval methods in HOL-LIGHT [Hales-Solovyev 13]

- **No free lunch:** SDP informal bottleneck

- 22 times slower than SDP: $q = q'$ formal bottleneck
Contribution

For more details on the formal side:

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Conclusion
Let \( f_1, f_2 \in \mathbb{R}_d[x] \) two conflicting criteria

Let \( S := \{ x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_m(x) \geq 0 \} \) a semialgebraic set

\[
(P) \left\{ \min_{x \in S} (f_1(x) f_2(x))^\top \right\}
\]

**Assumption**

The image space \( \mathbb{R}^2 \) is partially ordered in a natural way (\( \mathbb{R}_+^2 \) is the ordering cone).
Bicriteria Optimization Problems

\[\begin{align*}
g_1 &:= -(x_1 - 2)^3/2 - x_2 + 2.5 , \\
g_2 &:= -x_1 - x_2 + 8(-x_1 + x_2 + 0.65)^2 + 3.85 , \\
S &:= \{x \in \mathbb{R}^2 : g_1(x) \geq 0, g_2(x) \geq 0\} . \\
f_1 &:= (x_1 + x_2 - 7.5)^2/4 + (-x_1 + x_2 + 3)^2 , \\
f_2 &:= (x_1 - 1)^2/4 + (x_2 - 4)^2/4 .
\end{align*}\]
Parametric sublevel set approximation

Inspired by previous research on multiobjective linear optimization [Gorissen-den Hertog 12]

Workaround: reduce $P$ to a parametric POP

$$(P_\lambda) : \quad f^*(\lambda) := \min_{x \in S} \{ f_2(x) : f_1(x) \leq \lambda \} ,$$
A Hierarchy of Polynomial underestimators

Moment-SOS approach [Lasserre 10]:

\[
(D_d) \left\{ \begin{array}{l}
\max_{q \in \mathbb{R}_{2d}[\lambda]} \sum_{k=0}^{2d} q_k / (1 + k) \\
\text{s.t. } f_2(x) - q(\lambda) \in Q_{2d}(K).
\end{array} \right.
\]

- The hierarchy \((D_d)\) provides a sequence \((q_d)\) of polynomial underestimators of \(f^*(\lambda)\).

- \(\lim_{d \to \infty} \int_0^1 (f^*(\lambda) - q_d(\lambda)) d\lambda = 0\)
A Hierarchy of Polynomial underestimators

Degree 4
A Hierarchy of Polynomial underestimators

Degree 6
A Hierarchy of Polynomial underestimators

Degree 8
Contributions

- Numerical schemes that avoid computing finitely many points.

- Pareto curve approximation with polynomials, convergence guarantees in $L_1$-norm

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Approximation of sets defined with “∃”

Let $\mathbf{B} \subset \mathbb{R}^m$ be the unit ball and assume that $\mathbf{F} = f(\mathbf{S}) \subseteq \mathbf{B}$.

- Another point of view:

$$F = \{\mathbf{y} \in \mathbf{B} : \exists \mathbf{x} \in \mathbf{S} \text{ s.t. } h(\mathbf{x}, \mathbf{y}) \geq 0\} ,$$

with

$$h_f(\mathbf{x}, \mathbf{y}) := -\|\mathbf{y} - f(\mathbf{x})\|_2^2 .$$

- Approximate $\mathbf{F}$ as closely as desired by a sequence of sets of the form:

$$F_k := \{\mathbf{y} \in \mathbf{B} : q_k(\mathbf{y}) \geq 0\} ,$$

for some polynomials $q_k \in \mathbb{R}_{2k}[\mathbf{y}]$. 
A hierarchy of outer approximations of \( f(S) \)

- Let \( K = S \times B, g_0 := 1 \) and \( Q_k(K) \) be the \( k \)-truncated quadratic module generated by \( g_0, \ldots, g_m \):

\[
Q_k(K) = \left\{ \sum_{l=0}^{m} \sigma_l(x, y)g_l(x), \text{ with } \sigma_l \in \Sigma_{k-v_l}[x, y] \right\}
\]

