Symbolic-Numeric Algorithms for Computing Validated Results

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Joint work with E. Kaltofen, M. Safey El Din, A. Greuet, F. Guo, Q. Guo
S. Hutton, B. Li, N. Li, Y. Ma, C. Wang, Z. Yang and Y. Zhu

What is Symbolic-Numeric Computation?

- Definition: the use of software that **combines symbolic and numeric methods** to solve problems [Wikipedia]

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- Definition: the use of software that **combines symbolic and numeric methods** to solve problems [Wikipedia]
- Objective: compute **reliable** results **faster**.
- Challenge: solve mathematical problems that today are **not solvable** by numerical or symbolic methods **alone** [Corless,Kaltofen,Watt 2003]

Computing Validated Results via Symbolic-numeric Algorithm

- Compute an approximate solution of good quality for a given problem using numeric algorithms.

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Validated Results for Two Problems

- Certification using sum-of-squares [Peyrl, Parrilo'07,08; Kaltofen, Li, Yang, Zhi'08,09; Ma, Zhi'10; Monniaux, Corbineau'11; Guo, Kaltofen, Zhi'12; Greuet, Guo, Safey El Din, Zhi'12]
- Verification of solutions of polynomial systems [Beltran, Leykin'12; Hauenstein, Sottile'12; Kanzawa, Oishi'99, Mantzaflaris, Mourrain'11; Rump, Graillat'09, Li, Zhi'12,13,14; Yang, Zhi, Zhu'13]

Certification Using Sum-Of-Squares

Emil Artin's 1927 Theorem (Hilbert's 17th Problem)

$$\forall \xi_1, \ldots, \xi_n \in \mathbb{R}\colon f(\xi_1, \ldots, \xi_n) \geq 0, \quad f \in \mathbb{Q}[X_1, \ldots, X_n]$$

$$\Updownarrow$$

$$\exists u_i, v_j \in \mathbb{Q}[X_1, \ldots, X_n]\colon f(X_1, \ldots, X_n) = \frac{\sum_{i=1}^m u_i^2}{\sum_{j=1}^m v_j^2}$$

$$\Updownarrow$$

$$\exists \textbf{rational } W^{[1]} \succeq 0, W^{[2]} \succeq 0\colon f = \frac{m_d^T \, W^{[1]} \, m_d}{m_e^T \, W^{[2]} \, m_e}$$

with $m_d(X_1, \ldots, X_n)$, $m_e(X_1, \ldots, X_n)$ vectors of terms

$W \succeq 0$ (positive semidefinite)

$\iff W = PL\, D\, L^T P^T$, D diagonal, $D_{i,i} \geq 0$ (Cholesky)

Theodore Motzkin's 1967 Polynomial

$$\begin{aligned}&(3\,\textbf{arithm. mean} - 3\,\textbf{geom. mean})(x^4y^2, x^2y^4, z^6)\\ &= x^4y^2 + x^2y^4 + z^6 - 3x^2y^2z^2\end{aligned}$$

is positive semidefinite (AGM inequality) but **not** a sum-of-squares.

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\end{aligned}
$$

is positive semidefinite (AGM inequality) but **not** a sum-of-squares.

However,

$$
\begin{aligned}
&(x^4y^2 + x^2y^4 + z^6 - 3x^2y^2z^2)(\mathbf{x^2} + \mathbf{y^2} + \mathbf{z^2}) = \\
&\qquad \left(z^4 - x^2y^2\right)^2 + 3\left(xyz^2 - \frac{xy^3}{2} - \frac{x^3y}{2}\right)^2 + \left(\frac{xy^3}{2} - \frac{x^3y}{2}\right)^2 \\
&\qquad + \left(xz^3 - xy^2z\right)^2 + \left(yz^3 - x^2yz\right)^2
\end{aligned}
$$

Theodore Motzkin's 1967 Polynomial

$$(3\,\textbf{arithm. mean} - 3\,\textbf{geom. mean})(x^4y^2, x^2y^4, z^6)$$
$$= x^4y^2 + x^2y^4 + z^6 - 3x^2y^2z^2$$

is positive semidefinite (AGM inequality) but **not** a sum-of-squares.

Moreover,

$$(x^4y^2 + x^2y^4 + z^6 - 3x^2y^2z^2)(\mathbf{x^2} + \mathbf{z^2}) =$$
$$\left(z^4 - x^2y^2\right)^2 + \left(xyz^2 - x^3y\right)^2 + \left(xz^3 - xy^2z\right)^2$$

[Kaltofen,Li,Yang,Zhi JSC 2012]

Semidefinite Programming: Block Form

$A^{[i,j]}, C^{[j]}, W^{[j]}$ are real **symmetric** matrix blocks

$W =$ block diagonal$(W^{[1]}, ..., W^{[k]})$

$$\min_{W^{[1]},\ldots,W^{[k]}} \quad C^{[1]} \bullet W^{[1]} + \cdots + C^{[k]} \bullet W^{[k]}$$

$$\text{s. t.} \quad \begin{bmatrix} A^{[1,1]} \bullet W^{[1]} + \cdots + A^{[1,k]} \bullet W^{[k]} \\ \vdots \\ A^{[m,1]} \bullet W^{[1]} + \cdots + A^{[m,k]} \bullet W^{[k]} \end{bmatrix} = b \in \mathbb{R}^m,$$

$$\boxed{W^{[j]} \succeq 0, W^{[j]} = (W^{[j]})^T, j = 1, \ldots, k}$$

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Note: the Hilbert-Artin form $f \times (m_e^T W^{[2]} m_e) = m_d^T W^{[1]} m_d$ is a feasible solution for $k = 2$; (pure) SOS polynomial has $k = 1$.

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Software: SeDuMi, YALMIP, SOSTOOLS, SparsePOP, SDPT3, VSDP, GloptiPoly

Exact Certification of Optima via Rational SOS

Problems with sum-of-squares certificates:

- Numerical sum-of-squares yields **"≥ 0" approximately**!
- **Exact** optimum is **high-degree/large-height** algebraic number.

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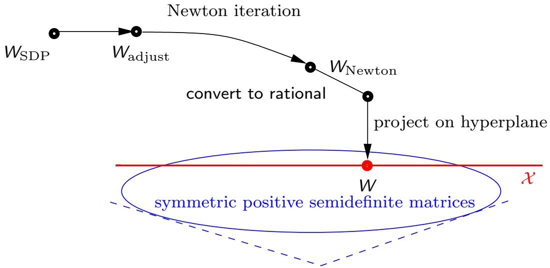
- **Exact** optimum is **high-degree/large-height** algebraic number.

We certify a **rational** lower bound $r \lessapprox r^* = \inf_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x})$ (of small size) via a **rational** matrix W so that the following conditions hold exactly:

$$f(\mathbf{X}) - r = m_d(\mathbf{X})^T \cdot W \cdot m_d(\mathbf{X}),$$
$$W \succeq 0,\ W^T = W$$

Rationalizing Sum-Of-Squares: “Easy Case” $W \succ 0$

[Harrison’07; Peyrl, Parrilo’07, ’08; Kaltofen, Li, Yang, Zhi,’08,’09]

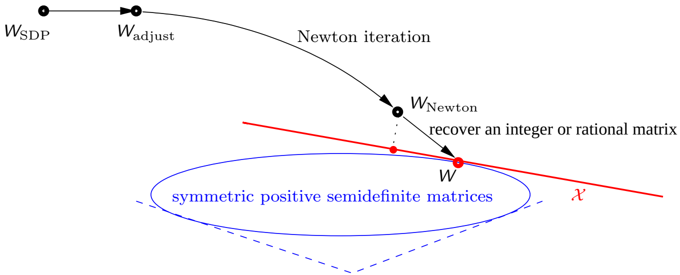


affine linear hyperplane is given by

$$\mathscr{X} = \{A \mid A^T = A, f(\mathbf{X}) - r = m_d(\mathbf{X})^T \cdot A \cdot m_d(\mathbf{X})\}$$

Rationalizing a Sum-Of-Squares: "Hard Case" $W \succeq 0$

[Kaltofen, Li, Yang, Zhi,'08,'09, Monniaux, Corbineau'11]



where the affine linear hyperplane is **tangent** to the cone boundary of singular W: **real optimizers, fewer squares, missing terms**

Rationalizing a Sum-Of-Squares

From **"Hard Case"** to **"Easy Case"**:

- Reducing the dimension of W by removing **extra monomials**.

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- Computing the **minimal number of squares** by matrix completion method.

Rationalizing a Sum-Of-Squares

From **"Hard Case"** to **"Easy Case"**:

- Reducing the dimension of W by removing **extra monomials**.
- Computing the **minimal number of squares** by matrix completion method.
- Computing a hyperplane $\mathscr{X} \subset \mathbb{R}^N$ such that

$$\mathfrak{S}(W) = \{\mathbf{x} \in \mathbb{R}^N \,|\, W(\mathbf{x}) \succeq 0\} \subset \mathscr{X}$$

Rationalizing a Sum-Of-Squares

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Siegfried Rump's 2006 Model Problem

For $n = 1, 2, 3, \ldots$ compute the global minimum μ_n:

$$\mu_n = \min_{P,Q} \frac{\|PQ\|_2^2}{\|P\|_2^2 \|Q\|_2^2}$$

$$\text{s. t. } P(Z) = \sum_{i=1}^{n} p_i Z^{i-1}, Q(Z) = \sum_{i=1}^{n} q_i Z^{i-1} \in \mathbb{R}[Z] \setminus \{0\}$$

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- $n \leq 8$ using Gröbner bases by Mohab Safey El Din.
- $n \leq 8$ using COSY package by Kyoko Makino.
- $n \leq 12$ using SOSTOOLS and INTLAB by Siegfried Rump.

