Combinatorial Conversion and Moment Bisimulation For Stochastic Rewriting Systems

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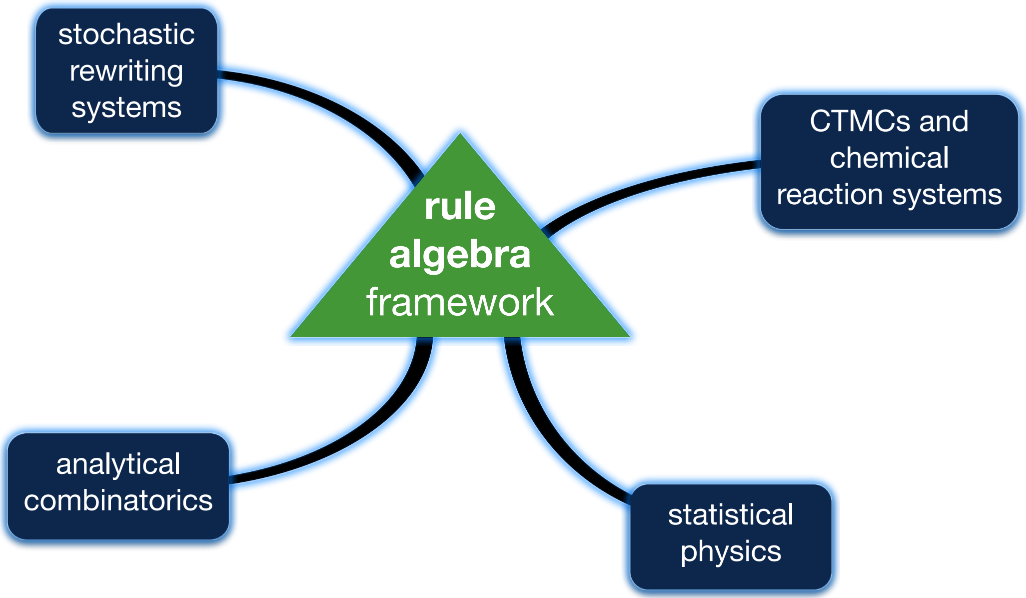
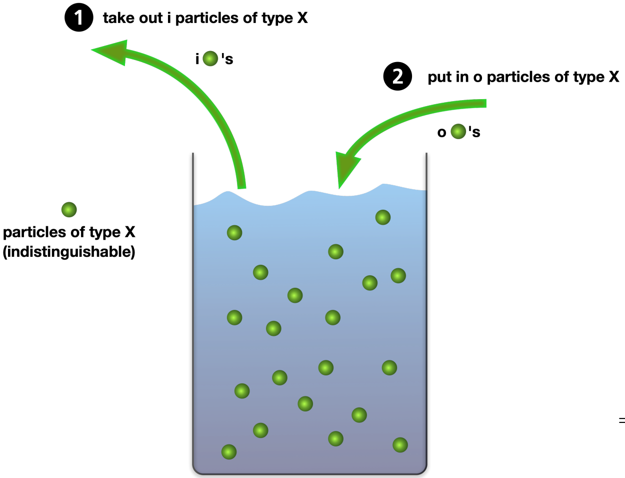
Overview


stochastic rewriting systems
CTMCs and chemical reaction systems
rule algebra framework
analytical combinatorics
statistical physics

The mathematical "blueprint": the Heisenberg-Weyl algebra

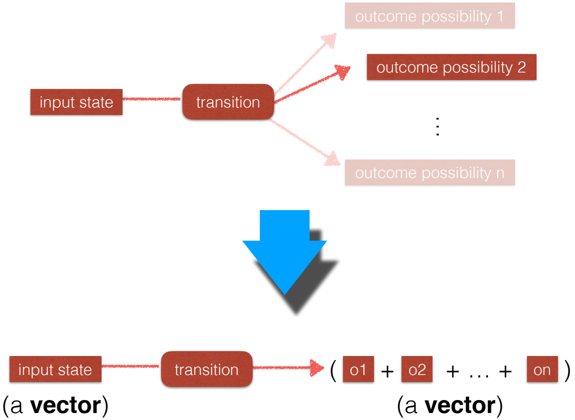


- **pure state:** a pool of n **indistinguishable particles** (of some **type** X)
- **generic operations: remove** i **particles of type** X from the pool, then **add** o **particles of type** X (with $i, o \in \mathbb{Z}_{\geqslant 0}$)
- **elementary operations:**
  - pick a particle of type X at random and **remove it**
  - **add a particle** of type X

$\Rightarrow$ **basic combinatorics:**

- $\mathbf{n}$ **possible ways** to **remove** a particle
- $\mathbf{1}$ **possible way** to **add** a particle

The mathematical “blueprint”: the Heisenberg-Weyl algebra



A possibility to encode non-determinism:

map **multiple possibilities** of transitions . . .

. . . into **“sum of possibilities”**

(via employing the notion of a **vector space of states** and of transitions as **linear operators** on this space)

The mathematical "blueprint": the Heisenberg-Weyl algebra

- from the theory of **bosonic Fock spaces:**

$$|n\rangle \quad \widehat{=} \quad \textbf{pure state of } n \text{ particles}$$

- **Ansatz:** encode the elementary operations in terms of (representations of) the **generators** of the **Heisenberg-Weyl algebra**:

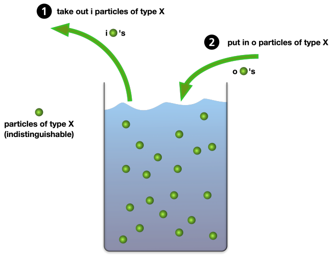
$$a\,|n\rangle := \begin{cases} n\,|n-1\rangle & \text{if } n>0 \\ 0 & \text{else} \end{cases}$$

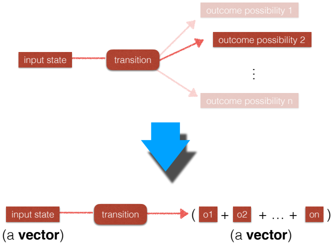
$$a^\dagger\,|n\rangle := |n+1\rangle \quad (n \geqslant 0)$$

- **canonical commutation relations:**

$$(aa^\dagger - a^\dagger a)\,|n\rangle = \big((n+1)-(n)\big)\,|n\rangle = |n\rangle$$

$$\Leftrightarrow \quad [a,a^\dagger] = aa^\dagger - a^\dagger a = \mathbb{1}$$





Multi-species variant

- **multi-species Heisenberg-Weyl algebra:** defined via **generators $a_i, a_j^\dagger$** and the **canonical commutation relations**

$$[a_i, a_j] = 0 = [a_i^\dagger, a_j^\dagger]\,, \quad [a_i, a_j^\dagger] = \delta_{i,j}\,,$$

where $i,j \in \{1,\ldots,N\}$ (with N the **number of species**)

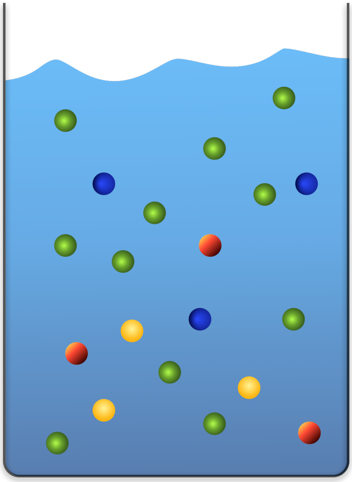
- **pure states:**

$$|\underline{n}\rangle \equiv |n_1,\ldots,n_N\rangle$$

- **canonical representation:**

$$a_i\,|\underline{n}\rangle := \begin{cases} n_i\,|\underline{n}-\underline{\Delta}_i\rangle & \text{if } n_i > 0 \\ 0 & \text{else} \end{cases}$$

$$a_i^\dagger\,|\underline{n}\rangle := |\underline{n}+\underline{\Delta}_i\rangle$$



Stochastic transition systems and continuous time Markov chain (CTMC) theory

- **Standard CTMC theory** [1]: one way to describe the CTMC's dynamics is to give a **probability distribution** (with $\mathbf{S}$ the **set of pure states**)

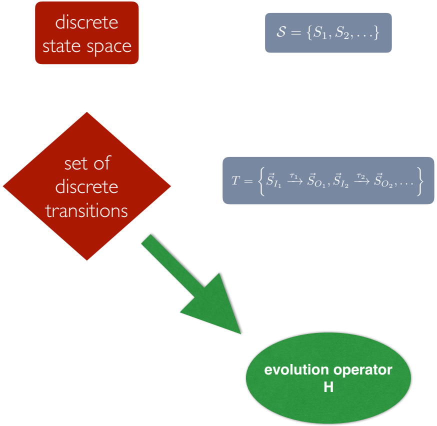
$$|\Psi(t)\rangle := \sum_{S\in\mathbf{S}} p_S(t)|S\rangle$$

  of being in one of the pure states (represented by basis vectors $|S\rangle$), and specifying the **Master equation** (aka **Kolmogorov forward 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 will be intimately related to the concept of **rule algebras** in our formalism!



[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 [2][3] aka “**stochastic mechanics**” [4] for studying CTMCs:

- **Observables** $\mathscr{O}$ are linear operators under which each pure state is an Eigenstate,

$$\mathscr{O}|S\rangle = \omega_{\mathscr{O}}(S)|S\rangle\,.$$

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

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

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

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

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

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

- Additional property of the evolution operator H:

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

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

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

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

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

[2] M Doi. “Second quantization representation for classical many-particle system”. In: *Journal of Physics A: Mathematical and General* 9.9 (Sept. 1976), pp. 1465–1477

[3] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Stochastic mechanics of graph rewriting”. In: *Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016)* (2016), pp. 46–55

[4] John Baez and Jacob D Biamonte. *Quantum Techniques in Stochastic Mechanics*. WORLD SCIENTIFIC, May 2017

A first hint at the practical advantages and potential of the framework

- **Proposition ([5], Prop. 3.35):** For **linear operators** $A, B \in End_{\mathbb{K}}(\mathscr{V})$ (with $\mathscr{V}$ a $\mathbb{K}$-vector space) and λ a formal variable,

$$e^{\lambda A} B e^{-\lambda A} = e^{ad_{\lambda A}} B \,,$$

where

$$ad_A B := [A, B] = AB - BA \,,\; ad_A^0 B := B \,.$$

[5] Brian C. Hall. *Lie Groups, Lie Algebras, and Representations*. Springer International Publishing, 2015

[6] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Stochastic mechanics of graph rewriting”. In: *Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016)* (2016), pp. 46–55

[7] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

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- **Application:** suppose H is an evolution operator, and let

$$\underline{\lambda} \cdot \underline{\mathscr{O}} \equiv \sum_i \lambda_i \mathscr{O}_i$$

denote a **formal linear combination** of **observables** $\mathscr{O}_i$.

