Real-Time Computability of Real Numbers by Chemical Reaction Networks

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Introduction and Motivation

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Hydrazine Combustion

$$\begin{aligned} 3N_2H_4 &\longrightarrow 4NH_3 + N_2 \\ N_2H_4 &\longrightarrow N_2 + 2H_2 \\ 4NH_3 + N_2H_4 &\longrightarrow 3N_2 + 8H_2 \\ 2H_2 + O_2 &\longrightarrow 2H_20 \end{aligned}$$

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Abstract CRN

$$3A \longrightarrow 4B + C$$
$$A \longrightarrow C + 2D$$
$$4B + A \longrightarrow 3C + 8D$$
$$2D + E \longrightarrow 2F$$

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- How powerful are they?
- Benchmark: we are asking which real numbers can be computed by CRNs.
- In fact, which real numbers can be computed **quickly by CRNs**?

Main Result

Today's Theorem
Every algebraic number can be computed by a CRN in real time.

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algebraic	**not algebraic (transcendental)**
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Outline

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- Large Population Protocol
- Transendental Number

Real-time Computability

More about CRNs

$$A + 2B \xrightarrow{r} A + C$$
$$\emptyset \xrightarrow{s} X$$

A, B, C, X are **species** (abstract molecule types). r, s are **rate constants**. The **rates** of these two reactions at time t are

$$r \cdot a(t) \cdot b(t)^2$$

and

$$s.$$

where $a(t) =$ the **concentration** of A at time t, etc.

CRN and its ordinary differential equations

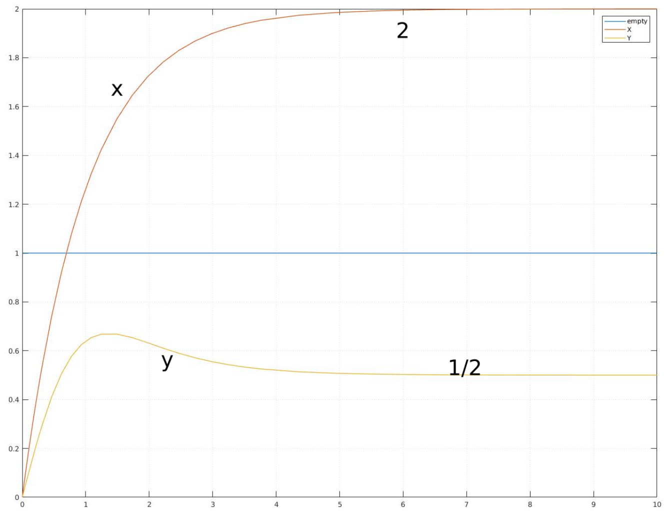
Once we have the definition for rates of reactions, we can write a CRN into a system of ordinary differential equations (ODEs).

Example:

$$\begin{aligned} \emptyset &\xrightarrow{2} X \\ X &\xrightarrow{1} \emptyset \\ \emptyset &\xrightarrow{1} Y \\ X + Y &\xrightarrow{1} X \end{aligned} \qquad \Longleftrightarrow \qquad \begin{aligned} x' &= 2 - x \\ y' &= 1 - xy \end{aligned}$$

with initial value $x(0) = 0$, $y(0) = 0$.

Plot



Streamplot

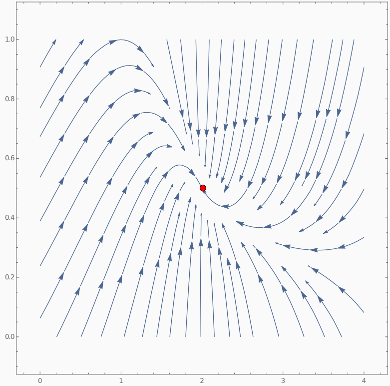
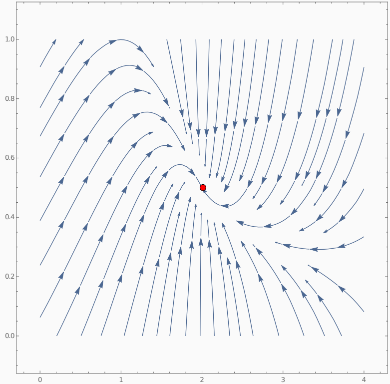