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Let $f(\mathbf{X}) = \|PQ\|_2^2$, $g(\mathbf{X}) = \|P\|_2^2 \|Q\|_2^2$,

$$\left.\begin{array}{lll} \mu_n^\star := \sup\limits_{r \in \mathbb{R}, W} & r & \\ \text{s. t.} & f(\mathbf{X}) - r g(\mathbf{X}) = m_d(\mathbf{X})^T \cdot W \cdot m_d(\mathbf{X}) & \\ & W \succeq 0, W^T = W & \end{array}\right\}$$

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- $\mathbf{X} = \{p_1, \ldots, p_{\lceil n/2 \rceil}\} \cup \{q_1, \ldots, q_{\lceil n/2 \rceil}\}$, because P, Q achieving μ_n must be **symmetric or skew-symmetric.** [Rump and Sekigawa'06]

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  - $m_d(\mathbf{X})$ is a monomial vector restricted to $p_i q_j$.

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  - Exact W has corank 1 when n is even and corank 2 when n is odd.

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  - $m_d(\mathbf{X})$ is a monomial vector restricted to $p_i q_j$.
  - Exact W has corank 1 when n is even and corank 2 when n is odd.
  - Certify a **slightly perturbed** lower bound with a W of **full rank**.

Certified Lower Bounds by Multiple Precision SDP

[Kaltofen,Li,Yang,Zhi'12, Guo'10]

n	k	# iter	prec.	secs/iter	lower bound r_n	upper bound
4	2	50	4×15	0.71	0.0174291733214326528**8**	0.0174291733214326528**9**
5	1	50	4×15	2.03	0.0023395955481555911**2**	0.0023395955481555911**3**
6	2	50	4×15	1.76	0.0002897318752796819**2**	0.0002897318752796819**3**
7	1	75	5×15	11.36	0.0000341850698000828**4**	0.0000341850698000828**5**
8	2	75	5×15	12.49	0.0000039054356497557**2**	0.0000039054356497557**3**
9	1	75	5×15	84.12	0.43600165391810484613e–06	0.43600165391810484613e–06
10	2	75	5×15	92.79	0.47839395687709759327e–07	0.47839395687709759327e–07
11	1	85	5×15	622.03	0.51787490974469905331e–08	0.51787490974469905331e–08
12	2	85	5×15	634.48	0.554588183116313476**1e–09**	0.554588183116313476**2e–09**
13	1	100	5×15	3800.0	0.58866880811866093130e–10	0.58866880811866093130e–10
14	2	100	5×15	3800.00	0.62024449920539050**219e–11**	0.62024449920539050**220e–11**
15	1	120	6×15	15000.00	0.64943654185809512880e–12	0.64943654185809512880e–12
16	2	120	6×15	23000.00	0.6763604255822137905**7e–13**	0.6763604255822137905**8e–13**
17	1	70	6×15	72400.00	0.70112631**896355325150e–14**	0.70112631**970143741585e–14**
18	2	50	6×15	95720.00	0.7**1154604865069396988e–15**	0.7**2383944796943875862e–15**

Rationalizing a Sum-Of-Squares

From **"Hard Case"** to **"Easy Case"**:

- Reducing the dimension of W by removing extra monomials.
- Computing the **minimal number of squares** by matrix completion method.

Example: *Voronoi2* [Everett,Lazard,Lazard,Safey El Din'07]

Voronoi2(a,α,β,X,Y) has 253 monomials

$$a^{12}\alpha^6 + a^{12}\alpha^4 - 4a^{11}\alpha^5 Y + 10a^{11}\alpha^4\beta X + \underbrace{\cdots}_{248 \text{ terms}} + 20a^{10}\alpha^2 X^2.$$

- The singular values of the computed Gram matrix $W_{118\times 118}$:

$$196, 152.78, 152.29, 107.36, 68.64, 61.48, \mathbf{43.05}, 42.58, 25.06, \cdots$$

- Compute the truncated Cholesky decomposition of $W \approx \hat{L}\hat{L}^T$ w.r.t. tolerance $\mathbf{43}$ and obtain

$$\textit{Voronoi2} \approx \mathbf{g_1^2} + \mathbf{g_2^2} + \cdots + \mathbf{g_7^2} \qquad (*)$$

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$$\textit{Voronoi2} \approx \mathbf{g_1^2}+\mathbf{g_2^2}+\cdots+\mathbf{g_7^2} \qquad (*)$$

- Apply Gauss-Newton iterations to refine $(*)$, after 30 iterations, we truncate $\tilde{L}\,\tilde{L}^T$ to an **integer matrix** $W=LDL^T$:

$$\textit{Voronoi2}=\mathbf{f_1^2}+\frac{\mathbf{1}}{\mathbf{16}}\mathbf{f_2^2}+\mathbf{f_3^2}+\frac{\mathbf{1}}{\mathbf{28}}\mathbf{f_4^2}+\frac{\mathbf{7}}{\mathbf{27}}\mathbf{f_5^2},$$

where $f_i \in \mathbb{Q}[a,\alpha,\beta,X,Y]$.

Sum of Minimal Number of Squares

Represent $f(X_1,\dots,X_n)$ as a sum of **minimal number** of squares of polynomials in $\mathbb{Q}[X_1,\dots,X_n]$

$$\exists \text{ minimal number of } u_i\colon f(X_1,\dots,X_n) = \sum_{i=1}^{\min\ k} u_i(X_1,\dots,X_n)^2$$

$$\Updownarrow$$

$$\exists\, W \succeq 0 \text{ of minimal rank}\colon f = m_d(X_1,\dots,X_n)^T \cdot W \cdot m_d(X_1,\dots,X_n)$$

$$= \sum_{i=1}^{\min\ \text{rank}\ W} (\sqrt{D_{i,i}}\, L_i \cdot m_d(X_1,\dots,X_n))^2$$

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Note: SDP solvers based on interior point method return matrices with **maximum rank** [Klerk, Roos and Terlaky'97].

Low-rank Gram Matrix Completion Problem

Find a Gram matrix of the **lowest rank** satisfying
$f = m_d(\mathbf{X})^T\, W\, m_d(\mathbf{X})$

Rank Minimization:

$$\begin{array}{ll} \min & \operatorname{rank}(W) \\ \text{s. t.} & \mathbb{A}(W) = b \\ & W \succeq 0,\, W^T = W \end{array}$$

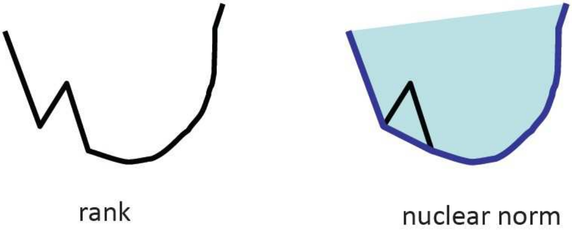
Nuclear Norm Minimization:

$$\begin{array}{ll} \min & \|W\|_* \\ \text{s. t.} & \mathbb{A}(W) = b \\ & W \succeq 0,\, W^T = W \end{array}$$

- $\mathbb{A} : \mathbb{S}^n \to \mathbb{R}^m,\ b \in \mathbb{R}^m$.
- $\|W\|_* = \Sigma_i \sigma_i$, $\sigma_i = i$-th singular value of the matrix W.
  When $W \succeq 0$, $\|W\|_* = \Sigma_i \lambda_i = \mathrm{Tr}(W)$, $\lambda = i$-th eigenvalue of W.

Why is the Nuclear Norm Relevant?

- Bad **nonconvex** problem $\Longrightarrow$ **Convex** problem!
- Nuclear norm is the **"best"** convex approximation of the rank function. [Fazel's PhD thesis'02]
- [Parrilo'10]



Nuclear Norm Regularized Least Squares

Nuclear norm minimization:

$$\begin{array}{ll} \min & \|W\|_* \\ \text{s. t.} & \mathbb{A}(W) = b \\ & W \succeq 0, W^T = W \end{array}$$

The constraints $\mathbb{A}(W) = b$ can be relaxed, resulting the nuclear norm regularized LS problem

$$\min_{W \in \mathbb{S}_+^n} \ \mu \|W\|_* + \frac{1}{2}\|\mathbb{A}(W) - b\|_2^2$$

where $\mathbb{S}_+^n$ is the set of symmetric positive semidefinite matrices and $\mu > 0$ is a given parameter.

Modified Fixed Point Iterative Method

Starting with $X^0 = 0$, inductively define for $k = 1, 2, \ldots$

$$\begin{cases} Z^k & = & X^k + \frac{t_{k-1}-1}{t_k}(X^k - X^{k-1}) \\ Y^k & = & Z^k - \tau_k \mathbb{A}^*(\mathbb{A}(Z^k) - b) \\ X^{k+1} & = & \mathscr{T}_{\tau\mu}(Y^k) \\ t_{k+1} & = & \frac{1+\sqrt{1+4t_k^2}}{2} \end{cases}$$

where $\mathbb{A}^* : \mathbb{R}^m \to \mathbb{S}^n$ is the adjoint of $\mathbb{A}$ and $\tau, \mu > 0$.