- Define the **moment-generating function** $\mathscr{M}(t; \underline{\lambda})$ of the CTMC as

$$\mathscr{M}(t; \underline{\lambda}) := \left\langle e^{\underline{\lambda} \cdot \underline{\mathscr{O}}} \right\rangle (t)\,,$$

whence formally

$$\left[\partial_{\lambda_{i_1}}^{n_1} \cdots \partial_{\lambda_{i_k}}^{n_k} \mathscr{M}(t; \underline{\lambda}) \right] \Big|_{\underline{\lambda} \to \underline{0}} = \langle \mathscr{O}_{i_1}^{n_1} \cdots \mathscr{O}_{i_k}^{n_k} \rangle (t)\,.$$

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Formal all-order moment evolution equation [6] [7]:

$$\begin{aligned}
\frac{d}{dt} \mathscr{M}(t; \underline{\lambda}) &= \left\langle \middle| e^{\underline{\lambda} \cdot \underline{\mathscr{O}}} H \middle| \Psi(t) \right\rangle \\
&= \left\langle \middle| \left(e^{\underline{\lambda} \cdot \underline{\mathscr{O}}} H e^{-\underline{\lambda} \cdot \underline{\mathscr{O}}} \right) e^{\underline{\lambda} \cdot \underline{\mathscr{O}}} \middle| \Psi(t) \right\rangle \\
&= \left\langle \middle| \left(e^{ad_{\underline{\lambda} \cdot \underline{\mathscr{O}}}} H \right) e^{\underline{\lambda} \cdot \underline{\mathscr{O}}} \middle| \Psi(t) \right\rangle .
\end{aligned}$$

[5] Brian C. Hall. *Lie Groups, Lie Algebras, and Representations*. Springer International Publishing, 2015

[6] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Stochastic mechanics of graph rewriting”. In: *Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016)* (2016), pp. 46–55

[7] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Delbrück's insight: probability generating functions

Bargmann-Fock representation [8]

$$
\begin{aligned}
|\underline{n}\rangle \quad &\leftrightarrow \quad \prod_{i=1}^{N} x_i^{n_i} \\
a_i^\dagger \quad &\leftrightarrow \quad \hat{x}_i \quad \text{(multiplication by } x_i\text{)} \\
a_i \quad &\leftrightarrow \quad \frac{\partial}{\partial_{x_i}} \quad \text{(derivation by } x_i\text{)}
\end{aligned}
$$

- **normal-ordering relation:** for all formal power series $f \equiv f(x_1, \ldots, x_N)$,

$$
\left(\hat{x}_i \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_j} \hat{x}_i\right) f = \delta_{i,j} f
$$

- **probability generating function:** given a probability distribution $|\psi\rangle = \sum_{\underline{n} \geqslant 0} p_{\underline{n}} |\underline{n}\rangle$,

$$
|\psi\rangle \quad \leftrightarrow \quad P(x) := \sum_{\underline{n} \geqslant 0} p_{\underline{n}} \underline{x}^{\underline{n}}
$$

Delbrück [9]

The **master equation** for a chemical reaction system with reactions

$$
\underline{i} \cdot \underline{X} \xrightarrow{r_{\underline{i},\underline{o}}} \underline{o} \cdot \underline{X}
$$

reads in the Bargmann-Fock representation

$$
\frac{\partial}{\partial t} P(t; \underline{x}) = \sum_{\underline{i},\underline{o}} r_{\underline{i},\underline{o}} \left((\hat{\underline{x}})^{\underline{o}} - (\hat{\underline{x}})^{\underline{i}} \right) \left(\frac{\partial}{\partial \underline{x}} \right)^{\underline{i}} P(t; \underline{x})
$$

[8] V Fock. "Verallgemeinerung und Lösung der diracschen statistischen Gleichung". In: *Zeitschrift für Physik A Hadrons and Nuclei* 49.5 (1928), pp. 339–357; Valentine Bargmann. "On a Hilbert space of analytic functions and an associated integral transform part I". In: *Communications on pure and applied mathematics* 14.3 (1961), pp. 187–214

[9] Max Delbrück. "Statistical fluctuations in autocatalytic reactions". In: *The Journal of Chemical Physics* 8.1 (1940), pp. 120–124

A seminal result on normal-ordering techniques

Theorem [10]

Let $\mathscr{H}$ be a **semi-linear operator** (in the Bargmann-Fock basis for N **species**),

$$\mathscr{H} = v(\hat{\underline{x}}) + \sum_{i=0}^{N} q_i(\hat{\underline{x}})\, \partial_{x_i} \,,$$

with $q_i(\hat{\underline{x}})$ and $v(\hat{\underline{x}})$ some functions in the operators $\hat{x}_i$. Let $F(0;\underline{x})$ be an entire function in the indeterminates x_i. Define the formal power series (with formal variable λ)

$$F(\lambda;\underline{x}) := e^{\lambda\mathscr{H}}\, F(0;\underline{x})\,.$$

Then $F(\lambda;\underline{x})$ may be expressed in **closed form** as follows:

$$F(\lambda;\underline{x}) = g(\lambda;\underline{x})F\big(0;\underline{T}(\lambda;\underline{x})\big)\,, \qquad \begin{cases} \frac{\partial}{\partial\lambda} T_i(\lambda;\underline{x}) & = q_i(\underline{T}(\lambda;\underline{x}))\,, \quad T_i(0;\underline{x}) = x_i \\ \ln g(\lambda;\underline{x}) & = \int_0^\lambda v(\underline{T}(\kappa;\underline{x}))d\kappa \end{cases}$$

Moreover, $e^{\lambda\mathscr{H}}$ induces a **one-parameter group** of transformations due to

$$\underline{T}(\lambda+\mu;\underline{x}) = \underline{T}(\mu;\underline{T}(\lambda;\underline{x}))\,, \qquad g(\lambda+\mu;\underline{x}) = g(\lambda;\underline{x})g(\mu;\underline{T}(\lambda;\underline{x}))\,,$$

[10] G. Dattoli et al. "Evolution operator equations: Integration with algebraic and finite-difference methods: Applications to physical problems in classical and quantum mechanics and quantum field theory". In: *Riv. Nuovo Cim.* 20N2 (1997), pp. 1–133; P Blasiak et al. "Boson normal ordering via substitutions and Sheffer-Type Polynomials". In: *Physics Letters A* 338.2 (2005), pp. 108–116

Result: exact actions of evolution semi-groups

From [11]:

Table 3 Closed-form results for the time-dependent probability generating functions $P(t;\underline{x})$ for reaction systems of N species with a single non-binary elementary reaction; here, $S_1,\ldots,S_N$ denote the N different species, while $\underline{\Delta}_i$ ($i\in\{1,\ldots,N\}$ denotes the N-vector with coordinates $(\underline{\Delta}_i)=\delta_{i,j}$.

reaction	$\mathscr{H}=\underline{q}(\underline{x})\cdot\partial_{\underline{x}}+v(\underline{x})$	$P(t;\underline{x})=g(t;\underline{x})P(0;\underline{T}(t;\underline{x})$	comments
$\emptyset\xrightarrow{\alpha}S_i$	$\alpha\,(\hat{x}_i-1)$	$Pois(\alpha t;x_i)\cdot P(0;\underline{x})$	$Pois(\mu;x):=e^{\mu(x-1)}$
$\emptyset\xrightarrow{\alpha}S_i+S_j$	$\alpha\,(\hat{x}_i\hat{x}_j-1)$	$\left(e^{\alpha t(x_ix_j-1)}\right)\cdot P(0;\underline{x})$	(Poisson distribution, $0\leq\mu<\infty$)
$S_i\xrightarrow{\alpha}\emptyset$	$\alpha\,(1-\hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x}+(-x_i+Bern(e^{-\alpha t};x_i))\underline{\Delta}_i)$	$Bern(\mu;x):=(1-\mu)+x\mu$
$S_i\xrightarrow{\alpha}S_j\quad(i\neq j)$	$\alpha\,(\hat{x}_j-\hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x}+(-x_i+(x_j(1-e^{-\alpha t})+x_ie^{-\alpha t})\underline{\Delta}_i)$	(Bernoulli distribution, $0\leq\mu\leq 1$)
$S_i\xrightarrow{\alpha}2S_i$	$\alpha\left(\hat{x}_i^2-\hat{x}_i\right)\frac{\partial}{\partial x_i}$	$P(0;\underline{x}+(-x_i+Geom(e^{-\alpha t};x_i))\underline{\Delta}_i)$	$Geom(\mu;x):=\frac{x\mu}{1-x(1-\mu)}$
$S_i\xrightarrow{\alpha}S_i+S_j\quad(i\neq j)$	$\alpha\,(\hat{x}_i\hat{x}_j-\hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x}+(-x_i+x_iPois(\alpha t;x_j)))\underline{\Delta}_i)$	(Geometric distribution, $0<\mu\leq 1$)
$S_i\xrightarrow{\alpha}S_j+S_k\quad(i\neq j\neq k)$	$\alpha\,(\hat{x}_j\hat{x}_k-\hat{x}_i)\,\frac{\partial}{\partial x_i}$	$P(0;\underline{x}+(-x_i+x_jx_k(1-e^{-\alpha t})+x_ie^{-\alpha t})\underline{\Delta}_i)$	

[11] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. “Combinatorics of Chemical Reaction Systems”. In: *arXiv:1712.06575* (2017)

On the evolution equation for the moment generating functions [10]

- **Well-known fact**: there exists a **change of variables**

$$\mathcal{M}(t;\underline{\lambda}) = P(t;\underline{e^{\lambda}})$$

that allows to determine the **moment generating function** $\mathcal{M}(t;\underline{\lambda})$ directly from $P(t;\underline{x})$ (i.e. $x_i \to e^{\lambda_i}$)

- **Idea:** apply this change of variables also to **Delbrück's evolution equation**

$$\frac{\partial}{\partial t}P(t;\underline{x}) = \sum_{\underline{i},\underline{o}} r_{\underline{i},\underline{o}}\left((\underline{\hat{x}})^{\underline{o}} - (\underline{\hat{x}})^{\underline{i}}\right)\left(\frac{\partial}{\partial \underline{x}}\right)^{\underline{i}} P(t;\underline{x})$$

Moment generating function evolution equation ([11], Theorem 5)

$$\frac{\partial}{\partial t}\mathcal{M}(t;\underline{\lambda}) = \mathbb{D}(\underline{\lambda},\partial_{\underline{\lambda}})\mathcal{M}(t;\underline{\lambda})$$

$$\mathbb{D}(\underline{\lambda},\partial_{\underline{\lambda}}) = \sum_{\underline{i},\underline{o}} r_{\underline{i},\underline{o}}\left(e^{\underline{\lambda}\cdot(\underline{o}-\underline{i})} - 1\right)\sum_{\underline{k}=\underline{0}}^{\underline{i}} \underline{s}_1(\underline{i},\underline{k})\left(\frac{\partial}{\partial \underline{\lambda}}\right)^{\underline{k}}$$

$$\underline{s}_1(\underline{i},\underline{k}) := \prod_{j\in\mathbf{S}} s_1(i_j,k_j)\,,$$

with $\mathbf{S}$ the **set of species**, and with $s_1(i,k)$ denoting the **(signed) Stirling numbers of the first kind**.

[10] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: *arXiv:1712.06575* (2017)

Combinatorics of chemical reaction systems

Nicolas Behr[a], **Gérard H. E. Duchamp**[b] **and Karol A. Penson**[c]

We propose a concise stochastic mechanics framework for chemical reaction systems that allows to formulate evolution equations for three general types of data: the probability generating functions, the exponential moment generating functions and the factorial moment generating functions. This formulation constitutes an intimate synergy between techniques of statistical physics and of combinatorics. We demonstrate how to analytically solve the evolution equations for all six elementary types of single-species chemical reactions by either combinatorial normal-ordering techniques, or, for the binary reactions, by means of Sobolev-Jacobi orthogonal polynomials. The former set of results in particular highlights the relationship between infinitesimal generators of stochastic evolution and parametric transformations fo probability distributions. Moreover, we present exact results for generic single-species non-binary reactions, hinting at a notion of compositionality of the analytic techniques.

