Compositional frameworks for open systems

Blake S. Pollard
Department of Physics and Astronomy
University of California, Riverside

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Idea: View open systems as morphisms in categories

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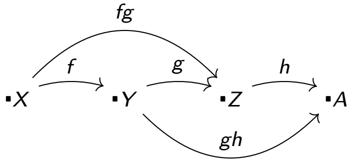
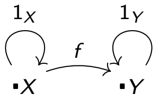
A category $\mathcal{C}$ consists of

- **objects** $X, Y \in Ob(\mathcal{C})$ and
- **morphisms** $f : X \to Y \in Mor(\mathcal{C})$

equipped with an **associative composition** operation

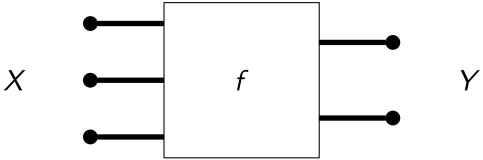


together with **identity morphisms** $1_X : X \to X$ satisfying the **left/right identity laws**

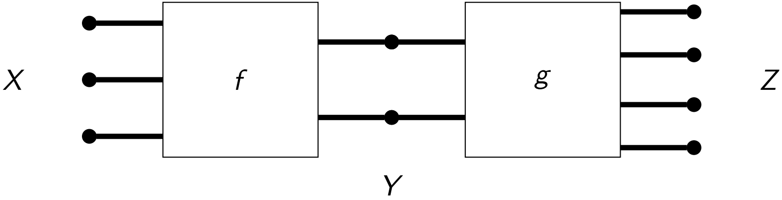


Open systems as morphisms in a category

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



Composition corresponds to connecting systems.



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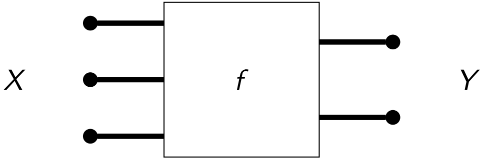

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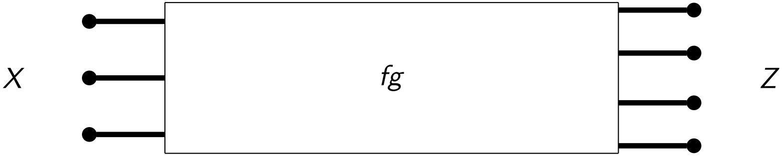


Markov processes as labelled graphs

Definition

A continuous-time, discrete-state Markov chain, or **Markov process** $M = (V, E, s, t, r)$ is

$$(0, \infty) \xleftarrow{r} E \underset{t}{\overset{s}{\rightrightarrows}} V$$

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

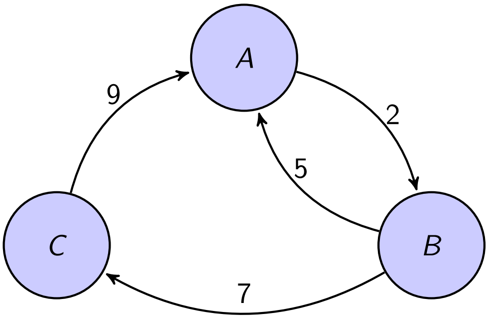
The master equation

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

$$\frac{dp}{dt} = Hp.$$

$$H = \begin{pmatrix} -2 & 5 & 9 \\ 2 & -12 & 0 \\ 0 & 7 & -9 \end{pmatrix}$$

$$p = \begin{pmatrix} p_A \\ p_B \\ p_C \end{pmatrix}$$



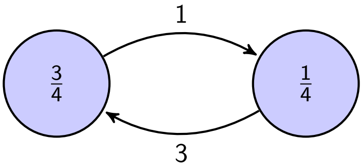
Steady-states and detailed balance

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

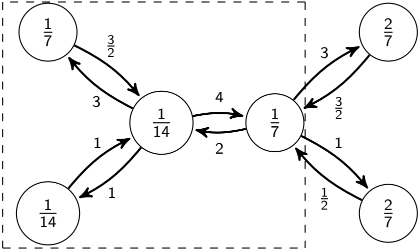
$$H_{ij} q_j = H_{ji} q_i \text{ for all } i, j \in V.$$



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.

