NLCertify: A Tool for Formal Nonlinear Optimization

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Abstract. NLCertify is a software package for handling formal certification of nonlinear inequalities involving transcendental multivariate functions. The tool exploits sparse semialgebraic optimization techniques with approximation methods for transcendental functions, as well as formal features. Given a box and a transcendental multivariate function as input, NLCertify provides OCAML libraries that produce nonnegativity certificates for the function over the box, which can be ultimately proved correct inside the Coq proof assistant.

Keywords: Formal Nonlinear Optimization, Hybrid Symbolic-Numeric Certification, Proof Assistant, Sparse SOS, Maxplus Approximation

1 Introduction

A variety of tools for solving nonlinear systems are being adapted for the field of formal reasoning. One way to import the technology available inside an *informal* tool is the *skeptical* approach: the tool yields a form of certificate which can be verified on the *formal* side, i.e. inside a theoretical prover such as Coq [7]. A recent illustration [4] is the integration of the computational features of SAT/SMT solvers in Coq. The NLCertify¹ tool has informal nonlinear optimization features and enables formal verification in a skeptical way. An ambitious application is to automatically verify real numbers inequalities occurring by thousands in Thomas Hales' proof of Kepler's conjecture [8]. In the present article, nonlinear functions include polynomials, semialgebraic functions obtained by composition of polynomials with some basic operations (including the square root, sup, inf, +, ×, -, /, etc.) and composition of semialgebraic functions with transcendental functions (arctan, cos, exp, etc.) or basic operations.

Polynomial inequalities over a finite set of polynomial constraints can be certified using a hierarchy of sums of squares (SOS) relaxations [10]. Several variants of these relaxations are implemented in some MATLAB toolboxes: GLOPTIPOLY 3 [9] solves the Generalized Problem of Moments while SPARSE-POP takes sparsity into account [16], YALMIP [12] is a high-level parser for

¹ The source code is available at https://forge.ocamlcore.org/frs/?group_id=351. See also the documentation at http://nl-certify.forge.ocamlcore.org.

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nonlinear optimization problems and has a built-in module for SOS calculations. These toolboxes rely on external SOS solvers for solving the relaxations (e.g. SDPA [17]). However, the validity of the bounds obtained with these numerical tools can be compromise, due to the rounding error of the SOS solver. The tool² mentioned in [13] allows to handle some degenerate situations. For a more general class of problems (when the functions are not restricted to polynomials), one can combine SOS software with frameworks that approximate transcendental functions. Sollya [6] returns safe tight bounds for the approximation error obtained when computing minimax estimators of nonlinear univariate functions.

On the formal side, recent efforts have been done to verify nonlinear inequalities with theorem provers. A tool³ in HOL-LIGHT combines formal interval arithmetic computation and quadratic Taylor approximation [15]. The features of the METITARSKI [1] theorem prover include continued fractions expansions of univariate transcendental functions such as log, arctan, etc. PVS incorporates nonlinear optimization libraries relying on Bernstein polynomial approximation [14]. The interval⁴ tactic can assert the validity of interval enclosures of nonlinear functions over a finite set of box constraints inside COQ. The micromega tactic returns emptiness certificates for basic semialgebraic sets [5].

One specific challenge of the field of formal nonlinear optimization is to develop adaptive techniques to produce certificates with a reduced complexity. NLCertify provides efficient informal libraries by implementing the nonlinear maxplus method [2], which combines sparse SOS relaxations with maxplus quadratic approximation. In addition, the tool offers a secure certification framework for the bounds obtained with these semialgebraic relaxations [3]. These various features are placed in a unified framework extending to about 15000 lines of OCAML code and 3600 lines of COQ code. The NLCertify package can solve successfully non-trivial inequalities from the Flyspeck project (essentially tight inequalities, involving both semialgebraic and transcendental expressions of 6 to 12 variables) as well as significant global optimization benchmarks. The running tests for the verification of polynomial inequalities (Section 2) and transcendental inequalities (Section 3) are performed on Intel Core i5 CPU (2.40 GHz)⁵.

2 Certified Polynomial Optimization

One particular problem among certification of nonlinear problems is to verify the inequality $\forall \mathbf{x} \in \mathbf{K}, f_{\text{pop}}(\mathbf{x}) \geq 0$, where f_{pop} is an *n*-variate positive polynomial, $\mathbf{K} := {\mathbf{x} \in \mathbb{R}^n : g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0}$ is a semialgebraic set obtained with polynomials g_1, \ldots, g_m . One way to convexify this polynomial optimization problem is to find sums of squares of polynomials $\sigma_0, \sigma_1, \ldots, \sigma_m$ satisfying $f_{\text{pop}}(\mathbf{x}) = \sigma_0 + \sum_{j=1}^m \sigma_j(\mathbf{x})g_j(\mathbf{x})$ and $\deg \sigma_0 \leq 2k, \deg(\sigma_1g_1)\ldots, \deg(\sigma_mg_m) \leq 2k$, for a fixed positive integer k (called the *relaxation* order). When k increases,

