Compositional modelling of open reaction networks

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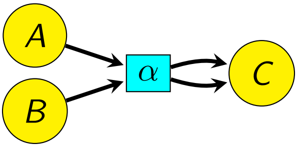
Reaction networks

Definition

A **reaction network with rates** (S, T, s, t, r) *consists of:*

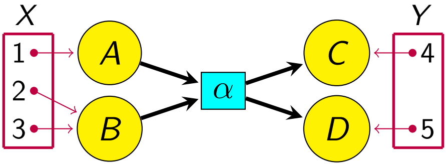
- *a finite set* S *of* **species**,
- *a finite set* T *of* **transitions**,
- *functions* $s, t \colon T \to \mathbb{N}^S$ *assigning* **source** *and* **target complexes**, *and*
- *a function* $r \colon T \to (0, \infty)$, *assigning* **rates** *to each transition.*



Open reaction networks

Open reaction networks are generalizations of reaction networks in which certain species are labelled as **input** and **output** species.

$$R\colon X \to Y$$



Black-boxing open reaction networks

$$\mathtt{RxNet} \xrightarrow{\color{lightgray}\blacksquare} \mathtt{Dynam} \xrightarrow{\blacksquare} \mathtt{Rel}$$

The category of open reaction networks

Definition

An **open reaction network** $R\colon X \to Y$ *consists of a cospan of finite sets*

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

together with a reaction network $R = (S, T, s, t, r)$ *on* S.

Theorem (Baez, P.)

There is a category `RxNet` *whose objects are finite sets and whose morphisms are isomorphism classes of open reaction networks.*

Reaction networks as decorations

$$F\colon (\mathtt{FinSet}, +) \to (\mathtt{Set}, \times)$$

$$F(S) = \{\text{all reaction networks on } S\}$$

$$f\colon S \to S'$$

$$\begin{array}{rccc} F(f)\colon & F(S) & \to & F(S') \\ & (S, T, s, t, r) & \mapsto & (S', T, f_*(s), f_*(t), r) \end{array}$$

$$f_*(s(\tau))(\sigma') = \sum_{\{\sigma | f(\sigma) = \sigma'\}} s(\tau)(\sigma)$$

Reaction networks as decorations

$$F\colon (\mathtt{FinSet}, +) \to (\mathtt{Set}, \times)$$

$$F(S) = \{\text{all reaction networks on } S\}$$

$$\Phi_{S,S'}\colon F(S) \times F(S') \to F(S+S')$$

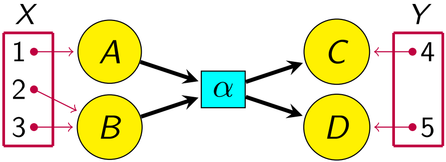
$$(S, T, s, t, r) \times (S', T', s', t', r') \mapsto (S+S', T+T', s+s', t+t', [r, r']\ )$$

$$s+s', t+t'\colon\ T+T' \to \mathbb{N}^{S+S'}$$

$$[r, r']\colon\ T+T' \to (0, \infty)$$

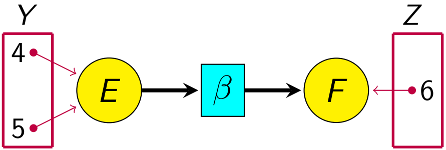
Composition of open reaction networks

$$R\colon X \to Y$$



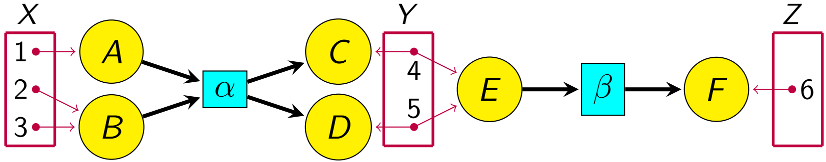
Composition of open reaction networks

$$R' \colon Y \to Z$$



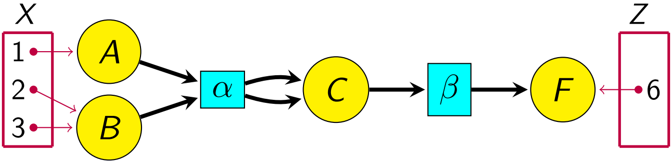
Composition of open reaction networks

To compose $R\colon X \to Y$ and $R'\colon Y \to Z$ we first combine them



Composition of open reaction networks

Then, we identify any species which are in the image of the same point in Y

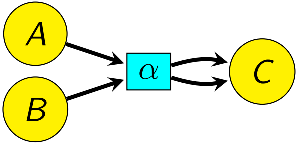


This gives a new open reaction network $RR' \colon X \to Z$.

