Certification of Roundoff Errors with SDP Relaxations and Formal Interval Methods

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SWIM

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Errors and Proofs

Mathematicians and Computer Scientists want to eliminate all the uncertainties on their results. Why?

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- U.S. Patriot missile killed 28 soldiers from the U.S. Army's
- Internal clock: 0.1 sec intervals
- Roundoff error on the binary constant "0.1"

Errors and Proofs

GUARANTEED OPTIMIZATION

Input : Linear problem (LP), geometric, semidefinite (SDP)

Output : solution + **certificate** numeric-symbolic $\rightsquigarrow$ formal

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Guaranteed Optimization

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Verification of critical systems

Reliable software/hardware embedded codes

Aerospace control

molecular biology, robotics, code synthesis, ...

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Efficient Verification of Nonlinear Systems

- Automated precision tuning of systems/programs
  analysis/synthesis
- Efficiency sparsity correlation patterns
- Certified approximation algorithms

Roundoff Error Bounds

Real : $f(\mathbf{x}) := x_1 \times x_2 + x_3$

Floating-point : $\hat{f}(\mathbf{x}, \mathbf{e}) := [x_1 x_2 (1 + e_1) + x_3](1 + e_2)$

Input variable constraints $\mathbf{x} \in \mathbf{X}$
Finite precision $\rightsquigarrow$ bounds over $\mathbf{e} \in \mathbf{E}$: $\mid e_i \mid \leqslant 2^{-53}$ (double)
Guarantees on absolute round-off error $\mid \hat{f} - f \mid$?

$\downarrow$ **Upper** Bounds $\downarrow$

$\max \hat{f} - f$ ———————— $\max \hat{f} - f$

$\uparrow$ **Lower** Bounds $\uparrow$

$\downarrow$ **Lower** Bounds $\downarrow$

$\min \hat{f} - f$ ———————— $\min \hat{f} - f$

$\uparrow$ **Upper** Bounds $\uparrow$

Nonlinear Programs

- Polynomials programs : $+, -, \times$

$$x_2x_5 + x_3x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$$

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$$\frac{4x}{1 + \frac{x}{1.11}}$$

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$$\frac{4x}{1 + \frac{x}{1.11}}$$

- Transcendental programs: $\arctan, \exp, \log, \ldots$

$$\log(1 + \exp(x))$$

Existing Frameworks

Classical methods:

- Abstract domains [Goubault-Putot 11]

  FLUCTUAT: intervals, octagons, zonotopes

- Interval arithmetic [Daumas-Melquiond 10]

  GAPPA: interface with COQ proof assistant

Existing Frameworks

Recent progress:

- Affine arithmetic + SMT [Darulova 14]

  `rosa`: sound compiler for reals (SCALA)

- Symbolic Taylor expansions [Solovyev 15]

  `FPTaylor`: certified optimization (OCAML/HOL-LIGHT)

- Guided random testing `s3fp` [Chiang 14]

Contributions

Maximal Roundoff error of the program implementation of f:

$$r^\star := \max |\hat{f}(\mathbf{x}, \mathbf{e}) - f(\mathbf{x})|$$

Decomposition: **linear** term l w.r.t. $\mathbf{e}$ + nonlinear term h

$$\max |l(\mathbf{x}, \mathbf{e})| + \max |h(\mathbf{x}, \mathbf{e})| \geqslant r^\star \geqslant \max |l(\mathbf{x}, \mathbf{e})| - \max |h(\mathbf{x}, \mathbf{e})|$$

- Coarse bound of h with interval arithmetic
- **Semidefinite programming** (SDP) bounds for l:

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$\uparrow$ **Upper** Bounds $\uparrow$

Sparse SDP relaxations | **Robust SDP relaxations**

Contributions

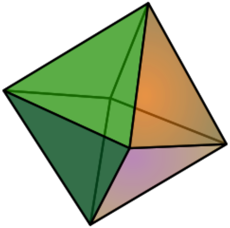
1. General **SDP** framework for upper and lower bounds
2. Comparison with SMT and linear/affine/Taylor arithmetic:
   $\rightsquigarrow$ **Efficient** optimization $\bigoplus$ **Tight** upper bounds
3. Extensions to transcendental/conditional programs
4. Formal verification of SDP bounds
5. Open source tool `Real2Float` (in OCAML and COQ)

What is Semidefinite Programming?