Matrix Thresholding Operator: Assume $W = Q \cdot \Lambda \cdot Q^T$, where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$. For any $\nu \geq 0$,

$$\mathscr{T}_\nu(W) := Q \cdot \text{diag}(\{\lambda_i - \nu\}_+) \cdot Q^T,$$

where $t_+ = \max(t, 0)$.

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Matrix Thresholding Operator: Assume $W = Q \cdot \Lambda \cdot Q^T$, where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. For any $\nu \geq 0$,

$$\mathscr{T}_\nu(W) := Q \cdot \mathrm{diag}(\{\lambda_i - \nu\}_+) \cdot Q^T,$$

where $t_+ = \max(t, 0)$.

We **only** compute eigenvalues which are **larger** than $\tau\mu$.

Exact SOS certificates: $m_d(x)$ is dense

Examples			Results				Gauss-Newton iteration		
n/r	p	FR	solvers	rank	θ	time (s)	rank	θ	time (s)
200/ 5	1221	0.81	AFPC-BB	14	3.63e+0	1.07e+1	5	6.95e-10	4.02e+2
			SDPNAL	21	2.83e+0	1.06e+1	5	6.91e-10	5.57e+2
			SeDuMi	200	2.58e-1	5.56e+1	5	7.18e-10	1.10e+3
300/ 5	1932	0.77	AFPC-BB	14	2.23e+1	2.32e+1	5	1.38e-9	5.61e+2
			SDPNAL	25	2.51e+0	2.69e+1	5	1.08e-9	7.05e+2
			SeDuMi	300	4.75e-1	2.62e+2	5	1.13e-9	6.89e+2
400/ 5	2610	0.76	AFPC-BB	15	1.25e+1	6.23e+1	5	5.83e-7	1.22e+3
			SDPNAL	27	2.09e+0	8.69e+1	5	2.34e-8	5.03e+3
			SeDuMi	399	3.38e-1	4.88e+2	5	4.39e-8	5.03e+3
500/ 5	5124	0.48	AFPC-BB	17	2.48e+1	5.33e+1	5	1.48e-5	7.92e+3
			SDPNAL	38	6.33e+0	2.53e+2	5	4.91e-8	1.84e+4
			SeDuMi	–	–	–	–	–	–

SDPNAL: [Zhao,Sun,Toh'10]; SeDuMi: [Sturm'99, Löfberg'04];
n the dimension, r the rank, p the number of linear constrains;
$FR = r(2n-r+1)/2p$ degrees of freedom ratio;
$\theta = \|f(x) - m_d(x)^T \cdot W \cdot m_d(x)\|_2$ the error.

Exact SOS certificates: $m_d(\mathbf{X})$ is sparse

Problems				AFPC-BB			SDPNAL		
n	r	p	FR	rank	θ	time (s)	rank	θ	time (s)
500	20	24240	0.40	20	1.50e+1	4.48e+1	113	4.23e+1	6.72e+2
1000	10	27101	0.36	10	2.21e+1	3.70e+2	99	8.80e+1	2.70e+3
1000	50	95367	0.51	50	1.01e+1	6.56e+2	218	9.20e+1	9.92e+3
1500	10	45599	0.32	10	3.31e+1	1.00e+3	121	3.41e+1	3.72e+4
1500	50	122742	0.60	50	1.51e+1	3.84e+3	226	3.79e+1	1.36e+4

For the problem with $n = 1500, r = 50$, f has **122402** monomials

$$f = 498w^{34}x^4z^2 - 160w^{31}x^3y^2z^3 + 58x^6z^2 + \underbrace{\cdots}_{122399 \text{ terms}}$$

We can recover the **exact SOS** certificate **without G-N refinement**.

Rationalizing a Sum-Of-Squares

From **"Hard Case"** to **"Easy Case"**:

- Reducing the dimension of W by removing extra monomials.
- Computing the minimal number of squares by matrix completion method.
- Computing a **hyperplane** $\mathscr{X} \subset \mathbb{R}^N$ such that

$$\mathfrak{S}(W) = \{\mathbf{x} \in \mathbb{R}^N \,|\, W(\mathbf{x}) \succeq 0\} \subset \mathscr{X}$$

Certificates for Low Dimensionality of $\mathfrak{S}(\mathsf{W})$

- Let $W \in \mathbb{S}^n$, then $\mathfrak{S}(\mathsf{W})$ has an **empty** interior

$$\Longleftrightarrow \exists \mathbf{u}_1, \ldots, \mathbf{u}_s \in \mathbb{R}^n \backslash \{\mathbf{0}\}, s \leq n, \ s.t. \ \sum_{i=1}^{s} \mathbf{u}_i^T \cdot \mathsf{W} \cdot \mathbf{u}_i = 0.$$

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$$\mathsf{W}' = \mathsf{P}^T \cdot \mathsf{W} \cdot \mathsf{P} = \begin{bmatrix} \mathscr{L}_1 & \mathscr{L}_2 & \cdots & \mathscr{L}_n \\ \mathscr{L}_2 & & & \\ \vdots & & \widehat{\mathsf{W}} & \\ \mathscr{L}_n & & & \end{bmatrix}.$$

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- For any $\mathscr{L}_i \neq 0$, there exists $A \succeq 0$ s.t. $-\mathscr{L}_i^2 = \mathrm{tr}(AW)$. Therefore

$$(a_1, \ldots, a_k) \in \mathfrak{S}(\mathsf{W}) \Longrightarrow \mathscr{L}_i(a_1, \ldots, a_k) = 0$$

$$\Longrightarrow \mathfrak{S}(\mathsf{W}) \subset \mathscr{X} = \{\mathscr{L}_1, \ldots, \mathscr{L}_n\}$$

[Klep,Schweighofer'13, Guo,Safey El Din,Zhi'13]

Infeasibility Certificates of SOS over $\mathbb{R}[\mathbf{X}]$

Given $y = (y_\alpha) \in \mathbb{R}^{\mathbb{N}^n}$, for $f = \sum_\alpha f_\alpha \mathbf{X}^\alpha \in \mathbb{R}[\mathbf{X}] = \mathbb{R}[X_1, \ldots, X_n]$, define

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[Guo,Kaltofen,Zhi'12] The following are equivalent:

1. $f \notin SOS/SOS_{\deg \leq 2e} = \left\{ \sum u_i^2 / \sum v_j^2 \mid u_i, v_j \in \mathbb{R}[\mathbf{X}],\ \deg v_j \leq e \right\}$.
2. $\exists y' \in \mathbb{Q}^m$, *s.t.* $\forall v, u \in \mathbb{R}[\mathbf{X}]$ *with* $\deg v \leq e$, $\deg u \leq e + (\deg f)/2$, *we have* $L_{y'}(u^2) \geq 0$ *and* $L_{y'}(f v^2) < 0$.

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Special case: $e = 0$ [Ahmadi and Parrilo'09]

Even Symmetric Sextics [Choi et al.1987]

Let $M_r(\mathbf{X}) = \sum_{i=1}^{n} X_i^r$, for integer $0 \le k \le n-1$, we define forms $f_{n,k}$ by

$$\begin{cases} f_{n,0} &= -nM_6 + (n+1)M_2M_4 - M_2^3, \\ f_{n,k} &= (k^2+k)M_6 - (2k+1)M_2M_4 + M_2^3,\ 1 \le k \le n-1. \end{cases}$$

For $n = 4, 5, 6$, we can certify that the polynomials

$$f_{4,2}, f_{5,2}, f_{6,2} \notin \mathsf{SOS}/\mathsf{SOS}_{\deg \le 2}$$

and

$$f_{5,3}, f_{6,3}, f_{6,4} \notin \mathsf{SOS}/\mathsf{SOS}_{\deg \le 4}$$

To our knowledge, they are the **first** PSD polynomials which can not be written as $\sum_i u_i^2 / \sum_j v_j^2$ with $\deg \sum_j v_j^2 = 4$!

An Ill-Posed Polynomial

Consider polynomial $f(X,Y) = X^2 + Y^2 - 2XY = (X-Y)^2$.

$$\forall \varepsilon > 0,\ f_\varepsilon(X,Y) = (1-\varepsilon^2)X^2 + Y^2 - 2XY$$

is not **SOS**. Take $x = y = C$, $f_\varepsilon(x,y) = -\varepsilon^2 C^2 \Rightarrow \inf \mathbf{f}_\varepsilon = -\infty$. **Ill-posed!**

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- For $\varepsilon = 10^{-1},\ 10^{-2},\ 10^{-3},\ 10^{-4}$, SDP solver SeDuMi in Matlab can **numerically** detect f_ε is not SOS. But for $\varepsilon = 10^{-5}$ or smaller, it **fails!**

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- Our method in Maple can give **exact** certificate of f_ε being **not SOS** for $\varepsilon = 10^{-8}$ or smaller!

  [Guo,Kaltofen,Zhi'12]

Infeasibility Certificates of SOS over $\mathbb{Q}[\mathbf{X}]$

Sturmfels' question

Let $f \in \mathbb{Q}[Y_1, \ldots, Y_n]$ s.t. $f = g_1^2 + \cdots + g_s^2$ (with $g_i \in \mathbb{R}[Y_1, \ldots, Y_n]$). Do there exist $h_1, \ldots, h_p \in \mathbb{Q}[Y_1, \ldots, Y_n]$ s.t. $f = h_1^2 + \cdots + h_p^2$?

