Applying category theory to real life (for real)

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Outline

- The characters
- The model
- What is this good for?

(based on work by John Baez and Blake Pollard)

The characters – Chemical reaction networks

Things that look like $2H_2 + O_2 \xrightarrow{\tau} 2H_2O$

The characters – Chemical reaction networks

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More formally:

Defn. A chemical reaction network is $R = (S, T, s, t, r)$ where

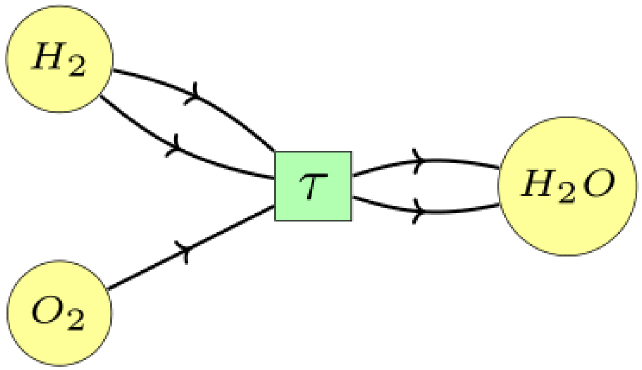
- S is a finite set of ***species***
- T is a finite set of ***transitions***
- functions $s, t : T \to \mathbb{N}^S$ indicating ***source*** and ***target*** of transitions
- a function $r : T \to (0, \infty)$ indicating the ***rate*** of transitions

