Stochastic mechanics of graph rewriting

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Concept

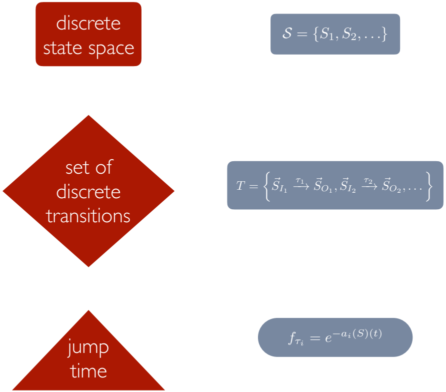
- **TOPIC: continuous time Markov chains (CTMCs) for graph rewriting systems**
- **THE SPECIAL TWIST:**
  - link between **non-deterministic transitions** and **associative unital algebras**
  - **new** insights into the **combinatorics** of graph rewriting, **unification** of the formalisms of physics and mathematical combinatorics with the computer science formalism
  - powerful new formulae for **fragmentation**!
- **PLAN:** short motivation/introduction about **stochastic graph rewriting** (aka a particular class of CTMCs), then the new **rule algebraic formalism**

Graph rewriting and Markov chain theory

The basics of generic Markov chains

- **Idea:** consider a stochastic dynamical system with
  - a **discrete state space** (possibly ∞ many states though!)
  - the **memoryless property**, whence the transitions of the system can only depend on information available in the **current** state of the system (and not on the history of the state)
  - **transitions** are **discrete jumps** from one state to another – they happen instantaneuously, though at **random times**
- Closer analysis reveals that the jump times can then only be drawn from some **exponential jump time distribution** (that may be state-dependent)

$\Rightarrow$ characterization of a **continuous time Markov chain**!



The Master equation and other niceties

- **Standard CTMC theory**[1]: one way to describe the dynamics is to give a **probability distribution**

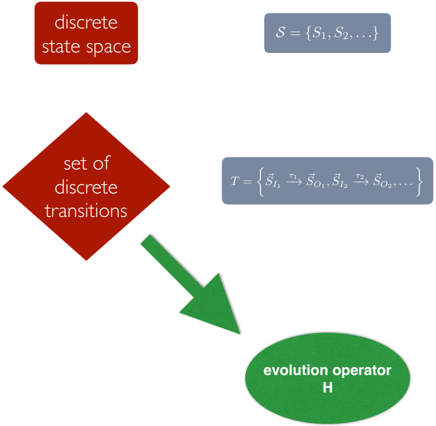
$$|\Psi(t)\rangle := \sum_{S\in\mathcal{S}} p_S(t)|S\rangle$$

of being in one of the discrete states (represented by basis vectors $|S\rangle$), and specifying the **Master equation** (aka **Schrödinger equation**)

$$\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle\,,$$

where H is the **evolution operator**.

- How precisely H is determined for a given system is one of the main questions in general!



[1] James R. Norris. *Markov Chains*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, 1998

The “stochastic mechanics” viewpoint

Benefits:

$\exists$ a full-blown formalism aka “**stochastic mechanics**”[2] for studying CTMCs:

- **Observables** O are linear operators under which each pure state is an Eigenstate,

$$O|S\rangle = \omega_O(S)|S\rangle\,.$$

- **Expectation values of observables** are computed by introducing the **dual projection vector**

$$\langle|S\rangle := 1 \quad \forall S \in \mathcal{S}\,,$$

such that for any state probability distribution $|\Psi(t)\rangle$

$$\mathbb{E}_{|\Psi(t)\rangle}(O) \equiv \langle O\rangle(t) := \langle|O|\Psi(t)\rangle\,.$$

$\Rightarrow$ **evolution of expectation values of observables** via Master equation:

$$\frac{d}{dt}\langle O\rangle(t) = \langle OH\rangle(t)\,.$$

- Additional property of the evolution operator H:

$$\langle|e^{tH}|\Psi(t)\rangle \stackrel{!}{=} 1 \quad \Rightarrow \quad \langle|H = 0\,,$$

i.e. H **preserves normalizations**.