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Scheiderer's counter example to Sturmfels' question (2012):

$$f = x^4 + xy^3 + y^4 - 3x^2yz - 4xy^2z + 2x^2z^2 + xz^3 + yz^3 + z^4$$

has **only** SOS decompositions over **the reals**:

$$\begin{aligned} f &= \left(x^2 + y^2\alpha - \frac{yz}{2} + \frac{1}{4}\frac{z^2(1+4\alpha)}{\alpha}\right)^2 \\ &\quad -2\alpha\left(xy - \frac{1}{4}\frac{y^2}{\alpha} + \frac{1}{2}\frac{xz}{\alpha} + yz\alpha - \frac{z^2}{2}\right)^2, \end{aligned}$$

where α is a **negative** real number satisfies $-1 - 8\alpha + 8\alpha^3 = 0$.

Scheiderer's Counter Example

Suppose

$$f = [x^2, xy, y^2, xz, yz, z^2] \cdot \mathsf{W} \cdot [x^2, xy, y^2, xz, yz, z^2]^T,$$

the Gram matrix W of f is a 6×6 symmetric matrix

$$\mathsf{W} = \begin{bmatrix} 1 & 0 & X_1 & 0 & -\frac{3}{2} - X_2 & X_3 \\ 0 & -2X_1 & \frac{1}{2} & X_2 & -2 - X_4 & -X_5 \\ X_1 & \frac{1}{2} & 1 & X_4 & 0 & X_6 \\ 0 & X_2 & X_4 & -2X_3 + 2 & X_5 & \frac{1}{2} \\ -\frac{3}{2} - X_2 & -2 - X_4 & 0 & X_5 & -2X_6 & \frac{1}{2} \\ X_3 & -X_5 & X_6 & \frac{1}{2} & \frac{1}{2} & 1 \end{bmatrix}$$

We have $\mathfrak{S}(\mathsf{W}) = \{\mathbf{x} \in \mathbb{R}^6 \,|\, \mathsf{W}(\mathbf{x}) \succeq 0\} \neq \emptyset$ but $\mathfrak{S}(\mathsf{W}) \cap \mathbb{Q}^6 = \emptyset$.

Find rational points in $\mathfrak{S}(\mathsf{W})$ [Guo,Safey El Din,Zhi'13]

Consider $\mathsf{W} = \mathsf{W}_0 + X_1\mathsf{W}_1 + \cdots + X_k\mathsf{W}_k \succeq 0$, $\mathsf{W}_0, \ldots, \mathsf{W}_k$ are $(D \times D)$ symmetric matrices with entries in $\mathbb{Q}$ of bit size $\leq \tau$.

- Decide if $\mathfrak{S}(\mathsf{W}) \cap \mathbb{Q}^k \neq \emptyset$ within $\mathbf{(k\tau)^{O(1)} 2^{O(\min(k,D)D^2)} D^{O(D^2)}}$ bit operations.
- Return **rational points** in $\mathfrak{S}(\mathsf{W})$ whose coordinates have bit length $\leq \boldsymbol{\tau}^{\mathbf{O(1)}} \mathbf{2}^{\mathbf{O(\min(k,D)D^2)}}$.

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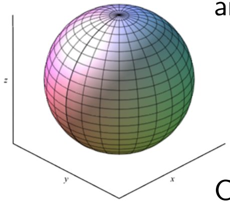
Certificates for SOS decompositions over $\mathbb{Q}$ [Guo,Safey El Din,Zhi'13]

Let $f \in \mathbb{Q}[Y_1, \ldots, Y_n]$ with coefficients of bit size $\leq \tau$ and $\deg(f) = 2d$.

- Decide if $f = \sum f_i^2, f_i \in \mathbb{Q}[Y_1, \ldots, Y_n]$ within $\tau^{\mathbf{O(1)}}\mathbf{2}^{\mathbf{O(M(d,n)^3)}}$ bit operations. ($\tau^{O(1)}\mathsf{M}(d,n)^{\mathsf{M}(d,n)^6}$ in [Safey El Din,Zhi'10])
- The bit lengths of rational coefficients of the f_i's: $\tau^{\mathbf{O(1)}}\mathbf{2}^{\mathbf{O(M(d,n)^3)}}$.
- **"Computer-validation"** for Scheiderer's counter example.

Full Dimensional Case



Let $W = W_0 + X_1 W_1 + \cdots + X_k W_k$ where $W_0, \ldots, W_k$ are $(D \times D)$ symmetric matrices with entries in $\mathbb{Q}$.

- **characteristic polynomial** of W: $y^D + m_{D-1} y^{D-1} + \cdots + m_0$
- $\Psi = \{(-1)^{(i+D)} m_i > 0,\ 0 \leq i \leq D-1\}$

Critical point method (Grigoriev, Vorobjov, Canny, Heintz, Solerno, Renegar, Basu, Pollack, Roy, Safey El Din)

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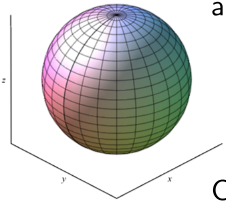

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Scheiderer's counter example

Ψ have 6 inequalities with 6 indeterminates, apply the routine HasRealSolutions in RAGLib (Safey El Din) to compute

$$\mathscr{U} = \mathrm{OpenDecision}(\Psi).$$

The set $\mathscr{U}$ is **empty** $\Longrightarrow$ $\mathfrak{S}(W)$ is **not full dimensional**.

Low Dimensional Case

Certificates for low dimensionality of $\mathfrak{S}(\mathsf{W})$ [Klep,Schweighofer'13]

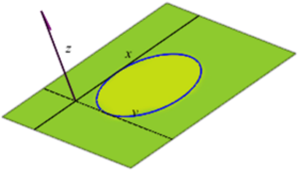
- Assume $\mathfrak{S}(\mathsf{W})$ has an **empty** interior, $\nexists\, \mathbf{u} \in \mathbb{R}^D \backslash \{\mathbf{0}\}$ s.t. $\mathsf{W} \cdot \mathbf{u} = \mathbf{0}$

$$\Longleftrightarrow \exists \mathbf{u}_1, \ldots, \mathbf{u}_s \in \mathbb{R}^D \backslash \{\mathbf{0}\}, 1 \leq s \leq D, s.t. \sum_{i=1}^{s} \mathbf{u}_i^T \cdot \mathsf{W} \cdot \mathbf{u}_i = 0.$$

- Assume $u_{11} \neq 0$, let $\mathsf{P} = [\mathbf{u}_1, \mathsf{e}_2, \ldots, \mathsf{e}_\mathsf{D}]$,

$$\mathsf{W}' = \mathsf{P}^T \cdot \mathsf{W} \cdot \mathsf{P} = \begin{bmatrix} \mathscr{L}_1 & \mathscr{L}_2 & \cdots & \mathscr{L}_D \\ \mathscr{L}_2 & & & \\ \vdots & & \widehat{\mathsf{W}} & \\ \mathscr{L}_D & & & \end{bmatrix}, \ \mathscr{L}_1, \ldots, \mathscr{L}_D \in \mathbb{R}[X_1, \ldots, X_k],$$

- $(a_1, \ldots, a_k) \in \mathfrak{S}(\mathsf{W}) \Longrightarrow \mathscr{L}_i(a_1, \ldots, a_k) = 0, i = 1, \ldots, D.$



Scheiderer's Counter Example (II)

- Using the routine RUR [Rouillier'99], we get a real algebraic vector

$$\mathbf{u} = \left[-1 + \frac{1}{2}\,\vartheta + \frac{1}{2}\,\vartheta^4, \frac{\vartheta^3}{2} + \frac{1}{2}, \vartheta^2, -2\,\vartheta + \frac{1}{2}\,\vartheta^2 + \frac{1}{2}\,\vartheta^5, \vartheta, 1\right]^T$$

$$\text{s.t. } \mathbf{u}^T \cdot \mathsf{W} \cdot \mathbf{u} = 0,\ \vartheta^6 - 4\,\vartheta^2 - 1 = 0.$$

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$$\text{s.t. } \mathbf{u}^T \cdot \mathsf{W} \cdot \mathbf{u} = 0,\ \vartheta^6 - 4\,\vartheta^2 - 1 = 0.$$

- Construct $\mathsf{P} = [\mathbf{u}, \mathsf{e}_2, \ldots, \mathsf{e}_6]$, $\mathsf{W}' = \mathsf{P}^T \cdot \mathsf{W} \cdot \mathsf{P}$, real linear forms $\mathscr{L}_1, \ldots, \mathscr{L}_6$ are the entries of the first column of W':

$$\begin{bmatrix} \mathscr{L}_1 \\ \mathscr{L}_2 \\ \mathscr{L}_3 \\ \mathscr{L}_4 \\ \mathscr{L}_5 \\ \mathscr{L}_6 \end{bmatrix} = \begin{bmatrix} & & 0 & \\ \frac{1}{2}\,X_2\,\vartheta^5 & & +\cdots & -X_1 - X_5 \\ \frac{1}{2}\,X_4\,\vartheta^5 & +\frac{1}{2}\,X_1\,\vartheta^4 & +\ldots & -X_1 + X_6 + \frac{1}{4} \\ (1 - X_3)\,\vartheta^5 & & +\ldots & +\frac{1}{2} + \frac{1}{2}\,X_2 \\ \frac{1}{2}\,X_5\,\vartheta^5 & -(\frac{3}{4} + \frac{1}{2}\,X_2)\,\vartheta^4 & +\ldots & +1 + X_2 - \frac{1}{2}\,X_4 \\ \frac{1}{4}\,\vartheta^5 & +\frac{1}{2}\,X_3\,\vartheta^4 & +\ldots & -X_3 + 1 - \frac{1}{2}\,X_5 \end{bmatrix}$$

