A characterisation of compatible state space aggregations

Mate Puljiz
University of Birmingham

joint work with
Chris Good, David Parker, and Jonathan E. Rowe

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What are we studying?

- When can we *simplify* an iterated system

$$\boldsymbol{x}_{n+1} = f(\boldsymbol{x}_n), \text{ where } f : \mathbb{R}^N \to \mathbb{R}^N?$$

- E.g.

$$\begin{aligned} x_{n+1} &= x_n^2, \\ y_{n+1} &= y_n^2 + 2x_n y_n, \\ z_{n+1} &= z_n + w_n, \\ w_{n+1} &= 0, \end{aligned}$$

can be simplified to

$$\begin{aligned} X_{n+1} &= X_n^2, \\ Y_{n+1} &= Y_n, \end{aligned}$$

where $X_i = x_i + y_i$ and $Y_i = z_i + w_i$.

Why are we studying this?

- Very general framework
- Simplifying real-life models (model reduction)
- Discovering underlying regularities of a model
- Efficient usage of computational resources

Our goal

- Identify a class of iterated systems of interest
- Interpret these as a parametrised set of models for artificial chemistries
- Given one such model, characterise its compatible aggregations in terms of the intrinsic parameters of the model

Notation

- Aggregation – a partition of the set of variables (sometimes the induced equivalence relation on $\{1, 2, \ldots, N\}$)
  - $\{\{x, y\}, \{z, w\}\}$ above
  - Can be encoded by a 0-1 column stochastic matrix
  - E.g. $\Xi = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$ above as $(X_i, Y_i)^T = \Xi \cdot (x_i, y_i, z_i, w_i)^T$
- Compatible aggregation – an aggregation for which the coarse grained description is well-defined

Class 1 – Markov Chains

Parameter set

M – an $N \times N$ column stochastic matrix

Iterated system

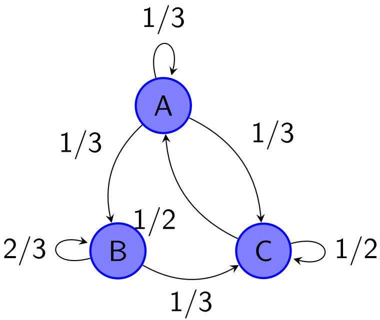
$$\boldsymbol{p}_{n+1} = M\boldsymbol{p}_n,$$

where $\boldsymbol{p} = (p^1, p^2, \ldots, p^N)$

Proposition (Folklore, see Kemeny & Snell [9])

An equivalence relation $\equiv$ on the set of states $\{1, 2\ldots, N\}$ is a compatible aggregation if and only if any two equivalent states have exactly the same outgoing transition probabilities towards any of the blocks of the (induced) partition.

A picture



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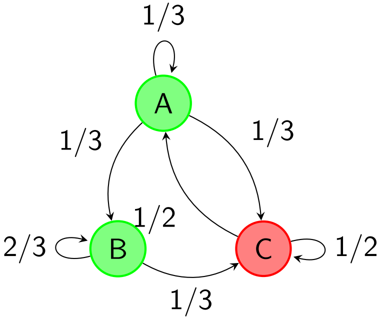

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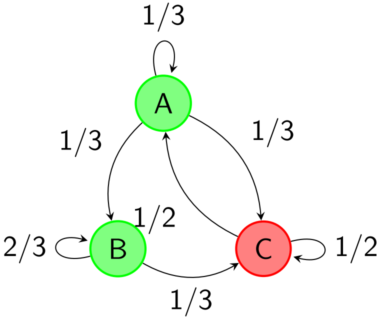

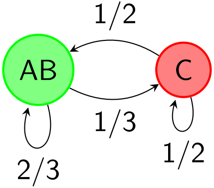

Proposition (Folklore, see Kemeny & Snell [9])

An equivalence relation $\equiv$ on the set of states $\{1, 2 \ldots, N\}$ is a compatible aggregation for M if and only if any two equivalent states have exactly the same outgoing transition probabilities towards any of the blocks of the (induced) partition.

