

Motivation: Flyspeck-Like Problems
Classical Approach: Taylor + SOS
Max-Plus Based Templates Approach
Certified Global Optimization with Coq

Certified Global Optimization using Max-Plus based Templates

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The Kepler Conjecture

Global Optimization Problems: Examples from the Literature
Global Optimization Problems: a Framework

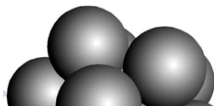
Motivation: Flyspeck-Like Problems

The Kepler Conjecture

Kepler Conjecture (1611):

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

- 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



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Inequalities issued from Flyspeck non-linear part involve:

- 1 Multivariate **Polynomials**:

$$x_1 x_4 (-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) + x_2 x_5 (x_1 - x_2 + x_3 + x_4 - x_5 + x_6) + \\ x_3 x_6 (x_1 + x_2 - x_3 + x_4 + x_5 - x_6) - x_2 (x_3 x_4 + x_1 x_6) - x_5 (x_1 x_3 + x_4 x_6)$$

- 2 **Semi-Algebraic** functions algebra \mathcal{A} : composition of polynomials with $|\cdot|$, $\sqrt{\cdot}$, $+$, $-$, \times , $/$, \sup , \inf , \dots
- 3 **Transcendental** functions \mathcal{T} : composition of semi-algebraic functions with \arctan , \exp , \sin , $+$, $-$, \times , \dots

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Global Optimization Problems: Examples from the Literature

- **H3:** $\min_{\mathbf{x} \in [0,1]^3} - \sum_{i=1}^4 c_i \exp \left[- \sum_{j=1}^3 a_{ij} (x_j - p_{ij})^2 \right]$
- **MC:** $\min_{\substack{x_1 \in [-3,3] \\ x_2 \in [-1.5,4]}} \sin(x_1 + x_2) + (x_1 - x_2)^2 - 0.5x_2 + 2.5x_1 + 1$
- **SBT:** $\min_{\mathbf{x} \in [-10,10]^n} \prod_{i=1}^n \left(\sum_{j=1}^5 j \cos((j+1)x_i + j) \right)$

Motivation: Flyspeck-Like Problems

Global Optimization Problems: a Framework

Given K a compact set, and f a **transcendental** function, minor

$$f^* = \inf_{\mathbf{x} \in K} f(\mathbf{x}) \text{ and prove } f^* \geq 0$$

- 1 f is underestimated by a **semialgebraic** function f_{sa}
- 2 We reduce the problem $f_{sa}^* := \inf_{\mathbf{x} \in K} f_{sa}(\mathbf{x})$ to a polynomial optimization problem in a lifted space K_{pop} (with lifting variables \mathbf{z})
- 3 We solve the POP problem $f_{pop}^* := \inf_{(\mathbf{x}, \mathbf{z}) \in K_{pop}} f_{pop}(\mathbf{x}, \mathbf{z})$ using

a hierarchy of SDP relaxations by Lasserre

Classical Approach: Taylor + SOS

Semialgebraic Optimization Problems

- Polynomial Optimization Problem (POP):

$p^* := \min_{\mathbf{x} \in K} p(\mathbf{x})$ with K the compact set of constraints:

$$K = \{\mathbf{x} \in \mathbb{R}^n : g_1(\mathbf{x}) \geq 0, \dots, g_m(\mathbf{x}) \geq 0\}$$

- Let $\Sigma[\mathbf{x}]$ be the cone of Sum-of-Squares (SOS) and consider the restriction $\Sigma_d[\mathbf{x}]$ to polynomials of degree at most $2d$:

$$\Sigma_d[\mathbf{x}] = \left\{ \sum_i q_i(\mathbf{x})^2, \text{ with } q_i \in \mathbb{R}_d[\mathbf{x}] \right\}$$

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Semialgebraic Optimization Problems
Semialgebraic Optimization Problems: examples
Taylor Approximation of Transcendental Functions