Rational Linear Forms

Let $\mathscr{L}_i = l_{i,\delta-1}(X_1,\ldots,X_k)\vartheta^{\delta-1} + \cdots + l_{i,0}(X_1,\ldots,X_k)$, we have

$$\{\mathbf{x} \in \mathbb{Q}^k \,|\, \mathscr{L}_i(\mathbf{x}) = 0\} \neq \emptyset \iff \{\mathbf{x} \in \mathbb{Q}^k \,|\, l_{i,0}(\mathbf{x}) = \ldots = l_{i,\delta-1}(\mathbf{x}) = 0\} \neq \emptyset$$

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[Guo,Safey El Din,Zhi'13]

- Set $L_j = [l_{1,j},\ldots,l_{D,j}]^T$, $[L_0,\ldots,L_{\delta-1}]=0$ has **no solutions** $\Longrightarrow \mathfrak{S}(\mathsf{W})$ has **no rational solutions**!
- Otherwise, apply Gaussian elimination, we obtain $\mathsf{W}' \longrightarrow \begin{bmatrix} 0 & \mathbf{0} \\ \mathbf{0} & \widetilde{\mathsf{W}} \end{bmatrix}$, $\mathfrak{S}(\widetilde{\mathsf{W}})\cap\mathbb{Q}^{k'} = \mathsf{proj}(\mathfrak{S}(\mathsf{W})\cap\mathbb{Q}^k)$, $k'\leq k$.

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A computer validation for Scheiderer's counter example

$$L_5 = \left[0, \frac{1}{2}X_2, \frac{1}{2}X_4, 1-X_3, \frac{1}{2}X_5, \frac{1}{4}\right]^T,$$

$L_5 = \mathbf{0}$ has **no solutions** $\Longrightarrow \mathfrak{S}(\mathsf{W})$ has **no rational solutions**!

SOS Certificates for Lower Bounds: Constraint Case

Let $V \subset \mathbb{R}^n$ be a real algebraic variety defined by

$$f_1(\mathbf{X}) = \cdots = f_p(\mathbf{X}) = 0$$

with $F = (f_1, \ldots, f_p) \subset \mathbb{Q}[X_1, \ldots, X_n]$.

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- When f^* is **reached** over V [Demmel, Nie, Powers, Sturmfels]:

$$f - f^* + \varepsilon = \mathsf{SOS} \mod \mathbf{F}, \mathsf{MaxMinors}(\mathrm{jac}([f, \mathbf{F}]))$$

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- When f^* is reached at **infinity** (generalized critical values):
  - [Schweighofer'06]: Gradient tentacle
  - [Hà,Pham'08,Hà,Pham'10]: Truncated tangency variety
  - [Greuet,Guo,Safey El Din,Zhi'12]: Modified polar variety

Polar Varieties [Bank, Giusti, Heintz, Mbakop, Pardo, Safey, Schost]

Let W_{n-i+1} be **zero-set** of $\mathbf{F}$ and $\mathrm{MaxMinors}(\mathrm{jac}(\mathbf{F},\mathbf{X}_{\geq i+1}))$. In generic coordinates, the polar variety W_{n-i+1} is the **critical locus** of

$$\pi_i : (X_1,\ldots,X_n) \longrightarrow (X_1,\ldots,X_i)$$

restricted to $V(\mathbf{F})$.

- $\mathrm{codim} W_{n-i+1} = n-i+1$ and $\dim(W_{n-i+1} \cap V(X_1,\ldots,X_{i-1})) = 0$
- $\bigcup_{i=1}^{n-s} (W_{n-i+1} \cap V(X_1,\ldots,X_{i-1})) \cap \mathbb{R}^n = \emptyset \Leftrightarrow V \cap \mathbb{R}^n = \emptyset$

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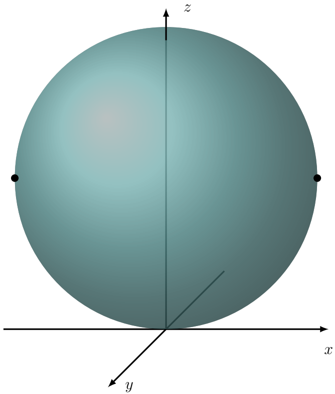
Modified Polar Varieties [Greuet,Guo,Safey El Din,Zhi'12]

Let W_{n-i+1} be **zero-set** of $\mathbf{F}, \text{MaxMinors}(\text{jac}([f, \mathbf{F}], \mathbf{X}_{\geq i+1}))$

- $W = \bigcup W_{n-i+1} \cap V(X_1, \ldots, X_{i-1})$ has dimension 1
- $f(V \cap \mathbb{R}^n) = f(W \cap \mathbb{R}^n)$

Polar Varieties: Example

- $f = x$, $g = x^2 + y^2 + (z-1)^2 - 1$,
- $V = V(g)$.



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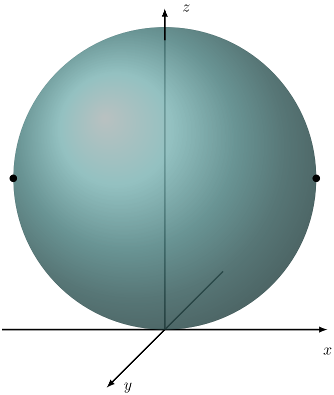
- $W_3 = V \rightarrow \dim 2$;



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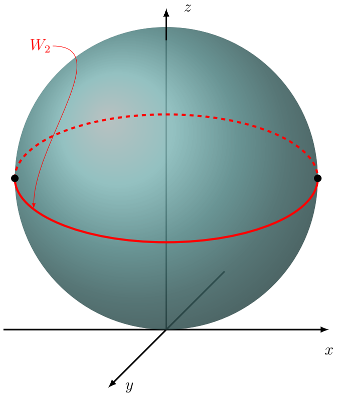

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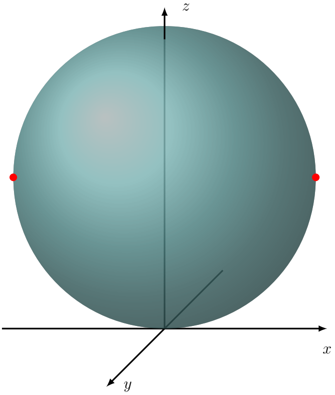

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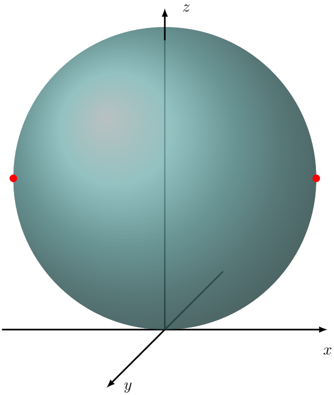
$\to f(V \cap \mathbb{R}^n)$ and $f(W_i \cap \mathbb{R}^n)$: same extrema



Existence of SOS certificates

Asymptotic values over S: $\{y \in \mathbb{R} \mid \exists x_k \subset S, \|x_k\| \to \infty, f(x_k) \to y\}$

Theorem (Schweighofer 2006)

$f, h_1, \ldots, h_m \in \mathbb{R}[X_1, \ldots, X_n]$, $S = \{\mathbf{x} \in \mathbb{R}^n \mid h_1(\mathbf{x}) \geq 0, \ldots, h_m(\mathbf{x}) \geq 0\}$ and

1. $f > 0$ over S and f bounded over S;
2. asymptotic values over $S \to$ finite subset of $]0, +\infty[$.