Note that if we denote by Ξ the associated 0-1 matrix, the condition above could be equally written as

$$\Xi(M_i) = \Xi(M_j) \quad \text{whenever} \quad i, j \in \{1, 2, \ldots, N\} \text{ such that } i \equiv j,$$

where M_k is the k$^{\text{th}}$ column of M.

Class 1 – Markov Chains

More abstractly

$\Xi(\boldsymbol{\alpha}_{\boldsymbol{v}}) = \Xi(\boldsymbol{\alpha}_{\boldsymbol{w}})$ whenever $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{Z}_+^N$ such that $\Xi(\boldsymbol{v}) = \Xi(\boldsymbol{w})$,

where $\boldsymbol{\alpha}_{\boldsymbol{v}} = \partial_{\boldsymbol{v}} M(0, \ldots, 0) = \begin{cases} M_i, & \text{if } \boldsymbol{v} = \boldsymbol{e_i}, \qquad (\partial_{\boldsymbol{e_i}} = \partial_i) \\ (0, \ldots, 0)^T, & \text{otherwise.} \end{cases}$

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$\Xi(M_i) = \Xi(M_j)$ whenever $i, j \in \{1, 2, \ldots, N\}$ such that $i \equiv j$,

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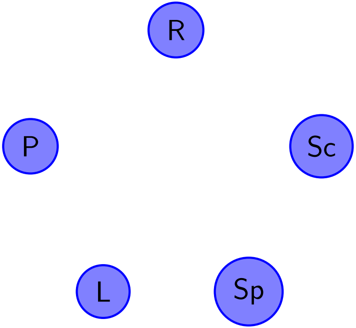
Class 2 – Binary Tournaments

Parameter set

$\leftharpoonup$ – an orientation on a complete graph on N vertices (a finite set of parameters)



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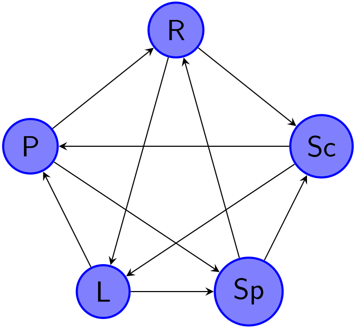


Class 2 – Binary Tournaments

Parameter set

$\leftharpoondown$ – an orientation on a complete graph on N vertices (a finite set of parameters)

Iterated system

$$p^i_{n+1} = (p^i_n)^2 + 2 \sum_{i \leftharpoondown k} p^k_n \cdot p^i_n = (T(p^1_n, \ldots, p^N_n))_i,$$

for $i \in \{1, 2, \ldots, N\}$

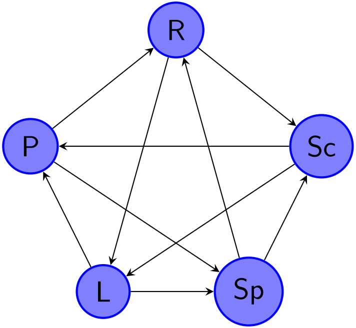
Class 2 – Binary Tournaments

Proposition

An equivalence relation $\equiv$ on $\{1, 2 \ldots, N\}$ is a compatible aggregation for the iterated system above if and only if

$$i \equiv j \equiv k \quad \textit{whenever} \quad i \equiv k \textit{ and } i \leftharpoonup j \leftharpoonup k.$$

A picture



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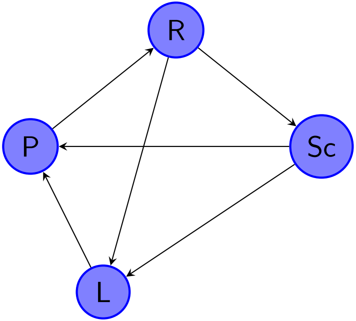

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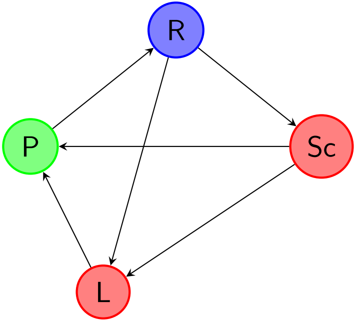

