Real-Time Computability of Real Numbers by Chemical Reaction Networks

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Overview

- Real-time computability
- Algebraic numbers and how to computer them
- Beyond algebraic numbers
- Hartmanis-Stearns conjecture: a discussion

Real-time computability

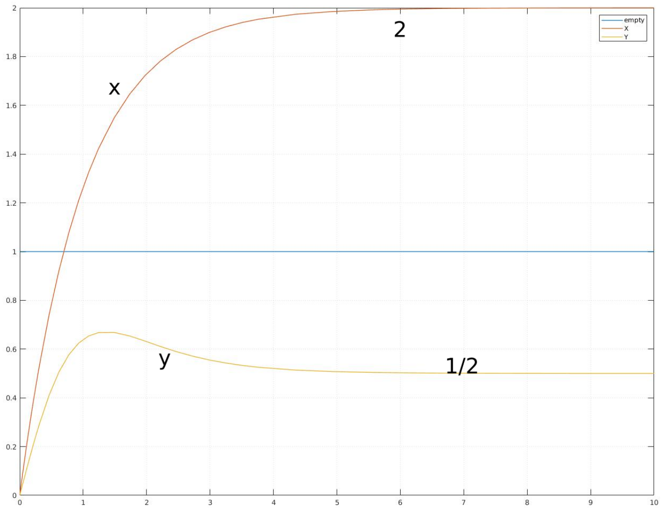
Real-time computability: an intuition

Example: Consider the following CRN and its corresponding ODE system:

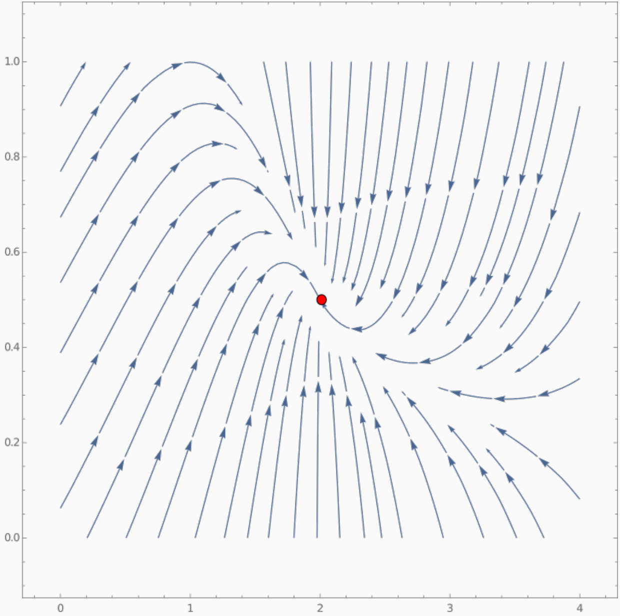
$$\begin{aligned} \emptyset &\xrightarrow{2} X \\ X &\xrightarrow{1} \emptyset \\ \emptyset &\xrightarrow{1} Y \\ X + Y &\xrightarrow{1} X \end{aligned} \quad \iff \quad \begin{aligned} x' &= 2 - x \\ y' &= 1 - xy \end{aligned}$$

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

Plot



Stream Plot



Real-time computability: the idea

We say a real number α is *real time computable by chemical reaction networks*, if there exist a chemical reaction network $N = (S, R)$ and a species $X \in S$, such that "X goes to α."

In the previous example, we say

- X computes 2
- Y computes $\frac{1}{2}$

Real-time computability: the definition

The Chemical reaction networks that we use here are under *deterministic mass action semantics* and satisfies the follows:

- *(integrality)*. All the rate constants of any reaction should be integers.
- *(boundedness)*. All the concentrations of any species are bounded.
- *(real time convergence)*. If N is initialized with $y(0) = 0$ for all $Y \in S$, then for all $t \in [1, \infty)$,

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

where $\{\alpha\} = \alpha - \lfloor \alpha \rfloor$ is the *fractional part* of α.

Integrality

Suppose we want to compute a real number α, if we do not have the integrality constraint. Then we 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".