The rate equation

A reaction network with rates specifies a set of coupled, non-linear differential equations called its **rate equation**:

$$
\begin{aligned}
\frac{dA(t)}{dt} &= -r(\alpha)A(t)B(t) \\
\frac{dB(t)}{dt} &= -r(\alpha)A(t)B(t) \\
\frac{dC(t)}{dt} &= 2r(\alpha)A(t)B(t)
\end{aligned}
$$



The rate equation

Given a reaction network with rates $R = (S, T, s, t, r)$, with species set $S = \{1, 2, \ldots, |S|\}$, let us denote a vector of **concentrations** of each species by $c = (c_1, c_2, \ldots, c_{|S|}) \in \mathbb{R}^S$. Concentrations are non-negative.

Introducing the notation

$$c^{s(\tau)} = \prod_{\sigma \in S} c_\sigma^{s_\sigma(\tau)},$$

we can write the rate equation of a general reaction network obeying mass-action kinetics as

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

The rate equation

Given a reaction network $R = (S, T, s, t, r)$, we can define a vector field

$$v(c) = \sum_{\tau \in T} r(\tau) \left(\ t(\tau) - s(\tau)\ \right) c^{s(\tau)}$$

generating the time evolution of the concentrations $c \in \mathbb{R}^S$ via

$$\frac{dc}{dt} = v(c).$$

For mass-action kinetics, the vector field $v \colon \mathbb{R}^S \to \mathbb{R}^S$ is polynomial in the concentrations.

A category of open dynamical systems

Definition

An **open dynamical system** $D\colon X \to Y$ *on* S *consists of a cospan of finite sets*

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

together with an algebraic vector field v *on* $\mathbb{R}^S$*.*

Theorem (Baez, P.)

There is a category $\mathtt{Dynam}$ *where objects are finite sets and morphisms are isomorphism classes of open dynamical systems.*

Decorating with algebraic vector fields

$$D\colon (\mathtt{FinSet}, +) \to (\mathtt{Set}, \times)$$

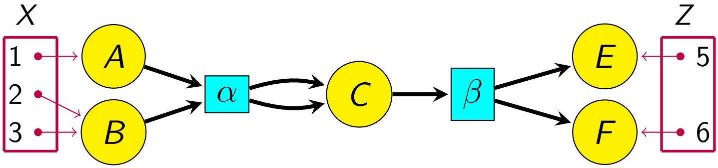
$$D(S) = \{v\colon \mathbb{R}^S \to \mathbb{R}^S \mid v \text{ is algebraic}\}$$

$$f\colon S \to S'$$

$$\begin{array}{cccc} D(f)\colon & D(S) & \to & D(S') \\ & v & \mapsto & f_* \circ v \circ f^* \end{array}$$

$$f^*(c')(\sigma) = (c' \circ f)(\sigma) \qquad f_*(v)(\sigma') = \sum_{\{\sigma \mid f(\sigma) = \sigma'\}} v(\sigma)$$

The gray-boxing functor

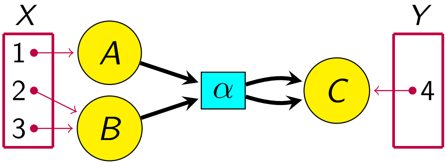


Theorem (Baez, P.)

There is a functor $\blacksquare$: $\mathtt{RxNet} \to \mathtt{Dynam}$ *sending an open reaction network to its corresponding open dynamical system.*

The gray-boxing functor

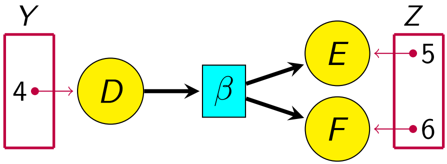
$\blacksquare(R\colon X \to Y)$



$$
\begin{aligned}
v_A &= -r(\alpha)A(t)B(t) \\
v_B &= -r(\alpha)A(t)B(t) \\
v_C &= 2r(\alpha)A(t)B(t)
\end{aligned}
$$

The gray-boxing functor

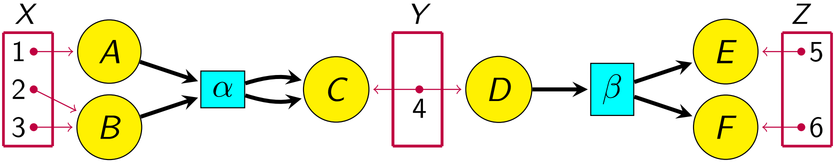
■$(R' \colon Y \to Z)$



$$
\begin{aligned}
v_D &= -r(\beta)D(t) \\
v_E &= r(\beta)D(t) \\
v_F &= r(\beta)D(t)
\end{aligned}
$$