- Linear Programming (LP):

$$\begin{aligned} \min_{\mathbf{z}} \quad & \mathbf{c}^\top \mathbf{z} \\ \text{s.t.} \quad & \mathbf{A}\,\mathbf{z} \geqslant \mathbf{d} \ . \end{aligned}$$

  - Linear cost $\mathbf{c}$
  - Linear inequalities "$\sum_i A_{ij}\, z_j \geqslant d_i$"

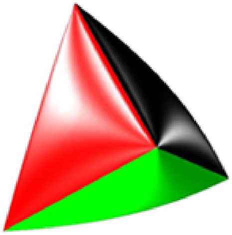


Polyhedron

What is Semidefinite Programming?

- Semidefinite Programming (SDP):

$$\min_{\mathbf{z}} \quad \mathbf{c}^\top \mathbf{z}$$
$$\text{s.t.} \quad \sum_i \mathbf{F}_i z_i \succcurlyeq \mathbf{F}_0 \ .$$



Spectrahedron

  - Linear cost $\mathbf{c}$
  - Symmetric matrices $\mathbf{F}_0, \mathbf{F}_i$
  - Linear matrix inequalities "$\mathbf{F} \succcurlyeq 0$" ($\mathbf{F}$ has nonnegative eigenvalues)

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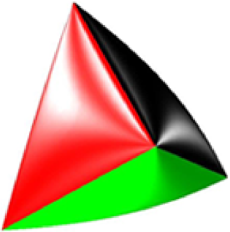

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Applications of SDP

- Combinatorial optimization
- Control theory
- Matrix completion
- Unique Games Conjecture (Khot '02) :
  "A *single concrete algorithm* provides **optimal guarantees** among all efficient algorithms for a large class of computational problems."
  (Barak and Steurer survey at ICM'14)
- Solving polynomial optimization (Lasserre '01)

SDP for Polynomial Optimization

- Prove **polynomial inequalities** with SDP:

$$f(a,b) := a^2 - 2ab + b^2 \geqslant 0 \ .$$

- Find $\mathbf{z}$ s.t. $f(a,b) = \begin{pmatrix} a & b \end{pmatrix} \underbrace{\begin{pmatrix} z_1 & z_2 \\ z_2 & z_3 \end{pmatrix}}_{\succcurlyeq 0} \begin{pmatrix} a \\ b \end{pmatrix}$.

- Find $\mathbf{z}$ s.t. $a^2 - 2ab + b^2 = z_1 a^2 + 2 z_2 ab + z_3 b^2 \qquad (\mathbf{A}\,\mathbf{z} = \mathbf{d})$

- $\begin{pmatrix} z_1 & z_2 \\ z_2 & z_3 \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_{\mathbf{F}_1} z_1 + \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\mathbf{F}_2} z_2 + \underbrace{\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}}_{\mathbf{F}_3} z_3 \succcurlyeq \underbrace{\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}}_{\mathbf{F}_0}$

SDP for Polynomial Optimization

- Choose a cost $\mathbf{c}$ e.g. $(1, 0, 1)$ and solve:

$$\begin{aligned} \min_{\mathbf{z}} \quad & \mathbf{c}^{\top} \mathbf{z} \\ \text{s.t.} \quad & \sum_i \mathbf{F}_i \, z_i \succcurlyeq \mathbf{F}_0 \ , \quad \mathbf{A} \, \mathbf{z} = \mathbf{d} \ . \end{aligned}$$

- Solution $\begin{pmatrix} z_1 & z_2 \\ z_2 & z_3 \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \succcurlyeq 0$ (eigenvalues 0 and 2)