The characters – Chemical reaction networks

Instead of equation-style notation

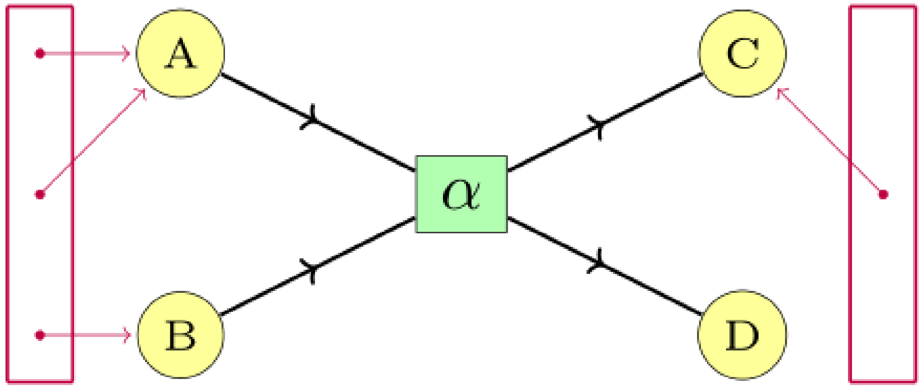
$$2H_2 + O_2 \xrightarrow{\tau} 2H_2O$$

we will use a graph-like notation



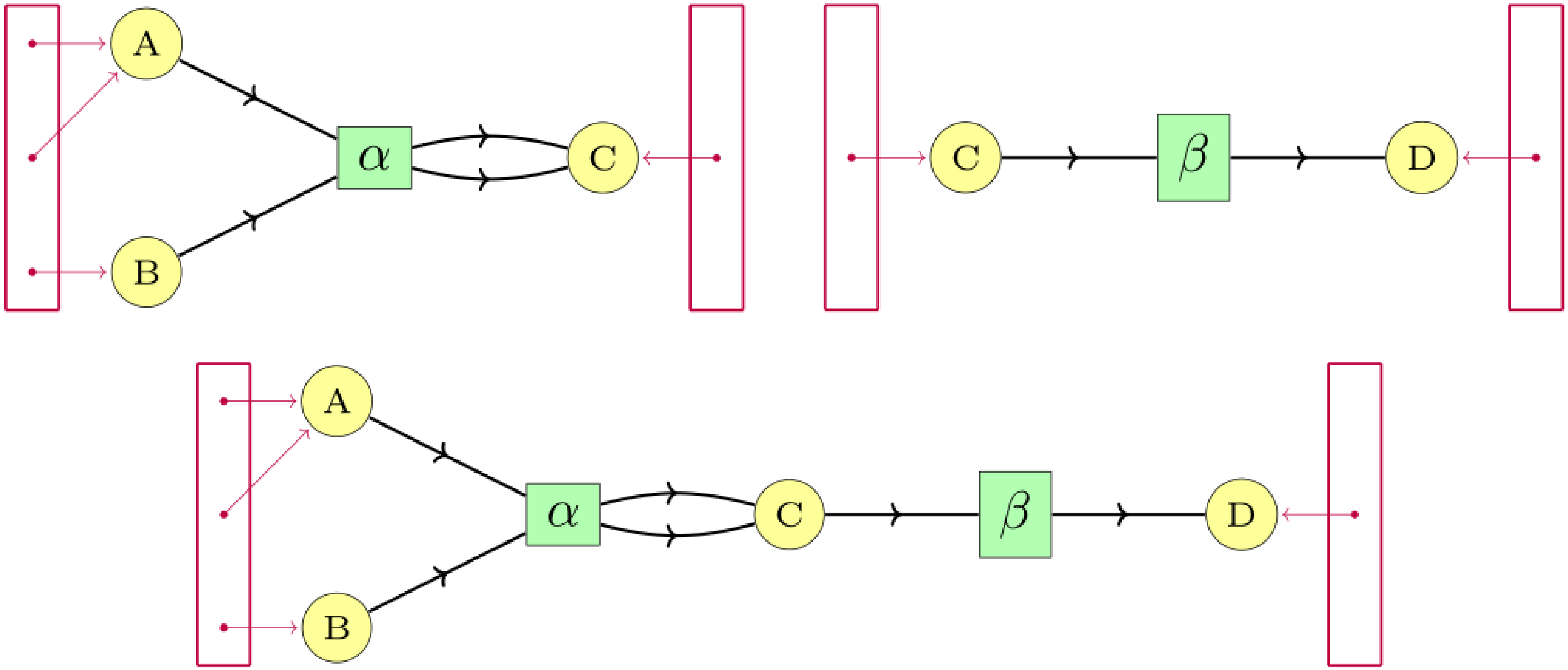
The characters – Chemical reaction networks

Our reactions have input and output “hoses” that allow us to manipulate the concentration of some species.



Important features – “Composition”

Can “connect” different containers by gluing along input/output hoses.



Important features – Associated dynamical system

The “rate equation”: describes the change in the concentrations of the species through time.

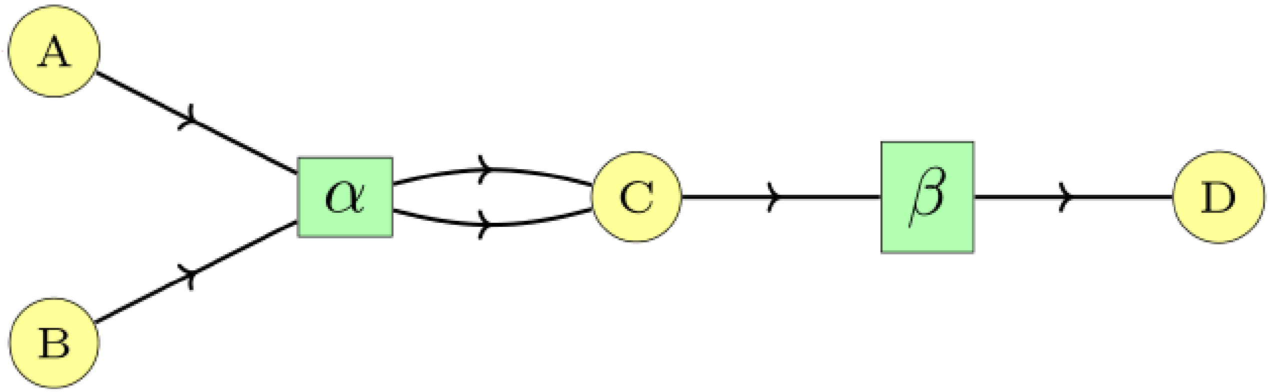
For $c: \mathbb{R} \to \mathbb{R}^S$ time-dependent concentrations,

$$\frac{dc(t)}{dt} = \sum_{\tau \in T} r(\tau)(t(\tau) - s(\tau))c(t)^{s(\tau)}$$