² Available from the pages http://bit.ly/fBNLhR and bit.ly/gPXNF8

³ http://flyspeck.googlecode.com/files/FormalVerifier.zip

⁴ https://www.lri.fr/~melquion/soft/coq-interval/

 $^{^5}$ With OCAML 4.01.0, Coq 8.4pl2, SSREFLECT 1.4, SDPA 7.3.6 and Sollya 3.0

one obtains progressively stronger relaxations. In this way, it is always possible to certify the inequality $\forall \mathbf{x} \in \mathbf{K}, f_{\text{pop}}(\mathbf{x}) \geq 0$ for a sufficiently large order (under certain assumptions [10]). These relaxations are implemented in NLCertify and numerically solved with the SOS solver SDPA. The tool performs a rational extraction from the SOS solver output with the LACAML⁶ library. Then the corresponding remainder ϵ_{pop} (the difference between the objective polynomial f_{pop} and the SOS representation) can be bounded on a box which contains **K**. More details can be found in [3].

Example 1. (caprasse) Here, we consider the degree 4 polynomial inequality $\forall \mathbf{x} \in [-0.5, 0.5]^4, -x_1x_3^3 + 4x_2x_3^2x_4 + 4x_1x_3x_4^2 + 2x_2x_4^3 + 4x_1x_3 + 4x_3^2 - 10x_2x_4 - 10x_4^2 + 5.1801 \ge 0$. The inequality is scaled on $[0, 1]^4$ with the solver option scale_pol = true and one adds the redundant constraints $x_1^2 \le 1, \ldots, x_4^2 \le 1$ by setting bound_squares_variables = true. The inequality can be solved numerically at the second SOS relaxation order (relax_order = 2). The correctness of the SOS representation is verified inside COQ (via the reflexive tactic ring) by setting check_certif_coq = true. Then the execution of NLCertify returns the following output:

Here, the caprasse inequality is formally proved in less than 1 second which is 8 times faster than the verification procedure in HOL-LIGHT with the framework described in [15] and 10 times faster than the tool based on Bernstein approximation in PVS [14].

3 Certificates for Nonlinear Transcendental Inequalities

Now, we consider a more general goal $\forall \mathbf{x} \in \mathbf{K}, f(\mathbf{x}) \geq 0$, where f is an n-variate transcendental function and $\mathbf{K} \subset \mathbb{R}^n$ is a box. NLCertify implements the nonlinear maxplus method [2], which can be summarized as follows. The tool builds first the abstract syntax tree t of f (see Figure 1 for an illustration). The leaves of t are semialgebraic functions. The other nodes can be either univariate transcendental functions or basic operations. NLCertify approximates t with means of semialgebraic estimators and provides lower and upper bounds of t over \mathbf{K} . When t represents a polynomial, the tool computes lower and upper

⁶ Linear Algebra with OCAML, this library implements BLAS/LAPACK routines

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bounds of t using a hierarchy of sparse SOS relaxations, as outlined in Section 2. The extension to the semialgebraic case is straightforward through the implementation of the Lasserre-Putinar lifting-strategy [11]. The user can choose to approximate transcendental functions with maxplus estimators as well as best uniform (or minimax) polynomials. The maxplus method derives lower (resp. upper) estimators using concave maxima (resp. convex infima) of quadratic forms (see Figure 2 for an example). Alternatively, univariate minimax polynomials are provided with an interface to the Sollya environment, in which the Remez iterative algorithm is implemented. In this way, NLCertify computes certified global estimators from approximations of primitive functions by induction over the syntax tree t.

Example 2 (from LEMMA 9922699028 Flyspeck ⁷). Let define the polynomial $\Delta \mathbf{x} := x_1 x_4 (-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) + x_2 x_5 (x_1 - x_2 + x_3 + x_4 - x_5 + x_6) + x_3 x_6 (x_1 + x_2 - x_3 + x_4 + x_5 - x_6) - x_2 x_3 x_4 - x_1 x_3 x_5 - x_1 x_2 x_6 - x_4 x_5 x_6$, the semialgebraic functions $r(\mathbf{x}) := \partial_4 \Delta \mathbf{x} / \sqrt{4x_1 \Delta \mathbf{x}}$ and $l(\mathbf{x}) := 1.6294 - \pi/2 - 0.2213(\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0) + 0.913(\sqrt{x_4} - 2.52) + 0.728(\sqrt{x_1} - 2.0)$, as well as the box $\mathbf{K} := [4, 2.1^2]^3 \times [2.65^2, 8] \times [4, 2.1^2]^2$. Note that for illustration purpose, the inequality has been modified by taking a sub-box of the original Flyspeck inequality box $[4, 2.52^2]^3 \times [2.52^2, 8] \times [4, 2.52^2]^2$.

