Compositional frameworks for open systems

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Idea: View open systems as morphisms in categories

A category \( \mathcal{C} \) consists of objects \( X, Y \in \text{Ob}(\mathcal{C}) \) and morphisms \( f : X \to Y \in \text{Mor}(\mathcal{C}) \), equipped with an associative composition operation:

\[
\begin{array}{ccc}
X & \xrightarrow{f} & Y \\
\downarrow & \searrow & \downarrow \\
Y & \xrightarrow{g} & Z \\
\downarrow & \nearrow & \downarrow \\
Z & \xrightarrow{h} & A
\end{array}
\]

Together with identity morphisms \( 1_X : X \to X \) satisfying the left/right identity laws:

\[
\begin{array}{ccc}
X & \xrightarrow{f} & Y \\
\downarrow & \searrow & \downarrow \\
Y & \xrightarrow{1_Y} & Y \\
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equipped with an **associative composition** operation

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  Y \\
\end{array}
\quad
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  Z \\
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  A \\
\end{array}
\quad
\begin{array}{c}
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  \downarrow g \\
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  A \\
\end{array}
\quad
\begin{array}{c}
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  \downarrow 1_X \\
  \downarrow f \\
  Y \\
\end{array}
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\end{array}
\]

together with **identity morphisms** \( 1_X : X \to X \) satisfying the **left/right identity laws**
Open systems as morphisms in a category

We can think of open systems as morphisms in a category.

Composition corresponds to connecting systems.
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Composition corresponds to connecting systems.
A continuous-time, discrete-state Markov chain, or Markov process $M = (V, E, s, t, r)$ is

$$(0, \infty) \xleftarrow{r} E \xrightarrow{\ s\ } \ x \xrightarrow{\ t\ } V$$

- where $V$ is a finite set of states,
- $E$ is a finite set of edges,
- $s, t : E \to V$ assign a source and target to each edge, and
- $r : E \to (0, \infty)$ assigns a rate constant $r_e$ to each edge $e \in E$. 
The master equation

From a Markov process $M = (V, E, s, t, r)$ we can construct a matrix $H: \mathbb{R}^V \to \mathbb{R}^V$, called its Hamiltonian which generates the time evolution of a probability distribution $p \in \mathbb{R}^V$ via the master equation

$$\frac{dp}{dt} = Hp.$$
Steady-states and detailed balance

A **steady state** is a distribution $q$ such that

$$\frac{dq_i}{dt} = \sum_j (H_{ij}q_j - H_{ji}q_i) = 0 \text{ for all } i \in V.$$

A **detailed balanced equilibrium** $q$ is a steady state which satisfies

$$H_{ij}q_j = H_{ji}q_i \text{ for all } i, j \in V.$$

An **detailed balanced Markov process** is a Markov process equipped with a detailed balanced equilibrium distribution.
Open detailed balanced Markov processes

Consider a subsystem of a larger Markov process as an open system itself:

Although probability is conserved in the whole process, probability can flow in and out of the subprocess.

Thus we consider non-normalized probabilities, taking arbitrary non-negative real values.
What are open detailed balanced Markov processes?

Open Markov processes are generalizations of Markov processes in which probability can flow in and out through certain input and output states.
What are open detailed balanced Markov processes?

Open Markov processes are generalizations of Markov processes in which probability can flow in and out through certain **input** and **output** states.
We thus equip a detailed balanced Markov process on the set $V$ with finite sets $X$, $Y$ and input and output maps $i: X \to V$ and $o: Y \to V$ specifying how the inputs and outputs are included in the set of states $V$.

We call the subset of states $B = i(X) \cup o(Y) \subseteq V$ the boundary of the process.
The open master equation

The probabilities $p \in \mathbb{R}^V$ of an open Markov process satisfy the **open master equation**

$$\frac{dp_i}{dt} = \sum_j H_{ij}p_j \text{ for } i \in V - B$$

$$p_i(t) = f_i(t) \text{ for } i \in B.$$  

To specify the dynamics of an open Markov process one must specify the **boundary probabilities** $f_i(t)$.  

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A steady state solution of the open master is equation is a solution $p : V \to [0, \infty)$ such that $\frac{dp}{dt} = 0$. 
Composing open detailed balanced Markov processes

If the outputs of one open Markov process match the inputs of another you can compose the two to get a new open Markov process.
Composition

If the outputs of one open Markov process match the inputs of another you can compose the two to get a new open Markov process.

