A Compositional structure for Reaction networks

* Reaction networks or Petrinets : To describe processes where entities of various kinds interact and turn into entities.

* We generalise the ideas of "open" reaction networks that allow entities to flow in and out. (inputs / outputs)

→ These are morphisms in the category. So composing connects output of one to the input of other.

→ Now, we use our dynamical system knowledge ($\mathcal{N}^{\partial}$) and construct a functor to our desired system.

"Compositional framework" for studying dynamical systems.

The functor is a "black-boxing" functor. (We can use it for "markov" chain.

→ Introduction: * These networks are used ~~to~~ as a framework for describing processes where entities interact and transform to other.

eg: $S + I \xrightarrow{i} 2I \qquad I \xrightarrow{r} R \xrightarrow{\lambda} S$

3 species ; 3 reactions here.

* Reaction network is a directed graph whose vertices are "complexes" and edges are "reactions"

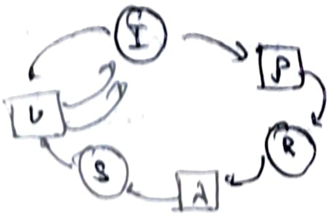
→ We can add a positive real number in each reactions called "rate constant" which will determine the rate equations.

for the given eg: $\frac{dS}{dt} = v_\lambda R - v_i SI$

• S, I, R stand for concentrations of species that are "smooth" functions $S, I, R : \mathbb{R} \to [0, \infty)$. Rate eqn is just law of mass action.

Keynote: This network ~~is~~ not just represents a rate equation, but we can infer the existence and uniqueness of steady state solutions irrespective of rate constants. → (∃ independent/disjoint sets such that the amoun)

Petri nets: It is a $\boxed{\text{bipartite}}$ directed graph. Here vertices of one kind represents elements and other kind represents transitions. Eg for the prev ex is



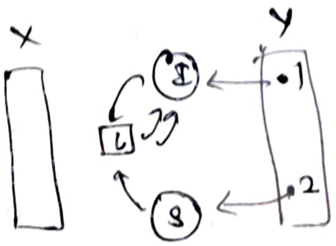
Here edges specify the inputs/outputs to the reactions.

petri nets ⇒ Place/-transition nets (Petri net with rate constant is stochastic petri nets)

* Petri net can be used to determine multiple steady states.

Open petri nets:

Pictorial representation:
(We have just added two boxes)

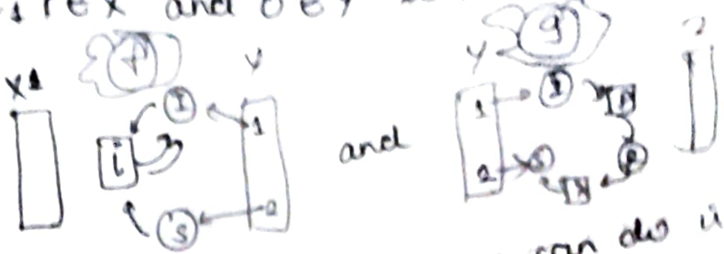


* The box at the left shows a set X of inputs and right ⇒ set Y of outputs.
* These points are where the entities can just flow in and out. The DE's will have $-o_1, -o_2$ term respectively.

⇒ We define this petrinet between two sets X, Y to be a category RxNet.

* We assume / given $i_1 \in X$ and $o \in Y$ to be arbitrary smooth functions.

Importance. Let



• We are having two open petri nets. What we can do is we can compose f and g to yield a petrinet with no input / output parameters / entities.

But wait? How easily can you compose it? - In this case it is just $i_1 = o_1 ; o_2 = i_2$.

* We will see the procedure to do it; It is basically a functor : RxNet → Dynam.

→ The category Dynam is a open dynamical system Dynamical system which means that a vector field $\mathbb{R}^n$ ~~th~~ used to define n. ODE. eg is just Petri net

* Open dynamical system means we can constant vector i.e having input / output ports ⇒ Open petri nets

(Monoidal categories)

$$\begin{tikzcd} \boxed{\text{Categ.}} \arrow[r, "\text{enrich}"] \arrow[d] & \boxed{?} \arrow[d] \\ \boxed{\text{Sets}} \arrow[r, "\text{enrich}"] & \boxed{\text{monoids}} \end{tikzcd}$$

? : Monoidal categories

Monoids: A set with elements having a binary oper obeying associativity neutral elements

→ We use symmetric monoidal categories that could be used to have series / parallel arrangement

Decorated cospans:

* Powerful general tool for describing open systems.

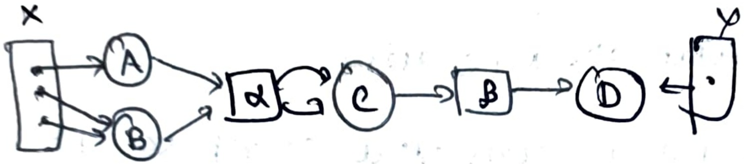
What is cospan? Any diagram of the form

$$\begin{tikzcd} & S & \\ X \arrow[ur, "i"] & & Y \arrow[ul, "o"'] \end{tikzcd}$$

. (We care about finite sets here)

Here 'S' is called "apex" of the cospan ⇒ set of states of an open system. X, Y are "legs" of the cospan. $i: X \to S$ and $o: Y \to S$

For



$S = \{A, B, C, D\}$
$X = \{\cdot\ \cdot\ \cdot\}$ $Y = \{\cdot\}$

∴ A open petrinet is basically a cospan of finite sets whose apex S is "decorated" with some extra