June 13, 2014

BIRS Conference on

Programming with Chemical Reaction Networks: Mathematical Foundations
June 8th - June 13, 2014

A discussion on the problem of: **complexity of distributions for CRNs**.

Overriding question: given a state space Γ, and a distribution π with support on Γ, can we come up with a chemical reaction network $\text{CRN}_\pi = \{\mathcal{S}, \mathcal{C}, \mathcal{R}, \kappa\}$ for which π is well approximated by a marginal of the stationary distribution of the network.

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We narrowed the problem to considering the following question: let $N \in \{0, 1, 2, \dots\}$, we want π defined on $\{0, 1, 2, \dots\}$ so that for some $\epsilon > 0$ small,

$$\pi(N) \geq 1 - \epsilon.$$

The solution to this particular problem is to consider the following model:

$$\begin{array}{c} \emptyset \\ K \cdot L \downarrow\uparrow L \\ C_{-M} \underset{L\cdot N}{\overset{L\cdot X}{\rightleftarrows}} C_{-M+1} \underset{L\cdot N}{\overset{L\cdot X}{\rightleftarrows}} \cdots \underset{L\cdot N}{\overset{L\cdot X}{\rightleftarrows}} C_0 \underset{L\cdot N}{\overset{L\cdot X}{\rightleftarrows}} \cdots \underset{L\cdot N}{\overset{L\cdot X}{\rightleftarrows}} C_{M-1} \underset{L\cdot N}{\overset{L\cdot X}{\rightleftarrows}} C_M \end{array}$$

$$\emptyset \overset{C_{-M}}{\rightarrow} X \qquad\qquad X \overset{C_M \cdot N^{-1}}{\rightarrow} \emptyset,$$

where $L \gg 1$ is a large constant dependent upon ϵ, the reactions in the chain are catalyzed by X, and the final two reactions are catalyzed by C_{-M} and C_M, respectively.

The stochastic equations for X satisfy

$$X(t) = X(0) + Y_1\left(\int_0^t C_{-M}(s)ds\right) - Y_2\left(\int_0^t N^{-1}C_M(s)X(s)ds\right).$$

Next, we note that the stationary distribution for the $\{C_i\}$, *under the assumption that* $X = x \geq 1$ *is fixed*, is a product of Poisson random variables with mean:

$$\overline{C}_0 = K,\ \ \overline{C}_1 = \overline{C}_0\frac{x}{N} = K\frac{x}{N}, \dots,\ \ \overline{C}_M = K\left(\frac{x}{N}\right)^M, \dots, \overline{C}_{-M} = K\left(\frac{N}{x}\right)^M$$

If $X = 0$, then the process very quickly sends C_{-M} to infinity. Thus, $X(t)$ is well approximated by the following model,

$$X(t) = X(0) + Y_1\left(\int_0^t K\left(\frac{N}{X(s)}\right)^M 1(X(s)\geq 1)\right) - Y_2\left(\int_0^t KN^{-1}\left(\frac{X(s)}{N}\right)^M X(s)1(X(s)\geq 2)ds\right).$$

High level summary. We considered the following problem: for which probability distributions are there CRNs which can generate, at least approximations to, those distributions as stationary distributions. We focussed on the well defined problem of constructing a point mass distribution. We think this problem is largely solved.

We then considered how to construct CRNs that give more complicated distributions. We believe we can use the construction of a point mass to construct any distribution.

The question then arrises as to how to construct distributions with CRNs with minimal "complexity", where complexity is loosely defined as the amount of information needed to describe the networks.