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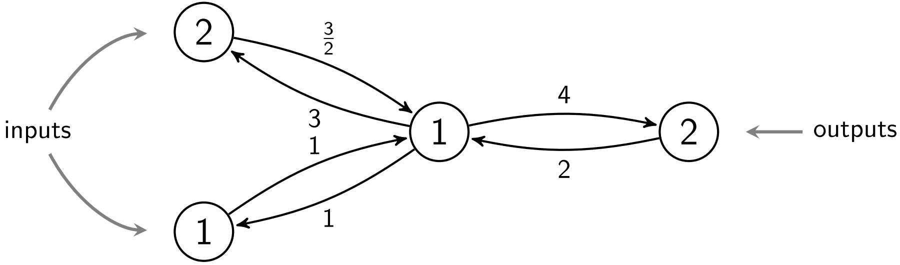
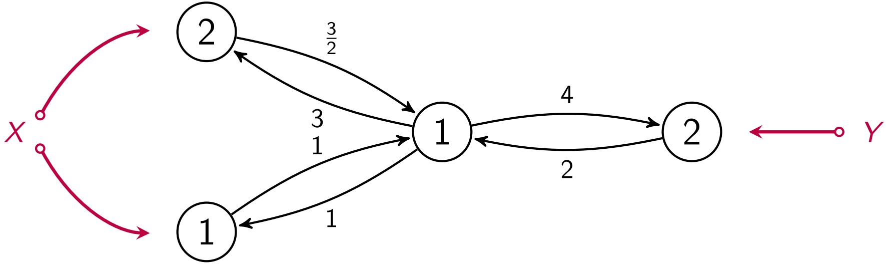


DetBalMark

We thus equip a detailed balanced Markov process on the set V with finite sets X, Y and **input** and **output** maps $i\colon X \to V$ and $o\colon Y \to V$ 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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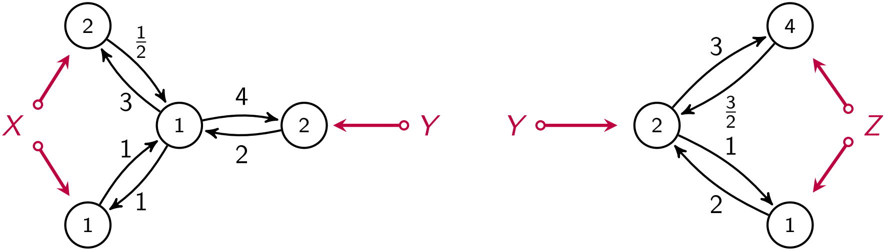
A **steady state** solution of the open master is equation is a solution $p\colon V \to [0, \infty)$ such that $\frac{dp}{dt} = 0$.

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

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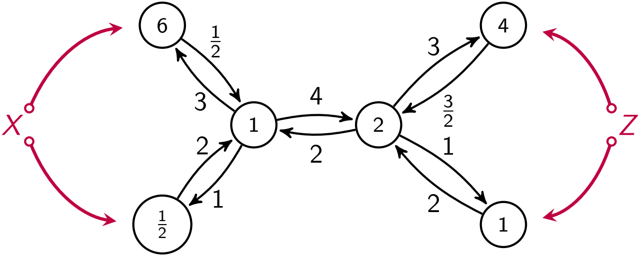


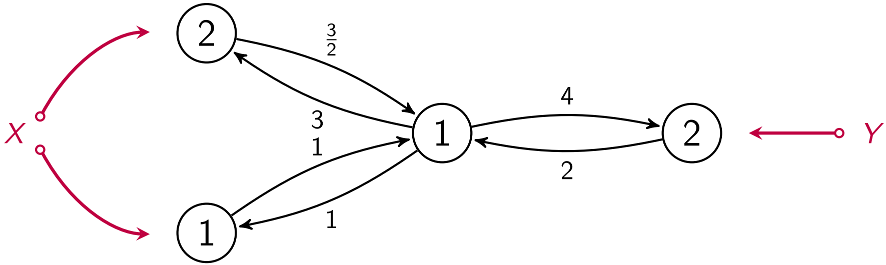
In our framework composition corresponds to gluing together the processes along their overlap.

DetBalMark

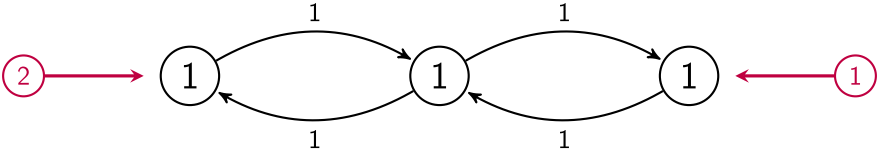
We thus have a category DetBalMark where

- an object is a finite set equipped with a non-normalized probability
- a morphism is an open detailed balanced Markov process.