1 Introduction

Intended as an invitation to interdisciplinary researchers and in particular to combinatorists, we present in this work an extension of the early work of Dellbrück [1] on probability generating functions for chemical reaction systems to a so-called stochastic mechanics framework. While the idea to study chemical reaction systems in terms of probability generating functions is thus not new and on the contrary one of the standard techniques of this field (see e.g. [2] for a historical overview), we believe that the reformulation of these techniques in terms of the stochastic mechanics formalism could lead to fruitful interaction of a broader audience of theoretical researchers. In the spirit of the ideas presented by M. Doi in his seminal paper [3], the main motivation for such a reformulation lies in a clear conceptual separation of (i) the state space of the system and (ii) the linear operators implementing the evolution of the system. Combined with insights obtained in a recent study of stochastic graph rewriting systems [4–6], one may add to this list (iii) the linear operators that implement observable quantities such as moments of number counts on states. It is only through combining this Ansatz with the standard notions of combinatorial generating functions that we find the true strengths of the stochastic mechanics approach: providing an avenue to obtain exact solutions to dynamical evolution equations. Combinatorists will recognize in our formulation of evolution equations intrinsic notions of normal-ordering problems, and indeed certain semi-linear normal-ordering techniques [7–10] will prove immensely fruitful in this direction. Chemists and other practitioners might appreciate that our solutions not only provide asymptotic information on the time-evolution of the reaction systems, but on the contrary full information on the evolution of reaction systems from any initial state at time $t = 0$ to any desired time $t = T$ (with $T > 0$). While many individual results on such time-evolutions are known in the literature [2, 11], we hope that our concise formalism may help to consolidate the knowledge on the mathematical

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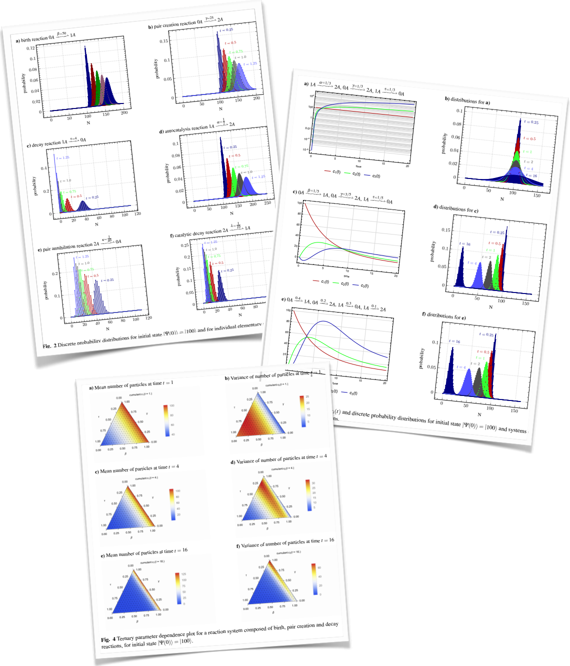

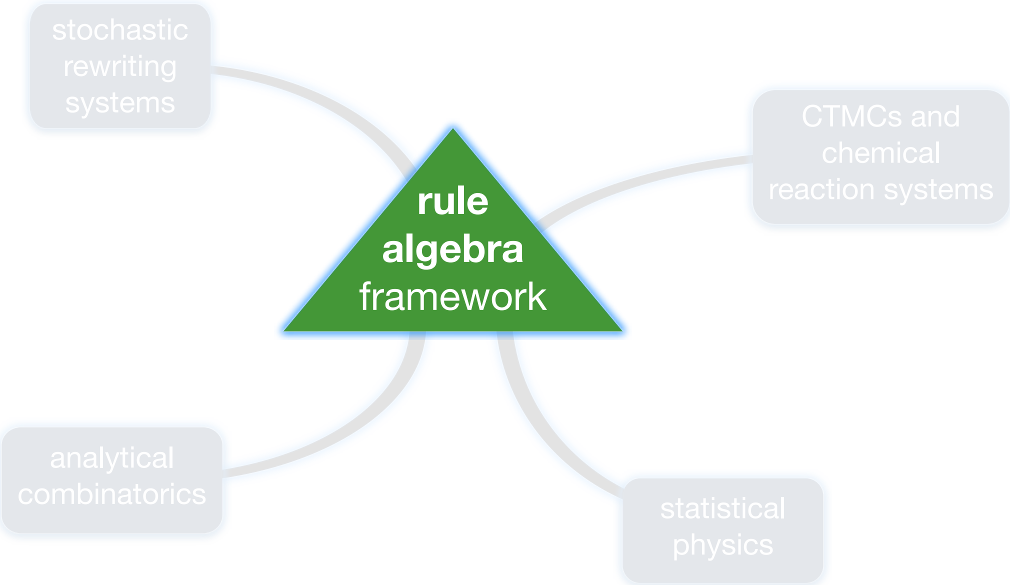
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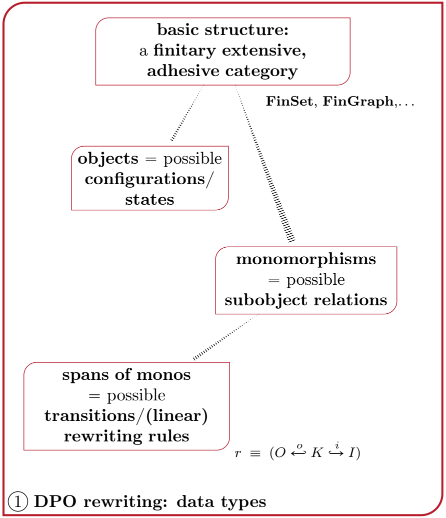
Overview: the DPO rule algebra framework [11] [12]



[11] Nicolas Behr and Pawel Sobocinski. “Rule Algebras for Adhesive Categories”. In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

[12] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Overview: the DPO rule algebra framework [11] [12]

$\mathcal{R}_{\mathbf{C}}$ – $\mathbb{K}$-**vector space**
spanned by basis vectors
$\delta(r) \equiv \delta(O \xleftarrow{o} K \xrightarrow{i} I)$

composition on $\mathcal{R}_{\mathbf{C}}$:
$\delta(r_2) *_{\mathcal{R}_{\mathbf{C}}} \delta(r_1) := \sum_m \delta(r_2 \overset{m}{\blacktriangleleft} r_1)$

m – matches
$.\overset{\cdot}{\blacktriangleleft}.$ – DPO rule composition

rule algebra:
$\mathcal{R}_{\mathbf{C}} \equiv (\mathcal{R}_{\mathbf{C}}, *_{\mathcal{R}_{\mathbf{C}}})$

state space:
$\hat{\mathbf{C}} := span_{\mathbb{K}}(\{|X\rangle \mid X \in \mathsf{obj}(\mathbf{C})_{\cong}\})$

canonical representation:
$\rho_{\mathbf{C}} : \mathcal{R}_{\mathbf{C}} \to End_{\mathbb{K}}(\hat{\mathbf{C}})$
such that
$\rho(\delta(r_2))\rho(\delta(r_1)) = \rho(\delta(r_2) *_{\mathcal{R}_{\mathbf{C}}} \delta(r_1))$

2 **DPO-type rule algebra**

[11] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

[12] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: *arXiv preprint 1904.07313* (2019)

Overview: the DPO rule algebra framework [11] [12]

set of transitions with base rates:

$$\left\{\left(\kappa_j, \left(O_j \xleftarrow{o_j} K_j \xrightarrow{i_j} I_j\right)\right)\right\}_{j\in J}$$

infinitesimal generator of a CTMC:

$$H = \sum_{j\in J} \kappa_j \left(\rho_{\mathbf{C}}\left(\delta(O_j \xleftarrow{o_j} K_j \xrightarrow{i_j} I_j)\right) - \rho_{\mathbf{C}}\left(\delta(I_j \xleftarrow{i_j} K_j \xrightarrow{i_j} I_j)\right)\right)$$

evolution equation:

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

$$\underbrace{|\Psi(t)\rangle}_{\in \mathsf{Prob}(\mathbf{C})} = \sum_{X\in \mathsf{obj}(\mathbf{C})_{\cong}} p_X(t)\,|X\rangle$$

(3) **stochastic DPO rewriting systems**

[11] Nicolas Behr and Pawel Sobocinski. “Rule Algebras for Adhesive Categories”. In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

[12] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Overview: the DPO rule algebra framework [11] [12]

basic structure: a **finitary extensive, adhesive category**

FinSet, **FinGraph**, ...

objects = possible **configurations/ states**

monomorphisms = possible **subobject relations**

spans of monos = possible **transitions/(linear) rewriting rules**

$r \equiv (O \overset{o}{\hookleftarrow} K \overset{i}{\hookrightarrow} I)$

① **DPO rewriting: data types**

$\mathcal{R}_{\mathbf{C}}$ – $\mathbb{K}$**-vector space** spanned by basis vectors $\delta(r) \equiv \delta(O \overset{o}{\leftarrow} K \overset{i}{\rightarrow} I)$

composition on $\mathcal{R}_{\mathbf{C}}$: $\delta(r_2) *_{\mathcal{R}_{\mathbf{C}}} \delta(r_1) := \sum_m \delta(r_2 \overset{m}{\blacktriangleleft} r_1)$

m – matches

$\blacktriangleleft$ – DPO rule composition

rule algebra: $\mathcal{R}_{\mathbf{C}} \equiv (\mathcal{R}_{\mathbf{C}}, *_{\mathcal{R}_{\mathbf{C}}})$

state space: $\hat{\mathbf{C}} := span_{\mathbb{K}}(\{|X\rangle \mid X \in \mathsf{obj}(\mathbf{C})_{\cong}\})$

canonical representation: $\rho_{\mathbf{C}} : \mathcal{R}_{\mathbf{C}} \to End_{\mathbb{K}}(\hat{\mathbf{C}})$ such that $\rho(\delta(r_2))\rho(\delta(r_1)) = \rho(\delta(r_2) *_{\mathcal{R}_{\mathbf{C}}} \delta(r_1))$

② **DPO-type rule algebra**

set of transitions with base rates:

$$\left\{\left(\kappa_j, \left(O_j \overset{o_j}{\hookleftarrow} K_j \overset{i_j}{\hookrightarrow} I_j\right)\right)\right\}_{j \in J}$$

infinitesimal generator of a CTMC:

$$H = \sum_{j \in J} \kappa_j \left(\rho_{\mathbf{C}}\left(\delta(O_j \overset{o_j}{\hookleftarrow} K_j \overset{i_j}{\hookrightarrow} I_j)\right) - \rho_{\mathbf{C}}\left(\delta(I_j \overset{i_j}{\hookleftarrow} K_j \overset{i_j}{\hookrightarrow} I_j)\right)\right)$$

evolution equation:

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

$$\underbrace{|\Psi(t)\rangle}_{\in \mathsf{Prob}(\mathbf{C})} = \sum_{X \in \mathsf{obj}(\mathbf{C})_{\cong}} p_X(t)\,|X\rangle$$

③ **stochastic DPO rewriting systems**

[11] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

[12] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: *arXiv preprint 1904.07313* (2019)

Background: adhesive and extensive categories

Adhesive and extensive categories (cf. [13], Def. 3.1 ff)

A category $\mathbf{C}$ is said to be **adhesive** if

(i) $\mathbf{C}$ has pushouts along **monomorphisms**,

(ii) $\mathbf{C}$ has pullbacks, and if

(iii) pushouts along monomorphisms are **van Kampen (VK) squares**.

If $\mathbf{C}$ in addition possesses a **strict initial object** $X_{\varnothing} \in ob(\mathbf{C})$, i.e. an object s.th. $\forall X \in ob(\mathbf{C}) : \exists! m_X : X_{\varnothing} \hookrightarrow X$, the category is said to be **extensive**.

- **Examples** [13]:
  - $\mathbf{Set}$, the category of **(finite) sets and set functions**
  - $\mathbf{Graph}$, the category of **(finite) directed multigraphs and graph homomorphisms** (and also **colored/typed graphs, attributed graphs, hypergraphs,...**)
  - any **presheaf topos** and any **elementary topos** [14]
- **Note:** One might further generalize by considering **quasi-adhesive categories** (see [13], [15]).