$\Rightarrow$ analogue of the **Ehrenfest equation** of quantum mechanics:

$$\frac{d}{dt}\langle O\rangle(t) = \langle[O,H]\rangle(t)\,,$$

where $[A,B] := AB - BA$ is the **commutator**

[2] John C Baez and Jacob Biamonte. “A course on quantum techniques for stochastic mechanics”. In: *s arXiv:1209.3632* (2012)

Specializing to graph rewriting systems

Basics:

- **State space:** $G_{\cong}$ — isomorphism classes of **finite directed multi-graphs**
- **Discrete transitions:** isomorphism classes (!) of **graph rewriting rules** $I \overset{r}{\Rightarrow} O$, with **input graph** $I \in G_{\cong}$, **output graph** $O \in G_{\cong}$, and where $r : I \rightharpoonup O$ is an **isomorphism class of a partial injective morphism of graphs**
- **Evolution operator** H: to be dtermined!

Insight from statistical physics/chemistry:

- Promote the discrete state space to a **vector space** (usually over $\mathbb{R}$) $\mathcal{S}$, with one basis vector per possible discrete state.
- The transitions themselves should form an **associative unital algebra**, implementing the action of transitions on states via a (choice of) **representation** of this algebra , where a representation is an **algebra homomorphism** from the algebra of transitions T to the **space of endomorphisms** $End(\mathcal{S})$ over the state vector space $\mathcal{S}$:

$$\rho : T \to End(\mathcal{S})$$

such that

$$\rho(t_1 * t_2) = \rho(t_1)\rho(t_2)\,.$$

The main objectives of this work

- **Implement the full CTMC/ stochastic mechanics formalism** for graph rewriting – this will require in particular to find the **state space**, **implementation of transitions** via a **transition algebra**, defining the **evolution operator**, and finally the construction of the **canonical representation** of the transition algebra.
- **Determine a description of the evolution of graph rewriting systems** in this formalism.
- Study the potential benefits of this approach!

Stochastic mechanics formalism

Step 1: Directed multigraphs and the graph state space

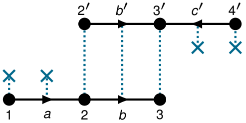
- A **finite directed multigraph** $G \equiv (V, E, s, t)$ is specified as a set of **vertices** V, a set of **edges** E, and **source and target maps** $s : E \to V$ and $t : E \to V$.
- The **graph state space** $\mathcal{G}$ is defined as the **span of the set of isomorphism classes of graphs** $G_{\cong}$,

$$\mathcal{G} := span_{\mathbb{R}}(G_{\cong})\,.$$

Step 2: Normal rule diagrams

- A **graph rewriting rule** $I \overset{r}{\Rightarrow} O$ consists of an **input graph** I, an **output graph** O, and an **injective partial morphism** $r : I \rightharpoonup O$. We will always consider such rules **up to isomorphism** (of I and O, and the induced effect on r).
- **Crucial idea:** encode rules as **normal rule diagrams** – draw I at the bottom, O at the top and r as dotted lines (with $\times\cdots$ to indicate which vertices and edges are not mapped)!

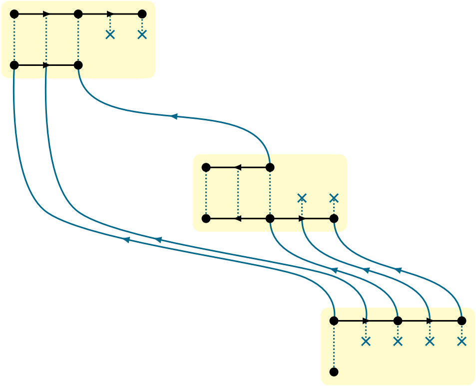
$$\left(\bullet_1 \underset{a}{\longrightarrow} \bullet_2 \underset{b}{\longrightarrow} \bullet_3 \quad \overset{r}{\rightharpoonup} \quad \bullet_{2'} \underset{b'}{\longrightarrow} \bullet_{3'} \underset{c'}{\longleftarrow} \bullet_{4'}\right) \;\widehat{=}$$



An example of a rule and its associated normal rule diagram.