Classical Approach: Taylor + SOS

Semialgebraic Optimization Problems

$$M(\mathbf{g}) = \left\{ \sum_{j=0}^m \sigma_j(\mathbf{x})g_j(\mathbf{x}), \text{ with } \sigma_j \in \Sigma[\mathbf{x}] \right\}$$

Proposition (Putinar)

Suppose $\mathbf{x} \in [\mathbf{a}, \mathbf{b}]$. $p(\mathbf{x}) - p^* > 0$ on $K \implies (p(\mathbf{x}) - p^*) \in M(\mathbf{g})$

- But the search space for $\sigma_0, \dots, \sigma_m$ is infinite so consider the truncated module $M_d(\mathbf{g})$:

Classical Approach: Taylor + SOS

Semialgebraic Optimization Problems: examples

Lasserre Hierarchy Convergence:

- Let $k \geq k_0 := \max\{f, 1, \lceil \deg g_1/2 \rceil, \dots, \lceil \deg g_m/2 \rceil\}$.
- The sequence $\inf(\mu_k)_{k \geq k_0}$ is non-decreasing. Under a certain (moderate) assumption, it converges to p^* .

- $$\min_{\mathbf{x} \in [4, 6.3504]^6} \Delta(\mathbf{x}) = x_1 x_4 (-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) + x_2 x_5 (x_1 - x_2 + x_3 + x_4 - x_5 + x_6) + x_3 x_6 (x_1 + x_2 - x_3 + x_4 + x_5 - x_6) - x_2 (x_3 x_4 + x_1 x_6) - x_5 (x_1 x_3 + x_4 x_6) = \mu_2 = 128$$

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Semialgebraic Optimization Problems: examples

b.s.a.l. lemma [Lasserre, Putinar] :

Let \mathcal{A} be the semi-algebraic functions algebra obtained by composition of polynomials with $|\cdot|$, $(\cdot)^{\frac{1}{p}}$ ($p \in \mathbb{N}_0$), $+$, $-$, \times , $/$, \sup , \inf . Then every well-defined $f_{sa} \in \mathcal{A}$ has a basic semi-algebraic lifting.

Example from Flyspeck:

$$z_1 := \sqrt{4x_1 \Delta \mathbf{x}}, m_1 = \inf_{\mathbf{x} \in [4, 6.3504]^6} z_1(\mathbf{x}), M_1 = \sup_{\mathbf{x} \in [4, 6.3504]^6} z_1(\mathbf{x}).$$

$$h_1 := z_1 = m_1$$

$$h_1 := z_1$$

Classical Approach: Taylor + SOS

Taylor Approximation of Transcendental Functions

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

Classical idea: approximate $\sin(\sqrt{\cdot})$ by a degree- d Taylor

Polynomial f_d , solve $\min_{\mathbf{x} \in [1, 500]^n} - \sum_{i=1}^n (x_i + x_{i+1}) f_d(x_i)$ (**POP**)

Issues:

- Lack of accuracy if d is not large enough \implies expensive
Branch and Bound

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Benchmarks: Flyspeck

Max-Plus Based Templates Approach

Main Purpose

Goals:

- Reduce the $O(n^{2k})$ polynomial dependency: decrease the number of lifting variables
- Reduce the $O(n^{2k})$ exponential dependency: use low degree approximations
- Reduce the Branch and Bound iterations: refine the approximations with an adaptive iterative algorithm

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Max-Plus Estimators and Semi-convexity

- Let $\hat{f} \in \mathcal{T}$ be a transcendental univariate elementary function such as `arctan`, `exp` defined on a real interval I .
- Convexity/semi-convexity properties and monotonicity of \hat{f}
- \hat{f} is semi-convex: there exists a constant $c_j > 0$ s.t.
 $a \mapsto \hat{f}(a) + c_j/2(a - a_j)^2$ is convex
- By convexity:
 $\forall a \in I, \hat{f}(a) \geq -c_j/2(a - a_j)^2 + \hat{f}'(a_j)(a - a_j) + \hat{f}(a_j) = \text{par}_{a_j}^-(a)$
- $\forall j, \hat{f} \geq \text{par}_{a_j}^- \implies \hat{f} \geq \max_j \{\text{par}_{a_j}^-\}$ **Max-Plus underestimator**

