Binomial Solutions to Smale's 17th Problem and their Application to Chemical Reaction Networks

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Smale's 17th Problem

Smale's 17th:

Can one approximate a root of a polynomial system in polynomial-time with a uniform algorithm, on average.

The development of algorithms that are solutions to this problem have applications in real-world polynomial system solving.

Previous Work:

1. Beltrán & Pardo (2008): Partial positive solution with uniform probabilistic algorithm that runs in time polynomial.
2. Cucker & Bürgisser (2012): Deterministic Algorithm running in time $N^{O(\log\log N)}$.

Key Words

Approximate Root: Smale defined an approximate root as

$$||\zeta - N_f^k(z)|| \leq \frac{1}{2^{2^k-1}}||\zeta - z||$$

Theorem

Define

$$\gamma(f,\zeta) = sup_{k\geq 2}\left|\frac{f'(\zeta)^{-1}f^k(\zeta)}{k!}\right|^{\frac{1}{k-1}}$$

Suppose that ζ *is a true root of* f *and* $f'(\zeta)^{-1}$ *exists. If*

$$|z-\zeta| \leq \frac{3-\sqrt{7}}{2\gamma(f,\zeta)},$$

then z *is an approximate root of* f *with associated true root* ζ.

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1. **Approximate**
2. **A**: The number of distinct roots of a polynomial system can be exponential in the number of variables.
3. **Polynomial-Time/On Average**: Computational complexity takes time polynomial in the input size (number of variables & degree). For a random polynomial, it would run in polynomial time.

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Binomial Case Solutions

Lemma

$x^d - c$ where $c > 0$, $c \in \mathbb{R}_+$, $d \in \mathbb{N}$, and $d \geq 2$ is a solution to Smale's 17th problem

1. For $c > 1$, choose interval $[0, c]$ and use bisection method
$$\left| x_n - |c|^{\frac{1}{d}} \right| < \frac{1}{3d} < \frac{3-\sqrt{7}}{d-1}|c|^{\frac{1}{d}}$$
2. For $c < 1$ choose interval $[0, 1]$ and use bisection method
$$\left| x_n - |c|^{\frac{1}{d}} \right| < \frac{3-\sqrt{7}}{d}|c| < \frac{3-\sqrt{7}}{d-1}|c|^{\frac{1}{d}}$$

Complexity: $O((\log(d)^2))(\log(d) \pm \log(c))$
For a random polynomial, the average value of c is constant.

Matrix Exponentiation and Smith Normal Form

$$x^A := (x_1^{A_{11}} \ldots x_n^{A_{n1}}, \ldots, x_1^{A_{1n}} \ldots x_n^{A_{nn}})$$

Then $x^A = c$ where $x = (x_1, x_2, \ldots x_n)$, $c = (c_1, c_2, \ldots c_n)$, and A is an $n \times n$ matrix, is written as:

$$x_1^{A_{11}} \ldots x_n^{A_{n1}} = c_1$$

$$\vdots$$

$$x_1^{A_{1n}} \ldots x_n^{A_{nn}} = c_n$$

The Form

Smith proved that any integer matrix can be diagonalized using elementary row and column operations. SNF will be utilized in the algorithm to solve binomial systems.

Smith Normal Form

Given

$$x_1^2 x_2^4 = 5$$

$$x_1^6 x_2^8 = 9$$

$$UAV = S$$

$$\begin{pmatrix} -1 & 1 \\ 2 & -1 \end{pmatrix} \begin{pmatrix} 2 & 6 \\ 4 & 8 \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}$$

$$(x^A = c) \Rightarrow (y^U = x) \Rightarrow (y^{UA} = c) \Rightarrow (y^{UAV} = y^S = c^V)$$

Then

$$(y_1)^2 = 5$$

$$(y_2)^4 = \frac{9}{5}$$

SNF $\Rightarrow$ Univariate binomials $\Rightarrow$ Previous algorithm $\Rightarrow$ $\tilde{y} \Rightarrow \tilde{y}^U = \tilde{x}$.