[13] Stephen Lack and Paweł Sobociński. "Adhesive and quasiadhesive categories". In: *RAIRO-Theoretical Informatics and Applications* 39.3 (2005), pp. 511–545

[14] Stephen Lack and Paweł Sobociński. "Toposes are adhesive". In: *Graph Transformations, Third International Conference, (ICGT 2006)*. Vol. 4178. LNCS. Springer, 2006, pp. 184–198

[15] Richard Garner and Stephen Lack. "On the axioms for adhesive and quasiadhesive categories". In: *Theor. App. Categories* 27.3 (2012), pp. 27–46

Brief comments on abstract category-theoretical structures:

- **pushout (PO) along monomorphisms** in the category $\mathbf{Set}$:

$$\begin{tikzcd} & A \arrow[dl, hook] \arrow[dr, hook] & \\ B \arrow[dr, hook] & \textbf{PO} & C \arrow[dl, hook] \\ & D & \end{tikzcd}$$

Interpretation:

A – **intersection** of B and C in D

D – **union** of B and C along A

- **pushout complement (POC)** of $D \hookleftarrow B \hookleftarrow A$: a set C and monomorphisms $D \hookleftarrow C \hookleftarrow A$ such that the square $\square(ABDC)$ is a **pushout**

- **pullback (PB) along monomorphisms** in the category $\mathbf{Set}$:

$$\begin{tikzcd} & A \arrow[dl, hook] \arrow[dr, hook] & \\ B \arrow[dr, hook] & \textbf{PB} & C \arrow[dl, hook] \\ & D & \end{tikzcd}$$

Interpretation: A – **intersection** of B and C in D

Brief comments on abstract category-theoretical structures:

- **from** [16]**:**

Definition 1. A van Kampen square is a pushout diagram as in Fig 1 which satisfies the following condition:

– for any commutative cube, as illustrated, of which Fig 1 forms the bottom face and the back faces are pullbacks: the front faces are pullbacks iff the top face is a pushout.

$$\begin{tikzcd}
& & C' \arrow[dll, "m'"'] \arrow[dr, "f'"] \arrow[ddd, "c"'] & \\
A' \arrow[dr, "g'"'] \arrow[ddd, "a"'] & & & B' \arrow[dll, "n'"] \arrow[ddd, "b"] \\
& D' \arrow[ddd, "d"] & & \\
& & C \arrow[dll, "m"'] \arrow[dr, "f"] & \\
A \arrow[dr, "g"'] & & & B \arrow[dll, "n"] \\
& D & &
\end{tikzcd}$$

The following lemma shows that, in categories with pushouts and pullbacks, van Kampen squares paste together to give van Kampen squares.

[16] Stephen Lack and Paweł Sobociński. “Toposes are adhesive”. In: *Graph Transformations, Third International Conference, (ICGT 2006)*. Vol. 4178. LNCS. Springer, 2006, pp. 184–198

Brief comments on abstract category-theoretical structures:

from [17]: in an adhesive category $\mathbf{C}$, for every object $Z \in ob(\mathbf{C})$ one may define the **subobject lattice** $\mathbf{Sub}(Z)$ via defining a preorder on the monomorphisms $x : X \hookrightarrow Z$ (with $x \prec y$ if there exists some monomorphism $i : X \hookrightarrow Y$ such that $y = i \circ x$)

Corollary 5.2 of [17]

The lattice $\mathbf{Sub}(Z)$ is **distributive**.

Proof: It is easy to verify that the front and back faces of the cube below are pullbacks. Because the bottom face is a pushout, we use adhesivity in order to conclude that the top face is a pushout, which in turn implies that $A \cap (B \cup C) = (A \cap B) \cup (A \cap C)$. □

$$
\begin{tikzcd}
 & & & A\cap B\cap C \arrow[dlll] \arrow[dr] \arrow[dd] & \\
A\cap B \arrow[dr] \arrow[dd] & & & & A\cap C \arrow[dlll] \arrow[dd] \\
 & A\cap(B\cup C) \arrow[dd] & & B\cap C \arrow[dlll] \arrow[dr] & \\
B \arrow[dr] & & & & C \arrow[dlll] \\
 & B\cup C & & &
\end{tikzcd}
$$

[17] Stephen Lack and Paweł Sobociński. “Adhesive and quasiadhesive categories”. In: *RAIRO-Theoretical Informatics and Applications* 39.3 (2005), pp. 511–545

DPO rewriting in extensive categories

Rewriting an object with a rule applied at a match (cf. [18], Def. 7.3)

Fix an **extensive category** $\mathbf{C}$. Let

- $X \in ob(\mathbf{C})$ be an **object**,
- $r \equiv (O \xleftarrow{o} K \xrightarrow{i} I)$ a **(linear) rule**, denoted $r \in Lin(\mathbf{C})$ (with **Input** I, **Kontext** K and **Output** O)
- $m : I \hookrightarrow X$ a **monomorphism**.

Then m is called an **admissible match**, denoted

$$m \in M_r(X)\,,$$

if and only if the diagram below is **constructible***:

$$\begin{tikzcd}
O \arrow[d, hook, dotted] \arrow[dr, phantom, "②"] & K \arrow[l, hook', "o"'] \arrow[r, hook, "i"] \arrow[d, hook, dashed] \arrow[dr, phantom, "①"] & I \arrow[d, hook, "m"] \\
r_m(X) & K' \arrow[l, hook', dotted] \arrow[r, hook, dashed] & X
\end{tikzcd}$$

① **pushout complement** (* **might fail to exist!**)

② **pushout** (which **always exists**!)

In that case, $r_m(X)$ is referred to as the **rewrite of X with rule r along the match m**.

[18] Stephen Lack and Paweł Sobociński. “Adhesive and quasiadhesive categories”. In: *RAIRO-Theoretical Informatics and Applications* 39.3 (2005), pp. 511–545

Composition of linear rules in DPO rewriting

Sequential composite of linear rules along a match (compare [19], Sec. 3)

Fix an **extensive category** $\mathbf{C}$. Let

- $r_j \equiv (O_j \xleftarrow{o_j} K_j \xrightarrow{i_j} I_j)$ $(j = 1,2)$ be two **(linear) rules**, and let
- $\mu \equiv (I_1 \xleftarrow{m_{12}} M_{12} \xrightarrow{m_{21}} O_2)$ be a **span of monomorphisms**.

μ is called an **admissible match**, denoted $\mu \in r_1 \Vdash r_2$, if and only if the diagram below (where all arrows are monomorphisms) is **constructible**:

$$
\begin{tikzcd}
 & & & K_{12} \arrow[dlll, bend right, "o_{12}"'] \arrow[dll, dashed] \arrow[drr, dashed] \arrow[drrr, bend left, "i_{12}"] \arrow[d, phantom, "\mathrm{PB}"] \arrow[dll, phantom, "=", bend right, near end] \arrow[drr, phantom, "=", bend left, near end] & & & \\
O_{12} & K'_1 \arrow[l, dotted] \arrow[rr] & & Y_{12} & & K'_2 \arrow[ll] \arrow[r, dotted] & I_{12} \\
O_1 \arrow[u, dotted] \arrow[ur, phantom, "\mathrm{PO}"] & K_1 \arrow[l, "o_1"'] \arrow[u] \arrow[r, "i_1"'] \arrow[ur, phantom, "\mathrm{POC}"] & I_1 \arrow[ur, bend left] & M_{12} \arrow[l, "m_{12}"'] \arrow[r, "m_{21}"'] \arrow[u, phantom, "\mathrm{PO}"] & O_2 \arrow[ul, bend right] & K_2 \arrow[l, "o_2"'] \arrow[u] \arrow[r, "i_2"'] \arrow[ul, phantom, "\mathrm{POC}"] & I_2 \arrow[u, dotted] \arrow[ul, phantom, "\mathrm{PO}"]
\end{tikzcd}
$$

Then the rule $r_1 \overset{\mu}{\blacktriangleleft} r_2 \equiv (O_{12} \xleftarrow{o_{12}} K_{12} \xrightarrow{i_{12}} I_{12})$ is referred to as **composite of r_1 with r_2 along the match μ**.

[19] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

DPO-type rule algebras [19]

Let $\mathbf{C}$ be an **extensive category**, and denote by $Lin(\mathbf{C})$ the **set of linear rules**. Define the **free $\mathbb{K}$-vector space**

$$\mathscr{R}_{\mathbf{C}} := span_{\mathbb{K}}\left(\left\{\delta(r)\middle| r \equiv (O \xleftarrow{o} K \xrightarrow{i} I) \in Lin(\mathbf{C})\right\}\right) \qquad \text{(for } \mathbb{K} \text{ a field, e.g. } \mathbb{K} = \mathbb{R}, \mathbb{C}\text{)}.$$

Then $\mathscr{R}_{\mathbf{C}}$ equipped with the bilinear **multiplication law**,

$$*_{\mathscr{R}_{\mathbf{C}}} : \mathscr{R}_{\mathbf{C}} \times \mathscr{R}_{\mathbf{C}} \to \mathscr{R}_{\mathbf{C}} : (\delta(r_1), \delta(r_2)) \mapsto \begin{cases} 0_{\mathscr{R}_{\mathbf{C}}} & \text{if } (r_1 \Vdash r_2) = \varnothing \\ \sum_{\mu \in (r_1 \Vdash r_2)} \delta(r_1 \overset{\mu}{\blacktriangleleft} r_2) & \text{otherwise} \end{cases}$$

is an **associative unital algebra**, referred to as **DPO-type rule algebra over $\mathbf{C}$**, with **unit** for $*_{\mathscr{R}_{\mathbf{C}}}$ given by $\delta(r_{\varnothing}) := \delta(\varnothing \hookleftarrow \varnothing \hookrightarrow \varnothing)$.

[19] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

Canonical representations of DPO-type rule algebras [19]

Let $\mathbf{C}$ be an **extensive category**, and define $\hat{\mathbf{C}}$ as the **free $\mathbb{K}$-vector space spanned by isomorphism classes of objects of $\mathbf{C}$**,

$$\hat{\mathbf{C}} := span_{\mathbb{K}}\left(\left\{ |X\rangle \middle| X \in ob(\mathbf{C})_{\cong} \right\}\right).$$

Then the **canonical representation $\rho_{\mathbf{C}}$ of $\mathscr{R}_{\mathbf{C}}$** is defined as

$$\rho_{\mathbf{C}} : \mathscr{R}_{\mathbf{C}} \to End_{\mathbb{K}}(\hat{\mathbf{C}}) : \rho_{\mathbf{C}}(r)\,|X\rangle := \begin{cases} 0_{\hat{\mathbf{C}}} & \text{if } M_r(X) = \varnothing \\ \sum_{m \in M_r(X)} |r_m(x)\rangle & \text{otherwise.} \end{cases}$$

[19] Nicolas Behr and Pawel Sobocinski. “Rule Algebras for Adhesive Categories”. In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

Stochastic rewriting systems as continuous-time Markov chains (CTMCs) [20] [21]

Input: · a set of **linear rules with base rates** $\{(\kappa_j, r_j \equiv (O_j \xleftarrow{o_j} K_j \xrightarrow{i_j} I_j)\}_{j\in J}$ (with $\kappa_j \in \mathbb{R}_{>0}$) and

· an **initial state** $|\Psi_0\rangle \in Prob(\mathbf{C})$ ($\leftarrow$ **probability distributions over the state space** $\hat{\mathbf{C}}$)

Output: a **CTMC** with **time-dependent state** $|\Psi(t)\rangle \in Prob(\mathbf{C})$ and **evolution equation** (with $t \geqslant 0$)

$$\tfrac{d}{dt}\,|\Psi(t)\rangle = H\,|\Psi(t)\rangle\,, \qquad |\Psi(0)\rangle = |\Psi_0\rangle$$

$$H = \sum_{j\in J} \kappa_j \left(\rho_{\mathbf{C}}\left(\delta(O_j \xleftarrow{o_j} K_j \xrightarrow{i_j} I_j)\right) - \rho_{\mathbf{C}}\left(\delta(I_j \xleftarrow{i_j} K_j \xrightarrow{i_j} I_j)\right)\right)$$

[22] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Stochastic mechanics of graph rewriting”. In: *Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016)* (2016), pp. 46–55

[23] Nicolas Behr and Pawel Sobocinski. “Rule Algebras for Adhesive Categories”. In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

Observables $=$ diagonal linear operators on $\hat{\mathbf{C}}$ [18] [19]

For all $I \in ob(\mathbf{C})$ and $i : K \hookrightarrow I \in mor(\mathbf{C})$, the operators $\mathscr{O}_I^i := \rho_{\mathbf{C}}(\delta(I \xleftarrow{i} K \xrightarrow{i} I))$ are **diagonal operators on $\hat{\mathbf{C}}$**, by virtue of the **symmetry** of the diagram below (if it is **constructible**):

$$\begin{tikzcd} I \arrow[d, dotted] & K \arrow[l, hook', "i"'] \arrow[r, hook, "i"] \arrow[d, dashed] & I \arrow[d, hook, "m"] \\ r_m(X) = X \arrow[ur, phantom, "②"] & K' \arrow[l, dotted, hook'] \arrow[r, dashed, hook] \arrow[ur, phantom, "①"] & X \end{tikzcd}$$

① **pushout complement** (**might fail to exist!**)

② **pushout** (which **always exists**!)