or for short

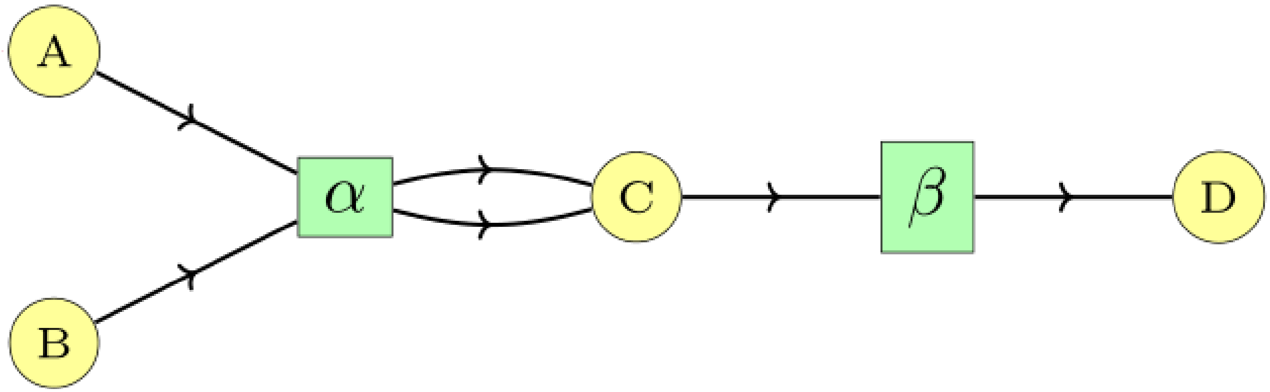
$$\frac{dc(t)}{dt} = v^R(c(t)) \qquad \text{for } v^R : \mathbb{R}^S \to \mathbb{R}^S.$$

Important features – Associated dynamical system



$$\frac{d[A]}{dt} = -[A][B]r(\alpha)$$

Important features – Associated dynamical system



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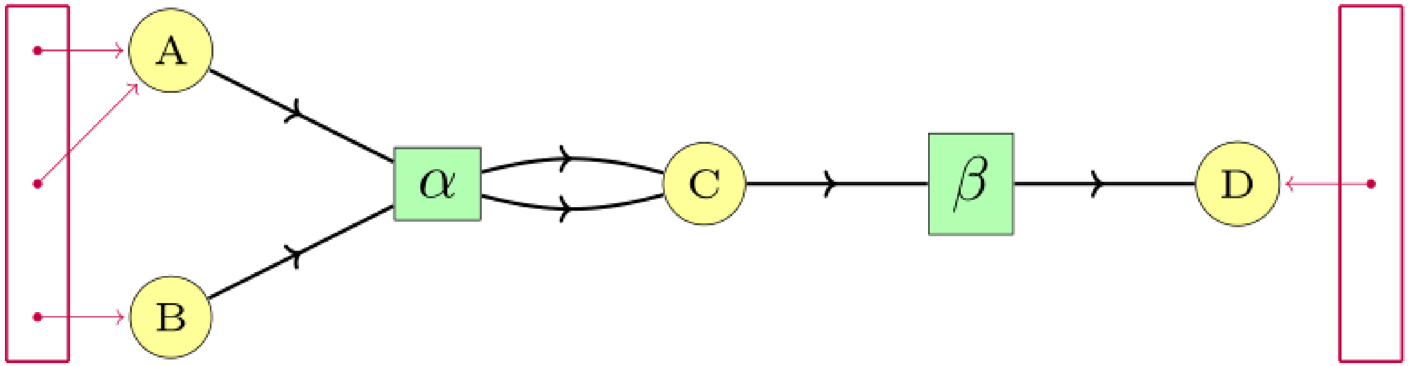
$$\frac{d[D]}{dt} = [C]r(\beta)$$

Important features – Associated dynamical system



$$\frac{d[A]}{dt} = -[A][B]r(\alpha) + I_A^1 + I_A^2$$

$$\frac{d[B]}{dt} = -[A][B]r(\alpha) + I_B$$

$$\frac{d[C]}{dt} = 2[A][B]r(\alpha) - [C]r(\beta)$$

$$\frac{d[D]}{dt} = [C]r(\beta) - O_D$$

The model – Preliminaries

Defn. A category consists of

- a collection of objects
- a collection of morphisms

such that

- each morphism has a source and a target
- we can compose: $f: X \to Y$ and $g: Y \to Z \rightsquigarrow gf: X \to Z$
- composition is associative
- identity morphisms are units for the composition