- Define \( h(y) := \sup_{x \in S} h(x, y) \)

- Hierarchy of Semidefinite programs:

\[
\rho_k := \min_{q \in \mathbb{R}_{2k}[y], \sigma_l} \left\{ \int_B (q - h)dy : q - h_f \in Q_k(K) \right\}
\]

Yet another SOS program with an optimal solution \( q_k \in \mathbb{R}_{2k}[y] \)!
A hierarchy of outer approximations of \( f(S) \)

From the definition of \( q_k \), the sublevel sets

\[
F_k := \{ y \in B : q_k(y) \leq 0 \} \supseteq F ,
\]

provide a sequence of certified outer approximations of \( F \).

It comes from the following:

\[
\forall (x, y) \in K, q_k(y) \geq h_f(x, y) \iff \forall y, q_k(y) \geq h(y) .
\]
Strong convergence property

**Theorem**

1. The sequence of underestimators $(q_k)_{k \geq k_0}$ converges to $h$ w.r.t the $L_1(B)$-norm:

$$\lim_{k \to \infty} \int_{B} |q_k - h| dy = 0.$$
Strong convergence property

**Theorem**

1. The sequence of underestimators \((q_k)_{k \geq k_0}\) converges to \(h\) w.r.t the \(L_1(B)\)-norm:

\[
\lim_{k \to \infty} \int_B |q_k - h| \, dy = 0.
\]

2. \[
\lim_{k \to \infty} \text{vol}(F_k \setminus F) = 0.
\]
Approximation for polynomial image of semialgebraic sets

Image of the unit ball $S := \{x \in \mathbb{R}^2 : \|x\|_2^2 \leq 1\}$ by

$$f(x) := \left( x_1 + x_1 x_2, x_2 - x_1^3 \right) / 2$$
Approximation for polynomial image of semialgebraic sets

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$$f(x) := \left( x_1 + x_1 x_2, x_2 - x_1^3 \right) / 2$$
Semialgebraic set projections

\[ f(x) = (x_1, x_2): \text{projection on } \mathbb{R}^2 \text{ of the semialgebraic set} \]

\[ S := \{ x \in \mathbb{R}^3 : \|x\|^2_2 \leq 1, 1/4 - (x_1 + 1/2)^2 - x_2^2 \geq 0, \]

\[ 1/9 - (x_1 - 1/2)^4 - x_2^4 \geq 0 \} \]

Graphical representation of the semialgebraic set projection.
Semialgebraic set projections

\[ f(x) = (x_1, x_2): \text{projection on } \mathbb{R}^2 \text{ of the semialgebraic set} \]

\[ S := \{ x \in \mathbb{R}^3 : \|x\|_2^2 \leq 1, 1/4 - (x_1 + 1/2)^2 - x_2^2 \geq 0, \\
1/9 - (x_1 - 1/2)^4 - x_2^4 \geq 0 \} \]
Semialgebraic set projections

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\[ 1/9 - (x_1 - 1/2)^4 - x_2^4 \geq 0 \} \]
Support function of a closed convex set

Assume that $F$ is strictly convex

- Let $q := \sup_{x \in F} \{b^\top x\}$ be the support function of $F$
- $q$ is degree-1 positive homogeneous, subadditive
- One can show that $f = \nabla q$
- For a convex homogeneous $\tilde{q}$, let $q(x) := \|x\| \tilde{q}(\frac{x}{\|x\|})$
- One can show that $\nabla q(x) = \nabla \tilde{q}(x)$, for each $x \in S^{n-1}$
Support function of a closed convex set

\[ \tilde{q}(x) := x_1^4 + x_2^4 + 2x_1^2x_2^2 + 7/2(x_1^2 + x_2^2) - (x_1x_2 + x_1 + x_2) \]
Support function of a closed convex set

\[ \tilde{q}(x) := x_1^4 + x_2^4 + 2x_1^2x_2^2 + \frac{7}{2}(x_1^2 + x_2^2) - (x_1x_2 + x_1 + x_2) \]
Approximating Pareto curves

Back our previous nonconvex example:
Approximating Pareto curves

Back our previous nonconvex example:

\[ F_2 \]
Approximating Pareto curves

Back our previous nonconvex example:
Approximating Pareto curves

“Zoom” on the region which is hard to approximate:

![Graph showing a Pareto curve with a zoomed-in view of a specific region.