Zero initial values

- This prevents the CRN coding too much information in its initial value.
- A very useful trick in CRN construction is to make a species Y having its concentration be the reciprocal of another species X all the time. The trick fails here because of the zero initial value.
- The very special “species” $\emptyset$ has initial value 1 and stays constant over time.

Boundedness

- A reasonable notion of reaction time is the arc length of trajectory. This constraint prevent the CRN “running” unrealistically fast.
- This also prevent a species vanish very fast.
- Again it add to the hardness of a lot of constructions.

Real-time convergence

- It require the CRN signal is a good *analog* approximation of $\{\alpha\}$.
- This does not require the CRN explicitly produce symbols in any sort of digital representation of $\{\alpha\}$.

Real-time computability of algebraic number

Rational number

Lemma

All rational numbers are CRN real-time computable.

Just need to consider:

$$\begin{aligned} \emptyset &\xrightarrow{p} X \\ X &\xrightarrow{q} \emptyset \end{aligned} \qquad \Longleftrightarrow \qquad x' = p - qx$$

This ODE has explicit solution. It is not hard to analyze the solution to conclude the above CRN computes $\frac{p}{q}$ in real time.

Algebraic number: an example

We try to compute $\sqrt{2}$. Consider $\sqrt{2}$ is a root of $x^2 - 2 = 0$. Rewrite the above to $2 - x^2 = 0$, and we want some function/species satisfies that:

$$\frac{dx}{dt} = 2 - x^2$$

Implement this with CRN:

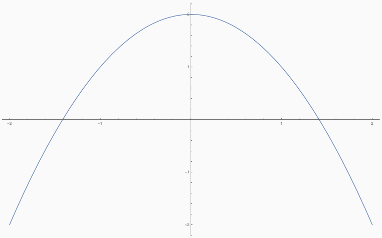
$$\emptyset \xrightarrow{2} X$$

$$2X \xrightarrow{1} X$$

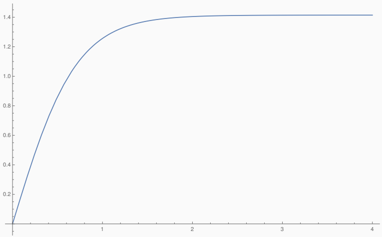
By the construction we know that this CRN has a fixed point of $\sqrt{2}$. Luckily we still have an explicit solution, hence we can do real-time analysis based on that, but this is not the case in general.

Note: the constant term must be positive.

Phase portrait and plot of previous example



(a) phase portrait of $x' = 2 - x^2$



(b) plot of the solution

Another example: Golden Ratio

Golden ration $\phi = \frac{1+\sqrt{5}}{2} = 1.618...$ is the root of

$$1 + \phi - \phi^2 = 0$$

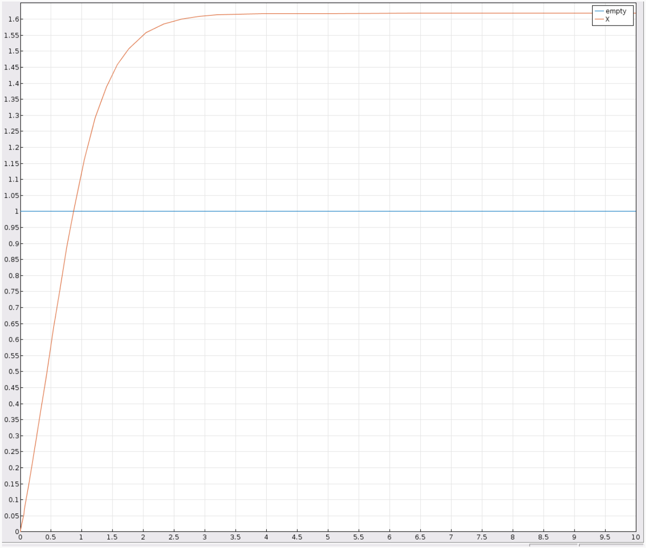
To turn this into a CRN, it will just be:

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

$$X \xrightarrow{1} 2X$$

$$2X \xrightarrow{1} X$$

Golden Ratio



Algebraic Number

Theorem

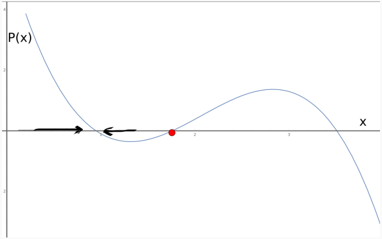
All algebraic numbers are CRN real-time computable.