The model – Preliminaries

Defn. A functor $F: C \to D$ between two categories consists of:

- for each object $X \in C$, an object $F(X) \in D$
- for each morphism $f: X \to Y \in C$, a morphism $F(f): F(X) \to F(Y) \in D$

such that

- $F(id_X) = id_{F(X)}$
- $F(gf) = F(g)F(f)$

The model – Preliminaries

Defn. A natural transformation $\tau : F \Rightarrow G$ between functors $F, G : C \to D$ consists of a morphism

$$\tau_X : F(X) \to G(X) \quad \text{for every } X \in C$$

such that, given $f : X \to X'$

$$\begin{array}{ccc} F(X) & \xrightarrow{\tau_X} & G(X) \\ {\scriptstyle F(f)}\downarrow & & \downarrow{\scriptstyle G(f)} \\ F(X') & \xrightarrow[\tau_{X'}]{} & G(X') \end{array}$$

The model – Cospans

GOAL: assemble chemical reaction networks into a category.

TOOL: cospans.

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TOOL: cospans.

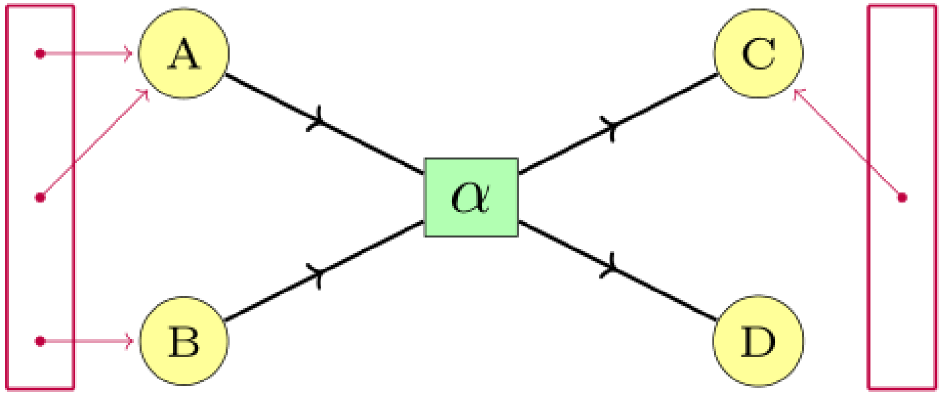
Defn. A cospan is a diagram

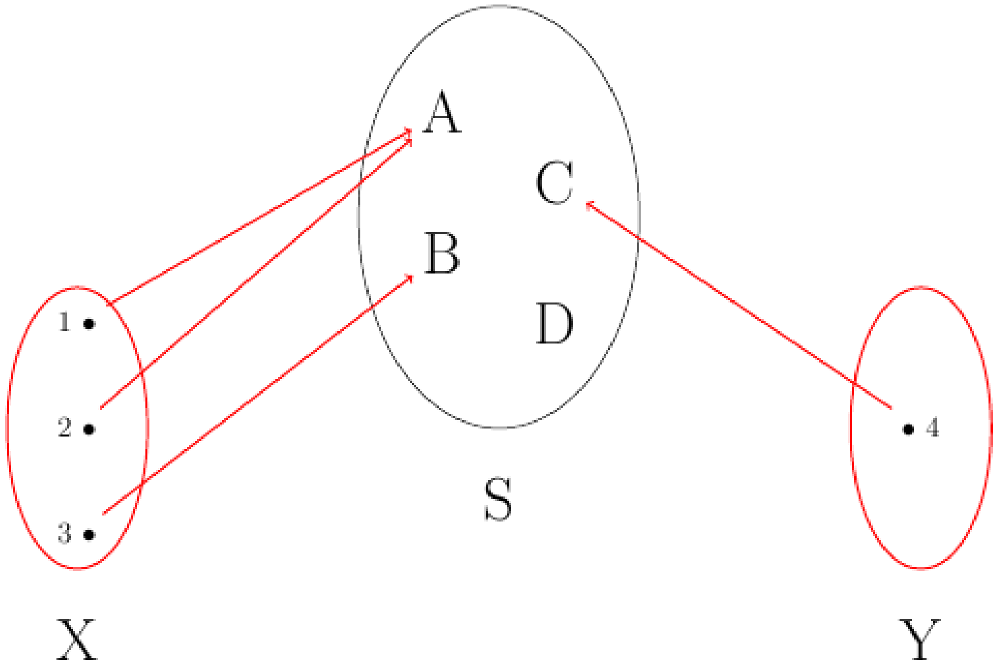
$$X \xrightarrow{\;i\;} S \xleftarrow{\;o\;} Y$$

where X, Y, S are finite sets and i, o are functions.