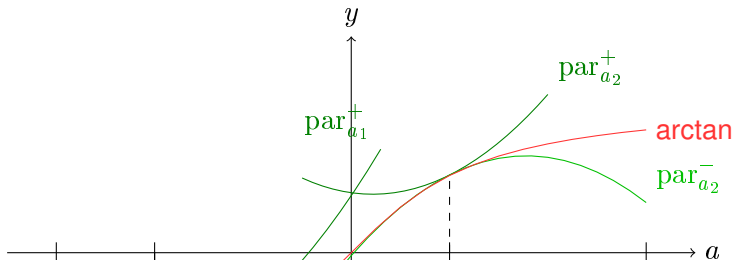
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Max-Plus Estimators for \arctan

Example with \arctan :



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Max-Plus Based Templates Approach

Max-Plus Estimators on a Flyspeck example

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

Lemma₉₉₂₂₆₉₉₀₂₈ from Flyspeck:

$$\forall \mathbf{x} \in [4, 6.3504]^6, \arctan\left(\frac{\partial_4 \Delta \mathbf{x}}{\sqrt{4x_1 \Delta \mathbf{x}}}\right) + l(\mathbf{x}) \geq 0$$

- Using **semialgebraic** optimization methods:

$$\forall x \in [4, 6.3504]^6, m < \frac{\partial_4 \Delta \mathbf{x}}{\sqrt{4x_1 \Delta \mathbf{x}}} < M$$

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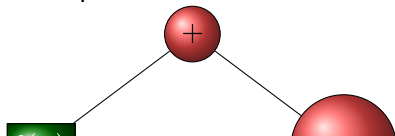
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Max-Plus Based Templates Approach

Semialgebraic Max-Plus Approximations Algorithm

Abstract syntax tree representations of multivariate transcendental function:

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



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Semialgebraic Max-Plus Approximations Algorithm

Recursive Algorithm `samp_approx`:

Input: tree t , box K , SDP relaxation order k , control points sequence

$$s = \mathbf{x}^1, \dots, \mathbf{x}^p \in K$$

Output: lower bound m , upper bound M , lower tree t^- , upper tree t^+

1: **if** $t \in \mathcal{A}$ **then**

2: $t^- := t, t^+ := t$

3: **else if** $r := \text{root}(t) \in \mathcal{T}$ parent of the single child c **then**

4: $m_c, M_c, c^-, c^+ := \text{samp_approx}(c, K, k, s)$

5: $\text{par}^-, \text{par}^+ := \text{build_par}(r, m_c, M_c, s)$



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Semialgebraic Max-Plus Optimization Algorithm

Iterative Algorithm `samp_optim`:

Input: tree t , box K , $iter_{\max}$ (optional argument)

Output: lower bound m , feasible solution \mathbf{x}_{opt}

1: $s := [\text{argmin}(\text{randeval } t)]$ $\triangleright s \in K$

2: $iter := 0$

3: $m := -\infty$

4: **while** $iter \leq iter_{\max}$ **do**

5: Choose an SDP relaxation order k

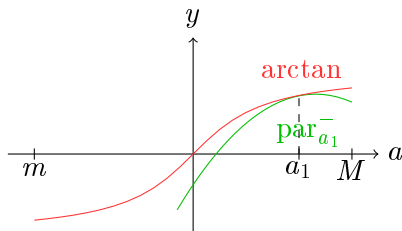
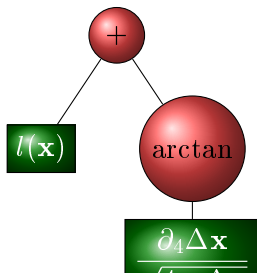
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Semialgebraic Max-Plus Optimization Algorithm