Then

$$f = \sum_{\delta \in \{0,1\}^m} \text{SOS } h_1^{\delta_1} \cdots h_m^{\delta_m}$$

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Modified Polar Varieties $\to W$ of **dimension** 1, $f(V \cap \mathbb{R}^n) = f(W \cap \mathbb{R}^n)$

Existence Theorem (Greuet,Guo,Safey El Din,Zhi'12)

Let $B > f^\star$, up to a **generic** linear change of coordinates

$$f - f^\star + \varepsilon = \text{SOS} + \text{SOS}(B - f) \bmod I(W) \text{ in } \mathbb{R}[X_1, \ldots, X_n]$$

Numerical Instabilities Coming from Asymptotic Values

Consider the problem $f^* = \inf_{x,y \in \mathbb{R}} f(x,y) := (1-xy)^2 + y^2$,

$$\left.\begin{array}{l} \sup\limits_{r \in \mathbb{R}} \quad r \\ f(X) - r \equiv m_{d_1}(X)^T \cdot W \cdot m_{d_1}(X) + m_{d_2}(X)^T \cdot V \cdot m_{d_2}(X) \cdot (M - f) \bmod \langle \ \dfrac{\partial f}{\partial x} \ \rangle \\ W \succeq 0, \quad W^T = W, \quad V \succeq 0, \quad V^T = V. \end{array}\right\}$$

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where $m_{d_1}(X) = m_{d_2}(X) := [1, x, y, x^2, xy, y^2]$. It dual problem is:

$$\inf_{y_\alpha\in\mathbb{R}} \quad \sum_\alpha f_\alpha y_\alpha, \quad P \succeq 0, \quad Q \succeq 0,$$

$$P = \begin{bmatrix} y_{0,0} & \cdot & \cdot & \cdot & \cdot & y_{0,2} \\ y_{1,0} & \cdot & \cdot & \cdot & \cdot & y_{1,2} \\ y_{0,1} & \cdot & \cdot & \cdot & \cdot & y_{0,3} \\ y_{2,0} & \cdot & \cdot & \cdot & \cdot & y_{2,2} \\ y_{1,1} & \cdot & \cdot & \cdot & \cdot & y_{1,3} \\ y_{0,2} & \cdot & \cdot & \cdot & \cdot & y_{0,4} \end{bmatrix} \quad Q = \begin{bmatrix} 4y_{0,0} + y_{1,1} - y_{0,2} & \cdot & \cdot & \cdot & 5y_{1,1} - y_{0,2} & \cdot \\ 4y_{1,0} - y_{0,1} + y_{2,1} & \cdot & \cdot & \cdot & 5y_{2,1} - y_{0,1} & \cdot \\ 5y_{0,1} - y_{0,3} & \cdot & \cdot & \cdot & 5y_{0,1} - y_{0,3} & \cdot \\ y_{3,1} - y_{1,1} + 4y_{2,0} & \cdot & \cdot & \cdot & 5y_{3,1} - y_{1,1} & \cdot \\ 5y_{1,1} - y_{0,2} & \cdot & \cdot & \cdot & 5y_{1,1} - y_{0,2} & \cdot \\ 5y_{0,2} - y_{0,4} & \cdot & \cdot & \cdot & 5y_{0,2} - y_{0,4} & \cdot \end{bmatrix}$$

Unbounded Moment Matrices

Denote the optimal point $p^* = (x^*, y^*)$ of $f = (1 - xy)^2 + y^2$,

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- $y_{i,j} \to \infty$ with $i > j$;
- The moment matrices P and Q are **unbounded** at the minimizer.

Exploit the Sparsity Structure

- Reduce to $m_{d_1} = [1, y, xy, y^2]$, $m_{d_2} = [1, y, xy]$

$$P = \begin{bmatrix} y_{0,0} & y_{0,1} & y_{1,1} & y_{0,2} \\ y_{0,1} & y_{0,2} & y_{1,2} & y_{0,3} \\ y_{1,1} & y_{1,2} & y_{2,2} & y_{1,3} \\ y_{0,2} & y_{0,3} & y_{1,3} & y_{0,4} \end{bmatrix}$$

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$$f_2^* \approx -4.029500408 \times 10^{-24}$$

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- The certified lower bound is

$$f_2^* = -4.02934120638315735552022956861251063 2 \times 10^{-24}$$

Verified Error Bounds for Real Solutions

Let $F(\mathbf{x}) = [f_1, \ldots, f_m]^T \in \mathbb{Q}[\mathbf{x}] = \mathbb{Q}[x_1, \ldots, x_n]$, $I = \langle f_1, \ldots, f_m \rangle$, $V \subset \mathbb{C}^n$ be the algebraic variety defined by:

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We verify the **existence of real solutions** on $V \cap \mathbb{R}^n$

- Zero dimensional case: regular or **singular** solutions
- Positive dimensional case: **radical** ideals

Verified Error Bounds for Isolated Regular Solutions

- [Krawczyk'1969, Moore'1977, Rump'1983]
  Let $F: \mathbb{R}^n \to \mathbb{R}^n$, $\tilde{\mathbf{x}} \in \mathbb{R}^n$, and $\mathbf{X} \in \mathbb{IR}^n$ with $\mathbf{0} \in \mathbf{X}$ and $A \in \mathbb{R}^{n\times n}$. Let $\mathbf{M} \in \mathbb{IR}^{n\times n}$ be given s.t.

$$\{\nabla f_i(\mathbf{y}) : \mathbf{y} \in \tilde{\mathbf{x}} + \mathbf{X}\} \subseteq \mathbf{M}_{i,:}, i = 1, \ldots, n.$$

  Denote by I_n the $n \times n$ identity matrix and assume

$$-AF(\tilde{\mathbf{x}}) + (I_n - A\mathbf{M})\mathbf{X} \subseteq \mathrm{int}(\mathbf{X}).$$

  There is a **unique** solution $\hat{\mathbf{x}} \in \tilde{\mathbf{x}} + \mathbf{X}$ satisfying $F(\hat{\mathbf{x}}) = \mathbf{0}$ and every matrix $\tilde{M} \in \mathbf{M}$ is **nonsingular**.

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  $$\{\nabla f_i(\mathbf{y}) : \mathbf{y} \in \tilde{\mathbf{x}} + \mathbf{X}\} \subseteq \mathbf{M}_{i,:}, i = 1, \ldots, n.$$

  Denote by I_n the $n \times n$ identity matrix and assume

  $$-AF(\tilde{\mathbf{x}}) + (I_n - A\mathbf{M})\mathbf{X} \subseteq \mathrm{int}(\mathbf{X}).$$

  There is a **unique** solution $\hat{\mathbf{x}} \in \tilde{\mathbf{x}} + \mathbf{X}$ satisfying $F(\hat{\mathbf{x}}) = \mathbf{0}$ and every matrix $\tilde{M} \in \mathbf{M}$ is **nonsingular**.
- Software: verifynlss in INTLAB [Rump'1999].

Verified Error Bounds for Isolated Regular Solutions

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- Software: verifynlss in INTLAB [Rump'1999].
- Limited to: **square** systems, isolated **regular** solutions.

Verified Error Bounds for Isolated Singular Solutions

An isolated solution $\hat{\mathbf{x}}$ is a **singular** solution of $F(\mathbf{x}) = \mathbf{0}$ iff

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- It is **not hard** to verify that a **perturbed** system $\widetilde{F}(\mathbf{x})$ within a **small verified** bound has a **singular** solution.

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- [Li and Zhi'12,14]: the existence of **breadth-one singular solutions** and the existence of **a singular solution** in general case of a perturbed system.

Deflation Technique

Let $\hat{\mathbf{x}}$ be a singular solution of $F(\mathbf{x}) = \mathbf{0}$ with $r = \operatorname{rank}(F_{\mathbf{x}}(\hat{\mathbf{x}})) < n$.

Minors

$\hat{\mathbf{x}}$ is a solution of

$$\begin{cases} F(\mathbf{x}) = \mathbf{0}, \\ \det(A) = 0, \forall A \in F_{\mathbf{x}}^{r+1}, \end{cases}$$

where $F_{\mathbf{x}}^{r+1}$ denotes the set of all $(r+1) \times (r+1)$ minors of $F_{\mathbf{x}}$.

Null Space

There exists a *unique* $\hat{\lambda}$ such that $(\hat{\mathbf{x}}, \hat{\lambda})$ is a solution of

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where $B \in \mathbb{C}^{n\times(r+1)}$, $\mathbf{h} \in \mathbb{C}^{r+1}$.

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Remark

The deflated regular system is an **over-determined system!**

Verification of Breadth-one Singular Solutions

- Suppose $\mathrm{corank}(F_{\mathbf{x}}(\hat{\mathbf{x}})) = 1$. Let μ be the multiplicity and $b_0, b_1, \ldots, b_{\mu-2}$ be **smoothing parameters**. Construct a **square and regular** system

$$G(\mathbf{x}, \mathbf{b}, \mathbf{a}) = \begin{pmatrix} F_0(\mathbf{x}, \mathbf{b}) = F(\mathbf{x}) + \left(\sum_{\nu=0}^{\mu-2} \frac{b_\nu x_1^\nu}{\nu!}\right) \mathbf{e}_1 \\ F_1(\mathbf{x}, \mathbf{b}, a_{1,2}, \ldots, a_{1,n}) \\ \vdots \\ F_{\mu-1}(\mathbf{x}, \mathbf{b}, a_{1,2}, \ldots, a_{1,n}, \ldots, a_{\mu-1,2}, \ldots, a_{\mu-1,n}) \end{pmatrix},$$

in $\underbrace{n}_{\mathbf{x}} + \underbrace{\mu - 1}_{\mathbf{b}} + \underbrace{(\mu-1)(n-1)}_{\mathbf{a}} = n\mu$ variables and

$$F_k(\mathbf{x}, \mathbf{b}, a_{1,2}, \ldots, a_{k,n}) := \sum_{j=1}^{k-1} \frac{j}{k} \cdot F_{k-j,\mathbf{x}} \cdot \mathbf{a}_j + F_{\mathbf{x}} \cdot \mathbf{a}_k,$$

$\mathbf{a}_1 = (1, a_{1,2}, \ldots, a_{1,n})^T$, $\mathbf{a}_i = (0, a_{i,2}, \ldots, a_{i,n})^T$, $i = 2, \ldots, \mu - 1$.

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- Suppose $\hat{\mathbf{x}}$, $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ are verified inclusions for G, then $\hat{\mathbf{x}}$ is a **breadth-one singular** root of $\widetilde{F}(\mathbf{x},\hat{\mathbf{b}})$ of **multiplicity** μ [Li,Zhi'12].