The model – Cospans

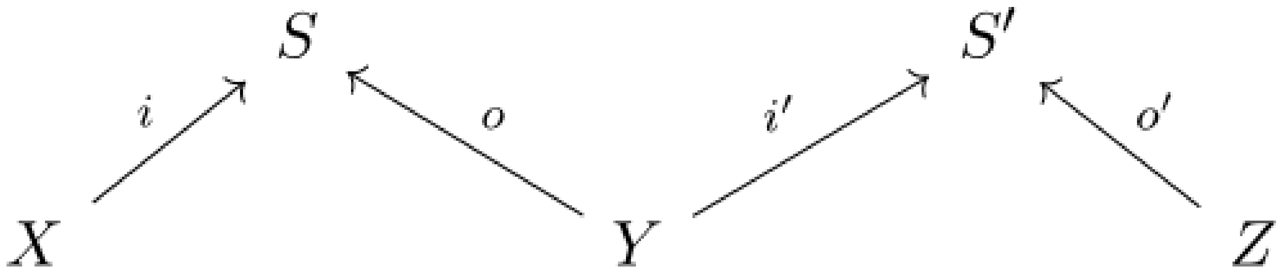
IDEA: S is the set of species in the reaction, i and o mark the input/output hoses.





The model – Cospans

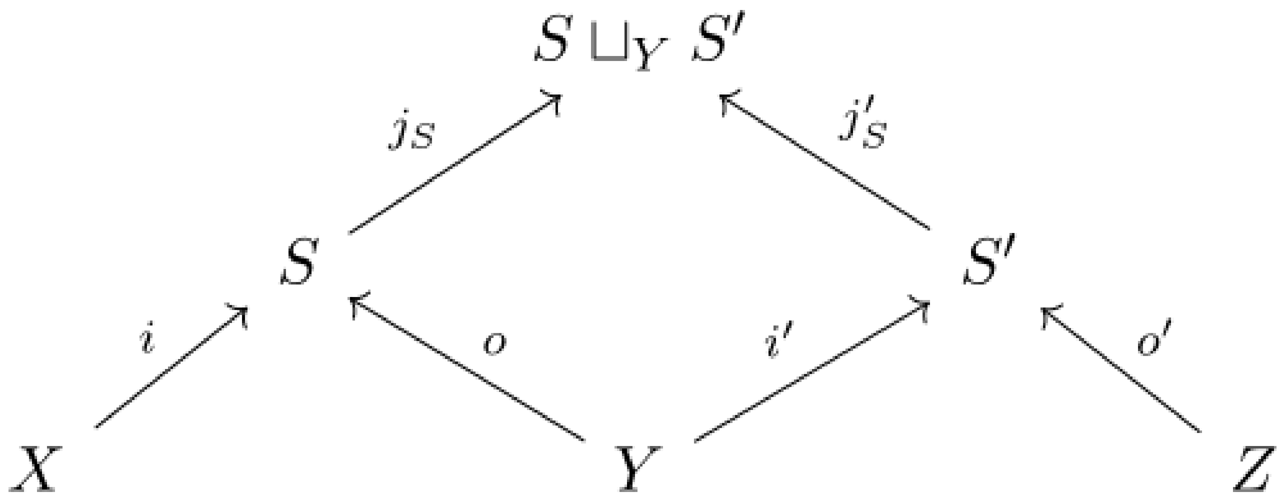
FEATURES RECOVERED: Cospans compose



Let $S \sqcup_Y S' = S \sqcup S'/\!\sim$ where $s \sim s'$ if $o(y) = s$ and $\mathrm{i}'(y) = s'$ for some $y \in Y$.