`samp_optim` First iteration:



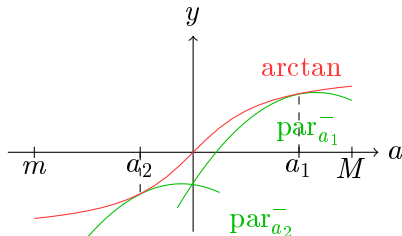
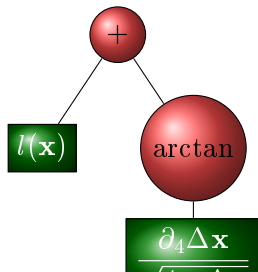
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`samp_optim` Second iteration:



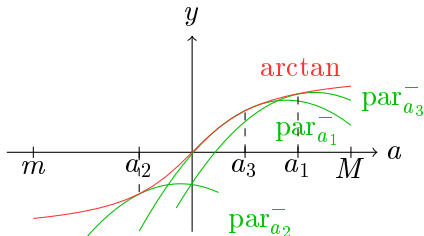
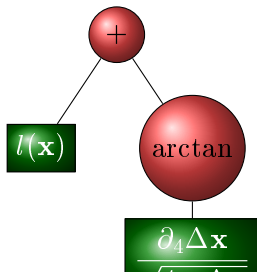
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`samp_optim` Second iteration:



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Semialgebraic Max-Plus Optimization Algorithm

- For $k = 3$, $m_3 = -0.0333 < 0$, obtain a new minimizer \mathbf{x}_{opt}^4 and iterate again...

Theorem: Convergence of Semialgebraic underestimators

Let f be a multivariate transcendental function that can be represented by such syntactic abstract trees.

Let $(\mathbf{x}_{opt}^p)_{p \in \mathbb{N}}$ be a sequence of control points obtained to define the hierarchy of underestimators in the algorithm `samp_optim` and \mathbf{x}^* be an accumulation point of $(\mathbf{x}_{opt}^p)_{p \in \mathbb{N}}$.

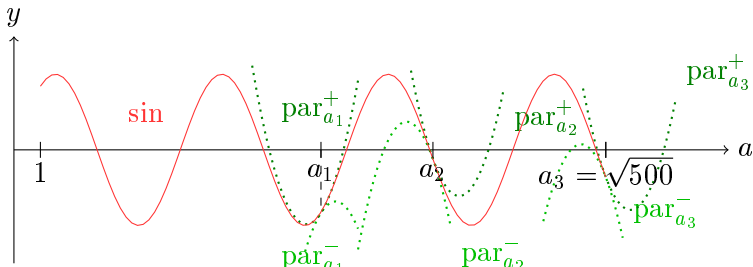
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Example with \sin :



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$$SWF: \min_{\mathbf{x} \in [1, 500]^n} - \sum_{i=1}^n (x_i + x_{i+1}) \sin(\sqrt{x_i}) \quad (\epsilon = 1)$$

- Use one lifting variable y_i to represent $x_i \mapsto \sqrt{x_i}$ and one lifting variable z_i to represent $x_i \mapsto \sin(x_i)$

$$\left\{ \begin{array}{l} \min_{\mathbf{x} \in [1, 500]^n, \mathbf{y} \in [1, \sqrt{500}]^n, \mathbf{z} \in [-1, 1]^n} - \sum_{i=1}^n (x_i + x_{i+1}) z_i \\ \text{s.t.} \quad z_i \leq \text{par}_{a_{ji}}^+(y_i), j \in \{1, 2, 3\} \end{array} \right.$$

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Polynomial Estimators using Semidefinite Programming

With `samp_optim`: the number of lifting variables is not bounded

Remedy: select some subcomponents of f and compute estimators involving less lifting variables