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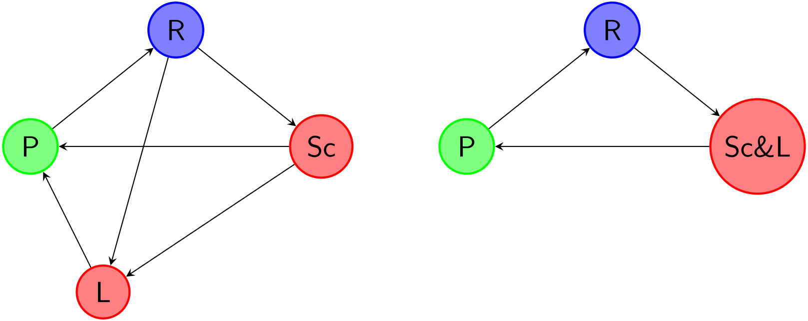

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More abstractly

$$\Xi(\boldsymbol{\alpha}_{\boldsymbol{v}}) = \Xi(\boldsymbol{\alpha}_{\boldsymbol{w}}) \quad \text{whenever} \quad \boldsymbol{v}, \boldsymbol{w} \in \mathbb{Z}_+^N \text{ such that } \Xi(\boldsymbol{v}) = \Xi(\boldsymbol{w}),$$

where

$$\boldsymbol{\alpha}_{\boldsymbol{v}} = \partial_{\boldsymbol{v}} T(0, \ldots, 0) = \begin{cases} 2\boldsymbol{e_i}, \text{ if } \boldsymbol{v} = 2\boldsymbol{e_i}, & (\partial_{2\boldsymbol{e_i}} = \partial_{ii}) \\ 2\boldsymbol{e_i}, \text{ if } \boldsymbol{v} = \boldsymbol{e_i} + \boldsymbol{e_k} \text{ and } i \leftharpoondown k, & \\ (0, \ldots, 0)^T, \text{ otherwise.} & (\partial_{\boldsymbol{e_i}+\boldsymbol{e_k}} = \partial_{ik}) \end{cases}$$

Class 2 v2 – 2nd order Chemistry

Parameter set

$\alpha_{\boldsymbol{v}}$ – $2\times$ the vector of probabilities of getting a certain product in a reaction represented by $\boldsymbol{v}$, where $\boldsymbol{v} \in \mathbb{Z}_+^N$ s.t. $|\boldsymbol{v}| = 2$

Iterated system

$$\boldsymbol{p_{n+1}} = T(\boldsymbol{p_n}),$$

where $\boldsymbol{p} = (p^1, p^2, \ldots, p^N)$ and

$$T(\boldsymbol{p}) = \sum_{\boldsymbol{v} \in \mathbb{Z}_+^N : |\boldsymbol{v}|=2} \frac{1}{\boldsymbol{v}!} \cdot \boldsymbol{\alpha_v} \cdot \boldsymbol{p}^{\boldsymbol{v}}$$

Class 2 v2 – 2[nd] order Chemistry

Proposition

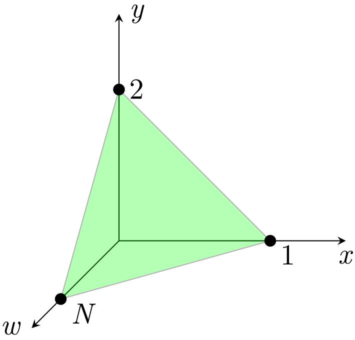
An equivalence relation $\equiv$ *on* $\{1, 2 \ldots, N\}$ *is a compatible aggregation for the iterated system above if and only if*

$$\Xi(\boldsymbol{\alpha}_{\boldsymbol{v}}) = \Xi(\boldsymbol{\alpha}_{\boldsymbol{w}}) \quad \textit{whenever} \quad \boldsymbol{v}, \boldsymbol{w} \in \mathbb{Z}_+^N \textit{ such that } \Xi(\boldsymbol{v}) = \Xi(\boldsymbol{w}).$$

Note that $\boldsymbol{\alpha}_v = \partial_v T(0, \ldots, 0)$.