The model – Cospans

FEATURES RECOVERED: Cospans compose

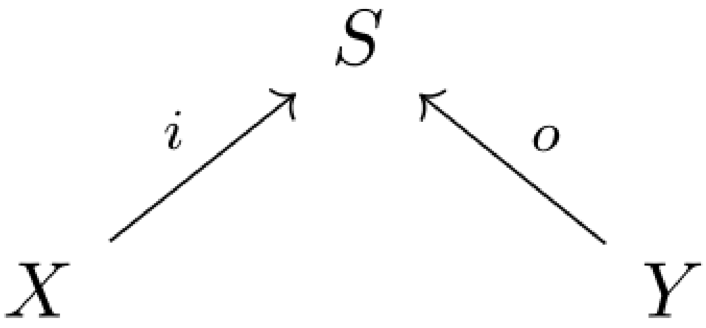


Let $S \sqcup_Y S' = S \sqcup S'/\sim$ where $s \sim s'$ if $o(y) = s$ and $i'(y) = s'$ for some $y \in Y$.

In reaction-land, this identifies a species of S with one of S' whenever both are connected to the same hose.

The model – Cospans

WHY COSPANS ARE GOOD: It's known that there exists a category, $Cospan$, whose objects are finite sets and whose morphisms from X to Y are cospans with X and Y as foots.



However…

The model – Cospans

FEATURES NOT RECOVERED: We have no record of transitions!

To fix that, we will "decorate" cospans: append the information of the reaction.

The model – ~~Cospans~~ Decorated cospans

These look like

$$\left(X \xrightarrow{\;i\;} S \xleftarrow{\;o\;} Y \quad , \quad R = (S, T, s, t, r) \right)$$

The model – ~~Cospans~~ Decorated cospans

These look like

$$\left(\begin{array}{ccc} & S & \\ & {\scriptstyle i}\nearrow \quad \nwarrow{\scriptstyle o} & \\ X & & Y \end{array} \quad , \quad R = (S, T, s, t, r) \right)$$

PROBLEM: Not obvious that these compose.

The model – ~~Cospans~~ Decorated cospans

SOLUTION:

Thm. [Fong]: If the decorations can be given through a functor

$$F: FinSet \to Set,$$

then we can form a category whose objects are finite sets and whose morphisms are cospans decorated by an element in the image under F of its apex.

The model – ~~Cospans~~ Decorated cospans

SOLUTION:

Thm. [Fong]: If the decorations can be given through a functor

$$F: FinSet \rightarrow Set,$$

then we can form a category whose objects are finite sets and whose morphisms are cospans decorated by an element in the image under F of its apex.

In this case: $F(S)$ is the set $\{(S, T, s, t, r)\}$ of all possible reaction networks using the species in S.

Claim: we can define F on morphisms so that everything works.

The model – ~~Cospans~~ Decorated cospans

Then, we get a category $RxNet$ with

- objects: finite sets
- morphisms $X \to Y$: decorated cospans

$$\left(\begin{array}{ccc} & S & \\ & {\scriptstyle i} \nearrow \quad \nwarrow {\scriptstyle o} & \\ X & & Y \end{array} \quad , \quad R = (S, T, s, t, r) \right)$$

that captures the same information as chemical reaction networks.

(Open) dynamical systems as decorated cospans

These look like

$$\left(\begin{array}{ccc} & S & \\ & {}^{i}\nearrow \quad \nwarrow^{o} & \\ X & & Y \end{array} \quad , \quad v \colon \mathbb{R}^S \to \mathbb{R}^S \right)$$

IDEA: S is the set of variables, v is the “intrinsic” vector field, and i and o mark the variables where we admit inflows/outflows.