Here we display and comment the output of NLCertify⁸ for the inequality $\forall \mathbf{x} \in \mathbf{K}, l(\mathbf{x}) + \arctan(r(\mathbf{x})) \geq 0$. The total (informal) computation time is about 20 seconds.

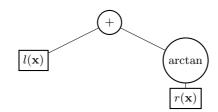


Fig. 1. The abstract syntax tree of the function f from LEMMA 9922699028 Flyspeck

```
% ./nlcertify 9922699028_modified
Proving that - 1.5708 + atan ... >= 0 over the box [(4, 4.41);
(4, 4.41); (4, 4.41); (7.0225, 8); (4, 4.41); (4, 4.41)] ...
Bounding semialgebraic components
Computing approximation of atan on [0.0297, 0.4165]
Minimizer candidate x = [4; 4; 4; 8; 4; 4]
Control points set: [0.3535] ...
Semialgebraic components bounded
Iteration 1
Lower bound = -0.00463
Minimizer candidate x = [4; 4; 4; 7.0225; 4; 4]
Iteration 2
Control points set: [0.1729; 0.3535] ...
```

 7 See the file available at http://code.google.com/p/flyspeck/source/browse/trunk/text_formalization/nonlinear formalization/nonlinear formalizati

 $^{^{8}}$ The parameter settings are samp_iters = 3, no branch and bound subdivisions (bb

⁼ false), xconvert_variables = true, check_certif_coq = false

```
Lower bound = -0.00006025
Minimizer candidate x = [4; 4; 4; 7.6622; 4; 4]
Iteration 3
Control points set: [0.1729; 0.2884; 0.3535] ...
Lower bound = 0.000004662
Minimizer candidate x = [4; 4; 4; 7.8083; 4; 4]
```

Lower and upper bounds for the semialgebraic components (i.e. r and l) are computed using SOS relaxations. An interval enclosure for r is [m, M], with m := 0.0297 and M := 0.4165. Multiple evaluations of f return a set of values and we obtain a first minimizer guess $\mathbf{x}_1 := (4, 4, 4, 8, 4, 4)$ of f over \mathbf{K} , which corresponds to the minimal value of the set. Then, the solver performs three iterations of the nonlinear maxplus algorithm.

- (1) The tool returns an underestimator par_{a_1} of $\arctan \operatorname{over} [m, M]$, with $a_1 := r(\mathbf{x}_1) = 0.3535$. Then, it computes $m_1 \leq \min_{\mathbf{x} \in \mathbf{K}} \{l(\mathbf{x}) + \operatorname{par}_{a_1}(r(\mathbf{x}))\}$. It yields $m_1 = -4.63 \times 10^{-3} < 0$ and $\mathbf{x}_2 := (4, 4, 4, 7.0225, 4, 4)$.
- (2) From the second control point, we get $a_2 := r(\mathbf{x}_2) = 0.1729$ and a tighter bound $m_2 \leq \min_{\mathbf{x} \in \mathbf{K}} \{l(\mathbf{x}) + \max_{1 \leq i \leq 2} \{ par_{a_i}(r(\mathbf{x})) \} \}$. We get $m_2 = -6.025 \times 10^{-5} < 0$ and $\mathbf{x}_3 := (4, 4, 4, 7.6622, 4, 4)$.
- (3) From the third control point, we get $a_3 := r(\mathbf{x}_3) = 0.2884$ and $m_3 \leq \min_{\mathbf{x} \in \mathbf{K}} \{l(\mathbf{x}) + \max_{1 \leq i \leq 3} \{ \operatorname{par}_{a_i}(r(\mathbf{x})) \} \}$. We obtain $m_3 = 4.662 \times 10^{-6} > 0$. Thus, the inequality is solved.

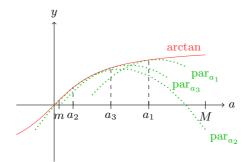


Fig. 2. A hierarchy of maxplus quadratic underestimators for arctan

4 Conclusion

NLCertify aims at combining the safety of the CoQ proof assistant with the efficiency of informal optimization algorithms, based on low degree maxplus estimators and sparse semialgebraic relaxations. This could allow to derive safe solutions for challenging problems that require to certify both approximation of transcendental functions and bounds for polynomial programs such as impulsive Rendezvous problems. Further developments on the formal side include the integration of a new reflexive tactic inside the CoQ standard library. Adding faster arithmetic for the polynomial coefficients ring would speedup the computation of the SOS checker. The current features could also be extended to handle noncommutative SOS certificates as well as discrete combinatorial optimization.

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