Step 3: Generic rule diagrams and diagram composition

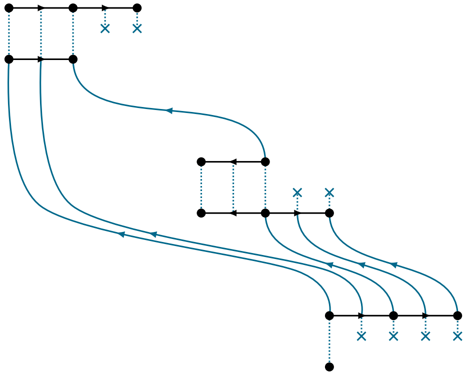
- The **composition** of rule diagrams may be understood visually as "threading together" normal rule diagrams along **diagram matches**, linking output vertices of one diagram to input vertices of another diagram, and similarly for the edges, subject to some **consistency conditions**:
  - **one-to-one** – any output vertex or edge is connected to at most one input vertex or edge
  - **acyclicity** – viewed in total, the rule diagram must not contain any cycles at all
  - **delayed edge morphism condition** – if an output edge is linked to an input edge of another diagram, its endpoint vertices must be linked, too, possibly via intermediate in-out vertex mappings
  - **totality** – see the paper!



Example for a composition of three normal rule diagrams (yellow boxes) into a composite rule diagram.

Step 4: Normalization of rule diagrams

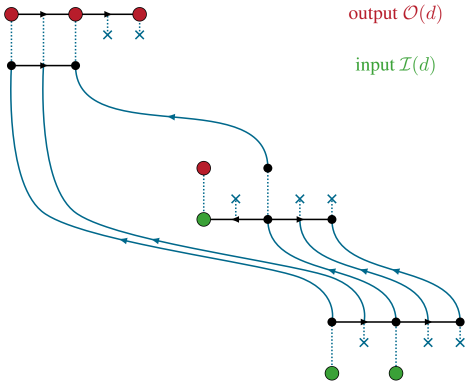
- Given a generic rule diagram d, its **normalization** $\partial(d)$ is defined as follows:



Example for a composition of three normal rule diagrams into a composite rule diagram.

Step 4: Normalization of rule diagrams

- Given a generic rule diagram d, its **normalization** $\partial(d)$ is defined as follows:
  - Determine the **input interface** $\mathcal{I}(d)$ and the **output interface** $\mathcal{O}(d)$ of d as those input and output graph parts that are not involved in the diagram matches of d.

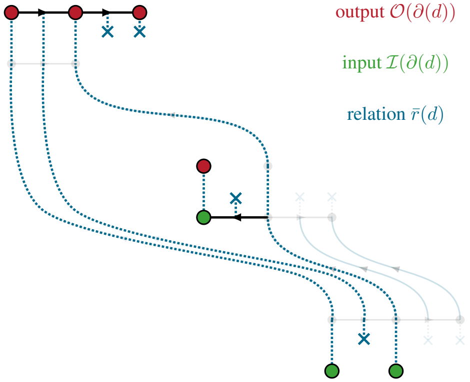


Input interface $\mathcal{I}(d)$ and **output interface** $\mathcal{O}(d)$ of the composite rule diagram d.

Step 4: Normalization of rule diagrams

- Given a generic rule diagram d, its **normalization** $\partial(d)$ is defined as follows:
  - Determine the **input interface** $\mathcal{I}(d)$ and the **output interface** $\mathcal{O}(d)$ of d as those input and output graph parts that are not involved in the diagram matches of d.
  - "Read out" the internal structure of $\partial(d)$ via following the **worldlines** from input to output parts – all complete paths from $\mathcal{I}(d)$ to $\mathcal{O}(d)$ will be part of the injective partial map $\bar{r}(d)$ of $\partial(d) \equiv (\mathcal{I}(d), \mathcal{O}(d), \bar{r}(d), \varnothing)$.
- Note that the normalized diagram $\partial(d)$ may again be interpreted as a **graph rewriting rule**, i.e.

$$\partial(d) \quad \widehat{=} \quad \bar{r}(d) : \mathcal{I}(d) \rightharpoonup \mathcal{O}(d)\,.$$



Normalization of the composite rule diagram.

Step 5: Rule diagram algebra

Rule diagram algebra

Denote by $\mathcal{D} := span_{\mathbb{R}}(D_{\cong})$ the **vector space of isomorphism classes of rule diagrams $D_{\cong}$**. Then one may define an **algebra composition** $*_{\mathcal{D}}$ as follows: given two rule diagrams $d_1, d_2 \in \mathcal{D}$, define

$$d_1 *_{\mathcal{D}} d_2 := \sum_{\text{all diagram matches } m} \text{iso-class of } d_1 \text{ composed with } d_2 \text{ along } m\,.$$

This compositon is then extended by linearity to all of $\mathcal{D}$. We call $\mathcal{D} \equiv (\mathcal{D}, +, \cdot, *_{\mathcal{D}})$ the **rule diagram algebra**.