Discretisation and Modelling issues

- Ω — $\{1, 2, \ldots, N\}$
- T — dynamics on $\Delta_N = M(\Omega)$
- R — size of a total population in simulation



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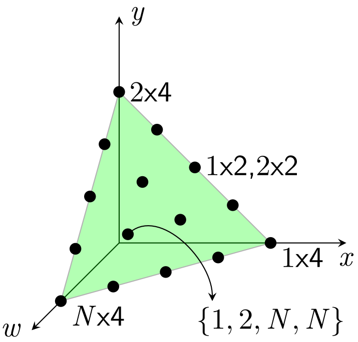

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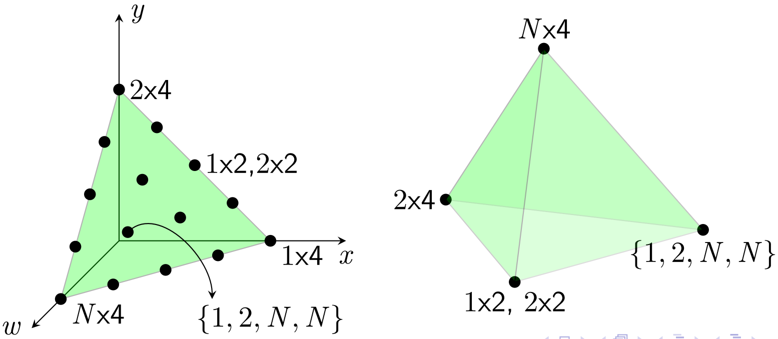
- $M(\frac{1}{R}X_N^R) = \Delta_{C(N,R)}$ — set of probabilities over finite populations



Different models

A countable family of independent random variables

$$\left\{ Z^{k,i}_{\boldsymbol{\alpha}},\, Y^{k,i}_{\boldsymbol{\beta}} : k \in \mathbb{N}, i \in \mathbb{N}, \boldsymbol{\alpha} \in T\left(\frac{1}{R} X^R_N\right), \boldsymbol{\beta} \in \frac{1}{R} X^R_N \right\},$$

where

$$Z^{k,i}_{\boldsymbol{\alpha}} \sim \begin{pmatrix} 1 & 2 & \dots & N \\ \alpha_1 & \alpha_2 & \dots & \alpha_N \end{pmatrix} \text{ and } Y^{k,i}_{\boldsymbol{\beta}} \sim \begin{pmatrix} 1 & 2 & \dots & N \\ \beta_1 & \beta_2 & \dots & \beta_N \end{pmatrix}$$

$$\frac{1}{R} V_k = F\left(\frac{1}{R} V_{k-1}; Z^{k,1}_{T\left(\frac{1}{R} V_{k-1}\right)}, Z^{k,2}_{T\left(\frac{1}{R} V_{k-1}\right)}, \dots; Y^{k,1}_{\frac{1}{R} V_{k-1}}, Y^{k,2}_{\frac{1}{R} V_{k-1}}, \dots \right),$$

for some $F \colon \frac{1}{R} X^R_N \times \Omega^\infty \times \Omega^\infty \to \frac{1}{R} X^R_N$ which is assumed to be compatible with $\Xi_\pi \times \pi^\infty \times \pi^\infty$ (for any quotient map $\pi \colon \Omega \to \tilde{\Omega}$)

Different models

Generational model

$$F_2\left(\frac{1}{R}\boldsymbol{v}; i_1, i_2, \ldots; j_1, j_2, \ldots\right) = \frac{1}{R}\left(\boldsymbol{e_{i_1}} + \boldsymbol{e_{i_2}} + \cdots + \boldsymbol{e_{i_R}}\right)$$

One at a time reaction

$$F_1\left(\frac{1}{R}\boldsymbol{v}; i_1, i_2, \ldots; j_1, j_2, \ldots\right) = \frac{1}{R}\left(\boldsymbol{v} + \boldsymbol{e_{i_1}} - \boldsymbol{e_{j_1}}\right)$$

Proposition

If Ξ is a compatible aggregation for T, then the Markov chains induced by the modelling functions F_1 (Vose [20]) or F_2 (or other compatible F) can be aggregated in the same way.