- Let t be such a subcomponent and \mathbf{x}^j be a control point and suppose that t is twice differentiable.
- Define the interval matrix \tilde{D} enclosing all the entries of $(\mathcal{D}^2(t)(\mathbf{x}) - \mathcal{D}^2(t)(\mathbf{x}_j))$ for $\mathbf{x} \in K$
- Define the quadratic form

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- Lower bound of $\min_{\mathbf{x} \in K} \{\lambda_{\min}(\mathcal{D}^2(t)(\mathbf{x}) - \mathcal{D}^2(t)(\mathbf{x}_j))\}$: $\lambda_{\min}(\tilde{D})$
 $\lambda^- := \lambda_{\min}(\tilde{D})$: minimal eigenvalue of an interval matrix
- For each interval $\tilde{D}_{ij} = [m_{ij}, M_{ij}]$, define the symmetric matrix entry $B_{ij} := \max\{|m_{ij}|, |M_{ij}|\}$
- Let \mathcal{S}^n be the set of diagonal matrices of sign.
 $\mathcal{S}^n := \{\text{diag}(s_1, \dots, s_n), s_1 = \pm 1, \dots, s_n = \pm 1\}$

Robust Optimization with Reduced Vertex Set [Calafiore, Dabbene]

The robust interval SDP problem $\lambda_{\min}(\tilde{D})$ is equivalent to the fol

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The Templates Algorithm

Previous Algorithm:

Input: tree t , box K , SDP relaxation order k , control points sequence

$$s = \mathbf{x}^1, \dots, \mathbf{x}^p \in K$$

Output: lower bound m , upper bound M , lower tree t^- , upper tree t^+

- 1: **if** $t \in \mathcal{A}$ **then**
- 2: $t^- := t, t^+ := t$
- 3: **else if** $r := \text{root}(t) \in \mathcal{T}$ parent of the single child c **then**
- 4: $m_c, M_c, c^-, c^+ := \text{samp_approx}(c, K, k, s)$
- 5: $\text{par}^-, \text{par}^+ := \text{build_par}(r, m_c, M_c, s)$



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The Templates Algorithm: `template_optim`

Input: tree t , box K , SDP relaxation order k , control points sequence
 $s = \mathbf{x}^1, \dots, \mathbf{x}^p \in K$

Output: lower bound m , upper bound M , lower tree t^- , upper tree t^+

```
1: if  $t \in \mathcal{A}$  then
2:   return  $\min(t, k), \max(t, k), t, t$ 
3: else if  $r := \text{root}(t) \in \mathcal{T}$  parent of the single child  $c$  then
4:    $m_c, M_c, c^-, c^+ := \text{template\_optim}(c, K, k, s)$ 
5:    $\text{par}^-, \text{par}^+ := \text{build\_par}(r, m_c, M_c, s)$ 
6:    $t^-, t^+ := \text{compose}(\text{par}^-, \text{par}^+, c^-, c^+)$ 
7:   return  $\min(t^-, k), \max(t^+, k), t^-, t^+$ 
```



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The Templates Algorithm: `build_template`

`build_template` builds quadratic forms by solving SDP problems.

Input: tree t , box K , SDP relaxation order k , control points sequence $s = \mathbf{x}^1, \dots, \mathbf{x}^p \in K$, lower/upper semialgebraic estimator t^-, t^+

- 1: **if** the number of lifting variables exceeds $n_{\text{lifting}}^{\max}$ **then**
- 2: **for** $\mathbf{x}^j \in s$ **do**
- 3: Compute the interval matrix \tilde{D}^j
- 4: $\lambda^- := \lambda_{\min}(\tilde{D}^j)$ $q_j^- := q_{\mathbf{x}^j, \lambda^-}$
- 5: $\lambda^+ := \lambda_{\max}(\tilde{D}^j)$ $q_j^+ := q_{\mathbf{x}^j, \lambda^+}$
- 6: **done**