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Binomial System Algorithm

Algorithm

Def binomial system

1. Before initiating algorithm, convert binomial system into form $x^A = c$

Input: $A = [a_{ij}] \in \mathbb{Z}^{n \times n}$
Conditions: $x = [x_1, x_2, \ldots, x_n]$ $y = [y_1, y_2, \ldots, y_n]$
$c = (c_1, c_2, \ldots, c_n) \in \mathbb{R}^n_+$
Output: Approximate Root

2. Calculate the Smith Normal Form of Matrix A. Store $U = [u_{ij}]$ $V = [v_{ij}]$ and $S = [s_{ij}]$
3. Perform a monomial change of variable. Let $y^U = x$, then $y^{UA} = c$ and $y^S = c^V$

Binomial System Algorithm

Algorithm

Def binomial system

4. Determine y^S and c^V with matrix exponentiation program. Hence, $y_1^{\alpha_1} = \beta_1 \ldots y_n^{\alpha_n} = \beta_n$ where $(\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$ and $(\beta_1, \ldots, \beta_n) \in \mathbb{R}^+$
5. Solve each equation with bisection method algorithm. Return vector $\tilde{y} \in \mathbb{Z}^n$
6. Calculate $\tilde{y}^U$ in order to return variable after monomial change, producing approximate root vector $\tilde{x}$
7. Test roots in $\tilde{x}$ versus approximate root theorem.
8. End

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Chemical Reaction Networks as Binomial Systems

Definition

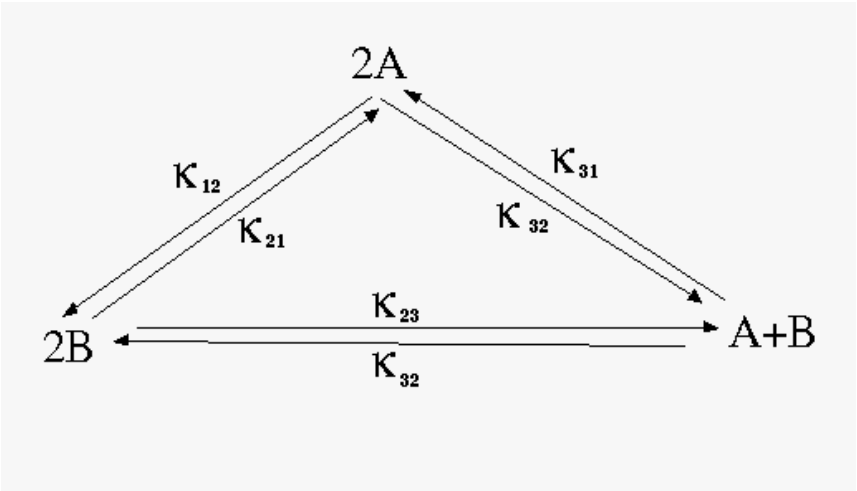
A **Chemical Reaction Network (CRN)** is an organized digraph of chemical reactions. Under the assumption of *mass-action kinetics*, chemical species react at a rate proportional to the product of their concentrations, where the proportionality constant is the rate constant κ.

Definition

In chemistry, a steady state is a situation in which all state variables are constant in spite of ongoing processes that strive to change them. It is called a **toric steady state** if the corresponding system of ODE's can be expressed as a binomial system and then solved.

A Chemical Reaction as ODE's

Reaction (Triangle Network): Let $s = 2$ and $m = 3$. Then $2A = x_1^2$, $2B = x_2^2$, and $A + B = x_1 x_2$



$$\frac{dx_1}{dt} = -\frac{dx_2}{dt} = (-2\kappa_{12} - \kappa_{13})x_1^2 + (2\kappa_{21} + \kappa_{23})x_2^2 + (\kappa_{31} - \kappa_{32})x_1 x_2$$

As only the coefficients of $x_1 x_2$ can be zero, this system has toric steady states iff $\kappa_{31} = \kappa_{32}$.

Chemical Reaction Networks as Binomial Systems

Millán et. al (2011) provided sufficient conditions for a reaction system to have toric steady states.

Condition 3.1, 3.4, 3.6

A chemical reaction system is given by a network G with m complexes and reaction rate constants κ_{ij}^*. These three conditions are essentially linear algebra conditions, which result from the concentrations of the chemical species changing over time (the κ values).

Application Results

Therefore, we can:

1. Find biomodels with defined paramaters (κ denotes reaction constants)
2. Convert these models' associated dynamical systems into binomial systems based on the work of Millán et. al
3. Use binomial system as input for developed binomial system algorithm

The solutions to such systems are of high importance to Computational & Systems Biologists.

References & Acknowledgements

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Thank You for Listening

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