- $a^2 - 2ab + b^2 = \begin{pmatrix} a & b \end{pmatrix} \underbrace{\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}}_{\succcurlyeq 0} \begin{pmatrix} a \\ b \end{pmatrix} = (a - b)^2 \, .$

- Solving **SDP** $\implies$ Finding **Sums of Squares** certificates

SDP for Polynomial Optimization

General case:

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

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

- Sums of squares (SOS) $\Sigma[\mathbf{x}]$ (e.g. $(x_1 - x_2)^2$)

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

- Fix the degree $2k$ of products:

$$\mathcal{Q}_k(\mathbf{X}) := \left\{ \sigma_0(\mathbf{x}) + \sum_{j=1}^m \sigma_j(\mathbf{x}) g_j(\mathbf{x}), \text{ with } \deg \sigma_j \, g_j \leqslant 2k \right\}$$

SDP for Polynomial Optimization

- **Hierarchy of SDP relaxations**:
$\lambda_k := \sup_{\lambda} \Big\{ \lambda : f - \lambda \in \mathcal{Q}_k(\mathbf{X}) \Big\}$

- Convergence guarantees $\lambda_k \uparrow f^*$ [Lasserre 01]

- Can be computed with SDP solvers (CSDP, SDPA)

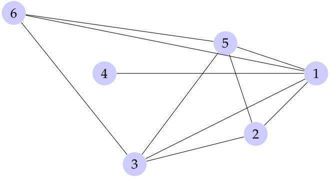
- **"No Free Lunch" Rule**: $\binom{n+2k}{n}$ SDP variables

- Extension to semialgebraic functions $r(\mathbf{x}) = p(\mathbf{x}) / \sqrt{q(\mathbf{x})}$ [Lasserre-Putinar 10]

Sparse SDP Optimization [Waki, Lasserre 06]

- Correlative sparsity pattern (csp) of variables

$$x_2x_5 + x_3x_6 - x_2x_3 - x_5x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$$



1. Maximal cliques $C_1, \ldots, C_l$
2. Average size $\kappa \rightsquigarrow \binom{\kappa+2k}{\kappa}$ variables

$C_1 := \{1, 4\}$
$C_2 := \{1, 2, 3, 5\}$
$C_3 := \{1, 3, 5, 6\}$
Dense SDP: 210 variables
Sparse SDP: 115 variables

Polynomial Programs

Input: exact $f(\mathbf{x})$, floating-point $\hat{f}(\mathbf{x}, \mathbf{e})$, $\mathbf{x} \in \mathbf{X}$, $\mid e_i \mid \leqslant 2^{-53}$
Output: Bound for $f - \hat{f}$

1: Error $r(\mathbf{x}, \mathbf{e}) := f(\mathbf{x}) - \hat{f}(\mathbf{x}, \mathbf{e}) = \sum_{\boldsymbol{\alpha}} r_{\boldsymbol{\alpha}}(\mathbf{e}) \mathbf{x}^{\boldsymbol{\alpha}}$

2: Decompose $r(\mathbf{x}, \mathbf{e}) = l(\mathbf{x}, \mathbf{e}) + h(\mathbf{x}, \mathbf{e})$, l **linear** in $\mathbf{e}$

3: $l(\mathbf{x}, \mathbf{e}) = \sum_{i=1}^{m} s_i(\mathbf{x}) e_i$

4: Maximal cliques correspond to $\{\mathbf{x}, e_1\}, \ldots, \{\mathbf{x}, e_m\}$

5: Bound $l(\mathbf{x}, \mathbf{e})$ with sparse SDP relaxations (and h with IA)

Dense relaxation: $\binom{n+m+2k}{n+m}$ SDP variables
Sparse relaxation: $m\binom{n+1+2k}{n+1}$ SDP variables