[20] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: *Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016)* (2016), pp. 46–55

[21] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

Key result: Combinatorial Conversion Theorem [22] [23]

- define the **"dual projection vector"** $\langle| : \hat{\mathbf{C}} \to \mathbb{K}$ via $\forall X \in ob(\mathbf{C}) : \quad \langle|X\rangle := 1_{\mathbb{R}}$

$\Rightarrow$ **Consequence:** so-called **jump-closure**, whereby for all linear rules $(O \xleftarrow{o} K \xrightarrow{i} I) \in Lin(\mathbf{C})$ one finds that

$$\langle|\rho_{\mathbf{C}}\left(\delta\left(O \xleftarrow{o} K \xrightarrow{i} I\right)\right) \equiv \langle|\rho_{\mathbf{C}}\left(\delta\left(I \xleftarrow{i} K \xrightarrow{i} I\right)\right) \equiv \langle|\mathcal{O}_I^i\,.$$

A stronger notion of closure: polynomial jump closure

Consider a stochastic rewriting system with evolution operator H. Then we refer to a set $\mathbb{O}$ of **connected observables**,

$$\mathbb{O} = \{\mathcal{O}_j \equiv \mathcal{O}_{M_j}^{r_j} \equiv \rho(M_j \xleftarrow{r_j} K_j \xrightarrow{r_j} M_j)\}_{j\in J}\,,$$

for some (possibly countably infinite) index set J as ***polynomially jump-closed*** if and only if it satisfies the **polynomial jump closure** (PJC) **condition**

$$(PJC) \quad \forall n \in \mathbb{Z}_{>0} : \exists \underline{N(n)} \in \mathbb{N}_0^{|J|}, \gamma_n(\underline{\lambda};\underline{k}) \in \mathbb{R} : \langle|ad_{\underline{\lambda}\cdot\underline{\mathcal{O}}}^{\circ\, n} H = \sum_{\underline{k}=\underline{0}}^{\underline{N(n)}} \gamma_n(\underline{\lambda};\underline{k})\langle|\underline{\mathcal{O}}^{\underline{k}}\,.$$

[22] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

[23] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: *arXiv preprint 1904.07313* (2019)

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A stronger notion of closure: polynomial jump closure

$$(PJC)\quad \forall n \in \mathbb{Z}_{>0} : \exists \underline{N(n)} \in \mathbb{N}_0^{|J|}, \gamma_n(\underline{\lambda};\underline{k}) \in \mathbb{R} : \langle| ad_{\underline{\lambda}\cdot\underline{\mathscr{O}}}^{\circ n} H = \sum_{\underline{k}=\underline{0}}^{\underline{N(n)}} \gamma_n(\underline{\lambda};\underline{k}) \langle| \underline{\mathscr{O}}^{\underline{k}} .$$

Combinatorial Conversion Theorem

For a **polynomially jump-closed set of connected observables** $\mathbb{O} = \{\mathscr{O}_j\}_{j\in J}$ of a system with evolution operator H, the evolution equation for the EGF $\mathscr{M}(t;\underline{\lambda})$ of the moments of the observables $\mathbb{O}$ may be **converted** from its explicit expression in the observables $\mathscr{O}_j$ into a **partial differential equation** of $\mathscr{M}(t;\underline{\lambda})$ itself w.r.t. the formal parameters $\{\lambda_j\}_{j\in J}$:

$$\frac{\partial}{\partial t}\mathscr{M}(t;\underline{\lambda}) = \mathbb{D}(\underline{\lambda},\partial_{\underline{\lambda}})\mathscr{M}(t;\underline{\lambda}), \qquad \mathbb{D}(\underline{\lambda},\partial_{\underline{\lambda}}) = \left(\left[\langle| \left(e^{ad_{\underline{\lambda}\cdot\underline{\mathscr{O}}}} H\right)\right]\Big|_{\mathscr{O}_j \to \frac{\partial}{\partial \lambda_j}}\right)|\varnothing\rangle .$$

Here, in the definition of the differential operator $\mathbb{D}$, we have made use of the assumption of polynomial jump-closure in converting the expression in square brackets into $\langle|$ applied to a formal series in the $\mathscr{O}_j$.

[22] Nicolas Behr and Pawel Sobocinski. "Rule Algebras for Adhesive Categories". In: *27th EACSL Annual Conference on Computer Science Logic (CSL 2018)*. Ed. by Dan Ghica and Achim Jung. Vol. 119. Leibniz International Proceedings in Informatics (LIPIcs). Dagstuhl, Germany: Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2018, 11:1–11:21

[23] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: *arXiv preprint 1904.07313* (2019)

Key result: Moment Bisimulations [24]

Definition of Moment Bisimulations

Consider two systems with evolution operators H_i and two **equinumerous** sets $\mathbb{O}_i$ of **connected graph observables polynomially jump-closed w.r.t.** H_i, respectively ($i \in 1,2$). Denote by $f : \mathbb{O}_1 \xrightarrow{\cong} \mathbb{O}_2$ a **bijection** of the two sets of observables. Then the pairs $(H_1, \mathbb{O}_1)$ and $(H_2, \mathbb{O}_2)$ are said to be ***moment bisimilar (via f)*** if the **moment bisimilarity** (MB) **condition** holds:

$$(MB) \qquad \left(\left[\langle | \left(e^{ad_{\underline{\lambda} \cdot \underline{O}}} H_1 \right) \right] \Big|_{O_i \to \frac{\partial}{\partial \lambda_i}} \right) |\varnothing\rangle = \left(\left[\langle | \left(e^{ad_{\underline{\lambda} \cdot \underline{f(O)}}} H_2 \right) \right] \Big|_{f(O_i) \to \frac{\partial}{\partial \lambda_i}} \right) |\varnothing\rangle \,.$$

Then by virtue of the **Combinatorial Conversion Theorem**,

$$\frac{\partial}{\partial t} \mathscr{M}_1(t; \underline{\lambda}) = \frac{\partial}{\partial t} \tilde{\mathscr{M}}_2(t; \underline{\lambda}) \,, \quad \tilde{\mathscr{M}}_2(t; \underline{\lambda}) := \langle | \, e^{\underline{\lambda} \cdot \underline{f(\mathscr{O})}} \, | \Psi_2(t) \rangle \,,$$

and whence for choices of initial states $|\Psi_1(0)\rangle \in Prob(\mathbf{C}_2), |\Psi_2(0)\rangle \in Prob(\mathbf{C}_2)$ such that $\mathscr{M}_1(0; \underline{\lambda}) = \tilde{\mathscr{M}}_2(0; \underline{\lambda})$ one finds that $\mathscr{M}_1(t; \underline{\lambda}) = \tilde{\mathscr{M}}_2(t; \underline{\lambda})$ for all $t \geqslant 0$ (if the solution exists).

[24] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Key result: The Discrete Moment Bisimulation Theorem [25]

Idea: consider moment bisimulations between some **generic** stochastic rewriting system (SRS) and a **discrete** SRS – we will see some explicit examples in a moment!

The Discrete Moment Bisimulation Theorem

Let $H = \sum_{k\in K} \kappa_k(\rho_{\mathbf{C}}(h_k) - \mathcal{O}_{\mathbf{C}}(h_k))$ be the evolution operator of a SRS, and let $\mathbb{O} = \{\mathcal{O}_j\}_{j\in J}$ be a **polynomially jump-closed set of observables for** H. Suppose the following **two conditions** (amounting to the **discrete moment bisimulation** (DMB) **condition**) are verified:

$$(DMB)\quad \begin{aligned} &(i) && \forall j\in J, k\in K : \exists \eta_{j,k}\in\mathbb{Z}: \quad ad_{\mathcal{O}_j}(\rho_{\mathbf{C}}(h_k)) = \eta_{j,k}\rho_{\mathbf{C}}(h_k)\\ &(ii) && \forall k\in K: \exists \alpha_k\in\mathbb{R}, \underline{\ell}_k\in\mathbb{N}_0^{|J|}: \quad \langle|\rho_{\mathbf{C}}(h_k) = \alpha_k\sum_{\underline{n}=\underline{0}}^{\underline{\ell}_k}\left(\prod_j s_1((\underline{\ell}_j)_i;n_j)\right)\langle|\underline{\mathcal{O}}^{\underline{n}}. \end{aligned}$$

Then for every isomorphism $F: J\xrightarrow{\cong}\mathscr{C}$ from J to a set of **vertex colors** $\mathscr{C}$, denoting by $\mathbb{O}_{discr} := \{\hat{n}_c\}_{c\in\mathscr{C}}$ a set of **discrete connected graph observables** (with $\hat{n}_c\in\mathcal{O}_{discr}$ **counting vertices of color** $c\in\mathscr{C}$) and by H_{discr} the evolution operator of a *discrete SRS* of **discrete graphs (**$\in ob(\mathbf{G}_0)$**) with vertices of colors** $\mathscr{C}$ defined as

$$H_{discr} := \sum_{k\in K}\alpha_k\kappa_k\left(\rho_{\mathbf{G}_0}\left(\delta\left(\underline{\bullet}^{(\underline{\eta}_k+\underline{\ell}_k)}\hookleftarrow\varnothing\hookrightarrow\underline{\bullet}^{\underline{\ell}_k}\right)\right)-\rho_{\mathbf{G}_0}\left(\delta\left(\underline{\bullet}^{\underline{\ell}_k}\hookleftarrow\varnothing\hookrightarrow\underline{\bullet}^{\underline{\ell}_k}\right)\right)\right),\quad \underline{\eta}_{k_j} := \eta_{j,k}.$$

the pair $(H,\mathbb{O})$ is **moment bisimilar** to $(H_{discr},\mathbb{O}_{discr})$ via the isomorphism $f(\mathcal{O}_j) := \hat{n}_{F(j)}$.

[25] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Application examples of the stochastic mechanics framework for graph rewriting systems

Comparison to normal-ordering style approaches to combinatorics

Some relevant results of [26]:

- **Fact:** The only elementary observables ($\approx$ connected motif observables in the general setting) are the **number operators** $\hat{n}_i$ (one for each species i),

$$\hat{n}_i := a_i^\dagger a_i\,, \quad \hat{n}_i\,|\underline{n}\rangle = n_i\,|\underline{n}\rangle \qquad (i \in \mathscr{I})\,.$$

- **Fact:** The **jump-closure property** specializes to (where $\underline{x}^{\underline{y}} := x_1^{y_1} x_2^{y_2} \cdots$)

$$\langle|\,(\underline{a}^\dagger)^{\underline{r}}\underline{a}^{\underline{s}} = \langle|\,(\underline{a}^\dagger)^{\underline{s}}\underline{a}^{\underline{s}} = \sum_{\underline{k}=\underline{0}}^{\underline{s}} s_1(\underline{s};\underline{k})\langle|\,\hat{\underline{n}}^{\underline{k}} \qquad (s_1(\underline{s};\underline{k}) - \textbf{Stirling numbers of the } 1^{st} \textbf{ kind})\,.$$

$\Rightarrow$ the Combinatorial Conversion Theorem entails that there **always exists a full closure**

$$\frac{\partial}{\partial t}\mathscr{M}(t;\underline{\lambda}) \equiv \frac{\partial}{\partial t}\left\langle e^{\underline{\lambda}\cdot\hat{\underline{n}}}\right\rangle(t) = \mathbb{D}(\underline{\lambda},\partial_{\underline{\lambda}})\mathscr{M}(t;\underline{\lambda})$$

without additional assumptions on the discrete rewriting system.

- This is **in stark contrast to generic rewriting systems**, where we typically have no Ansatz to determine interesting subsets of observables, and where closure is a delicate algebraic structure!

[26] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. “Combinatorics of Chemical Reaction Systems”. In: *arXiv:1712.06575* (2017)

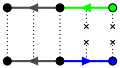
Notational convention: rule diagrams

- **An inconvenience:** in practice, explicitly providing the structure of a linear rule $r \equiv (O \overset{o}{\hookleftarrow} K \overset{i}{\hookrightarrow} I) \in \mathbf{Lin}(\mathbf{C})$ is notationally somewhat cumbersome…
- **Idea:** a span of monomorphisms such as $(O \overset{o}{\hookleftarrow} K \overset{i}{\hookrightarrow} I)$ encodes a *partial morphism* $O \overset{r}{\leftharpoondown} I$, whence it is a lot easier to represent r by the **graph of this partial function**, which we call **rule diagrams** [27] [28].

