Computing the real solutions of polynomial systems with the RegularChains library in MAPLE

Presented by Marc Moreno Maza[1]
joint work with
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Plan

1. Overview
2. Solver verification
3. Branch cut analysis
4. Biochemical network analysis
5. Reachibility problem for hybrid systems

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The RegularChains library in MAPLE

Design goals

- Solving polynomial systems over $\mathbb{Q}$ and $\mathbb{F}_p$, including **parametric** systems and **semi-algebraic** systems.
- Offering tools to manipulate their solutions.
- Organized around the concept of a **regular chain**, accommodating all types of solving and providing space-and-time efficiency.

Features

- Use of types for algebraic structures: `polynomial_ring`, `regular_chain`, `constructible_set`, `quantifier_free_formula`, `regular_semi_algebraic_system`.
- Top level commands: `PolynomialRing`, `Triangularize`, `RealTriangularize` `SamplePoints`, ...
- Tool kits: `ConstructibleSetTools`, `ParametricSystemTools`, `FastArithmeticTools`, `SemiAlgebraicSetTools`, ...

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Solving for the real solutions of polynomial systems

Classical tools

- Isolating the real solutions of zero-dimensional polynomial systems: `SemiAlgebraicSetTools:-RealRootIsolate`
- Real root classification of parametric polynomial systems: `ParametricSystemTools:-RealRootClassification`
- Cylindrical algebraic decomposition of polynomial systems: `SemiAlgebraicSetTools:-CylindricalAlgebraicDecompose`

New tools

- Triangular decomposition of semi-algebraic systems: `RealTriangularize`
- Sampling all connected components of a semi-algebraic system: `SamplePoints`
- Set-theoretical operations on semi-algebraic sets: `SemiAlgebraicSetTools:-Difference`

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Regular semi-algebraic system

Notation

- Let $T \subset \mathbb{Q}[x_1 < \ldots < x_n]$ be a regular chain with $\mathbf{y} := \{\mathrm{mvar}(t) \mid t \in T\}$ and $\mathbf{u} := \mathbf{x} \setminus \mathbf{y} = u_1, \ldots, u_d$.
- Let P be a finite set of polynomials, s.t. every $f \in P$ is regular modulo $\mathrm{sat}(T)$.
- Let $\mathcal{Q}$ be a quantifier-free formula of $\mathbb{Q}[\mathbf{u}]$.

Definition

We say that $R := [\mathcal{Q}, T, P_>]$ is a regular semi-algebraic system if:

(i) $\mathcal{Q}$ defines a non-empty open semi-algebra ic set S in $\mathbb{R}^d$,

(ii) the regular system $[T, P]$ specializes well at every point u of S

(iii) at each point u of S, the specialized system $[T(u), P(u)_>]$ has at least one real solution.

$$Z_{\mathbb{R}}(R) = \{(u, y) \mid \mathcal{Q}(u), t(u, y) = 0, p(u, y) > 0, \forall (t, p) \in T \times P\}.$$

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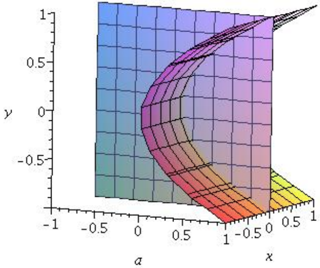
Example

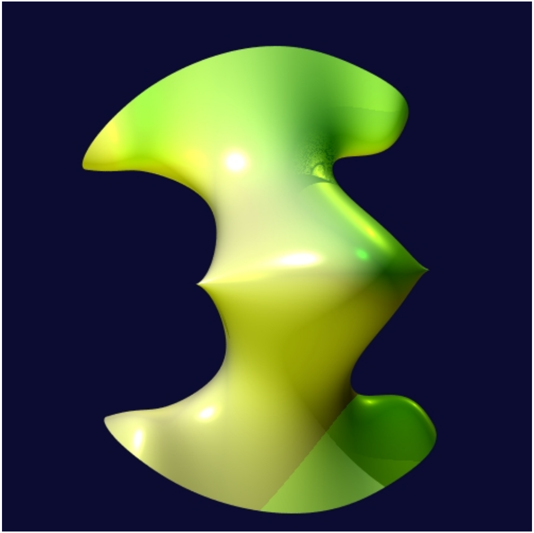
The system $[\mathcal{Q}, T, P_{>}]$, where

$$\mathcal{Q} := a > 0, \;\; T := \begin{cases} y^2 - a = 0 \\ x = 0 \end{cases}, \;\; P_{>} := \{y > 0\}$$

is a regular semi-algebraic system.



RealTriangularize applied to the *Eve* surface (1/2)



RealTriangularize applied to the *Eve* surface (2/2)

Applications Places System moreno

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$R := PolynomialRing([x, y, z]);\ F := [5*x\wedge 2 + 2*x*z\wedge 2 + 5*y\wedge 6 + 15*y\wedge 4 + 5*z\wedge 2 - 15*y\wedge 5 - 5*y\wedge 3];$

$$polynomial\_ring$$

$$[5x^2 + 2xz^2 + 5y^6 + 15y^4 + 5z^2 - 15y^5 - 5y^3]$$

$RealTriangularize(F, R, output = record);$

$$\left\{\begin{array}{c} 5x^2 + 2z^2x + 5y^6 + 15y^4 - 5y^3 - 15y^5 + 5z^2 = 0 \\ 25y^6 - 75y^5 + 75y^4 - z^4 - 25y^3 + 25z^2 < 0 \end{array}\right.,$$

$$\left\{\begin{array}{c} 5x + z^2 = 0 \\ 25y^6 - 75y^5 + 75y^4 - 25y^3 - z^4 + 25z^2 = 0 \\ 64z^4 - 1600z^2 + 25 > 0 \\ z \neq 0 \\ z - 5 \neq 0 \\ z + 5 \neq 0 \end{array}\right., \left\{\begin{array}{c} x = 0 \\ y - 1 = 0 \\ z = 0 \end{array}\right., \left\{\begin{array}{c} x = 0 \\ y = 0 \\ z = 0 \end{array}\right., \left\{\begin{array}{c} x + 5 = 0 \\ y - 1 = 0 \\ z - 5 = 0 \end{array}\right.,$$