Preliminary Comparisons

$$f(\mathbf{x}) := x_2x_5 + x_3x_6 - x_2x_3 - x_5x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$$

$$\mathbf{x} \in [4.00, 6.36]^6\,, \quad \mathbf{e} \in [-\epsilon, \epsilon]^{15}\,, \quad \epsilon = 2^{-53}$$

- Dense SDP: $\binom{6+15+4}{6+15} = 12650$ variables $\rightsquigarrow$ **Out of memory**

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- Interval arithmetic: 922ϵ ($10 \times$ less CPU)
- Symbolic Taylor `FPTaylor` tool: 721ϵ ($21 \times$ more CPU)

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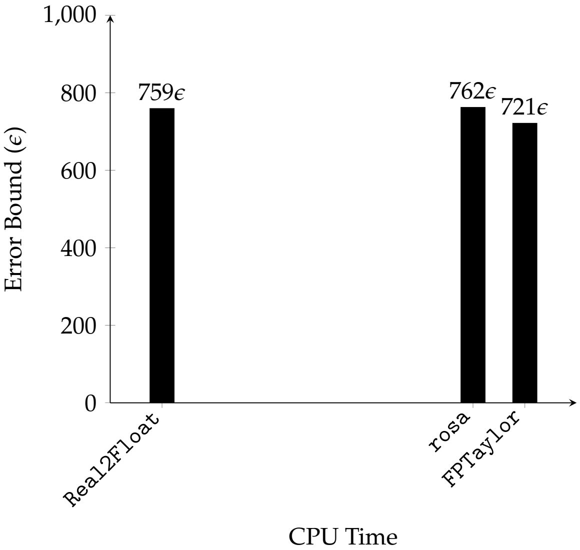
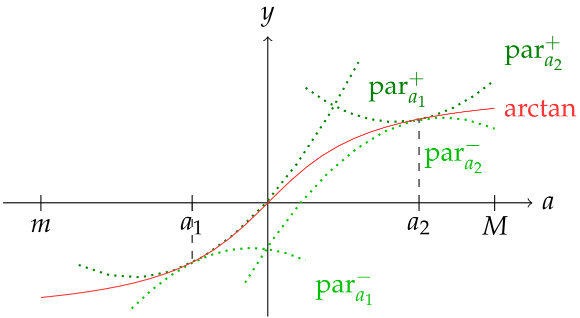
- Interval arithmetic: 922ϵ ($10\times$ less CPU)
- Symbolic Taylor `FPTaylor` tool: 721ϵ ($21\times$ more CPU)
- SMT-based `rosa` tool: 762ϵ ($19\times$ more CPU)

Preliminary Comparisons



Extensions: Transcendental Programs

Reduce $f^* := \inf_{\mathbf{x} \in \mathbf{K}} f(\mathbf{x})$ to semialgebraic optimization



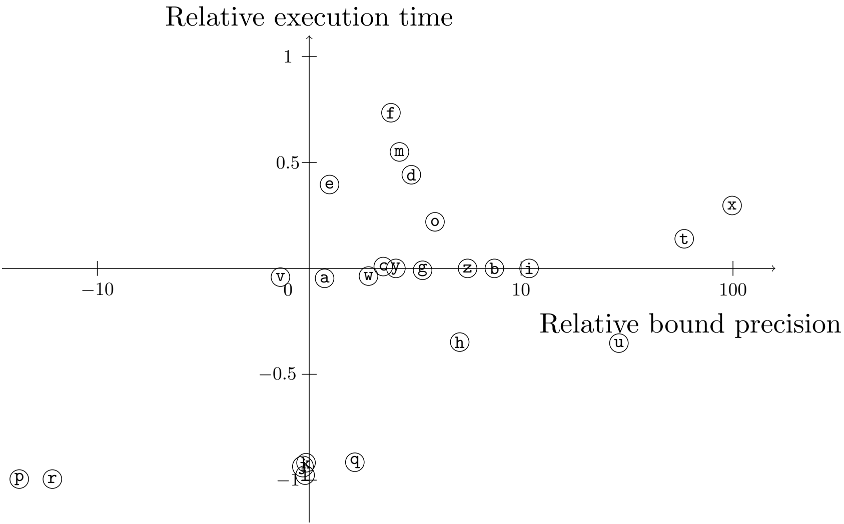
Extensions: Conditionals

$$\texttt{if } (p(\mathbf{x}) \leqslant 0)\ f(\mathbf{x});\ \texttt{else } g(\mathbf{x});$$