$F_4$}
Approximating Pareto curves

“Zoom” on the region which is hard to approximate:
Semialgebraic image of semialgebraic sets

Image of the unit ball $\mathbf{S} := \{ \mathbf{x} \in \mathbb{R}^2 : \| \mathbf{x} \|_2^2 \leq 1 \}$ by

$$f(\mathbf{x}) := (\min(x_1 + x_1 x_2, x_1^2), x_2 - x_1^3)/3$$
Image of the unit ball $S := \{ x \in \mathbb{R}^2 : \|x\|_2^2 \leq 1 \}$ by

$$f(x) := \left( \min(x_1 + x_1x_2, x_1^2), x_2 - x_1^3 \right) / 3$$
Semialgebraic image of semialgebraic sets

Image of the unit ball \( S := \{ x \in \mathbb{R}^2 : \| x \|_2^2 \leq 1 \} \) by

\[
f(x) := \left( \min(x_1 + x_1 x_2, x_1^2), x_2 - x_1^3 \right) / 3
\]
Image of the unit ball $S := \{ x \in \mathbb{R}^2 : \|x\|_2^2 \leq 1 \}$ by

$$f(x) := (\min(x_1 + x_1x_2, x_1^2), x_2 - x_3^3)/3$$
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One-loop with Conditional Branching

- \( r, s, T^i, T^e \in \mathbb{R}[x] \)

- \( x_0 \in X_0 \), with \( X_0 \) semialgebraic set

```
x = x_0;
while (r(x) \leq 0) {
    if (s(x) \leq 0) {
        x = T^i(x);
    }
    else {
        x = T^e(x);
    }
}
```
Well-representative Templates w.r.t. Properties

Sufficient condition to get **inductive invariant**:

\[
\alpha := \min_{q \in \mathbb{R}[x]} \sup_{x \in X_0} q(x)
\]

s.t. \( q - q \circ T^i \geq 0 \), \( q - q \circ T^e \geq 0 \), \( q - \kappa \geq 0 \).

\[
\bigcup_{k \in \mathbb{N}} X_k \subseteq \{ x \in \mathbb{R}^n : q(x) \leq \alpha \} \subseteq \{ x \in \mathbb{R}^n : \kappa(x) \leq \alpha \}
\]
Bounding Template using SOS

Sufficient condition to get bounding inductive invariant:

\[ \alpha := \min_{q \in \mathbb{R}[x]} \sup_{x \in X_0} q(x) \]

s.t. \[q - q \circ T^i \geq 0,\]
\[q - q \circ T^e \geq 0,\]
\[q - \| \cdot \|_2^2 \geq 0.\]

\[ \bigcup_{k \in \mathbb{N}} X_k \subseteq \{ x \in \mathbb{R}^n : q(x) \leq \alpha \} \subseteq \{ x \in \mathbb{R}^n : \|x\|^2 \leq \alpha \} \]
Bounds for $\bigcup_{k \in \mathbb{N}} X_k$

\[ X_0 := [0.9, 1.1] \times [0, 0.2] \quad r(x) := 1 \quad s(x) := 1 - \|x\|^2 \]

\[ T^i(x) := (x_1^2 + x_2^3, x_1^3 + x_2^2) \quad T^e(x) := \left( \frac{1}{2}x_1^2 + \frac{2}{5}x_2^3, -\frac{3}{5}x_1^3 + \frac{3}{10}x_2^2 \right) \]

$\kappa(x) = \|x\|^2$
Bounds for $\bigcup_{k \in \mathbb{N}} X_k$

$X_0 := [0.9, 1.1] \times [0, 0.2]$ \quad $r(x) := 1$ \quad $s(x) := 1 - \|x\|^2$

$T^i(x) := (x_1^2 + x_2^3, x_1^3 + x_2^2)$ \quad $T^e(x) := \left( \frac{1}{2} x_1^2 + \frac{2}{5} x_2^3, -\frac{3}{5} x_1^3 + \frac{3}{10} x_2^2 \right)$