Figure 1: Streamplot

Streamplot



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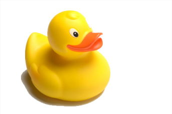
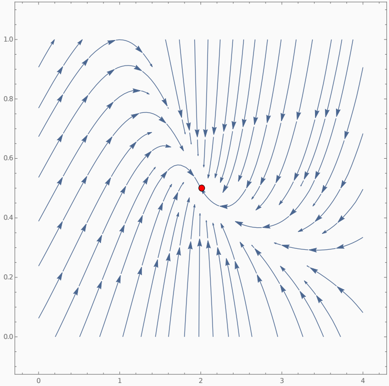


Figure 2: duck

Streamplot



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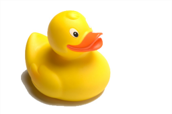

Figure 2: duck

Put a rubber duck at point $(0, 0)$ at time 0. It will eventually reach the red spot, i.e., $(2, \frac{1}{2})$.

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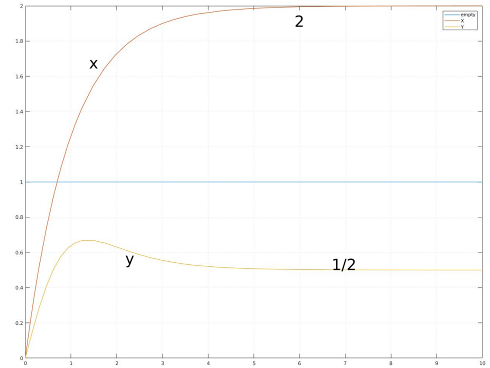

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- *(integrality)*. All the rate constants of any reaction should be integers.
- *(boundedness)*. All the concentrations of any species are bounded.
- *(real-time convergence)*. There is a species X, such that for all $t \in [\tau, \infty)$ for some τ,

$$|x(t) - |\alpha|| \leq 2^{-t} \tag{1}$$

.

Zero initial values

- This prevents the CRN from coding too much (infinite) information in its initial values.
  For example, encode an uncomputable number in the initial value to "compute" it.

Integer Rate

Suppose we want to compute a real number α, without the constraint, one can use the following simple CRN

$$\begin{aligned} \emptyset &\xrightarrow{\alpha} X \\ X &\xrightarrow{1} \emptyset \end{aligned}$$

to compute α, which is just like "cheating".

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Lyapunov CRN-Computable Reals: A Bridge

A Bridge Crosses Nonlinearity

- It is not easy to show real-time computability directly, due to the high nonlinearity of CRNs.

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- It is not easy to show real-time computability directly, due to the high nonlinearity of CRNs.
- However, we can take advantage of Lyapunov's **exponential stability theorem**[1], which requires only derivative and eigenvalue analysis.
- The path: instead of showing

$$\textbf{Algebraic} \subseteq \mathbb{R}_{RTCRN},$$

we define a new set $\mathbb{R}_{LCRN}$ in between and show

$$\textbf{Algebraic} \subseteq \mathbb{R}_{LCRN} \subseteq \mathbb{R}_{RTCRN},$$

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Jacobian Matrix

If $N = (S, R)$ is a CRN with $S = \{Y_1, \ldots, Y_n\}$, then the ODEs of each species can be written as

$$\begin{aligned} y_1' &= f_1(y_1, \ldots, y_n), \\ &\vdots \\ y_n' &= f_n(y_1, \ldots, y_n), \end{aligned}$$

where $f_1, \ldots, f_n : \mathbb{R}^n \to \mathbb{R}$ are polynomials.