(Open) dynamical systems as decorated cospans

Explicitly: Given

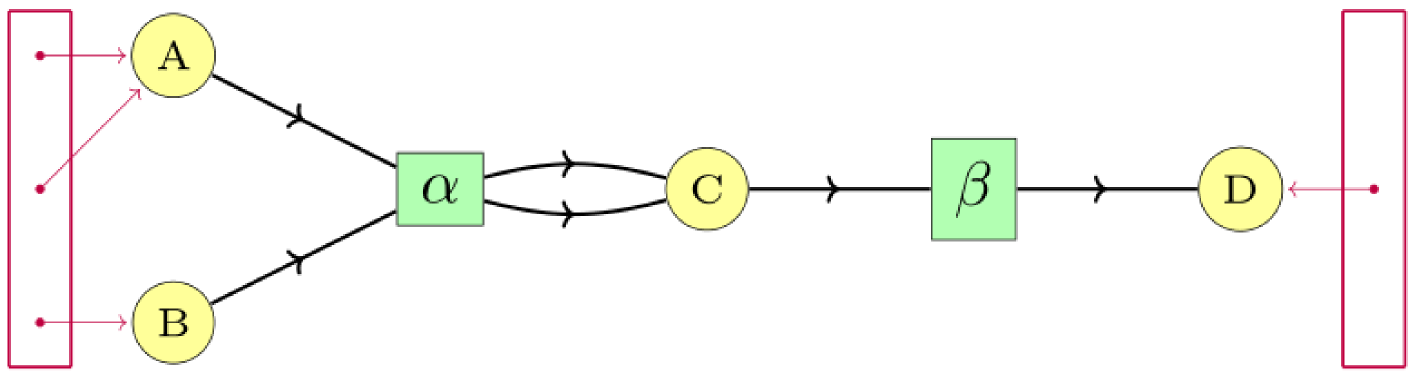
- an inflow $I: \mathbb{R} \to \mathbb{R}^X$
- an outflow $O: \mathbb{R} \to \mathbb{R}^Y$
- a vector $c: \mathbb{R} \to \mathbb{R}^S$

we let

$$\frac{dc(t)}{dt} = v(c(t)) + i_*(I(t)) - o_*(O(t))$$

where $i_*(I) : \mathbb{R} \to \mathbb{R}^S$ is $i_*(I)(t)(s) = \sum_{x:i(x)=s} I(t)(x)$

Important features – Associated dynamical system



$$\frac{d[A]}{dt} = -[A][B]r(\alpha) + I_A^1 + I_A^2 \qquad \frac{d[C]}{dt} = 2[A][B]r(\alpha) - [C]r(\beta)$$

$$\frac{d[B]}{dt} = -[A][B]r(\alpha) + I_B \qquad \frac{d[D]}{dt} = [C]r(\beta) - O_D$$

Here $I = (I_A^1, I_A^2, I_B)$ and $i_*(I) = (I_A^1 + I_A^2, I_B, 0, 0)$

(Open) dynamical systems as decorated cospans

Thm. [Fong]: If the decorations can be given through a functor

$$F: FinSet \to Set,$$

then we can form a category whose objects are finite sets and whose morphisms are cospans decorated by an element in the image under F of its apex.

In this case: $\mathrm{D}(S)$ is the set $\{\, \mathrm{v}: \mathbb{R}^S \to \mathbb{R}^S \,\}$ of all possible algebraic vector fields.

Claim: we can define D on morphisms so that everything works.

(Open) dynamical systems as decorated cospans

Then, we get a category **Dynam** with

- objects: finite sets
- morphisms $X \to Y$: decorated cospans

$$\left(X \xrightarrow{i} S \xleftarrow{o} Y \quad , \quad v\colon \mathbb{R}^S \to \mathbb{R}^S \right)$$

that captures the information of (open) dynamical systems.

From reactions to dynamical systems

GOAL: Get a functor $\mathrm{Sys}\colon RxNet \to Dynam$ taking a reaction network to its associated dynamical system.

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Thm. [Fong]: A natural transformation between the functors giving the decorations yields a functor between the decorated cospan categories.

In this case, for each finite set S,

$$\theta_S : F(S) \to D(S)$$

$$\theta_S(R = (S, T, s, t, r)) = v^R$$

From reactions to dynamical systems

So θ induces a functor $Sys\colon RxNet \to Dynam$ such that

- Sys is identity on objects
- On morphisms,

$$f = \left(X \xrightarrow{i} S \xleftarrow{o} Y \,,\; (\mathrm{S},\mathrm{T},\mathrm{s},\mathrm{t},\mathrm{r}) \right) \rightsquigarrow Sys\,(f) = \left(X \xrightarrow{i} S \xleftarrow{o} Y \,,\; v^{(S,T,s,t,r)} \right)$$