$\kappa(x) = \|x\|^2$
Bounds for $\bigcup_{k \in \mathbb{N}} X_k$

\[X_0 := [0.9, 1.1] \times [0, 0.2] \quad r(x) := 1 \quad s(x) := 1 - \|x\|^2\]

\[T^i(x) := (x_1^2 + x_2^3, x_1^3 + x_2^2) \quad T^e(x) := \left( \frac{1}{2}x_1^2 + \frac{2}{5}x_2^3, -\frac{3}{5}x_1^3 + \frac{3}{10}x_2^2 \right)\]

\[\kappa(x) = \|x\|^2\]
Does $\bigcup_{k \in \mathbb{N}} X_k$ avoid unsafe region?

$X_0 := [0.5, 0.7]^2$, $r(x) := 1$, $s(x) := \|x^2\|$

$T^i(x) := (x_1^2 + x_2^3, x_1^3 + x_2^2)$, $T^e(x) := (\frac{1}{2}x_1^2 + \frac{2}{5}x_2^3, -\frac{3}{5}x_1^3 + \frac{3}{10}x_2^2)$

$\kappa(x) = \frac{1}{4} - (x_1 + \frac{1}{2})^2 - (x_2 + \frac{1}{2})^2$

Degree 6
Does $\bigcup_{k \in \mathbb{N}} X_k$ avoid unsafe region?

$X_0 := [0.5, 0.7]^2 \quad r(x) := 1 \quad s(x) := \|x^2\|$ 

$T^i(x) := (x_1^2 + x_2^3, x_1^3 + x_2^2) \quad T^e(x) := \left(\frac{1}{2}x_1^2 + \frac{2}{5}x_2^3, -\frac{3}{5}x_1^3 + \frac{3}{10}x_2^2\right)\,$

$\kappa(x) = \frac{1}{4} - (x_1 + \frac{1}{2})^2 - (x_2 + \frac{1}{2})^2$
Does $\bigcup_{k \in \mathbb{N}} X_k$ avoid unsafe region?

$X_0 := [0.5, 0.7]^2 \quad r(x) := 1 \quad s(x) := \|x^2\|

T^i(x) := (x_1^2 + x_2^3, x_1^3 + x_2^2) \quad T^e(x) := (\frac{1}{2}x_1^2 + \frac{2}{5}x_2^3, -\frac{3}{5}x_1^3 + \frac{3}{10}x_2^2)

\kappa(x) = \frac{1}{4} - (x_1 + \frac{1}{2})^2 - (x_2 + \frac{1}{2})^2$
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Conclusion

- Formal nonlinear optimization: NLCertify
- Safe solutions for challenging problems, e.g. Flyspeck
- Approximation of Pareto Curves, images and projections of semialgebraic sets
- Program Analysis with polynomial templates
Conclusion

Further research:

- OCAML API
- Alternative Polynomials bounds using geometric programming (T. de Wolff, S. Iliman)
- COQ tactic
- Improve formal polynomial checker
- Semialgebraic/transcendental program analysis
Conclusion

Further research:

Generalized problem of moments

(Moment) \[
\inf \int_K p_0 \, d\mu \geq \sup \lambda_0 + \sum_i \lambda_i b_i
\]

(s.t.) \[
\int_K p_i \, d\mu \leq b_i
\]

\[
\mu \in \mathcal{M}_+(K)
\]

(SOS) \[
p_0 - \lambda_0 - \sum_i \lambda_i p_i \in \mathcal{Q}_k(K)
\]

Formal bounds using SDP and ring
Conclusion

Further research at IC:

1 Tuning FPGA hardware by performing program analysis
   - Krivine-Handelman representation of positive polynomials

   - Extension using Putinar representations

   - Mixed LP/SOS certificates
Conclusion

Further research at IC:

1. Adapting existing framework in GPU Verification
   - Verification of race/divergence freedom
   - Built in top of Boogie, interface with Z3
   - Recent features to handle nonlinearity
Thank you for your attention!

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