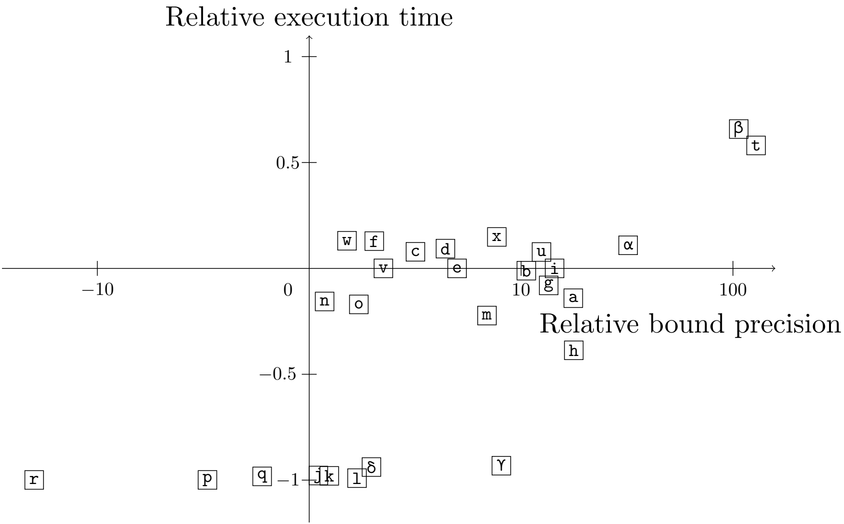
DIVERGENCE PATH ERROR:

$$
\begin{aligned}
r^\star := \max\{ & \\
& \max_{p(\mathbf{x})\leqslant 0, p(\mathbf{x},\mathbf{e})\geqslant 0} |\hat{f}(\mathbf{x},\mathbf{e}) - g(\mathbf{x})| \\
& \max_{p(\mathbf{x})\geqslant 0, p(\mathbf{x},\mathbf{e})\leqslant 0} |\hat{g}(\mathbf{x},\mathbf{e}) - f(\mathbf{x})| \\
& \max_{p(\mathbf{x})\geqslant 0, p(\mathbf{x},\mathbf{e})\geqslant 0} |\hat{f}(\mathbf{x},\mathbf{e}) - f(\mathbf{x})| \\
& \max_{p(\mathbf{x})\leqslant 0, p(\mathbf{x},\mathbf{e})\leqslant 0} |\hat{g}(\mathbf{x},\mathbf{e}) - g(\mathbf{x})| \\
& \}
\end{aligned}
$$

Comparison with `rosa`



Comparison with `FPTaylor`



Method 1: `geneig` [Lasserre 11]

Generalized eigenvalue problem:

$$f^* := \min_{\mathbf{x} \in \mathbf{X}} f(\mathbf{x}) \leqslant \lambda_k := \sup_{\lambda} \quad \lambda$$
$$\text{s.t.} \quad \mathbf{M}_k(f\,\mathbf{y}) \succcurlyeq \lambda \mathbf{M}_k(\mathbf{y}).$$