Verification of Breadth-one Singular Solutions

- The system $F = \{x_1^2 x_2 - x_1 x_2^2, x_1 - x_2^2\}$ has a singular solution $(0,0)$ of multiplicity 4 [Rump, Graillat'09].

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- Construct an augmented system

$$G(\mathbf{x},\mathbf{b},\mathbf{a}) = \begin{pmatrix} x_1^2 x_2 - x_1 x_2^2 - \mathbf{b_0} - \mathbf{b_1 x_2} - \frac{\mathbf{b_2}}{\mathbf{2}}\mathbf{x_2^2} \\ x_1 - x_2^2 \\ 2a_1 x_1 x_2 - a_1 x_2^2 + x_1^2 - 2x_1 x_2 - \mathbf{b_1} - \mathbf{b_2 x_2} \\ a_1 - 2x_2 \\ a_1^2 x_2 + 2a_1 x_1 - 2a_1 x_2 + 2a_2 x_1 x_2 - a_2 x_2^2 - \mathbf{x_1} - \mathbf{b_2} \\ a_2 - 1 \\ a_1^2 + a_1 a_2 x_2 - a_1 + 2a_2 x_1 - 2a_2 x_2 + 2a_3 x_1 x_2 - a_3 x_2^2 \\ a_3 \end{pmatrix}.$$

Verification of Breadth-one Singular Solutions

- Applying INTLAB function verifynlss to G with

$$\tilde{\mathbf{x}} = (0.002, 0.003, 0.002, 1.001, -0.01, 0, 0, 0),$$

we **prove** that

$$\widetilde{F}(\mathbf{x}, \hat{\mathbf{b}}) = \begin{pmatrix} x_1^2 x_2 - x_1 x_2^2 - \hat{\mathbf{b}}_0 - \hat{\mathbf{b}}_1 \mathbf{x}_2 - \frac{\hat{\mathbf{b}}_2}{2} \mathbf{x}_2^2 \\ x_1 - x_2^2 \end{pmatrix}$$

for

$$-10^{-14} \leq \hat{\mathbf{b}}_{\mathbf{i}} \leq 10^{-14}, \; i = 0, 1, 2$$

has a **4-fold breadth-one** root $\hat{\mathbf{x}}$ within

$$-10^{-14} \leq \hat{x}_i \leq 10^{-14}, \; i = 1, 2.$$

Verified Error Bounds for Singular Solutions (General Case)

- Let $\hat{\mathbf{x}} \in \mathbb{R}^n$ be an *isolated singular solution* of $F(\mathbf{x}) = \mathbf{0}$ with

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- Let $F_{\mathbf{x}}^{\mathbf{c}}(\hat{\mathbf{x}})$ be obtained from $F_{\mathbf{x}}(\hat{\mathbf{x}})$ by *deleting its $\mathbf{c}$-th columns*,
$$\text{s.t. } \mathrm{rank}(F_{\mathbf{x}}^{\mathbf{c}}(\hat{\mathbf{x}})) = n - d, \text{ for } \mathbf{c} = \{c_1, c_2, \ldots, c_d\}.$$

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- We introduce d smoothing parameters $\mathbf{b} = (b_1, \ldots, b_d)$ and consider
$$G(\mathbf{x}, \lambda, \mathbf{b}) = \begin{cases} F(\mathbf{x}) - \sum_{i=1}^{d} b_i \mathbf{e}_{k_i} = \mathbf{0}, \\ F_{\mathbf{x}}(\mathbf{x}) \mathbf{v}_1 = \mathbf{0}, \end{cases}$$
where $\mathbf{v}_1 = (\lambda_1, \ldots, \underset{c_1}{1}, \ldots, \underset{c_d}{1}, \ldots, \lambda_{n-d})_n^T$.

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Therefore, $(\hat{\mathbf{x}}, \hat{\lambda}, \mathbf{0})$ is an isolated solution of $G(\mathbf{x}, \lambda, \mathbf{b}) = \mathbf{0}$.

Verified Error Bounds for Isolated Singular Solutions

- In general, we construct **a square and regular** system via deflations [Li,Zhi'12,13]

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- Software: verifynlss2 by Rump for verifying double roots.
  viss by Li and Zhu for verifying arbitrary singular roots.

Verified Error Bounds for Isolated Singular Solutions

The system F has $(0,0,0,0)$ as a 131-fold isolated zero [Dayton and Zeng'05]

$$F = \{x_1^4 - x_2x_3x_4, x_2^4 - x_1x_3x_4, x_3^4 - x_1x_2x_4, x_4^4 - x_1x_2x_3\}.$$

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- Starting from $(0.003, 0.010, 0.003, 0.007)$, by deflation we derive

$$\tilde{F}(\mathbf{x}, \mathbf{b}) = \left\{ \begin{array}{l} x_1^4 - x_2x_3x_4 - b_1 - b_5x_1 \\ x_2^4 - x_1x_3x_4 - b_2 - b_6x_2 \\ x_3^4 - x_1x_2x_4 - b_3 - b_7x_3 \\ x_4^4 - x_1x_2x_3 - b_4 - b_8x_4 \end{array} \right\}.$$

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- Apply INTLAB function verifynlss, it yields inclusions

$$-10^{-321} \leq \hat{x}_i, \hat{b}_j \leq 10^{-321},$$

  which **proves** that $\tilde{F}(\mathbf{x},\hat{\mathbf{b}})$ $(|\hat{b}_j| \leq 10^{-321}, j = 1,2,\ldots,8)$ has an **isolated singular solution $\hat{\mathbf{x}}$** within $|\hat{x}_i| \leq 10^{-321}, i = 1,2,3,4$.

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Reduce **positive-dimensional** cases to **zero-dimensional** cases.

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A Naive Method: Fixing $n-m$ Variables

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- *Voronoi2* is a sum of 5 squares $\mathbb{Q}[a,\alpha,\beta,X,Y]$, 0 is attained on

  $$\{Y+a\alpha, 2a\beta X+4a^3\beta X+4a^4\alpha^2+4a^4+4a^2\alpha^2+4a^2-a^2X^2-\beta^2\}$$

  and

  $$\{aX+\beta, -4\beta^2-4-2a^3\alpha Y-4a\alpha Y+a^4\alpha^2+a^2Y^2-4a^2\beta^2-4a^2\}$$

  [Kaltofen,Li,Yang,Zhi'08]

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  $$\{aX+\beta, -4\beta^2-4-2a^3\alpha Y-4a\alpha Y+a^4\alpha^2+a^2Y^2-4a^2\beta^2-4a^2\}$$

  [Kaltofen,Li,Yang,Zhi'08]

- We can fix at most **three** variables, e.g. a,α,β.

Critical Point Method: a Radical & Equidimensional Ideal

Choose a point $\mathbf{u} \in \mathbb{R}^n$, $g = \frac{1}{2}(x_1 - u_1)^2 + \cdots + \frac{1}{2}(x_n - u_n)^2$ and

$$J_g(F) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_1} & \frac{\partial g}{\partial x_1} \\ \vdots & & \vdots & \vdots \\ \frac{\partial f_1}{\partial x_n} & \cdots & \frac{\partial f_m}{\partial x_n} & \frac{\partial g}{\partial x_n} \end{bmatrix}.$$

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Theorem (Aubry,Rouillier,Safey'02)

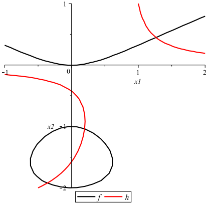
1. $C(V, \mathbf{u})$ *meets every semi-algebraically connected component of* $V \cap \mathbb{R}^n$*;*
2. $C(V, \mathbf{u}) = V_{sing} \cup V_{0,\mathbf{u}}$, *a variety defined by* $n - d + 1$ **minors** $\Delta_{\mathbf{u},d}(F)$ *of* $J_g(F)$ *and* $\dim(C(V, \mathbf{u})) < \dim(V)$.

$$F \longleftarrow F \cup \Delta_{\mathbf{u},d}(F)$$

Example: $f(x_1, x_2) = x_1^2 - x_2(x_2+1)(x_2+2)$

[Mork, Piene'08]

- Choose a random point $\mathbf{u} = [1,1]^T$, define h by the critical point method: $h = 16x_1x_2 + 6x_2^2x_1 - 6x_2^2 - 12x_2 - 4$



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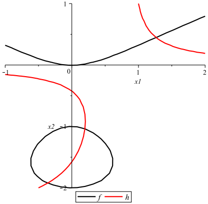

- Applying verifynlss to $\{f, h\}$ and 3 roots computed by HOM4PS-2.0, we prove that f has 3 verified real solutions

x_1	x_2
$-0.3656608 \pm 1.0 \times 10^{-15}$	$-1.9248972 \pm 5.6 \times 10^{-16}$
$0.1962544 \pm 2.6 \times 10^{-16}$	$-1.0385732 \pm 2.2 \times 10^{-16}$
$1.2624706 \pm 3.3 \times 10^{-16}$	$0.4490963 \pm 1.1 \times 10^{-16}$

The Low-rank Moment Matrix Completion Method

Given a truncated sequence $y = (y_\alpha)_{\alpha \in \mathbb{N}^n_{2t}} \in \mathbb{R}^{\mathbb{N}^n_{2t}}$, if $\exists$ a measure μ, $y_\alpha = \int x^\alpha d\mu$, then y is called a truncated moment sequence. Consider the truncated moment matrix

$$M_t(y) := (y_{\alpha+\beta})_{\alpha,\beta \in \mathbb{N}^n_t}$$

with rows and columns indexed by monomials x^α of degree $\leq t$.