Theorem

The rule diagram algebra is a **noncommutative, unital associative algebra**, with unit the **empty rule diagram $d_{\varnothing}$**.

Step 6: Rule algebra

Rule algebra

Denote by $\mathcal{R} := span_{\mathbb{R}}(R_{\cong})$ the **vector space of isomorphism classes of normal rule diagrams** $R_{\cong}$. Then one may define an **algebra composition** $*_{\mathcal{R}}$ as follows: given two normal rule diagrams $r_1, r_2 \in \mathcal{R}$, define

$$r_1 *_{\mathcal{R}} r_2 := \partial(\psi(r_1) *_{\mathcal{D}} \psi(r_2)) \,,$$

where $\psi : \mathcal{R} \hookrightarrow \mathcal{D}$ is the natural inclusion. This compositon is then extended by linearity to all of $\mathcal{R}$. We call $\mathcal{R} \equiv (\mathcal{R}, +, \cdot, *_{\mathcal{R}})$ the **rule algebra**.

Theorem

The rule algebra is a **noncommutative, unital associative algebra**, with unit the **empty rule diagram $d_{\varnothing}$**.

- **Note:** The proof is based on demonstrating that $\bar{\varphi} := \partial \circ (\psi \otimes \psi)$ is an **algebra homomorphism** from the rule diagram algebra $\mathcal{D}$ to the rule algebra $\mathcal{R}$.

Step 7: Canonical representation of the rule algebra

- Let $|G\rangle$ denote the basis vectors of the vector space $\mathcal{G}$ of **isomorphism classes of finite directed multigraphs**.

Canonical representation of the rule algebra

Taking inspiration from the **canonical representation** of the so-called **heisenberg-Weyl algebra**, one may easily define the **canonical representation of the rule algebra** as follows:

$$\rho(O \overset{r}{\Leftarrow} I)|\varnothing\rangle := \begin{cases} |O\rangle\,, & \text{if } I = \varnothing \\ 0 \cdot |\varnothing\rangle\,, & \text{else.} \end{cases}$$

Moreover, for $G \neq \varnothing$, we define

$$\rho(O \overset{r}{\Leftarrow} I)|G\rangle := \rho((O \overset{r}{\Leftarrow} I) *_{\mathcal{R}} (G \Leftarrow \varnothing))|\varnothing\rangle\,.$$

Theorem

This definition yields a proper representation.

Step 8: Stochastic mechanics

Core definition: the evolution operator

Given a **stochastic graph rewriting system** T in the form of a **set of graph rewriting rules** $I \stackrel{r}{\Rightarrow} O$ and a set of **base rates** $\kappa_r \in \mathbb{R}_{\geqslant 0}$, we may define the **evolution operrator** H as follows:

$$H := \sum_{r \in T} \kappa_r \left(\rho(r) - \rho(I \xleftarrow{id_{dom(r)}} I) \right) .$$

Theorem

H thus defined

- is an **infinitesimal stochastic operator**
- captures the dynamics of the system via the **Master equation** $\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$.

Consistency check

Specializing to **discrete graph rewriting**, we recover precisely the evolution operator of **chemical reaction systems**, as described in the **Doi-Peliti formalism**![3] [4] [5]

[3] Masao Doi. “Second quantization representation for classical many-particle system”. In: *Journal of Physics A: Mathematical and General* 9.9 (1976), p. 1465

[4] Masao Doi. “Stochastic theory of diffusion-controlled reaction”. In: *Journal of Physics A: Mathematical and General* 9.9 (1976), p. 1479

[5] L Peliti. “Path integral approach to birth-death processes on a lattice”. In: *Journal de Physique* 46.9 (1985), pp. 1469–1483

Harvesting of results

Unification

- We identified a formalism in which a stochastic graph rewriting system is described in a fashion completely standard in both CTMC and statistical physics theory!