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Uniform distribution moments: $\mathbf{y}_\alpha := \int_{\mathbf{X}} \mathbf{x}^\alpha d\mathbf{x}$
Localizing matrices $\mathbf{M}_k(f\ \mathbf{y})$:

$$\mathbf{M}_1(f\ \mathbf{y}) = \begin{array}{c c} & \begin{array}{ccc} 1 & x_1 & x_2 \end{array} \\ \begin{array}{c} 1 \\ x_1 \\ x_2 \end{array} & \begin{pmatrix} \int_{\mathbf{X}} f(\mathbf{x}) d\mathbf{x} & \int_{\mathbf{X}} f(\mathbf{x}) x_1 d\mathbf{x} & \int_{\mathbf{X}} f(\mathbf{x}) x_2 d\mathbf{x} \\ \int_{\mathbf{X}} f(\mathbf{x}) x_1 d\mathbf{x} & \int_{\mathbf{X}} f(\mathbf{x}) x_1^2 d\mathbf{x} & \int_{\mathbf{X}} f(\mathbf{x}) x_1 x_2 d\mathbf{x} \\ \int_{\mathbf{X}} f(\mathbf{x}) x_2 d\mathbf{x} & \int_{\mathbf{X}} f(\mathbf{x}) x_2 x_1 d\mathbf{x} & \int_{\mathbf{X}} f(\mathbf{x}) x_2^2 d\mathbf{x} \end{pmatrix} \end{array}$$

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Theorem [Lasserre 11]

$\lambda_k \downarrow f^*$

Method 2: `mvbeta` [DeKlerk et al. 16]

Elementary calculation with $f(\mathbf{x}) = \sum_\alpha f_\alpha \mathbf{x}^\alpha$:

$$f^* := \min_{\mathbf{x} \in \mathbf{X}} f(\mathbf{x}) \leqslant f_k^H := \min_{|\eta+\beta| \leqslant 2k} \quad \sum_\alpha f_\alpha \frac{\gamma_{\eta+\alpha,\beta}}{\gamma_{\eta,\beta}}$$

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Multivariate beta distribution moments:

$$\gamma_{\eta,\beta} := \int_{\mathbf{X}} \mathbf{x}^\eta (1 - \mathbf{x})^\beta d\mathbf{x} \,.$$

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Theorem [DeKlerk et al. 16]

$f_k^H \downarrow f^*$

Method 3: `robustsdp`

Robust SDP with $l(\mathbf{x}, \mathbf{e}) = \sum_{i=1}^{m} s_i(\mathbf{x}) e_i$:

$$l^* := \min_{(\mathbf{x},\mathbf{e}) \in \mathbf{X} \times \mathbf{E}} l(\mathbf{x}, \mathbf{e}) \leqslant \lambda'_k := \sup_{\lambda} \quad \lambda$$

$$\text{s.t.} \quad \forall \mathbf{e} \in \mathbf{E}\,, \; \mathbf{M}_k(l\, \mathbf{y}) \succcurlyeq \lambda \mathbf{M}_k(\mathbf{y}).$$

Method 3: `robustsdp`

Robust SDP with $l(\mathbf{x}, \mathbf{e}) = \sum_{i=1}^{m} s_i(\mathbf{x}) e_i$:

$$l^* := \min_{(\mathbf{x},\mathbf{e}) \in \mathbf{X} \times \mathbf{E}} l(\mathbf{x}, \mathbf{e}) \leqslant \lambda'_k := \sup_{\lambda} \quad \lambda$$

$$\text{s.t.} \quad \forall \mathbf{e} \in \mathbf{E}\,, \ \mathbf{M}_k(l\ \mathbf{y}) \succcurlyeq \lambda \mathbf{M}_k(\mathbf{y}).$$

Linearity $\rightsquigarrow$ $\mathbf{M}_k(l\ \mathbf{y}) = \sum_{i=1}^{m} e_i \mathbf{M}_k(s_i\ \mathbf{y})$

Factorize $\mathbf{M}_k(s_i\ \mathbf{y}) = \mathbf{L}_k^i \mathbf{R}_k^i$, $\mathbf{L}_k := [\mathbf{L}_k^1 \cdots \mathbf{L}_k^m]$, $\mathbf{R}_k := [\mathbf{R}_k^1 \cdots \mathbf{R}_k^m]^T$