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The **Jacobian matrix** of the CRN N is the $n \times n$ matrix

$$J_N = \begin{pmatrix} \frac{\partial f_1}{\partial y_1} & \cdots & \frac{\partial f_1}{\partial y_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial y_1} & \cdots & \frac{\partial f_n}{\partial y_n} \end{pmatrix}.$$

The Bridge: $\mathbb{R}_{LCRN}$

We define the set of real $\mathbb{R}_{LCRN}$ basically like $\mathbb{R}_{RTCRN}$:, but instead of requiring exponential convergence, we require:

- $x \in \mathbb{R}_{LCRN}$ then all eigenvalues of the Jacobian at x must have **negative real part**.
- x is a limit point of the system (in our rubber duck sense).

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Figure 3: whirlpool

Algebraic Numbers

Algebraic are in $\mathbb{R}_{NECRN}$

A real number $\alpha \in \mathbb{R}$ is **algebraic** if there is a polynomial $P(x)$ with integer coefficients such that α is a root of P, i.e., $P(\alpha) = 0$. Here we demonstrate by an example of how to compute algebraic numbers. Actually, along this path, one can show that algebraic numbers are in $\mathbb{R}_{LCRN}$.

Example: $\alpha = 2 - \sqrt{3}$ is a root of

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- constant term i.e., $P(0)$, of the polynomial should be positive.

First positive root

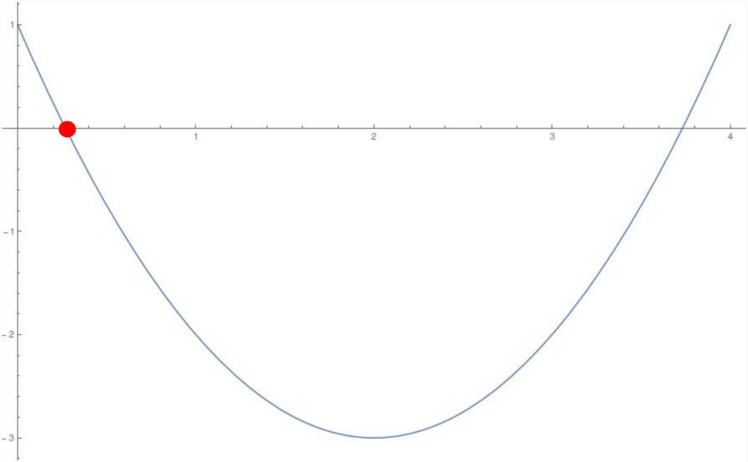

Figure 4: First positive root

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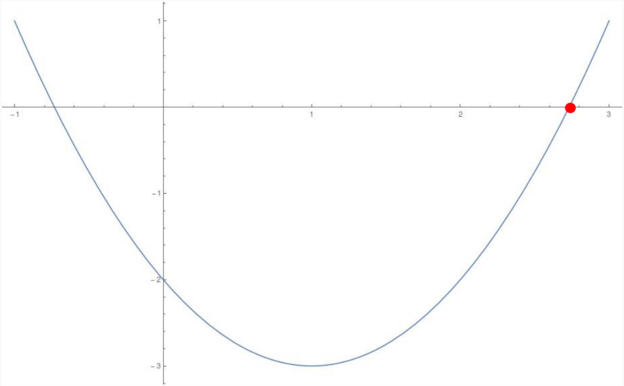

Figure 5: Other roots

Other roots: shift and flip

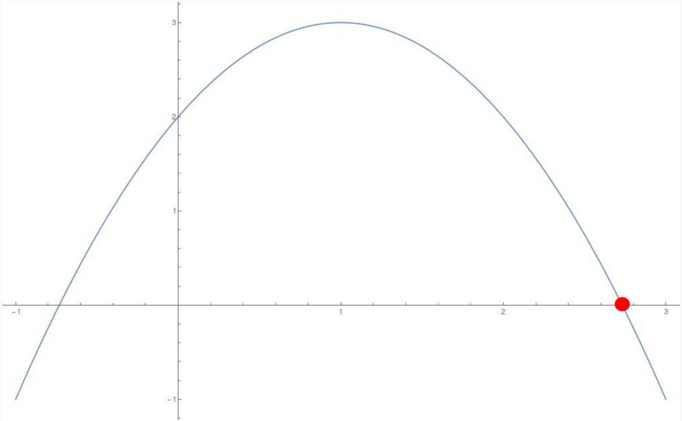

Figure 6: Other roots

$\mathbb{R}_{LCRN}$ is a field

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That is, we add the follows reaction to the original network.