Fragmentation theorem rederivation

Lemma

For any rules $O_1 \overset{r_1}{\Leftarrow} I$ and $O_2 \overset{r_2}{\Leftarrow} I$ with $dom(r_1) = dom(r_2)$, we have that

$$\langle|\rho(O_1 \overset{r_1}{\Leftarrow} I) = \langle|\rho(O_2 \overset{r_2}{\Leftarrow} I) = \langle|\rho(I \overset{r_I}{\Leftarrow} I)\,,$$

with $r_I := id_{dom(r_1)} = id_{dom(r_2)}$.

Theorem: Jump-closure of observables (compare [6])

Let H be the evolution operator of a stochastic graph rewriting system. Then for any observable $O_I := I \overset{r_I}{\Leftarrow} I$ we have that

$$\langle|O_I H = \sum_{O_{I'} \in \mathcal{F}(O_I)} \alpha_{O_I, O_{I'}, H} \langle|O_{I'}\,,$$

for some constants $\alpha_{O_i, O_{I'}, H} \in \mathbb{R}$, and with $\mathcal{F}(O_I)$ a finite family of observables.

Corollary: Fragmentation Theorem (compare [6])

$$\frac{d}{dt}\langle O_I\rangle(t) = \sum_{O_{I'} \in \mathcal{F}(O_I)} \alpha_{O_I, O_{I'}, H} \langle O_{I'}\rangle(t)\,.$$

[6]

New result: Generalized Fragmentation Theorem

- Any **evolution operator** H admits a **unique decomposition** $H = \hat{H} + \mathring{H}$, with the **non-observable part** $\hat{H}$ and **observable part** $\mathring{H}$

$$\hat{H} = \rho(\hat{r}) : \quad \hat{r} \in \mathcal{R} \backslash \mathcal{O}\,, \quad \mathring{H} = \rho(\mathring{r}) : \quad \mathring{r} \in \mathcal{O}\,,$$

where $\mathcal{O} \subset \mathcal{R}$ denotes the subalgebra of **observables**.

Theorem: Generalized Fragmentation Theorem

For any evolution operator H and any observables $O_1, \ldots, O_n \in \mathcal{O}$, we have that

$$\frac{d}{dt}\langle O_1 \ldots O_n \rangle(t) = \sum_{\sigma \in S_n} \frac{1}{n!} \sum_{m=1}^{n} \binom{n}{m} \langle \mathrm{C}(\mathcal{O}_m^\sigma, \hat{H}) \prod_{i>m} O_{\sigma(i)} \rangle(t)\,,$$

where

$$\mathcal{O}_m^\sigma := \{O_{\sigma(i)}\}_{1 \leqslant i \leqslant m}\,,$$

and with the **nested commutators**

$$\mathrm{C}(\mathcal{O}_m^{sigma}, \hat{H}) := [O_{\sigma(1)}, [O_{\sigma(2)}, [\ldots, [O_{\sigma(m)}, \hat{H}] \ldots]]\,.$$

Conclusion and outlook

Summary

- We defined a full **stochastic mechanics framework** for graph rewriting (of DPO type).
- Based on the new formulae, we were able to achieve not only a standard formulation of the so-called **Fragmentation Theorem**, but more importantly found a compact expression for a **Generalized Fragmentation Theorem** for arbitrary moments of observables.
- The full formalism is an autonomous, mathematically well-posed framework for graph rewriting.

Outlook

- All results presented strictly speaking are only fully well-behaved for **finite** systems; while practical experience would suggest applicability also for infinite systems with suitable properties, this remains an open research question!
- Study mathematical properties of the rule diagram algebra more closely[7].
- Generalization of the rule algebra idea to other types of rewriting (e.g. SPO types[7], Kappa, biological tissue models. . .).
- The **combinatorics** of rewriting is in principle accessible along the lines of the **analytical combinatorics formalism**[8].
- Generalization of the formalism to **branching and fusing rewriting** (and also a proper analysis of the category-theoretical foundations of graph rewriting) – project with V. Danos, I. Garnier and P. Sobocinski!

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[7] Nicolas Behr, Vincent Danos, Ilias Garnier, and Tobias Heindel. "The algebras of graph rewriting". In: ($\approx$ Q4 2016)

[8] Philippe Flajolet and Robert Sedgewick. *Analytic combinatorics*. Cambridge University Press, 2009

Thank you!

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