For instance, in $\mathbb{R}^2$

$$M_1(y) = \begin{pmatrix} y_{00} & | & y_{10} & y_{01} \\ - & - & - & - \\ y_{10} & | & y_{20} & y_{11} \\ y_{01} & | & y_{11} & y_{02} \end{pmatrix}$$

The Low-rank Moment Matrix Completion Method

Similarly, given $g(x) = \sum_{\gamma \in \mathbb{N}^n} g_\gamma \, x^\gamma \in \mathbb{R}[x]$, the localizing matrix with respect to g is also indexed by monomials x^α of degree $\leq t$

$$M_t(gy) := \Big(\sum_{\gamma \in \mathbb{N}^n} g_\gamma \, y_{\alpha+\beta+\gamma} \Big), \quad \alpha, \beta \in \mathbb{N}^n_t.$$

For instance, in $\mathbb{R}^2$, with $g(x_1, x_2) = 1 - x_1^2 - x_2^2$,

$$M_1(gy) = \begin{pmatrix} 1 - y_{20} - y_{02} & y_{10} - y_{30} - y_{12} & y_{01} - y_{21} - y_{03} \\ y_{10} - y_{30} - y_{12} & y_{20} - y_{40} - y_{22} & y_{11} - y_{31} - y_{13} \\ y_{01} - y_{21} - y_{03} & y_{11} - y_{31} - y_{13} & y_{02} - y_{22} - y_{04} \end{pmatrix}$$

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Note that, $\forall \; f \in \mathbb{R}[x], \; \deg(f) \leq t - 2d_j, \; d_j = \lceil \deg(g_j)/2 \rceil$,

$$g_j = 0 \Longrightarrow f^2 g_j = 0 \Longrightarrow M_{t-d_j}(g_j y) = 0, \quad j = 1, \ldots, s_1,$$
$$g_j \geq 0 \Longrightarrow f^2 g_j \geq 0 \Longrightarrow M_{t-d_j}(g_j y) \succeq 0, \quad j = s_1 + 1, \ldots, s_2.$$

The Low-rank Moment Matrix Completion Method

- Apply MMCRSolver [Ma, Zhi'12] for finding an approximate solution $\tilde{\mathbf{x}}$

$$\left\{\begin{array}{ll} \min & 1 \\ \text{s. t.} & f_1(\mathbf{x}) = 0, \\ & \quad\vdots \\ & f_m(\mathbf{x}) = 0. \end{array}\right. \Longrightarrow \left\{\begin{array}{ll} \min & ||M_t(y)||_* \\ \text{s. t.} & y_0 = 1, \\ & M_t(y) \succeq 0, \\ & M_{t-d_j}(f_j\, y) = 0, 1 \leq j \leq m \end{array}\right.$$

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- If $\operatorname{rank}(F_{\mathbf{x}}(\tilde{\mathbf{x}})) < n - d$, compute a null vector $\mathbf{v}$ of $F_{\mathbf{x}}(\tilde{\mathbf{x}})$:

$$F \longleftarrow F(\mathbf{x}) \cup F_{\mathbf{x}}(\mathbf{x})\mathbf{v}$$

Example (continued)

- MMCRSolver yields one approximate real solution

$$\tilde{\mathbf{x}} = [3.671518 \times 10^{-8}, -0.999902]^T.$$

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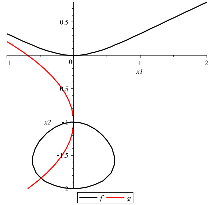

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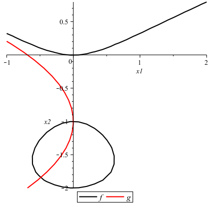

- Applying verifynlss to $\{f, g\}$, f has a verified real solution within the inclusion

x_1	x_2
$4.3211387 \times 10^{-8} \pm 2.7 \times 10^{-15}$	$-1 \pm 2.2 \times 10^{-15}$

Dense Random Hypersurfaces

Ex	*var*	*deg*	verifyrealrootpm		verifyrealrootpc		HasRealSolutions	
			time	*sol*	*time*	*sol*	*time*	*sol*
1	2	4	2.5	1	2.8	3	0.040	4
2	4	4	4.5	2	17.4	3	8.3	14
3	5	4	8.8	2	21.5	3	665.5	23
4	6	4	14.7	2	9.2	3	780	32
5	11	4	259	6	–	–	–	–
6	2	6	2.5	1	9.6	4	0.07	4
7	3	6	8.1	2	17.1	4	6.96	11
8	4	6	12.8	3	16.5	4	–	–
9	3	8	17.0	3	18.3	5	174	16
10	4	8	69.0	5	–	–	–	–

HasRealSolutions in RAGLib implemented by Safey El Din.

– denotes it is out of memory and no solutions are found.

Positive-dimensional Radical Ideals

system	*var*	*ctrs*	*deg*	verifyrealrootpm		verifyrealrootpc		HasRealSolutions	
				time	sol	*time*	sol	*time*	sol
curve0	2	1	12	9.28	$3_{\triangle}$	10.8	$4_{\triangle}$	0.30	12
butcher	4	2	3	3.41	1	319	30	0.89	7
gerdt2	5	3	4	4.82	1	506	31	0.27	6
hairer1	8	6	3	2.06	1	1.25	1	1.44	4
lanconelli	8	2	3	5.38	1	1.48	2	0.78	1
geddes2	5	4	6	18.9	1	5.43	11	1200	1
birkhoff	4	1	10	127	$1_{\triangle}$	7.72	7	31.2	6
Voronoi2	5	1	18	19.9	$1_{\triangle}$	587	$1_{\triangle}$	211	1

$\triangle$ denotes the singular solutions verified by verifynlss2 or viss

Existence of Real Solutions of Semi-algebraic Systems

Let $V \subset \mathbb{C}^n$ be a semi-algebraic set defined by:

$$f_1(\mathbf{x}) = \cdots = f_m(\mathbf{x}) = 0, \, g_1(\mathbf{x}) \geq 0, \ldots, g_s(\mathbf{x}) \geq 0$$

$f_i(\mathbf{x}), g_j(\mathbf{x}) \in \mathbb{Q}[\mathbf{x}] = \mathbb{Q}[x_1, \ldots, x_n]$ for $1 \leq i \leq m$ and $1 \leq j \leq s$.

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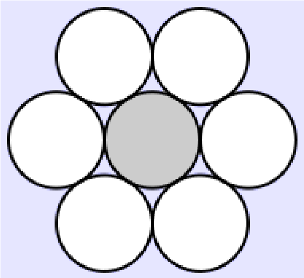
We verify the **existence of real solutions** on $V \cap \mathbb{R}^n$ using low-rank moment matrix completion method [Ma, Zhi'12]

$$\left\{ \begin{array}{ll} \min & 1 \\ \text{s. t.} & f_1(\mathbf{x}) = 0, \\ & \quad \vdots \\ & f_m(\mathbf{x}) = 0, \\ & g_1(\mathbf{x}) \geq 0, \\ & \quad \vdots \\ & g_s(\mathbf{x}) \geq 0. \end{array} \right. \Longrightarrow \left\{ \begin{array}{ll} \min & ||M_t(y)||_* \\ \text{s. t.} & y_0 = 1, \\ & M_t(y) \succeq 0, \\ & M_{t-d_i}(f_i\ y) = 0, 1 \leq i \leq m \\ & M_{t-d_j}(g_j\ y) \succeq 0, 1 \leq j \leq s \end{array} \right.$$

The Kissing Number Problems

The Kissing number is defined as the maximal number of non-overlapping unit spheres that can be arranged such that they each touch another given unit sphere.



The Kissing Number Problems

For $d = 2$, $n = 6$, the problem is reduced to verify

$$\begin{cases} x_i^2 + y_i^2 = 1, & 1 \le i \le 6, \\ (x_i - x_j)^2 + (y_i - y_j)^2 \ge 1, & 1 \le i < j \le 6, \end{cases}$$

has a real solution.

problem	*vars*	$\sharp eq$	$\sharp ineq$	*deg*	verifyrealrootpm			HasRealSolutions	
					time	*sol*	*width*	*time*	*sol*
Kissing21	2	1	0	2	0.53	2	$6.93e-18$	0.015	4
Kissing22	4	2	1	2	5.10	8	$1.98e-14$	0.171	2
Kissing23	6	3	3	2	21.01	$9_\triangle$	$1.19e-13$	4.851	16
Kissing24	9	4	6	2	62.24	5	$2.109e-14$	63.54	8
Kissing25	10	5	10	2	413.43	6	$8.03e-13$	2918	12
Kissing26	16	6	15	2	2671.96	$24_\triangle$	$4.74e-13$	–	-

Concluding Remarks

- Symbolic-numeric computation can be used to compute **reliable** results **faster**.
- Huge amount of works to develop at the **interface** of numeric computation and symbolic computations.

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Announcements:

- The 3rd Workshop on Hybrid Methodologies for Symbolic-Numeric Computation, August, 2015, Beijing, China.
- SIAM Conference on Applied Algebraic Geometry, August 3-7, 2015, Daejeon, South Korea.

Thanks to

- All my collaborators of these works
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- T. Yamaguchi, K. Nagasaka, F. Winkler and A. Szanto