In our framework composition corresponds to gluing together the processes along their overlap.
DetBalMark

We thus have a category DetBalMark where
  
  - an object is a finite set equipped with a non-normalized probability
  - a morphism is an open detailed balanced Markov process.

\[ f : X \rightarrow Y \]
An open detailed balanced Markov process in a non-equilibrium steady state

If we label our states \( V = \{A, B, C\} \), the open master equation says

\[
\frac{dp_B}{dt} = p_A - p_B + p_C - p_B
\]

Setting \( \frac{dp_B}{dt} = 0 \) together with \( p_A = 2 \) and \( p_C = 1 \) yields \( p_B = \frac{3}{2} \).

Generally we have a non-equilibrium steady state \( p = (p_A, \frac{p_A + p_C}{2}, p_C) \).
Functors

A functor is a map between categories which preserves identities and respects composition.

Given categories $\mathcal{C}$ and $\mathcal{D}$, a functor

$$F : \mathcal{C} \rightarrow \mathcal{D}$$

sends objects to objects and morphisms to morphisms such that:

$$F(fg) = F(f)F(g)$$

$$F(1_X) = 1_{F(X)}$$
We can use functors to study the ‘behaviors’ of open systems

\[ F : \text{OpenSys} \rightarrow \text{Behavior} \]
An object in LinRel is a real vector space and a morphism is a linear relation between finite-dimensional real vector spaces.

A linear relation $L: U \rightsquigarrow V$ is a linear subspace $L \subseteq U \oplus V$.

Given linear relations $L: U \rightsquigarrow V$ and $L': V \rightsquigarrow W$, their composite $LL': U \rightsquigarrow W$ is given by

$$LL' = \{(u, w): \exists v \in V \text{ with } (u, v) \in L \text{ and } (v, w) \in L'\}.$$ 

Composition in LinRel requires that the subspaces agree on their overlap.
Consider an open detailed balanced Markov process \( f : X \rightarrow Y \) on \( V \). For any state we can calculate the net inflow

\[
J_i(p) = \sum_j H_{ij}p_j - H_{ji}p_i.
\]

We define its **steady state behavior** to be the subspace of steady state boundary probability, flow pairs \((p_X, J_X, p_Y, -J_Y) \subseteq \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y\).
The black-box functor

\[ \bullet : \text{DetBalMark} \to \text{LinRel} \]

sends an open detailed balanced Markov process \( f : X \to Y \) to the subspace \((p_X, J_X, p_Y, -J_Y) \subseteq \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y\) thought of as a linear relation

\[ \bullet(f) : \mathbb{R}^X \oplus \mathbb{R}^X \rightsquigarrow \mathbb{R}^Y \oplus \mathbb{R}^Y. \]

Composition in \(\text{LinRel}\) requires that the probabilities agree on their overlap and that the outflow of one process matches the inflow of the other.
Black-boxing

\[ f : X \rightarrow Y \]

\[ f = (p_A, J_A, p_B, -J_B) = (p_A, p_B - p_A, p_B, p_B - p_A) \]
Black-boxing

\[ g : Y \to Z \]

\[ g = (p_B, J_B, p_C, -J_C) = (p_B, p_C - p_B, p_C, p_C - p_B) \]
Black-boxing

\[ fg : X \rightarrow Z \]

\[ fg = (p_A, J_A, p_C, -J_C) = (p_A, \frac{p_C - p_A}{2}, p_C, \frac{p_C - p_A}{2}) \]
Composition in LinRel

Alternatively we can compute

\[(f)\circ (g) = (p_A, J_A, p_B, -J_B)(p_B, J_B, p_C, -J_C) \]

\[(p_A, p_B - p_A, p_B, p_B - p_A)(p_B, p_C - p_B, p_C, p_C - p_B)\]

The current flowing out of \(f\) must equal the current flowing into \(g\)

\[p_B - p_A = p_C - p_B\]

or

\[p_B = \frac{p_A + p_C}{2}\]

giving the composite relation

\[\left( p_A, \frac{p_C - p_A}{2}, p_C, \frac{p_C - p_A}{2} \right).\]
Thanks!

For more on category theory applied to networks:

- Brendan Fong, *The Algebra of Open and Interconnected Systems*.
- John Baez and Brendan Fong, *A compositional framework for passive linear networks*.
- Blake Pollard *Open Markov processes: A compositional perspective on non-equilibrium steady states in biology*