Notational convention for the special case of linear rules of graphs

Let $\mathbf{G}$ denote the category of **finite directed vertex- and edge-colored multigraphs**. Then a linear rule $r \equiv (O \overset{r}{\leftharpoondown} I) \in \mathbf{Lin}(\mathbf{G})$ is represented by its **rule diagram**, where I is drawn **at the bottom**, O **at the top**, and where the internal **structure of the partial map** r is represented by **dotted lines**. We will also simplify the notation further by **dropping the symbol** δ (for elements $\delta(r)$ of the rule algebra) when writing the diagrams.

Example:



[27] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Stochastic mechanics of graph rewriting". In: *Proceedings of the 31st Annual ACM-IEEE Symposium on Logic in Computer Science (LICS 2016)* (2016), pp. 46–55

[28] Nicolas Behr, Vincent Danos, Ilias Garnier, and Tobias Heindel. "The algebras of graph rewriting". In: *arXiv:1612.06240* (2016)

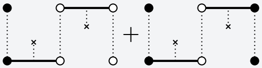
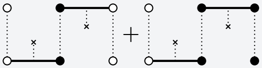
On the non-triviality of semi-linear processes: a variant of the Voter Model

Definition [29]:

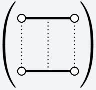
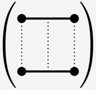
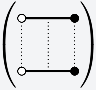
Consider a model defined on a **state space** of **bi-colored graphs** (with white ○ and black ● vertices, say), and with the following two transitions:

Here, the vertices marked ⊗ can be of **either black or white color**. The corresponding **evolution operator** H reads explicitly (with $\rho \equiv \rho_{\mathbf{G}}$)

$$H := \rho(h_{VM}) - \mathscr{O}(h_{VM})$$

$h_{VM} := \kappa_0 h_0 + \kappa_1 h_1$, $h_0 :=$  , $h_1 :=$  .

Consider the **edge observables**:

$\mathscr{O}_{00} := \frac{1}{2}\rho$  , $\mathscr{O}_{11} := \frac{1}{2}\rho$  , $\mathscr{O}_{01} := \rho$  .

[29] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

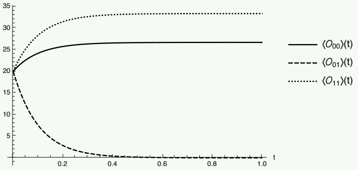
On the non-triviality of semi-linear processes: a variant of the Voter Model

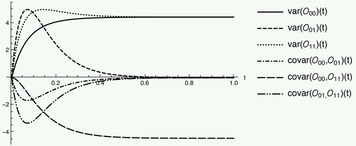
Evolution of means and (co-)variances of the edge observables

Starting from a **pure state** $|\Psi(0)\rangle = |G_0\rangle$ with initial counts N_X and parameters chosen as (with $N_V = N_0 + N_1$)

$$\kappa_0 = \frac{1}{30}\,,\ \kappa_1 = \frac{1}{10}\,,\ \left(N_V, N_0, N_{00}, N_{01}, N_{11}\right) = \left(100, 80, 20, 20, 20\right)\,,$$

one obtains the following **analytical results**:

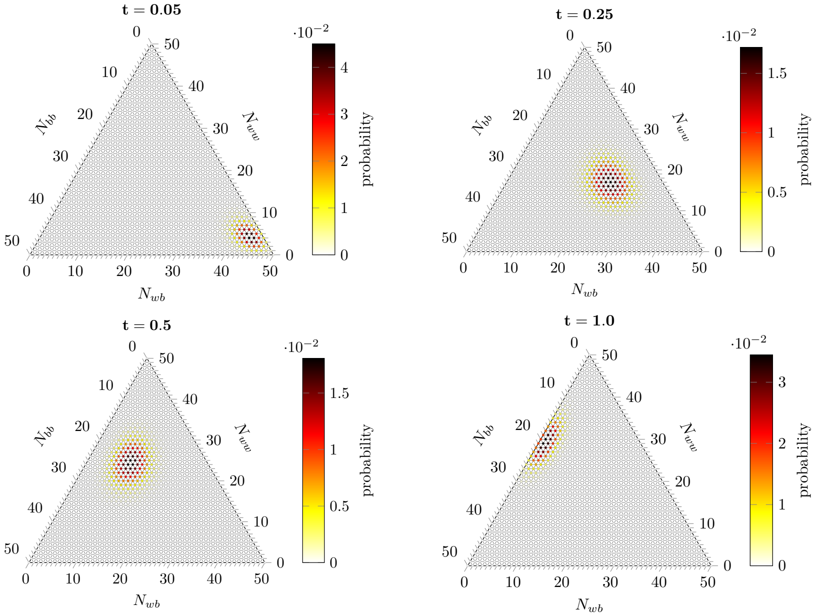




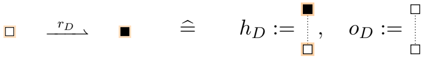
The plots illustrate the following **analytical result** on the **asymptotic limit** $t \to \infty$ **of the exponential moment generating function**:

$$\lim_{t\to\infty} \left\langle e^{\underline{\lambda}_E \cdot \underline{\mathcal{O}}_E} \right\rangle(t) = \left(\frac{\kappa_0 e^{\lambda_{00}} + \kappa_1 e^{\lambda_{11}}}{\kappa_0 + \kappa_1}\right)^{N_{01}} e^{\lambda_{00} N_{00} + \lambda_{11} N_{11}}\,.$$

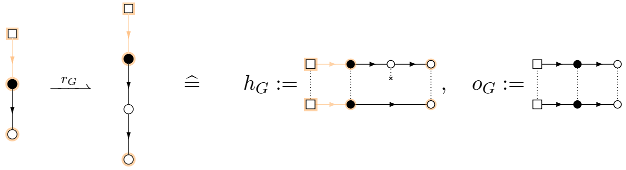
(a) Time-evolution of the edge observable count probability distribution



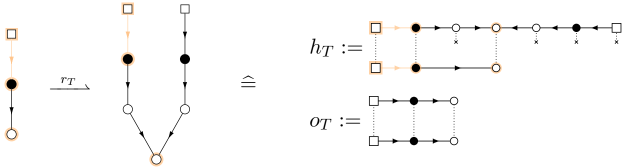
Taking advantage of discrete bisimulations: a cryptocurrency toy model [29]



(a) Ticket de-activation



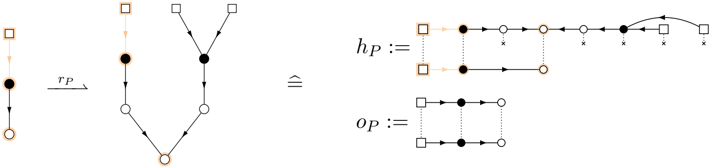
(b) Ledger growth



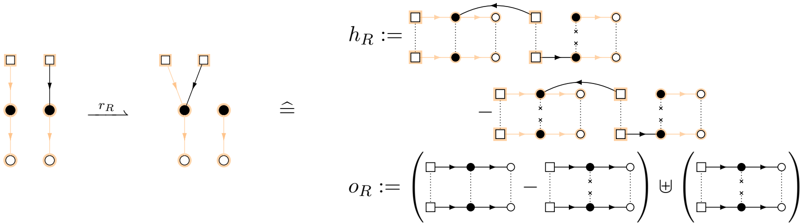
(c) Ticket production

[29] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Taking advantage of discrete bisimulations: a cryptocurrency toy model [29]



(d) Ticket pair production



(e) Ticket rearrangement

[29] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Taking advantage of discrete bisimulations: a cryptocurrency toy model [29]

The model is bisimilar to the following discrete rewriting system:

$$X_{\bullet_1} \xrightharpoonup{r_D} X_{\blacksquare_1} \qquad X_{\bullet_g} \xrightharpoonup{r_G} X_{\blacksquare_g}$$

$$X_{\bullet_1} \xrightharpoonup{r_G} X_{\bullet_1} + X_{\circ} \qquad X_{\bullet_g} \xrightharpoonup{r_G} X_{\bullet_g} + X_{\circ}$$

$$X_{\bullet_1} \xrightharpoonup{r_T} 2X_{\bullet_1} + X_t + 2X_{\circ} \qquad X_{\bullet_g} \xrightharpoonup{r_T} X_{\bullet_g} + X_{\bullet_1} + X_t + 2X_{\circ}$$

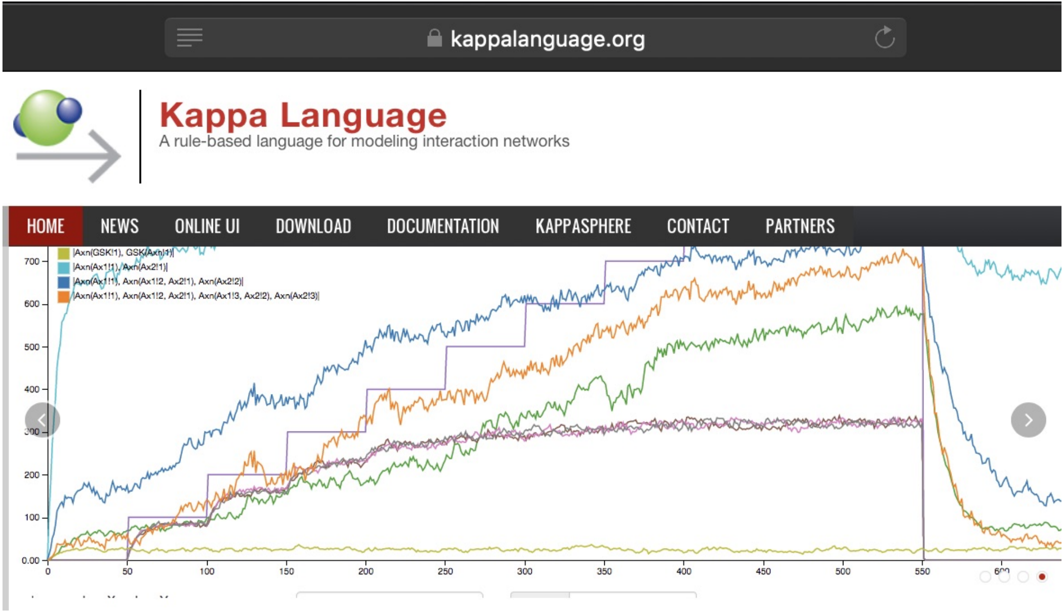
$$X_{\bullet_1} \xrightharpoonup{r_P} X_{\bullet_1} + 2X_{\bullet_g} + X_t + 2X_{\circ} \qquad X_{\bullet_g} \xrightharpoonup{r_P} 3X_{\bullet_g} + X_{\bullet_1} + X_t + 2X_{\circ}$$

$$X_{\bullet_1} + X_{\bullet_g} \xrightharpoonup{r_R} 2X_{\bullet_g}\,.$$

- $X_t\,,\ X_{\circ}\ \leftrightarrow$ observables counting **transaction nodes** resp. **ledger notes**
- $X_{\bullet_1}\,,\ X_{\bullet_g}\ \leftrightarrow$ observables counting **transaction nodes** with **exactly** 1 resp. **more than** 1 **active tickets attached** (with $X_{\blacksquare_1}$ and $X_{\blacksquare_g}$ the versions for **inactive tickets**)