Class 3 – A very general heuristic model

Parameter set

$\alpha_{\boldsymbol{v}}$ – $2\times$ the vector of probabilities of getting a certain product in a reaction represented by $\boldsymbol{v}$, where $\boldsymbol{v} \in \mathbb{Z}_+^N$ s.t. $|\boldsymbol{v}| = 2$

Iterated system

$$\boldsymbol{p_{n+1}} = T(\boldsymbol{p_n}),$$

where $\boldsymbol{p} = (p^1, p^2, \ldots, p^N)$ and

$$T(\boldsymbol{p}) = \sum_{\boldsymbol{v} \in \mathbb{Z}_+^N : |\boldsymbol{v}|=2} \frac{1}{\boldsymbol{v}!} \cdot \boldsymbol{\alpha}_{\boldsymbol{v}} \cdot \boldsymbol{p}^{\boldsymbol{v}}$$

Class 3 – A very general heuristic model

Parameter set

$\alpha_{\boldsymbol{v}}$ – $|\boldsymbol{v}|!\times$ the vector of probabilities of getting a certain product in a reaction represented by $\boldsymbol{v}$, where $\boldsymbol{v} \in \mathbb{Z}_+^N$ —

Iterated system

$$\boldsymbol{p_{n+1}} = T(\boldsymbol{p_n}),$$

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$$T(\boldsymbol{p}) = \sum_{\boldsymbol{v} \in \mathbb{Z}_+^N —} \frac{1}{\boldsymbol{v}!} \cdot \boldsymbol{\alpha}_{\boldsymbol{v}} \cdot \boldsymbol{p}^{\boldsymbol{v}}$$

Class 3 – Compatible aggregations

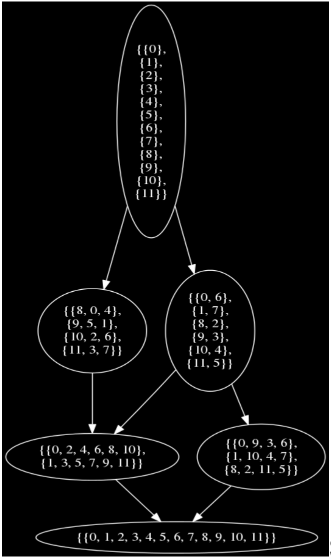
Theorem

An equivalence relation $\equiv$ *on* $\{1, 2 \ldots, N\}$ *is a compatible aggregation for the iterated system above if and only if*

$$\Xi(\boldsymbol{\alpha}_v) = \Xi(\boldsymbol{\alpha}_w) \quad \textit{whenever} \quad \boldsymbol{v}, \boldsymbol{w} \in \mathbb{Z}_+^N \textit{ such that } \Xi(\boldsymbol{v}) = \Xi(\boldsymbol{w}).$$

Note that $\boldsymbol{\alpha}_v = \partial_v T(0, \ldots, 0)$.

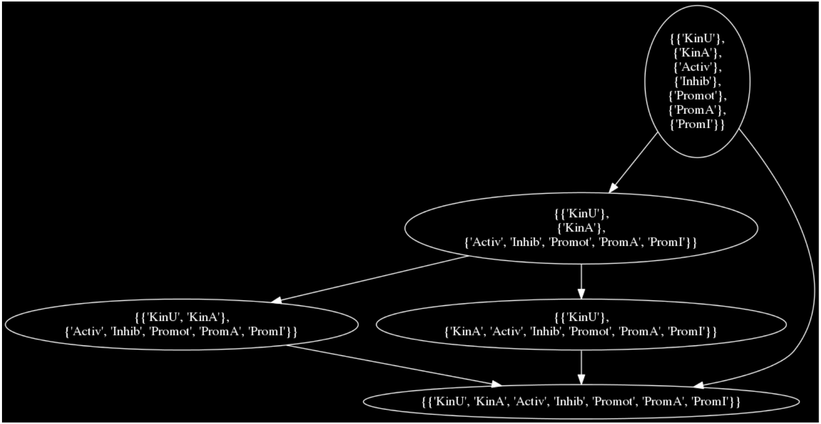
Modulo 12 Game



$x + y \to (x +_{12} y)$ $\Omega = \{0, 1, \ldots, 11\}$

An application to Kinetochore

Model by R. Henze, and B. Ibrahim



Acknowledgements

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Thank you for your attention!

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