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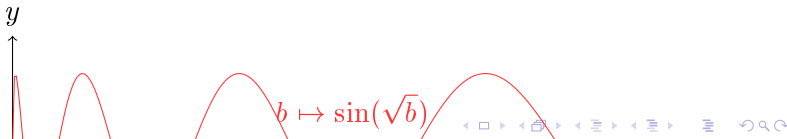
Max-Plus Based Templates Approach

The Templates Algorithm: *SWF*

When t is univariate, $\lambda^- = -c_j$ (the semi-convexity constant)

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

- Consider the univariate function $b \mapsto \sin(\sqrt{b})$ on $I = [1, 500]$



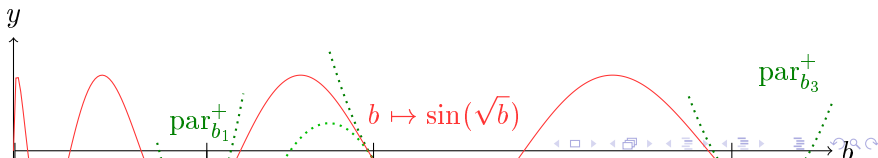
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Max-Plus Based Templates Approach

The Templates Algorithm: SWF

- $\forall j, \hat{f} \geq \text{par}_{b_j}^- \implies \hat{f} \geq \max_j \left\{ \text{par}_{b_j}^- \right\}$: **Max-Plus underestimator**
- $\forall j, \hat{f} \leq \text{par}_{b_j}^+ \implies \hat{f} \leq \min_j \left\{ \text{par}_{b_j}^+ \right\}$: **Max-Plus overestimator**



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The Templates Algorithm: *SWF*

- Use a lifting variable z_i to represent $x_i \mapsto \sin(\sqrt{x_i})$
- For each i , pick points b_{ji}
- With 3 points b_{ji} , we solve the **POP**:

$$\left\{ \begin{array}{l} \min_{\mathbf{x} \in [1,500]^n, \mathbf{z} \in [-1,1]^n} - \sum_{i=1}^n (x_i + x_{i+1}) z_i \\ \text{s.t.} \quad z_i \leq \text{par}_{b_{ji}}^+(x_i), j \in \{1, 2, 3\} \end{array} \right.$$

- **POP** with $n + n$ variables ($n_{\text{lifting}} = n$ variables), with

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Benchmarks: *SWF*

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

n	lower bound	n_{lifting}	#boxes	time
$10(\epsilon = 0)$	$-430n$	$2n$	16	40 s
$10(\epsilon = 0)$	$-430n$	0	827	177 s
$1000(\epsilon = 1)$	$-967n$	$2n$	1	543 s

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- SOS of degree $2k$
- $\#s$ control points (`template_optim` iterations)
- when $\#s = 0$, $n_{\text{lifting}} = 0$: interval arithmetic + SOS

Problem	n	lower bound	k	$\#s$	n_{lifting}	$\#boxes$	time
<i>H3</i>	3	-3.863	2	3	4	99	101 s
				0	0	1096	247 s
				2	1	17	18 s

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- $n = 6$ variables, SOS of degree $2k = 4$
- $n_{\mathcal{T}}$ univariate transcendental functions
- #boxes sub-problems

Inequality id	$n_{\mathcal{T}}$	n_{lifting}	#boxes	time
9922699028	1	9	47	241 s
9922699028	1	3	39	190 s

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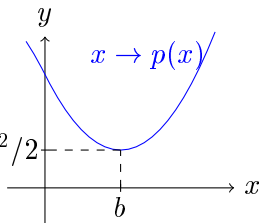
Certification Framework: who does what?