Steady states

Defn. Given an open dynamical system $(X \xrightarrow{i} S \xleftarrow{o} Y,\ v)$ together with an inflow $I \in \mathbb{R}^X$ and an outflow $O \in \mathbb{R}^Y$, a ***steady state*** with inflows I and outflows O is an element $c \in \mathbb{R}^S$ such that

$$v(c) + i_*(I) - o_*(O) = 0$$

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$$v(c) + i_*(I) - o_*(O) = 0$$

Want to study the relation between input concentrations, inflows, output concentrations and outflows in steady state (the **“externally observable steady state behavior”**)

$$\{(c \circ i, I, c \circ o, O) : v(c) + i_*(I) - o_*(O) = 0\} \subseteq \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y$$

Steady states

GOAL: Find a functor $St\colon Dynam \to ?$ that

- on objects: $St(S) = ?$
- on morphisms:

$$\left(X \xrightarrow{i} S \xleftarrow{o} Y \;,\quad v\colon \mathbb{R}^S \to \mathbb{R}^S \right) \rightsquigarrow \begin{array}{l} \{(c\circ i, I, c\circ o, O) : \\ \quad v(c) + i_*(I) - o_*(O) = 0\} \\ \qquad \subseteq \quad \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y \end{array}$$

Steady states

GOAL: Find a functor $St\colon Dynam \to ?$ that

- on objects: $St(S) = \mathbb{R}^S \oplus \mathbb{R}^S$
- on morphisms:

$$\left(X \xrightarrow{i} S \xleftarrow{o} Y \ , \quad v\colon \mathbb{R}^S \to \mathbb{R}^S \right) \rightsquigarrow \begin{aligned} &\{(c \circ i, I, c \circ o, O) : \\ &\quad v(c) + i_*(I) - o_*(O) = 0\} \\ &\qquad \subseteq \ \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y \end{aligned}$$

Steady states

? is the category Rel, whose

- objects: "based" vector space $\mathbb{R}^S \oplus \mathbb{R}^S$ for a finite set S
- morphisms $\mathbb{R}^X \oplus \mathbb{R}^X \to \mathbb{R}^Y \oplus \mathbb{R}^Y$ are linear subspaces

$$V \subseteq \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y$$

Steady states

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$$V \subseteq \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y$$

Composition? Given $V \subseteq (\mathbb{R}^X)^2 \oplus (\mathbb{R}^Y)^2$ and $W \subseteq (\mathbb{R}^Y)^2 \oplus (\mathbb{R}^Z)^2$ a pair $(x, z) \in (\mathbb{R}^X)^2 \oplus (\mathbb{R}^Z)^2$ belongs to the composition $W \circ V$ if there exists $y \in (\mathbb{R}^Y)^2$ such that $(x, y) \in V$ and $(y, z) \in W$.

Steady states

PROBLEM: Rel is not a decorated cospan category, so we can't use our magic theorems to prove $St\colon Dynam \to Rel$ is a functor.

SOLUTION: We can prove it by hand (some work involved).

Recap

- We built a category $RxNet$ encoding all the information of chemical reaction networks.
- We built a category $Dynam$ of (open) dynamical systems
- We have functors

$$Sys: RxNet \to Dynam$$

taking a chemical reaction to its associated open dynamical system, and

$$St: Dynam \to Rel$$

taking an open dyn. System to the space of all possible externally observable steady state behaviors.

What is this good for?

Interpreting the facts:

The correspondence that associates to an open chemical reaction the set of all its externally observable steady state behaviors **is functorial**, given by

$$\mathsf{RxNet} \xrightarrow{Sys} \mathsf{Dynam} \xrightarrow{St} \mathsf{Rel}$$

That means it respects composition.

Then, we can find the steady states of a big, complex system by composing the steady states of its smaller parts, which in theory should be much easier to study.

What is this good for?

Connections between areas:

With some imagination: this "decorated cospan" formalism can be applied to any sort of "open network".

Other examples of these are open electrical circuits, or open Markov processes.

THE HOPE: one can transfer intuition from one setting to the other and be able to make new connections.

Thanks for your time!

References

- J. C. Baez and B. S. Pollard, *A compositional framework for reaction networks*, Rev. Math. Phys. (2017)
- B. Fong, *Decorated cospans*, Theory Appl. Categ. (2015)