State transition models of biomolecular dynamics

A few research questions

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SIMAI 2006, Special Session S2
Baia Samuele (RG), 25/05/2006

Overview

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   - Basic concepts
   - Recurrence and attractors
   - Simple example
2. Metabolic P systems
   - Basic concepts
   - P metabolic algorithm
3. Research outlook
   - Research questions: state transition dynamics
   - Research questions: metabolic P system models
4. References
   - State transition dynamics
   - Metabolic P systems

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State transition dynamics: basic concepts

- **state transition (ST) dynamics**: (S, q)

  S : (discrete) **state space**

  $q : S \rightarrow \mathcal{P}(S)$: [total] transition **dynamics**

  $\mathbf{x} \rightarrow \mathbf{y} \stackrel{def}{=} \mathbf{y} \in \mathbf{q}(\mathbf{x})$: (binary) transition relation

  $q(X) \stackrel{def}{=} \bigcup_{s \in X} q(s)$: extension to **quasistates** $X \subseteq S$

- **orbit** : $(X_i | i \in \mathbb{N})$ t.c. $\forall i.\ X_{i+1} = q(X_i)$
- **eventually periodic** orbit of origin X :
  $\exists k \geq 0\ \exists n > 0.\ q^{k+n}(X) = q^k(X)$ (**periodic** orbit if $k = 0$)
- orbit **(eventually) included** in another one: $(\exists i \geq 0.) \forall j (\geq i) X_j \subseteq X'_j$
- **basin** B : $\emptyset \neq B \subseteq S$ s.t. $q(B) \subseteq B$
- s**-trajectory** : $\xi : \mathbb{N} \rightarrow S$ s.t. $\xi(0) = s$ and $\forall i \geq 0.\ \xi(i) \rightarrow \xi(i+1)$
- s**-flight** $\stackrel{def}{=}$ **injective** s**-trajectory**

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Deterministic ST dynamics: recurrence, attractors

Classical dynamics concepts:
attracting set, recurrence, attractor

- take **two distinct modal flavours** in the general, nondeterministic case, see [(Manca *et al.*, 2005), (Scollo *et al.*, 2006)]
- no modal difference in the **deterministic case** (where the concepts of orbit and trajectory practically coincide):

- state x is **recurrent** if $x \in q^n(x)$ for some $n > 0$
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ST dynamics: a contrived example

a simple model of epidemic propagation

as well as of unstable catalythic reaction:

$CG \longrightarrow GG$

$C \longrightarrow C$

$G \longrightarrow \lambda$

$G \longrightarrow K$

$G \longrightarrow G$

- **instability** of agent G: it either dies or recovers (becoming immune: K)
- **states** : $(|C|+|K|, |G|)$
- **transitions** can be determined by equipping rules with a measure of **relative strength**

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- **transitions** can be determined by equipping rules with a measure of **relative strength**

P systems: basic concepts

P systems: a computational model based on

- **multiset rewriting rules**
- workspace **compartmentalization**

- *biological counterparts*:
  - **biochemical reactions**
  - **membranes**
- evolution strategies in (variants of) P systems:
  - **maximal parallelism**, usually
  - or some other **fixed** strategy
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a possible way out: **metabolic** P systems [(Bianco *et al.*, 2006a), (Bianco *et al.*, 2006b), (Manca, 2006)]:

- **metabolic rules**: multiset rewriting rules equipped with **reaction maps**:

  real-valued functions of the system state, that tell the **competitive strength** of each metabolic rule
- each metabolic rule:
  - **consumes** finite amounts of those biochemical resources whose **types** occur in the **pattern** (the lhs)
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P metabolic algorithm

generalizing Avogadro's molar units:

- only finite amounts of biochemical resources are available: their allocation to rules obeys a **mass partition principle**, where each rule gets an amount of each needed resource that is an integer multiple of the rule's **reaction unit**
- the latter depends on the reaction map and on the number of occurrences of resource types in the pattern
- **PMA** [(Manca, 2006)] is the simple algorithm that, at each state, computes the resource allocation to metabolic rules according to their reaction maps and reaction units

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Moving from structureless to topological state spaces:

- definability of **weaker** notions of **recurrence**

  that is: replace **exact** occurrence of a state in its own trajectory with **approximate** occurrence

- definability of **weaker** notions of **attraction**

  that is: replace **exact** inclusion of orbits in the attracting set with **approximate** inclusion

- **generalization** of the characterization results obtained in [(Scollo *et al.*, 2006)], linking recurrence and attractors, under the aforementioned weakings

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two levels in metabolic P system modeling of biochemical dynamics:

- **stoichiometry:** the metabolic rules
- **regulation:** the reaction maps

- basic question (roughly): **how to get those models. . .**

  . . . for a given biochemical behaviour?
  This is the general **simulation problem**

- easier (?) question: assume the rules are given, how to get their **reaction maps?**

  This may be called the **regulation problem**

- even easier (??) question: assumes the rules are given and the **form** of reaction maps is nown (polynomial, say), how to get the values of their **unknown parameters** (the coefficients, say)?

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