Recall that we say a number is **algebraic** if it is a root $P(x) = 0$, where $P(x)$ is of a polynomial with integer coefficients.

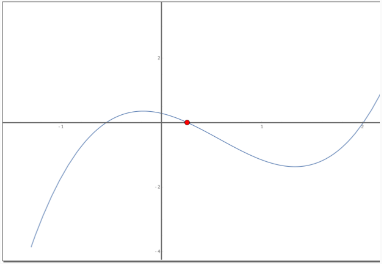
Proof idea:

- To compute α, we find the minimum polynomial $P(x)$ of it.. If needed, we may have to shift the polynomial by some rational number.
- Turn the ODE $x' = P(x)$ into a CRN.
- We need some stability analysis to establish real-time computability.

Shift and flip



(d) phase portrait of $x' = P(x)$



(e) shift and flip

Note that our construction seems to always compute the **first positive root** of a polynomial. If we want to "compute" the second root of a minimum polynomial $P(x)$, we need to first shift $P(x)$ by some rational $\frac{p}{q}$ between the first and the second root, i.e. take $P(x + \frac{p}{q})$. Then we add $\frac{p}{q}$ back.

This require some closure properties.

Real-time convergence of the construction

The rest of the things to show:

- The first positive root of $P(x)$ is CRN real-time computable.
- $\frac{p}{q}$ is CRN real-time computable.**(Done)**
- The sum of the previous two is also real-time computable.

The third bullet is not hard to implement.

Let x, y be two real number computed by X, Y in N_1 and N_2 respectively. The then addition operation can be done by adding a species Z, such that,

$$z' = x + y - z.$$

The proof of the first and third bullets will require some stability analysis.

Beyond algebraic numbers

More closure properties

We want more closure properties about CRN real-time computable numbers. Now we have if α, β are CRN real-time computable numbers, we have the constructions for the follows:

- $\alpha + \beta$
- $\alpha \times \beta$
- $\frac{1}{\alpha}$
- $\alpha - \beta$, suppose $\alpha \geq \beta$. **(Hard)**
- $\ln \alpha$, suppose $\alpha \geq 1$. **(Hard)**
- α^β **(Hard)**

By having algebraic numbers and exponentiation, we can get a lot of **transcendental** numbers that are also CRN real-time computable, e.g. $\sqrt{2}^{\sqrt{2}}$

A taste on why subtraction is hard

Let x, y be two real number computed by X, Y in N_1 and N_2 respectively. The then subtraction operation can be done by adding a species Z, such that,

$$z' = x - yz\bar{z} - z$$
$$\bar{z}' = 1 - z\bar{z}$$

In this construction, the ODE is very non-linear and not easy to analyze. Hence it not easy to reach the real-time computability conclusion.

A CRN/ODE that computes e

The number e in ODE and deterministic CRN, is just like one in nature number system. To compute e by CRN, one just need to consider

$$e = e^1.$$

The initial idea: consider

$$y(t) = e^t - 1$$

can be implement in CRN. If we can "substitute" t with some function $x(t)$, and make $x(t) \to 1$ in the limit.

Then we can get

$$y(1) = e^1 - 1$$

in the limit.