Method 3: `robustsdp`

Robust SDP with $l(\mathbf{x}, \mathbf{e}) = \sum_{i=1}^{m} s_i(\mathbf{x}) e_i$:

$$l^* := \min_{(\mathbf{x},\mathbf{e}) \in \mathbf{X} \times \mathbf{E}} l(\mathbf{x}, \mathbf{e}) \leqslant \lambda_k' := \sup_{\lambda} \quad \lambda$$
$$\text{s.t.} \quad \forall \mathbf{e} \in \mathbf{E}, \ \mathbf{M}_k(l\, \mathbf{y}) \succcurlyeq \lambda \mathbf{M}_k(\mathbf{y}).$$

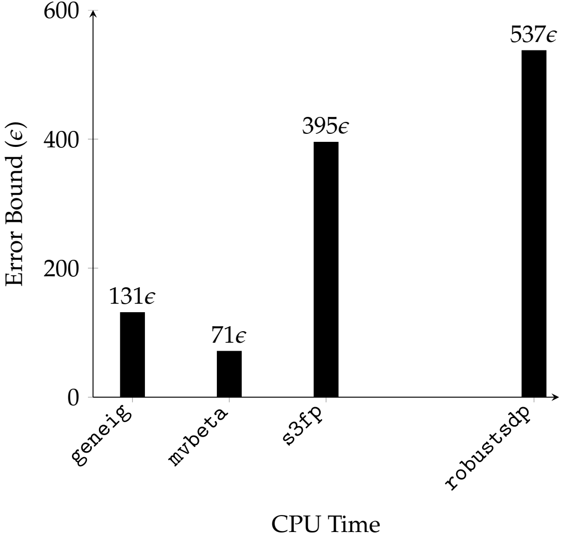
Linearity $\rightsquigarrow \mathbf{M}_k(l\, \mathbf{y}) = \sum_{i=1}^{m} e_i \mathbf{M}_k(s_i\, \mathbf{y})$

Factorize $\mathbf{M}_k(s_i\, \mathbf{y}) = \mathbf{L}_k^i \mathbf{R}_k^i$, $\mathbf{L}_k := [\mathbf{L}_k^1 \cdots \mathbf{L}_k^m]$, $\mathbf{R}_k := [\mathbf{R}_k^1 \cdots \mathbf{R}_k^m]^T$

Theorem following from [El Ghaoui et al. 98]

$$\lambda_k' \downarrow l^* \text{ and } \lambda_k' = \sup_{\lambda, \mathbf{S}, \mathbf{G}} \quad \lambda$$
$$\text{s.t.} \quad \begin{pmatrix} -\lambda \mathbf{M}_k(\mathbf{y}) - \mathbf{L}_k\, \mathbf{S}\, \mathbf{L}_k{}^T & \mathbf{R}_k{}^T + \mathbf{L}_k\, \mathbf{G} \\ \mathbf{R}_k - \mathbf{G}\, \mathbf{L}_k{}^T & \mathbf{S} \end{pmatrix} \succcurlyeq 0,$$
$$\mathbf{S}^T = \mathbf{S}, \mathbf{G}^T = -\mathbf{G}.$$

Benchmark `kepler0` with $k = 2$



Conclusion

Sparse/Robust SDP relaxations for NONLINEAR PROGRAMS:

- Polynomial and transcendental programs
- Certified $\leadsto$ Formal roundoff error bounds
  (Joint work with T. Weisser and B. Werner)
- `Real2Float` open source tool:

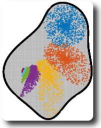
  `http://nl-certify.forge.ocamlcore.org/real2float.html`

Conclusion

Further research:

- Automatic **FPGA** code generation

- Roundoff error analysis with `while`/`for` loops



Master / PhD Positions Available !

End

Thank you for your attention!

http://www-verimag.imag.fr/~magron

- V. Magron, G. Constantinides, A. Donaldson. Certified Roundoff Error Bounds Using Semidefinite Programming, arxiv.org/abs/1507.03331