Formal Proofs, Program Analysis and Moment-SOS Relaxations

Victor Magron, Postdoc LAAS-CNRS

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Imperial College Department of Electrical and Electronic Eng.







Formal Proofs, Program Analysis and Moment-SOS Relaxations

- 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, ...)

 Possible workaround: proof assistants COQ (Coquand, Huet 1984)
 HOL-LIGHT (Harrison, Gordon 1980)
 Built in top of OCAML ¹/₁₀

Computer Science and Mathematics

- PhD on Formal Proofs for Global Optimization: Templates and Sums of Squares
- 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.



T. Hales, A Proof of the Kepler Conjecture, 1994.



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

Multivariate Polynomials:

$$\Delta \mathbf{x} := x_1 x_4 (-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) + x_2 x_5 (x_1 - x_2 + x_3 + x_4 - x_5 + x_6) + x_3 x_6 (x_1 + x_2 - x_3 + x_4 + x_5 - x_6) - x_2 (x_3 x_4 + x_1 x_6) - x_5 (x_1 x_3 + x_4 x_6)$$

■ Semialgebraic functions: composition of polynomials with | · |, √, +, -, ×, /, sup, inf, ...

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

$$l(\mathbf{x}) := -\frac{\pi}{2} + 1.6294 - 0.2213 \left(\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0\right) + 0.913 \left(\sqrt{x_4} - 2.52\right) + 0.728 \left(\sqrt{x_1} - 2.0\right)$$

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■ Transcendental functions *T*: composition of semialgebraic functions with arctan, exp, sin, +, -, ×,...

■ Feasible set **K** := [4, 6.3504]³ × [6.3504, 8] × [4, 6.3504]²

Lemma₉₉₂₂₆₉₉₀₂₈ from Flyspeck:

$$\forall \mathbf{x} \in \mathbf{K}, \arctan\left(\frac{p(\mathbf{x})}{\sqrt{q(\mathbf{x})}}\right) + l(\mathbf{x}) \ge 0$$

New Framework (in my PhD thesis)

- Certificates for lower bounds of Global Optimization Problems using SOS and new ingredients in Global Optimization:
 - Maxplus approximation (Optimal Control)
 - Nonlinear templates (Static Analysis)
- Verification of these certificates inside CoQ
- Implementation: NLCertify http://nl-certify.forge.ocamlcore.org/

Introduction

Moment-SOS relaxations and Maxplus approximation

Formal Nonlinear Optimization

Pareto Curves and Images of Semialgebraic Sets

Program Analysis with Polynomial Templates

Conclusion

- Semialgebraic set $\mathbf{K} := \{\mathbf{x} \in \mathbb{R}^n : g_1(\mathbf{x}) \ge 0, \dots, g_m(\mathbf{x}) \ge 0\}$
- $p^* := \min_{\mathbf{x} \in \mathbf{K}} p(\mathbf{x})$: NP hard
- Sums of squares Σ[x]

•
$$\mathcal{Q}(\mathbf{K}) := \left\{ \sigma_0(\mathbf{x}) + \sum_{j=1}^m \sigma_j(\mathbf{x}) g_j(\mathbf{x}), \text{ with } \sigma_j \in \Sigma[\mathbf{x}] \right\}$$

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• $\mathcal{M}_+(\mathbf{K})$: space of probability measures supported on \mathbf{K}



• Truncated quadratic module $Q_k(\mathbf{K}) := Q(\mathbf{K}) \cap \mathbb{R}_{2k}[\mathbf{x}]$



- Hierarchy of SOS relaxations: $\lambda_k := \sup_{\lambda} \{\lambda : p - \lambda \in Q_k(\mathbf{K})\}$
- Convergence guarantees $\lambda_k \uparrow p^*$ [Lasserre 01]
- Can be computed with SOS solvers (CSDP, SDPA)
- Extension to semialgebraic functions $r(\mathbf{x}) = p(\mathbf{x}) / \sqrt{q(\mathbf{x})}$ [Lasserre-Putinar 10]

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- Given **K** a compact set and *f* a transcendental function, bound $f^* = \inf_{\mathbf{x} \in \mathbf{K}} f(\mathbf{x})$ and prove $f^* \ge 0$
 - f is underestimated by a semialgebraic function f_{sa}
 - Reduce the problem *f*^{*}_{sa} := inf_{x∈K}*f*_{sa}(**x**) to a polynomial optimization problem (POP)

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



Nonlinear Function Representation



Nonlinear Function Representation



Abstract syntax tree representations of multivariate transcendental functions:

- leaves are semialgebraic functions of \mathcal{A}
- nodes are univariate functions of *D* or binary operations