Polynomial Optimization (POP): $\min_{x \in \mathbb{R}} p(x) = 1/2x^2 - bx + c$

- 1 A program written in OCaml/C provides the **SOS** decomposition:

$$1/2(x - b)^2$$

- 2 A program written in Coq checks:
 $\forall x \in \mathbb{R}, p(x) = 1/2(x - b)^2 + c - b^2/2$



- 3 Sceptical approach: obtain *certificates* of positivity with

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Coq tactics: `field`, `interval`

Formal proofs for lower bounds of POP:

- The oracle returns floating point certificate: $\mu, \sigma_0, \dots, \sigma_m$
- Check equality of polynomials: $f(\mathbf{x}) - \mu = \sum_{i=0}^m \sigma_i(\mathbf{x})g_i(\mathbf{x})$

with the Coq `field` tactic.

- The equality test often fails. Two solutions:
 - 1 Rounding and Projection of the certificate (Peyrl and Parillo, Kaltofen) until we get the equality

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Polynomial Underestimators of Semialgebraic functions using SDP

- Let t be a **semialgebraic** leaf of the abstract syntactic tree of f
- Let $\mathbf{x}^j \in K$ a control point
- Let λ denote the Lebesgue measure distributed on K

Consider the following optimization problem with optimal solution

h_d^* :

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

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Polynomial Underestimators of Semialgebraic functions using SDP

- There exist lifting variables z_1, \dots, z_p and polynomials $g_j \in \mathbb{R}[\mathbf{x}, \mathbf{z}]$, $j = 1, \dots, m$ defining the semialgebraic set: $K_{\text{pop}} := \{(\mathbf{x}, \mathbf{z}) \in \mathbb{R}^{n+p} : \mathbf{x} \in K, g_1(\mathbf{x}, \mathbf{z}) \geq 0, \dots, g_m(\mathbf{x}, \mathbf{z}) \geq 0\}$ such that $\Psi_t := \{(\mathbf{x}, t(\mathbf{x})) : \mathbf{x} \in K\} = \{(\mathbf{x}, z_p) : (\mathbf{x}, \mathbf{z}) \in K_{\text{pop}}\}$
- Then we can rewrite the previous optimization problem:

$$\left\{ \begin{array}{l} \min_{h \in \mathbb{R}_d[\mathbf{x}]} \int_{K_{\text{pop}}} (z_p - h) d\lambda \\ \text{s.t.} \quad z_p - h(\mathbf{x}) \geq 0 \text{ on } K_{\text{pop}} \end{array} \right.$$

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Polynomial Underestimators of Semialgebraic functions using SDP

- $K := \{\mathbf{x} \in \mathbb{R}^n : f_1(\mathbf{x}) \geq 0, \dots, f_{2n}(\mathbf{x}) \geq 0\}$
- Let $g_0 := 1$ and $\omega_0 := \deg(g_0), \dots, \omega_m := \deg(g_m)$
- For $k \geq k_0 = \max\{\lceil d/2 \rceil, \lceil \omega_1/2 \rceil, \dots, \lceil \omega_m/2 \rceil\}$, introduce the following SDP relaxation F_{dk} :

$$\left\{ \begin{array}{l} \max_{h \in \mathbb{R}_d[\mathbf{x}], \sigma, \phi} \int_K h d\lambda \\ \text{s.t.} \quad \forall \mathbf{x}, \mathbf{z}, z_p - h(\mathbf{x}) = \sum_{i=0}^m \sigma_i(\mathbf{x}, \mathbf{z}) g_i(\mathbf{x}) + \sum_{i=1}^{2n} \phi_i(\mathbf{x}, \mathbf{z}) f_i(\mathbf{x}) \end{array} \right.$$

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Exploiting System Properties

- Templates preserve system properties: Sparsity / Symmetries
- Implementation in OCaml of the sparse variant of SDP relaxations (Kojima) for POP and semialgebraic underestimators
- Reducing the size of SDP input data has a positive domino effect:
 - 1 on the global optimization oracle to decrease the $O(n^{2d})$ complexity
 - 2 to check SOS with `field` and `interval` Coq tactics

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End

Thank you for your attention!
Questions?