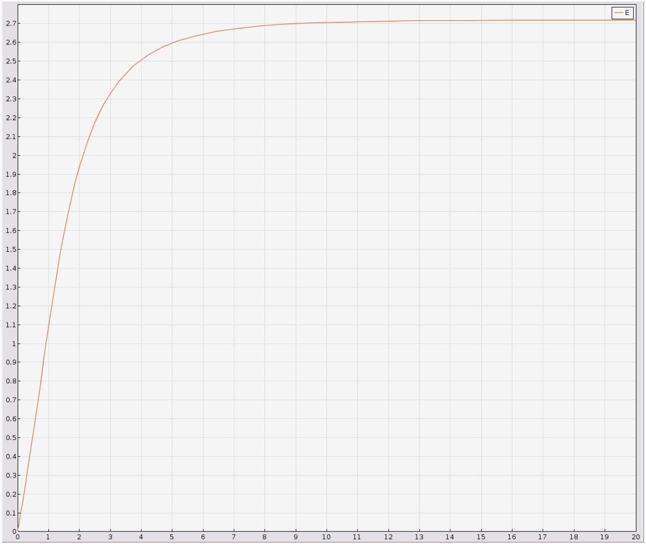
The rest of the thing need to do is just add back 1.

A CRN/ODE that computes e

The following CRN/ODE computes e by species E.

$$
\begin{aligned}
E' &= y + 1 - E \\
y' &= (y + 1)(1 - y\bar{y}x) \\
x' &= 1 - y\bar{y}x \\
\bar{y}' &= 1 - y\bar{y}
\end{aligned}
$$

Simulation for e



A CRN/ODE that computes π

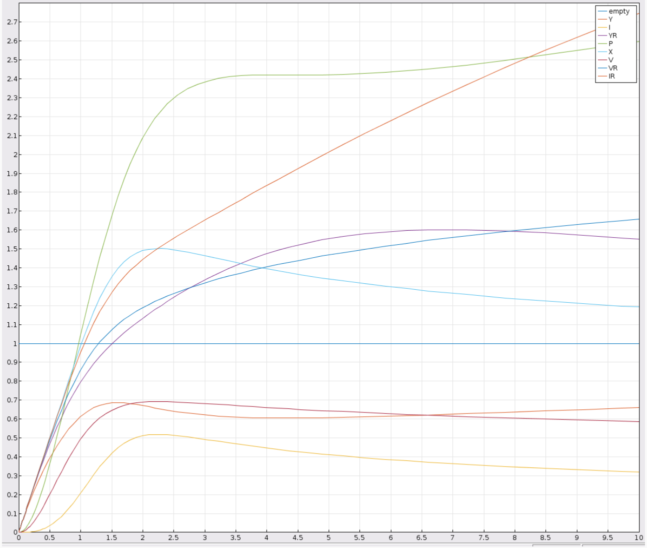
The following CRN/ODE computes π by species p. It takes 21 reactions to implement this system in CRN.

$$
\begin{aligned}
p' &= 4y - p \\
y' &= 1 - fy\bar{y} - y \\
v' &= 2x(1-v)^2(1 - v\bar{v}f\bar{f}x) \\
\bar{v}' &= 1 - v\bar{v} \\
\bar{x}' &= 1 - v\bar{v}f\bar{f}x \\
f' &= v(1 - v\bar{v}f\bar{f}x) \\
\bar{f}' &= 1 - f\bar{f} \\
\bar{y}' &= 1 - y\bar{y}
\end{aligned}
$$

Do not be fooled by this ODE system, it is just a fancy way to write

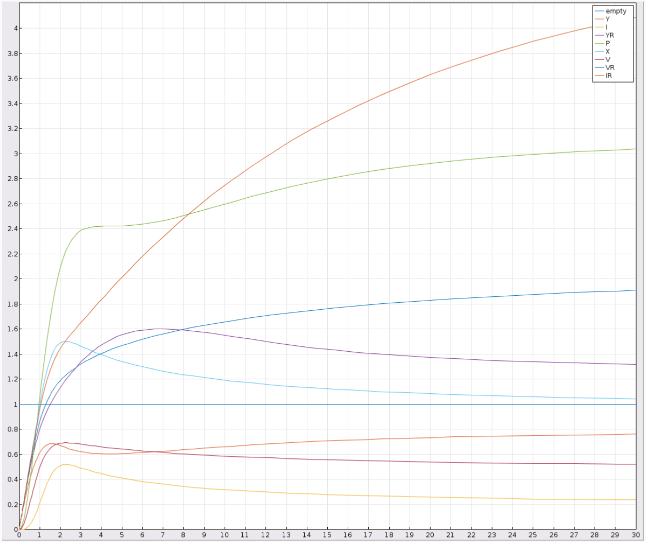
$$\int_0^1 \frac{1}{1+x^2}\,dx = \frac{\pi}{4}$$