Nonlinear Function Representation

• For the "Simple" Example from Flyspeck:



Maxplus Optimization Algorithm



1 1 control point $\{a_1\}$ SOS Computation: $m_1 = -0.746$

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Maxplus Optimization Algorithm



2 2 control points $\{a_1, a_2\}$: $m_2 = -0.112$

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Maxplus Optimization Algorithm



3 3 control points $\{a_1, a_2, a_3\}$: $m_3 = -0.04$

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Contributions

For more details:

- X. Allamigeon, S. Gaubert, V. Magron, and B. Werner. Certification of inequalities involving transcendental functions: combining sdp and max-plus approximation. In *Proceedings of the European Control Conference (ECC) Zurich*, pages 2244-2250, 2013.
- X. Allamigeon, S. Gaubert, V. Magron, and B. Werner. Certification of bounds of non-linear functions: the templates method. In *Proceedings of Conferences on Intelligent Computer Mathematics, CICM Calculemus, Bath,* pages 51-65. LNAI 7961 Springer, 2013.

In revision:

X. Allamigeon, S. Gaubert, V. Magron, and B. Werner. Certification of Real Inequalities – Templates and Sums of Squares. Submitted for publication. arxiv:1403.5899, March 2014

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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 $q \in Q(\mathbf{K})$, σ_0 , ..., σ_m is a positivity certificate for qCheck **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

Benchmarks for Flyspeck Inequalities

т 1%	<i>u</i> 1	1	2
Inequality	#boxes	Time	Time
9922699028	39	190 <i>s</i>	2218 <i>s</i>
3318775219	338	1560 <i>s</i>	19136 <i>s</i>

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



Bottleneck of informal optimizer is SOS solver

22 times slower! \implies Current bottleneck is to check polynomial equalities

Contribution: Publications and Software

For more details:

- X. Allamigeon, S. Gaubert, V. Magron and B. Werner. Formal Proofs for Nonlinear Optimization. Submitted for publication, arxiv:1404.7282
- X. Allamigeon, S. Gaubert, V. Magron, and B. Werner. Certification of bounds of non-linear functions: the templates method. In *Proceedings of Conferences on Intelligent Computer Mathematics, CICM Calculemus, Bath,* pages 51-65. LNAI 7961 Springer, 2013.

Contribution: Publications and Software

Software Implementation NLCertify:

- https://forge.ocamlcore.org/projects/nl-certify/
- 🕅 15 000 lines of OCAML code
 - P
- 4000 lines of COQ code
- V. Magron NLCertify: A Tool for Formal Nonlinear Optimization. To appear in the *Proceedings of the 4th International Congress on Mathematical Software*, ICMS 2014, Séoul, arxiv:1405.5668

- 1 Approximating Pareto curves, image of semialgebraic sets. With people from LAAS-CNRS:
 - Didier Henrion
 - Jean-Bernard Lasserre
- 2 Static analysis. With people from Onera:
 - Assalé Adjé
 - Pierre-Loic Garoche

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Bicriteria Optimization Problems

• Let $f_1, f_2 \in \mathbb{R}_d[\mathbf{x}]$ two conflicting criteria

• Let $\mathbf{S} := {\mathbf{x} \in \mathbb{R}^n : g_1(\mathbf{x}) \ge 0, \dots, g_m(\mathbf{x}) \ge 0}$ a semialgebraic set

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

Assumption

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

Bicriteria Optimization Problems

$$\begin{split} g_1 &:= -(x_1-2)^3/2 - x_2 + 2.5 \ , \\ g_2 &:= -x_1 - x_2 + 8(-x_1 + x_2 + 0.65)^2 + 3.85 \ , \\ \mathbf{S} &:= \{\mathbf{x} \in \mathbb{R}^2 : g_1(\mathbf{x}) \ge 0, \, g_2(\mathbf{x}) \ge 0\} \ . \end{split}$$

$$\begin{split} f_1 &:= (x_1+x_2-7.5)^2/4 + (-x_1+x_2+3)^2 \ , \\ f_2 &:= (x_1-1)^2/4 + (x_2-4)^2/4 \ . \end{split}$$



Parametric sublevel set approximation

- Inspired by previous research on multiobjective linear optimization [Gorissen-den Hertog 12]
- Workaround: reduce **P** to a **parametric POP**

$$(\mathbf{P}_{\lambda}): \quad f^*(\lambda) := \min_{\mathbf{x} \in \mathbf{S}} \left\{ f_2(\mathbf{x}) : f_1(\mathbf{x}) \leqslant \lambda \right\} ,$$

