A Compositional Framework for Reaction Networks

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Reaction networks, or equivalently Petri nets, are a general framework for describing processes in which entities of various kinds interact and turn into other entities. In chemistry, where the reactions are assigned 'rate constants', any reaction network gives rise to a nonlinear dynamical system called its 'rate equation'. Here we generalize these ideas to 'open' reaction networks, which allow entities to flow in and out at certain designated inputs and outputs. We treat open reaction networks as morphisms in a category. Composing two such morphisms connects the outputs of the first to the inputs of the second. We construct a functor sending any open reaction network to its corresponding 'open dynamical system'. This provides a compositional framework for studying the dynamics of reaction networks. We then turn to statics: that is, steady state solutions of open dynamical systems. We construct a 'black-boxing' functor that sends any open dynamical system to the relation that it imposes between input and output variables in steady states. This extends our earlier work on black-boxing for Markov processes.

1 Introduction

Reaction networks, first formally defined by Aris (1) in 1965, are a framework for describing processes whereby entities interact and transform into other entities. While they first arose in chemistry, and are often called 'chemical reaction networks', their applications are widespread. For example, a basic model of infectious disease, the SIRS model, is described by this reaction network:

$$S + I \xrightarrow{\iota} 2I \xrightarrow{\rho} R \xrightarrow{\lambda} S$$

We see here three types of entity, called 'species':

- S: **susceptible**,
- I: **infected**,
- R: **resistant**.

We also have three 'reactions':

- ι: $S + I \to 2I$: **infection**, in which a susceptible individual meets an infected one and becomes infected;
- ρ: $I \to R$: **recovery**, in which an infected individual gains resistance to the disease;
- λ: $R \to S$: **loss of resistance**, in which a resistant individual becomes susceptible.

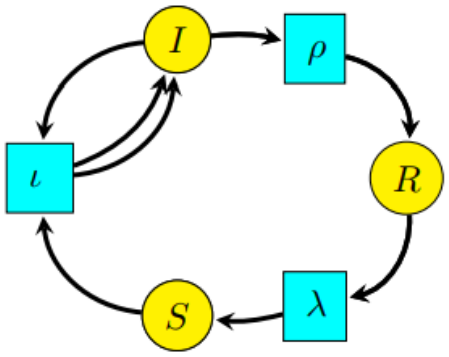
In general, a reaction network involves a finite set of species, but reactions go between 'complexes', which are finite linear combinations of these species with natural number coefficients. The reaction network is a directed graph whose vertices are certain complexes and whose edges are called 'reactions'. If we attach a positive real number called a 'rate constant' to each reaction, a reaction network determines a system of differential equations saying how the concentrations of the species change over time. This system of equations is usually called the 'rate equation'. In the example above, the rate equation is

$$\begin{aligned} \frac{dS}{dt} &= r_\lambda R - r_\iota SI \\ \frac{dI}{dt} &= r_\iota SI - r_\rho I \\ \frac{dR}{dt} &= r_\rho I - r_\lambda R \end{aligned} \quad (1)$$

Here r_ι, r_ρ and r_λ are the rate constants for the three reactions, and S, I, R now stand for the concentrations of the three species, which are treated in a continuum

approximation as smooth functions $S, I, R : \mathbb{R} \to [0, \infty)$. The rate equation can be derived from the 'law of mass action', which says that any reaction occurs at a rate equal to its rate constant times the product of the concentrations of the species entering it as inputs. A reaction network is more than just a stepping-stone to its rate equation. Interesting qualitative properties of the rate equation, such as existence and uniqueness of steady state solutions, can often be determined simply by examining the reaction network, independent of any particular choice of rate constants. Results in this direction began with Feinberg and Horn's seminal work in the 1960's (2, 5), leading to the Deficiency Zero and Deficiency One Theorems (3, 4) and more recently to a proof of the Global Attractor Conjecture [11]. In this paper we present a 'compositional framework' for reaction networks: that is, a way to build up a reaction network from smaller pieces, in such a way that its rate equation can be determined from those of the pieces. However, this framework requires that we view reaction networks in a somewhat different way, as 'Petri nets'.

Petri nets were invented by Carl Petri in 1939, when he was just a teenager, for the purposes of chemistry [32]. Much later, they became popular in theoretical computer science [23, 31], biology [26, 27, 36], and other fields [3, 22, 29]. A Petri net is a bipartite directed graph; vertices of one kind represent species, while those of the other kind represent reactions. The edges into a transition specify which species are inputs to that transition, while the edges out specify its outputs. One can easily turn a reaction network into a Petri net and vice versa. For example, the reaction network above translates into this Petri net:



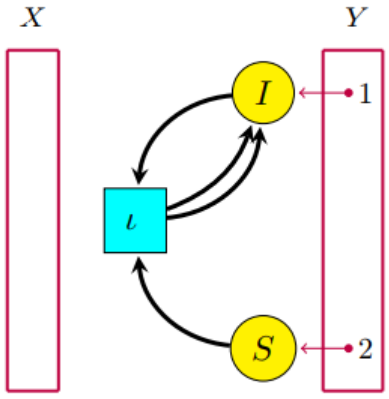
One should beware that the terminology is diverse, since it comes from several communities. In the Petri net literature, species are called 'places' and reactions are called 'transitions'. Indeed, Petri nets are sometimes called 'place-transition nets' or 'P/T nets'. On the other hand, chemists call them 'species-reaction graphs' or 'SR-graphs'. When each reaction of a Petri net has a rate constant attached to it, it is often called a 'stochastic Petri net'.

While some qualitative properties of a rate equation can be read off from a reaction network, others are more easily read from the corresponding Petri net. For example, properties of a Petri net can be used to determine whether its rate equation has the capacity to admit multiple steady states [6, 12, 17].

Petri nets are also better suited to a compositional framework. The key new concept required is that of an 'open' Petri net. Here is an example:

The box at left shows a set X of 'inputs' (which happens to be empty), while the box at right shows a set Y of 'outputs'. Both inputs and outputs are points at which entities of various species can flow in or out of the Petri net. We say the open Petri net goes from X to Y , and we shall show how to treat it as a morphism $f : X \to Y$ in a category we call `RxNet`.

Given an open Petri net with rate constants assigned to each reaction, we explain how to systematically obtain its 'open



rate equation', which amounts to the usual rate equation with extra terms describing inflows and outflows. The above example has this open rate equation:

$$\frac{dS}{dt} = -r_\iota SI - o_1$$
$$\frac{dI}{dt} = r_\iota I - o_2 \quad (2)$$

Here $o_1, o_2 : \mathbb{R} \to \mathbb{R}$ are arbitrary smooth functions describing outflows as a function of time. Given another open Petri net $g : Y \to Z$, for example this:

2 Reaction networks versus Petri nets

We begin by precisely defining reaction networks and Petri nets, so we can see that they are two ways of presenting the same concept.

Definition 2.1. A reaction network (S, T, s, t) consists of

a finite set S,

a finite set T,

functions $s, t : T \to N^s$.

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