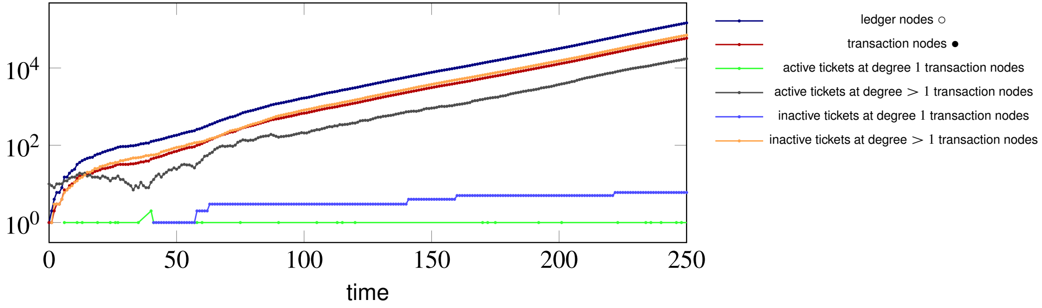
[29] Nicolas Behr, Vincent Danos, and Ilias Garnier. “Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems”. In: *arXiv preprint 1904.07313* (2019)

Alternative to exact solutions: numerical simulations [30]



[29] The Kappa language and KaSim simulation engine, https://kappalanguage.org

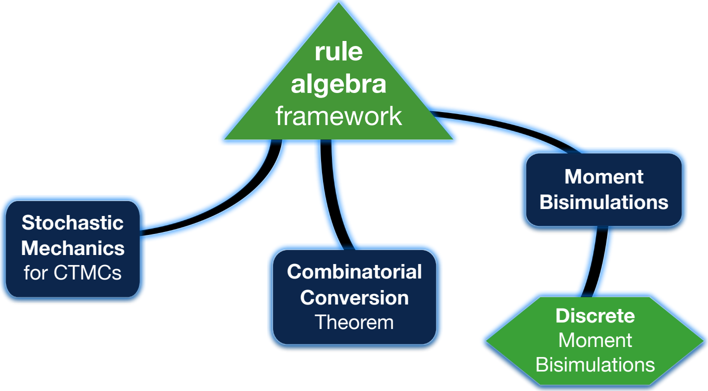
Taking advantage of discrete bisimulations: a cryptocurrency toy model [30]



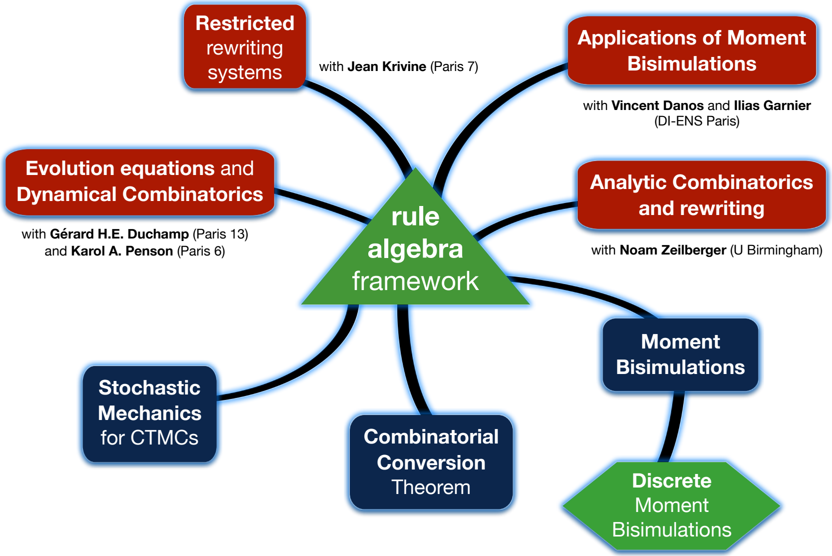
- While not analytically solvable, the discrete system may be studied by **numerical simulation algorithms** such as **Gillespie's SSA algorithm**.
- In comparison, a direct numerical simulation of this rewriting system is prohibitively complex!
- **Application:** one may use the results of the discrete model's simulation in order to study the dynamical properties of the system with respect to its parameters, and e.g. use these results to pick a particular candidate model for concrete practical applications.

[30] Nicolas Behr, Vincent Danos, and Ilias Garnier. "Combinatorial Conversion and Moment Bisimulation for Stochastic Rewriting Systems". In: *arXiv preprint 1904.07313* (2019)

Conclusion and Outlook



Conclusion and Outlook



Thank you!

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Appendix: Chemical reaction systems as discrete rewriting systems

The Heisenberg-Weyl algebra as the DPO discrete graph rewriting rule algebra

A first **consistency check** and **interesting special (and arguably simplest) case of rule algebras**:

The Heisenberg-Weyl algebra

Let $\mathscr{R}_0$ denote the rule algebra of DPO type rewriting for **discrete graphs**. Then the subalgebra $\mathscr{H}$ of $\mathscr{R}_0$ is defined as the algebra whose elementary **generators** are

$$x^{\dagger} := (\bullet \stackrel{\varnothing}{\Leftarrow} \varnothing)\,, \quad x := (\varnothing \stackrel{\varnothing}{\Leftarrow} \bullet)\,,$$

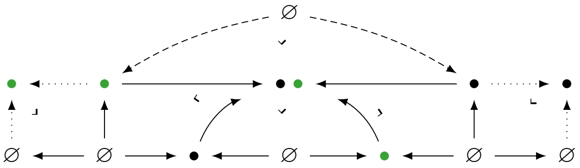
and whose elements are (finite) linear combinations of **words in $x^{\dagger}$ and x** (with concatenation given by the rule algebra multiplication $*_{\mathscr{R}_0}$) and of the **unit element** $R_{\varnothing} = (\varnothing \stackrel{\varnothing}{\Leftarrow} \varnothing)$. The canonical representation of $\mathscr{H}$ is the restriction of the canonical representation of $\mathscr{R}_0$ to $\mathscr{H}$.

The Heisenberg-Weyl algebra as the DPO discrete graph rewriting rule algebra

- famous property of the Heisenberg-Weyl algebra: with $a^\dagger := \rho(x^\dagger)$, $a := \rho(x)$, $\mathbb{1} := \rho(R_\varnothing)$,

$$[a, a^\dagger] := aa^\dagger - a^\dagger a = \mathbb{1}$$

- **realization/interpretation via the DPO rule algebra $\mathscr{R}_0$**: consider the following three **DPO-type compositions**



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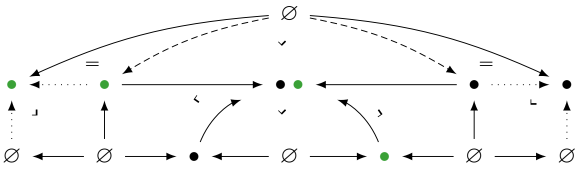

$$\hat{=} \qquad (\varnothing \xleftarrow{\varnothing} \bullet) \overset{\varnothing \leftarrow \varnothing}{\blacktriangleleft} (\bullet \xleftarrow{\varnothing} \varnothing) = (\bullet \xleftarrow{\varnothing} \bullet)$$

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- **realization/interpretation via the DPO rule algebra $\mathscr{R}_0$:** consider the following three **DPO-type compositions**

$$\begin{tikzcd}
 & & & \varnothing \arrow[dll, dashed, bend right] \arrow[drr, dashed, bend left] & & & \\
\varnothing & \varnothing \arrow[l, dotted] \arrow[rr] & & \bullet & & \varnothing \arrow[ll] \arrow[r, dotted] & \varnothing \\
\varnothing \arrow[u, dotted] & \varnothing \arrow[l] \arrow[r] \arrow[u] & \bullet \arrow[ur, bend left] & \bullet \arrow[l] \arrow[r] & \bullet \arrow[ul, bend right] & \varnothing \arrow[l] \arrow[r] \arrow[u] & \varnothing \arrow[u, dotted]
\end{tikzcd}$$

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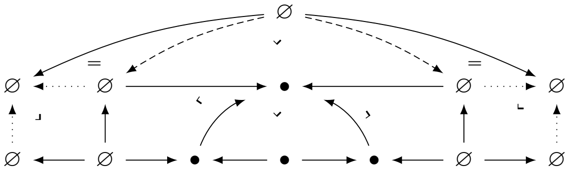

$$\hat{=} \qquad (\varnothing \xleftarrow{\varnothing} \bullet) \overset{\bullet \leftarrow \bullet}{\triangleleft} (\bullet \xleftarrow{\varnothing} \varnothing) = (\varnothing \xleftarrow{\varnothing} \varnothing)$$

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$$\begin{tikzcd}
 & & & \varnothing \arrow[dll, dashed] \arrow[drr, dashed] & & & \\
\bullet & \varnothing \arrow[l, dotted] \arrow[rr] & & \varnothing & & \varnothing \arrow[ll] \arrow[r, dotted] & \bullet \\
\bullet \arrow[u, dotted] & \varnothing \arrow[l] \arrow[r] \arrow[u] & \varnothing \arrow[ur, bend left] & \varnothing \arrow[l] \arrow[r] & \varnothing \arrow[ul, bend right] & \varnothing \arrow[l] \arrow[r] \arrow[u] & \bullet \arrow[u, dotted]
\end{tikzcd}$$

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$$\begin{tikzcd}
 & & & \varnothing \arrow[dlll, bend right] \arrow[dll, dashed, "="'] \arrow[drr, dashed, "="] \arrow[drrr, bend left] & & & \\
\bullet & \varnothing \arrow[l, dotted] \arrow[rr] & & \varnothing & & \varnothing \arrow[ll] \arrow[r, dotted] & \bullet \\
\bullet \arrow[u, dotted] & \varnothing \arrow[l] \arrow[r] \arrow[u] & \varnothing \arrow[ur, bend left] & \varnothing \arrow[l] \arrow[r] & \varnothing \arrow[ul, bend right] & \varnothing \arrow[l] \arrow[r] \arrow[u] & \bullet \arrow[u, dotted]
\end{tikzcd}$$

$$\widehat{=} \qquad (\bullet \xleftarrow{\varnothing} \varnothing) \overset{\varnothing \leftarrow \varnothing}{\blacktriangleleft} (\varnothing \xleftarrow{\varnothing} \bullet) = (\bullet \xleftarrow{\varnothing} \bullet)$$

The Heisenberg-Weyl algebra as the DPO discrete graph rewriting rule algebra

- it is straightforward to verify that

$$\underbrace{x^\dagger *_{\mathscr{R}_0} \ldots *_{\mathscr{R}_0} x^\dagger}_{m \text{ times}} = (\bullet^{\uplus\, m} \stackrel{\varnothing}{\Leftarrow} \varnothing)\,, \quad \underbrace{x *_{\mathscr{R}_0} \ldots *_{\mathscr{R}_0} x}_{n \text{ times}} = (\varnothing \stackrel{\varnothing}{\Leftarrow} \bullet^{\uplus\, n})$$

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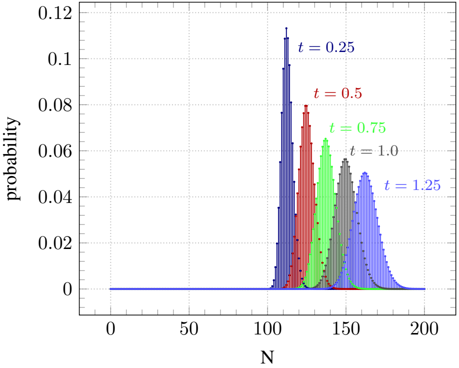
- analogously, we find the following:

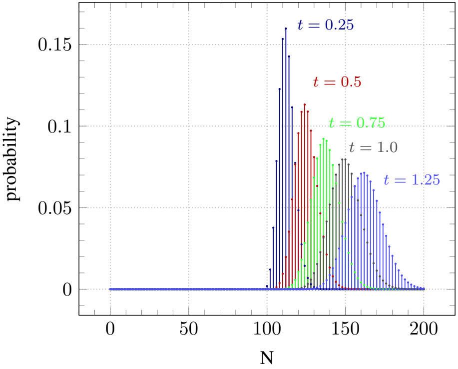
$$\begin{aligned}
\Bigg(\underbrace{x *_{\mathscr{R}_0} \ldots *_{\mathscr{R}_0} x}_{m \text{ times}}\Bigg) *_{\mathscr{R}_0} \Bigg(\underbrace{x^\dagger *_{\mathscr{R}_0} \ldots *_{\mathscr{R}_0} x^\dagger}_{n \text{ times}}\Bigg) &= (\varnothing \stackrel{\varnothing}{\Leftarrow} \bullet^{\uplus\, m}) *_{\mathscr{R}_0} (\bullet^{\uplus\, n} \stackrel{\varnothing}{\Leftarrow} \varnothing) \\
&\equiv \delta(A_m) *_{\mathscr{R}_0} \delta(B_n) \\
&= \sum_{\mathbf{m} \in A_m \Vdash B_n} \delta\left((\varnothing \stackrel{\varnothing}{\leftharpoondown} \bullet^{\uplus\, m}) \overset{\mathbf{m}}{\blacktriangleleft} (\bullet^{\uplus\, n} \stackrel{\varnothing}{\leftharpoondown} \varnothing) \right) \\
&= \sum_{k=0}^{min(m,n)} \underbrace{\left(\frac{1}{k!} \frac{m!}{(m-k)!} \frac{n!}{(n-k)!}\right)}_{\#\text{ of ways to pick } k \text{ vertices from } m \text{ and from } n \text{ vertices disregarding order}} \cdot \left(\bullet^{\uplus\, n-k} \stackrel{\varnothing}{\Leftarrow} \bullet^{\uplus\, m-k}\right)
\end{aligned}$$

Elementary nonary reactions – plots [30]

a) birth reaction $0A \xrightarrow{\beta=50} 1A$



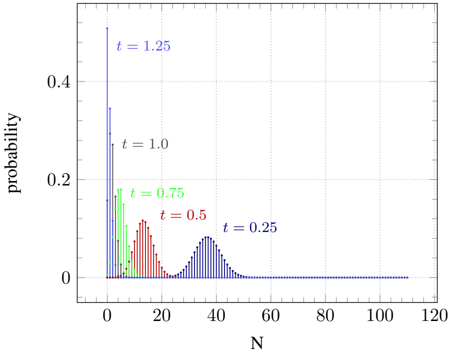
b) pair creation reaction $0A \xrightarrow{\gamma=25} 2A$



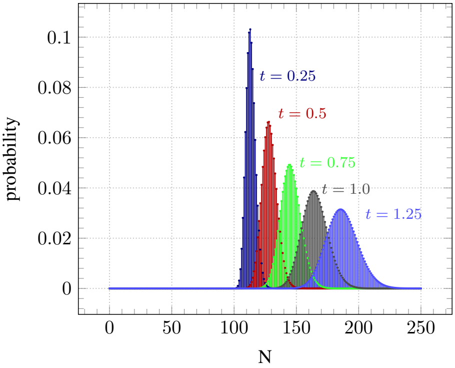
[30] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. “Combinatorics of Chemical Reaction Systems”. In: *arXiv:1712.06575* (2017)

Elementary unary reactions – plots [30]

c) decay reaction $1A \xrightarrow{\tau=4} 0A$



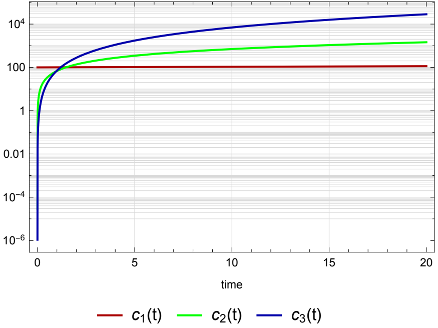
d) autocatalysis reaction $1A \xrightarrow{\alpha=\frac{1}{2}} 2A$



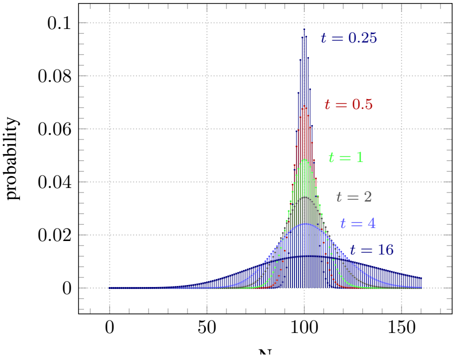
[30] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: *arXiv:1712.06575* (2017)

A hint of compositionality [30]

a) $1A \xrightarrow{\alpha=1/3} 2A,\ 0A \xrightarrow{\gamma=1/3} 2A,\ 1A \xrightarrow{\tau=1/3} 0A$



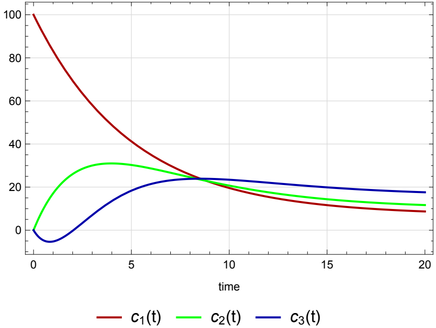
b) distributions for **a)**



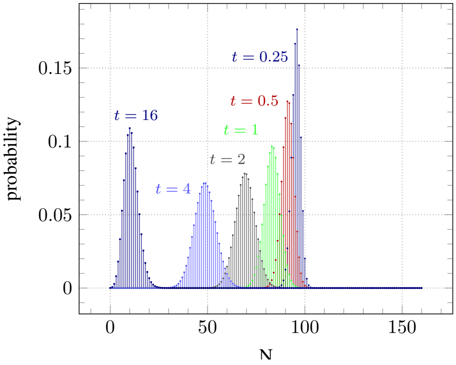
[30] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: *arXiv:1712.06575* (2017)

A hint of compositionality [30]

c) $0A \xrightarrow{\beta=1/5} 1A,\ 0A \xrightarrow{\gamma=3/5} 2A,\ 1A \xrightarrow{\tau=1/5} 0A$



d) distributions for **c)**

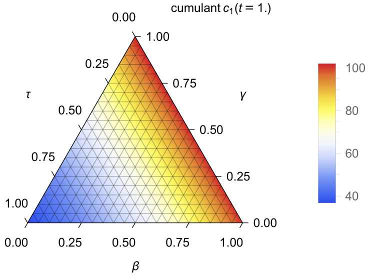


[30] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: *arXiv:1712.06575* (2017)

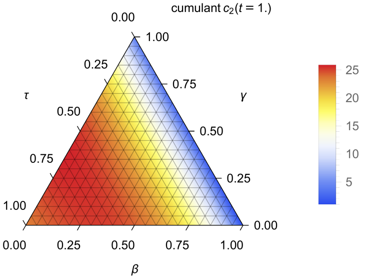
A hint of compositionality [30]

Example: ternary parameter dependence plot for a reaction system composed of **birth**, **pair creation** and **decay** reactions, for **initial state** $|\Psi(0)\rangle = |100\rangle$

a) Mean number of particles at time $t = 1$



b) Variance of number of particles at time $t = 1$

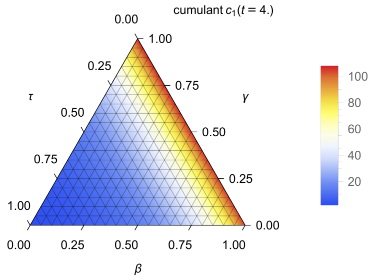


[30] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: *arXiv:1712.06575* (2017)

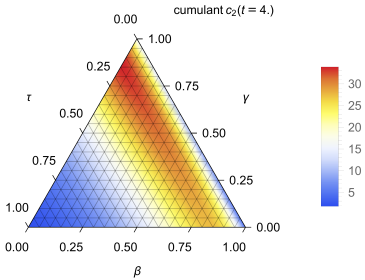
A hint of compositionality [30]

Example: ternary parameter dependence plot for a reaction system composed of **birth**, **pair creation** and **decay** reactions, for **initial state** $|\Psi(0)\rangle = |100\rangle$

c) Mean number of particles at time $t = 4$



d) Variance of number of particles at time $t = 4$

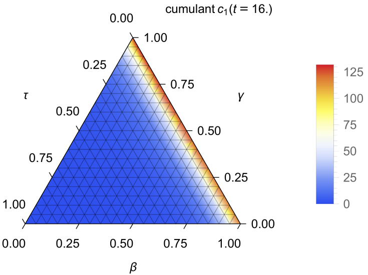


[30] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: *arXiv:1712.06575* (2017)

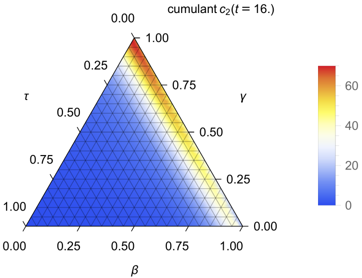
A hint of compositionality [30]

Example: ternary parameter dependence plot for a reaction system composed of **birth**, **pair creation** and **decay** reactions, for **initial state** $|\Psi(0)\rangle = |100\rangle$

e) Mean number of particles at time $t = 16$



f) Variance of number of particles at time $t = 16$



[30] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. "Combinatorics of Chemical Reaction Systems". In: *arXiv:1712.06575* (2017)

Binary reactions and Sobolev-Jacobi orthogonal polynomials

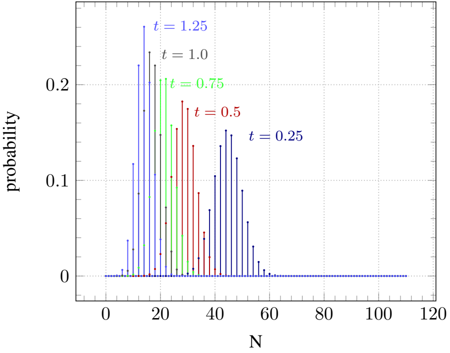
- The precise technical details are somewhat intricate, see the our paper!
- The **basic Ansatz** is the one of McQuarrie [31], **BUT** the original Ansatz had a mathematical error...
- **Problem:** McQuarrie suggested to use the Jacobi polynomials as eigenfunction basis of the infinitesimal generator, yet for the range of parameters of interest, these are ill-posed.
- **Our solution:** the mathematical problem has been successfully treated in the 1990's by Kwon & Littlejohn [32], who introduced so-called **Sobolev-Jacobi polynomials**.
- **Aside:** This is related **normal-ordering**, too! (But one of a new kind...)

[31] Donald A McQuarrie. "Kinetics of small systems. I". In: *The journal of chemical physics* 38.2 (1963), pp. 433–436; Donald A McQuarrie, CJ Jachimowski, and ME Russell. "Kinetics of small systems. II". In: *The Journal of Chemical Physics* 40.10 (1964), pp. 2914–2921; Donald A McQuarrie. "Stochastic approach to chemical kinetics". In: *Journal of applied probability* 4.3 (1967), pp. 413–478

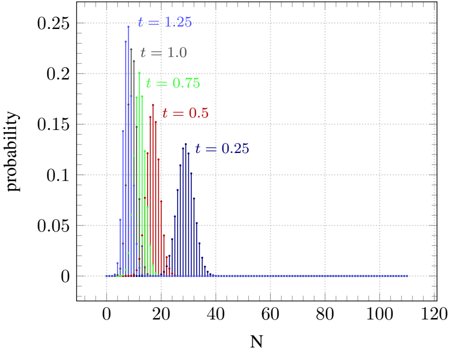
[32] KH Kwon, LL Littlejohn, and BH Yoo. "Characterizations of orthogonal polynomials satisfying differential equations". In: *SIAM Journal on Mathematical Analysis* 25.3 (1994), pp. 976–990; Kil H Kwon, LL Littlejohn, and BH Yoo. "New characterizations of classical orthogonal polynomials". In: *Indagationes Mathematicae* 7.2 (1996), pp. 199–213; Kil H Kwon and Lance L Littlejohn. "Classification of classical orthogonal polynomials". In: *J. Korean Math. Soc* 34.4 (1997), pp. 973–1008; Kil H Kwon and LL Littlejohn. "Sobolev orthogonal polynomials and second-order differential equations". In: *The Rocky Mountain journal of mathematics* (1998), pp. 547–594

Elementary binary reactions – plots [32]

e) pair annihilation reaction $2A \xrightarrow{\kappa=\frac{1}{40}} 0A$



f) catalytic decay reaction $2A \xrightarrow{\lambda=\frac{1}{10}} 1A$



[32] Nicolas Behr, Gerard HE Duchamp, and Karol A Penson. “Combinatorics of Chemical Reaction Systems”. In: *arXiv:1712.06575* (2017)