The gray-boxing functor

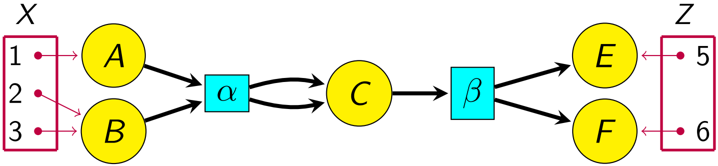
$\blacksquare(R\colon X \to Y)\blacksquare(R'\colon Y \to Z)$



$$
\begin{aligned}
v_A &= -r(\alpha)AB & \qquad v_D &= -r(\beta)D \\
v_B &= -r(\alpha)AB & \qquad v_E &= r(\beta)D \\
v_C &= 2r(\alpha)AB & \qquad v_F &= r(\beta)D
\end{aligned}
$$

The gray-boxing functor

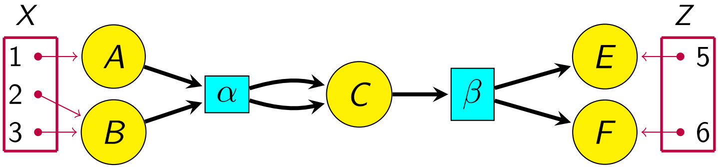
$\blacksquare(R\colon X \to Y)\blacksquare(R'\colon Y \to Z)$



$$\begin{aligned}
v_A &= -r(\alpha)AB \\
v_B &= -r(\alpha)AB \\
v_C + v_D &= 2r(\alpha)AB - r(\beta)D \text{ and } C = D \\
v_E &= r(\beta)D \\
v_F &= r(\beta)D
\end{aligned}$$

The gray-boxing functor

$\blacksquare(RR' \colon X \to Z)$



$$
\begin{aligned}
v_A &= -r(\alpha)AB \\
v_B &= -r(\alpha)AB \\
v_C &= 2r(\alpha)AB - r(\beta)C \\
v_E &= r(\beta)C \\
v_F &= r(\beta)C
\end{aligned}
$$

The gray-boxing functor

$$\blacksquare \colon \mathtt{RxNet} \to \mathtt{Dynam}$$

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

$$\begin{tikzcd}
F(S) \arrow[r, "F(f)"] \arrow[d, "\theta_S"'] & F(S') \arrow[d, "\theta_{S'}"] \\
D(S) \arrow[r, "D(f)"'] & D(S')
\end{tikzcd}$$

$$f \colon S \to S'$$

$$R = (S, T, s, t, r) \qquad R' = (S', T, f_*(s), f_*(t), r)$$

$$D(f)(v^R) = v^{R'}$$

$$f_* \circ v^R \circ f^* = v^{R'}$$

$$v^{R'}(c') = \sum_{\tau \in T} r(\tau)(f_*(t)(\tau) - f_*(s)(\tau))\; {c'}^{f_*(s)(\tau)}$$

The calculation

$$
\begin{aligned}
{c'}^{f_*(s)(\tau)} &= \prod_{\sigma' \in S'} {c'_{\sigma'}}^{f_*(s)(\tau)(\sigma')} \\
&= \prod_{\sigma' \in S'} {c'_{\sigma'}}^{\sum_{\{\sigma:\, f(\sigma)=\sigma'\}} s(\tau)(\sigma)} \\
&= \prod_{\sigma' \in S'} \prod_{\{\sigma:\, f(\sigma)=\sigma'\}} {c'_{\sigma'}}^{s(\tau)(\sigma)} \\
&= \prod_{\sigma \in S} {c'_{f(\sigma)}}^{s(\tau)(\sigma)} \\
&= \prod_{\sigma \in S} {f^*(c')_\sigma}^{s(\tau)(\sigma)} \\
&= f^*(c')^{s(\tau)}.
\end{aligned}
$$

And then!

$$
\begin{aligned}
v^{R'}(c') &= \sum_{\tau \in T} r(\tau)(f_*(t)(\tau) - f_*(s)(\tau))\, f^*(c')^{s(\tau)} \\
&= f_*(v^R(f^*(c'))).
\end{aligned}
$$

So $v^{R'} = f_* \circ v^R \circ f^*$ as desired.

Recap

$$\mathtt{RxNet} \xrightarrow{\quad\blacksquare\quad} \mathtt{Dynam} \xrightarrow{\quad\blacksquare\quad} \mathtt{Rel}$$

Open Markov processes

$$\begin{tikzcd}
\mathtt{RxNet} \arrow[r, "\color{gray}\blacksquare"] & \mathtt{Dynam} \arrow[r, "\blacksquare"] & \mathtt{Rel} \\
\mathtt{Mark} \arrow[u, "I"]
\end{tikzcd}$$

Thank you!

For more:

- John C. Baez and Blake S. Pollard, A compositional framework for reaction networks, *Reviews in Mathematical Physics*.
- John C. Baez, Brendan Fong and Blake S. Pollard, A compositional framework for Markov processes, *Journal of Mathematical Physics*.
- Blake S. Pollard, Open Markov processes: A compositional perspective on non-equilibrium steady states in biology, *Entropy*.
- Blake S. Pollard, A Second Law for open Markov processes, *Open Systems and Information Dynamics*.