Simulation for π



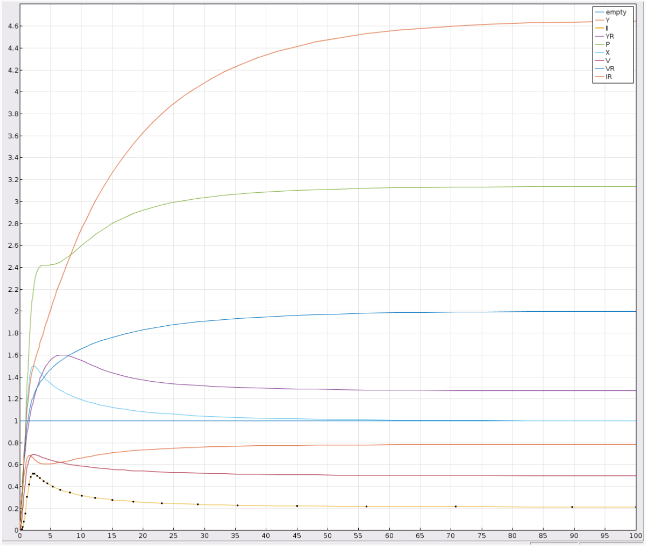
(g) Run time= 10

Simulation for π



(h) Run time= 30

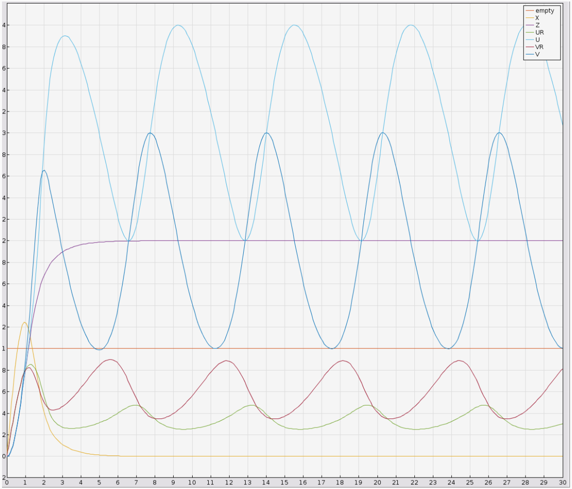
Simulation for π



(i) Run time= 100

Oscillator

Not every ODE/CRN converges to a fixed point. It may just oscillate.



(j) Run time= 30

Hartmanis-Stearns conjecture: a discussion

Hartmanis-Stearns conjecture

- Hartmanis-Stearns conjecture: no irrational algebraic number is real-time computable by a Turing machine.
- Our main theorem: every algebraic number is real-time computable by a CRN.

Our main theorem does not disprove Hartmanis-Stearns conjecture. They seems to be telling different stories.

- Turing machine is a discrete computation model.
- CRN is a analog computation model.

Open question 1

What if we can make our CRN behave like a digital/discrete machine, i.e. produce in linear time the individual digits of a real number in real time?

- If yes, then Hartmanis-Stearns conjecture fails for **analog** computation.
- If not, Hartmanis-Stearns conjecture holds for analog computation and is essentially about producing the individual digits.

Open question 2

Can we find a reasonable **discrete** model of computation on which some algebraic irrational can be compute in real time?

- If yes, then the Hartmanis-Stearns conjecture either false or model-dependent.
- If not, then the Hartmanis-Stearns conjecture is true in a strong, model-independent way, at least for discrete computation.

Thank you!