Moment-SOS approach [Lasserre 10]:

$$(D_d) \begin{cases} \max_{q \in \mathbb{R}_{2d}[\lambda]} & \sum_{k=0}^{2d} q_k / (1+k) \\ \text{s.t.} & f_2(\mathbf{x}) - q(\lambda) \in \mathcal{Q}_{2d}(\mathbf{K}) \end{cases}$$

 The hierarchy (D_d) provides a sequence (q_d) of polynomial underestimators of f^{*}(λ).

$$\lim_{d\to\infty}\int_0^1 (f^*(\lambda) - q_d(\lambda))d\lambda = 0$$

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- Numerical schemes that avoid computing finitely many points.
- Pareto curve approximation with polynomials, convergence guarantees in L₁-norm
- V. Magron, D. Henrion, J.B. Lasserre. Approximating Pareto Curves using Semidefinite Relaxations. Accepted pending minor revisions in *Operations Research Letters*. arxiv:1404.4772, April 2014.

Approximation of sets defined with " \exists "

Let $\mathbf{B} \subset \mathbb{R}^2$ be the unit ball and assume that $f(\mathbf{S}) \subset \mathbf{B}$.

Another point of view:

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

with

$$h(\mathbf{x}, \mathbf{y}) := \|\mathbf{y} - f(\mathbf{x})\|_2^2 = (y_1 - f_1(\mathbf{x}))^2 + (y_2 - f_2(\mathbf{x}))^2$$
.

Approximate *f*(**S**) as closely as desired by a sequence of sets of the form :

$$\Theta_d := \{\mathbf{y} \in \mathbf{B} : q_d(\mathbf{y}) \leqslant 0\}$$
 ,

for some polynomials $q_d \in \mathbb{R}_{2d}[\mathbf{y}]$.

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One-loop with Conditional Branching

 \bullet $r, s, T^i, T^e \in \mathbb{R}[\mathbf{x}]$

• $\mathbf{x}_0 \in \mathbf{X}_0$, with \mathbf{X}_0 semialgebraic set

 $\begin{array}{l} \mathbf{x} = \mathbf{x}_0 \, ; \\ \text{while } (r(\mathbf{x}) \leqslant 0) \, \{ \\ \quad \text{if } (s(\mathbf{x}) \leqslant 0) \, \{ \\ \quad \mathbf{x} = T^i(\mathbf{x}) \, ; \\ \quad \} \\ \quad \text{else} \, \{ \\ \quad \mathbf{x} = T^e(\mathbf{x}) \, ; \\ \quad \} \\ \} \end{array}$

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Bounding Template using SOS

Sufficient condition to get bounding inductive invariant:

$$\begin{split} \alpha &:= \min_{q \in \mathbb{R}[\mathbf{x}]} \quad \sup_{\mathbf{x} \in \mathbf{X}_0} q(\mathbf{x}) \\ \text{s.t.} \quad q - q \circ T^i \ge 0 \ , \\ q - q \circ T^e \ge 0 \ , \\ q - \| \cdot \|_2^2 \ge 0 \ . \end{split}$$

Nontrivial correlations via polynomial templates q(x)

•
$$\{\mathbf{x}: q(\mathbf{x}) \leq \alpha\} \supset \bigcup_{k \in \mathbb{N}} \mathbf{X}_k$$

Bounds for $\bigcup_{k \in \mathbb{N}} \mathbf{X}_k$

$$\begin{aligned} \mathbf{X}_0 &:= [0.9, 1.1] \times [0, 0.2] \quad \mathbf{r}(\mathbf{x}) := 1 \quad \mathbf{s}(\mathbf{x}) := 1 - x_1^2 - x_2^2 \\ T^i(\mathbf{x}) &:= (x_1^2 + x_2^3, x_1^3 + x_2^2) \quad T^e(\mathbf{x}) := (\frac{1}{2}x_1^2 + \frac{2}{5}x_2^3, -\frac{3}{5}x_1^3 + \frac{3}{10}x_2^2) \end{aligned}$$



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Bounds for $\bigcup_{k \in \mathbb{N}} \mathbf{X}_k$





Formal Proofs, Program Analysis and Moment-SOS Relaxations

Bounds for $\bigcup_{k \in \mathbb{N}} \mathbf{X}_k$







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- New framework for nonlinear optimization
- Formal nonlinear optimization: NLCertify 1000
- Approximation of Pareto Curves, images and projections of semialgebraic sets
- Program Analysis with polynomial templates

Further research:

- Improve formal polynomial checker
- Alternative Polynomials bounds using geometric programming (T. de Wolff, S. Iliman)
- Programs analysis with transcendental assignments/conditions

Thank you for your attention!

http://homepages.laas.fr/vmagron/