$$f : X \to Y$$



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

$$F\colon \mathcal{C} \to \mathcal{D}$$

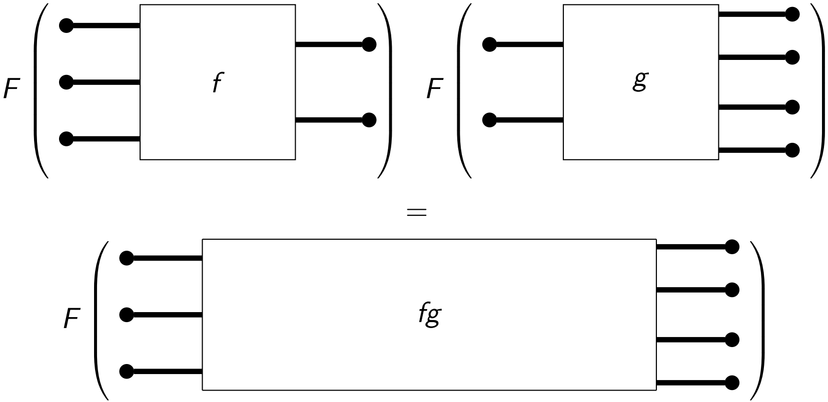
sends objects to objects and morphisms to morphisms such that:

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

$$F(1_X) = 1_{F(X)}$$

We can use functors to study the 'behaviors' of open systems

$$F\colon \mathtt{OpenSys} \to \mathtt{Behavior}$$



LinRel

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 $L \colon U \rightsquigarrow V$ is a linear subspace $L \subseteq U \oplus V$.

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

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

Composition in LinRel requires that the subspaces agree on their overlap.

The behavior of an open detailed balanced Markov process

Consider an open detailed balanced Markov process $f\colon X \to Y$ 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

The black-box functor

$$\blacksquare\colon \mathtt{DetBalMark} \to \mathtt{LinRel}$$

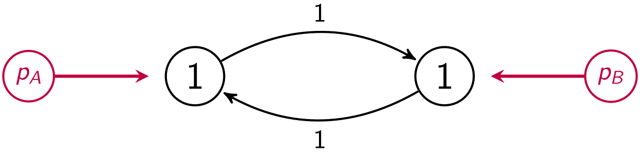
sends an open detailed balanced Markov process $f\colon X \to Y$ to the subspace $(p_X, J_X, p_Y, -J_Y) \subseteq \mathbb{R}^X \oplus \mathbb{R}^X \oplus \mathbb{R}^Y \oplus \mathbb{R}^Y$ thought of as a linear relation

$$\blacksquare(f)\colon \mathbb{R}^X \oplus \mathbb{R}^X \leadsto \mathbb{R}^Y \oplus \mathbb{R}^Y.$$

Composition in LinRel requires that the probabilities agree on their overlap and that the outflow of one process matches the inflow of the other.

Black-boxing

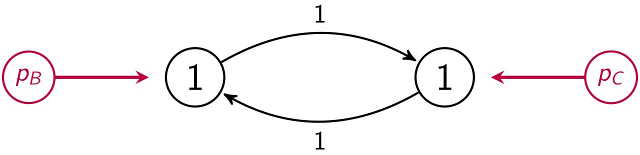
$f: X \to Y$



$\blacksquare f = (p_A, J_A, p_B, -J_B) = (p_A, p_B - p_A, p_B, p_B - p_A)$

Black-boxing

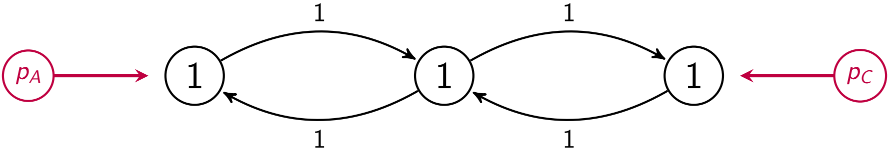
$$g\colon Y \to Z$$



$$\blacksquare g = (p_B, J_B, p_C, -J_C) = (p_B, p_C - p_B, p_C, p_C - p_B)$$

Black-boxing

$$fg : X \to Z$$



$$\blacksquare fg = (p_A, J_A, p_C, -J_C) = (p_A, \frac{p_C - p_A}{2}, p_C, \frac{p_C - p_A}{2}))$$

Composition in LinRel

Alternatively we can compute

$$\blacksquare(f)\blacksquare(g) =$$

$$(p_A, J_A, p_B, -J_B)(p_B, J_B, p_C, -J_C)$$

$$(p_A, p_B - p_A, p_B, p_B - p_A)(p_B, p_C - p_B, p_C, p_C - p_B)$$

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.
- John Baez, Brendan Fong and Blake Pollard, A compositional framework for Markov processes.
- Blake Pollard Open Markov processes: A compositional perspective on non-equilibrium steady states in biology
- John Baez and Blake Pollard, A compositional framework for reaction networks (in preparation).