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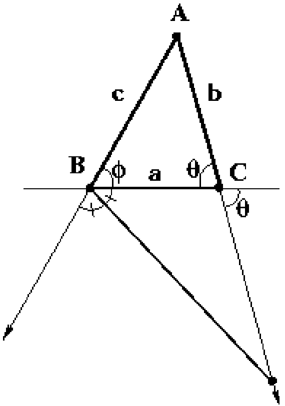
Plan

Are these two different output equivalent?



Given a triangle with edge lengths a, b, c (denoting the respective edges a, b, c too) the following two conditions S_1, S_2 are both characterizing the fact that the external bisector of the angle of a, c intersects with b on the other side of a than the triangle:

$$S_1 = a > 0 \wedge b > 0 \wedge c > 0 \wedge a < b + c \wedge b < a + c \wedge c < a + b \wedge \left(b^2 + a^2 - c^2 \leq 0\right) \quad \vee \quad \left(c(b^2 + a^2 - c^2)^2 < ab^2(2ac - (c^2 + a^2 - b^2))\right),$$

$$S_2 = a > 0 \wedge b > 0 \wedge c > 0 \wedge a < b + c \wedge b < a + c \wedge c < a + b \wedge c - a > 0.$$

Plan

Is this simplification correct?

The original problem

The branch cut of $\sqrt{z}$ is conventionally:

$$\{z \in \mathbb{C} \mid \Re(z) < 0 \ \wedge \ \Im(z) = 0\}.$$

Do the following equations hold for all $z \in \mathbb{C}$:

$$\sqrt{z-1}\sqrt{z+1} = \sqrt{z^2-1} \ \text{ and } \ \sqrt{1-z}\sqrt{1+z} = \sqrt{1-z^2}.$$

Turning the question to sampling

- The branch cuts of each formula is a semi-algebraic system $\mathcal{S}$ given as the disjunction of 3 others $\mathcal{S}_1$, $\mathcal{S}_2$, $\mathcal{S}_3$ (one per $\sqrt{}$).
- Consider CAD-cells $C_1, \ldots, C_e$, forming an intersection-free basis refining the connected components of $\mathcal{S}_1$, $\mathcal{S}_2$, $\mathcal{S}_3$.
- By virtue of the *Modromy Theorem*, it is sufficient to check whether the formula holds at a sample point of each of $C_1, \ldots, C_e$.

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Is there a unique positive equilibrium?

Allosteric enzym

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C$$

$$E + C \underset{k_4}{\overset{k_3}{\rightleftharpoons}} F$$

$$\begin{array}{rcl}
\frac{1}{2}\, C - \frac{1}{2}\, E + S - \frac{1}{2}\, C_0 + \frac{1}{2}\, E_0 - S_0 & = & 0 \\
\frac{1}{2}\, C + \frac{1}{2}\, E + F - \frac{1}{2}\, C_0 - \frac{1}{2}\, E_0 - F_0 & = & 0 \\
k_1\, ES - k_2\, C - k_3\, EC + k_4\, F & = & 0 \\
-2\, k_3\, EC + 2\, k_4\, F & = & 0 \\
E, S, C, F, E_0, S_0, C_0, F_0, k_1, k_2, k_3, k_4 & > & 0.
\end{array}$$

Cascad of polymerisation

$$P_1 + P_1 \underset{k_2^-}{\overset{k_2}{\rightleftharpoons}} P_2$$

$$P_1 + P_2 \underset{k_3^-}{\overset{k_3}{\rightleftharpoons}} P_3$$

$$\vdots$$

$$P_1 + P_{n-1} \underset{k_n^-}{\overset{k_n}{\rightleftharpoons}} P_n$$

- Each system is viewed as parametric in the initial concentrations and kinetic velocities.
- We show that, generically, there is a unique positive equilibrium.

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Which states can be reached from the intial one?

Hybrid systems with linear control

- Given $A \in \mathbb{R}^{n\times n}, B \in \mathbb{R}^{n\times m}$ consider $\dot{\xi} = A\xi + Bu$ where $\xi(t) \in \mathbb{R}^n$ is the state of the system at time t and $u : \mathbb{R} \to \mathbb{R}^m$ is a piecewise continuous function which is called the control input.
- With $x = \xi(0)$ and a control input u, we have:
$$\xi(t) = \Phi(x, u, t) = e^{At}x + \int_0^t e^{A(t-\tau)}Bu(\tau)d\tau.$$
- Question: Given $x = \xi(0)$, which values $\xi(t)$ can the reached?

The (Lafferriere et al. 2001) example

$$\Phi(x_1, x_2, u, t) = \left(x_1 e^{2t} + \frac{2}{3}u(-e^{2t} + e^{\frac{1}{2}t}), x_2 e^{-t} + \frac{1}{2}u(e^t - e^{-t})\right).$$

Let $z = e^{\frac{1}{2}t}$, the problem reduces to compute the (y_1, y_2) such that:

$$\exists u \exists z (0 \leq u \wedge z \geq 1 \wedge p_1 = 0 \wedge p_2 = 0) \quad \text{where}$$
$$p_1 = y_1 - \frac{2}{3}u(-z^4 + z) \quad \text{and} \quad p_2 = y_2 z^2 - \frac{1}{2}u(z^4 - 1).$$

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