$$\emptyset \xrightarrow{1} Y$$

$$X + Y \xrightarrow{1} X$$

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Let X computes α, Y computes β in a CRN. How to compute $\alpha - \beta$?

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Addition and multiplication can also be implemented easily.

Compare to Other Similar Models

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[2] *Computing with Large Populations Using Interactions*

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Generalized Ehrenfest urns:

- A restricted model of LPP
- Reactions look like $X + Y \to Z + Z$
- It can not compute all the algebraic numbers, specifically, it can not compute some *rationals*.

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LPP Cont.

But what if we have infinitely many equilibrium points? A continuum of them?

LPP Cont.

But what if we have infinitely many equilibrium points? A continuum of them?

Well, then we can compute transcendental numbers! The following CRN uses species U, V, such that $\lim_{t\to\infty} U(t) - V(t) = e - 1$. Actually, it is just a fancy way to encode $y = e^{1-e^{-t}} - 1$ in CRN.

$$\emptyset \xrightarrow{1} X \qquad X \xrightarrow{1} \emptyset$$

$$U \xrightarrow{1} 2U \qquad \emptyset \xrightarrow{1} U$$

$$X + U \xrightarrow{1} X \qquad V \xrightarrow{1} 2V$$

$$X \xrightarrow{1} X + V \qquad X + V \xrightarrow{1} X$$

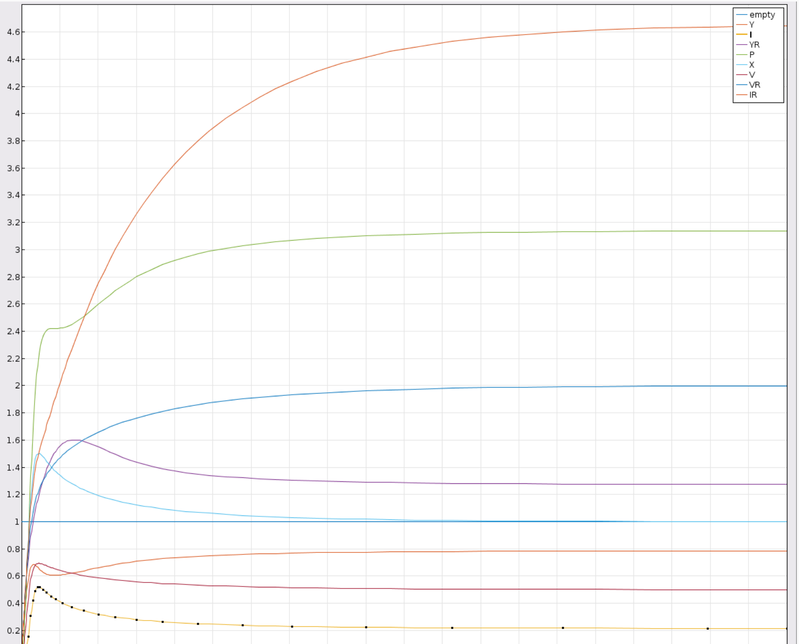
$$U + V \xrightarrow{1} \emptyset$$

The ODE for the previous CRN is:

$$x' = 1 - x$$
$$u' = 1 + u - xu - uv$$
$$v' = x + v - xv - uv$$

Its equilibrium points are on the curve $\{x = 1, uv = 1\}$.

Simulation by Simbiology



Thank you