Master 2 MPRI course 2-19 Biochemical Programming
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Written examination 3 hours
All printed documents allowed
Any electronic devide prohibited
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Abstract

We study the notion of contextual symmetry on the differential semantics of three variants of a model.

We consider a model with only one kind of agent and three sites which can be phosphorylated, or not. Each kind of site is identified by its position, (on the top, on the left, on the right). Unphosphorylated sites carry a white circular while phosphorylated ones carry a black one.

1 First variant of the model

The first variant of the model is described in Fig. 1.

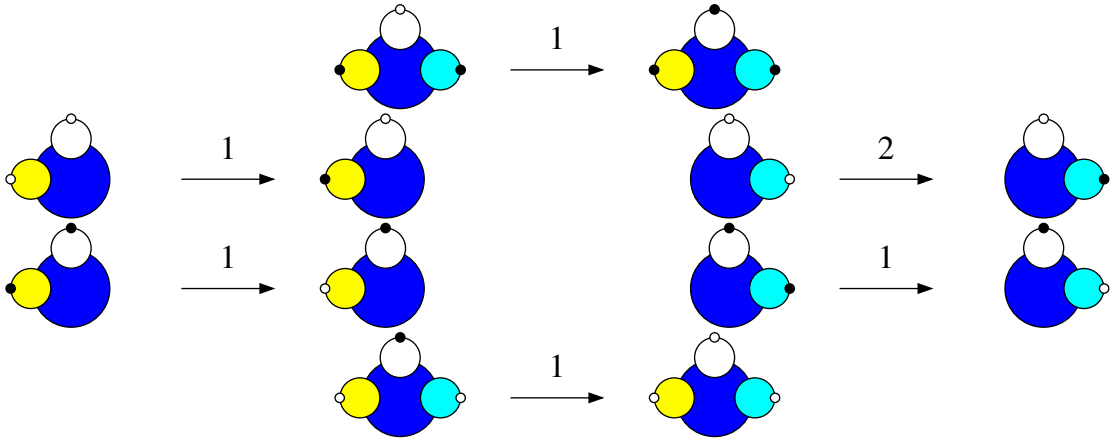

Figure 1: First case study.

It is worth noticing that when the site on the top is phosphorylated, the site on the left and the site on the right exhibit the same behavior in the sense that they share the same phosphorylation rate. We say that these sites are symmetric when the site on the top is phosphorylated. We call this a contextual symmetry.

Our goal is to investigate the consequence of contextual symmetries on the behavior of models.

Question 1 (Configuration space) *Enumerate all the configurations the protein can take ?*

We denote by $\mathcal{V}$ the set of the configurations of the protein.

Question 2 (Differential semantics) *Write the system of ordinary differential equations that describes the evolution of the concentration of each potential configuration of the protein.*

This system takes the form:

$$\frac{d\vec{X}(t)}{dt} = \mathbb{F}(\vec{X}(t))$$

where $\vec{X}(t)$ is the function mapping each configuration $x \in \mathcal{V}$ of the protein to its concentration at time t and $\mathbb{F}$ is a function from $\mathbb{R}^{\mathcal{V}}$ into itself.

We propose to ignore the distinction between both following configurations of the protein:

which comes down to replace the variables standing for the concentration of these configurations with a single one standing for the sum of their values.

Question 3 (Abstraction) *Introduce a set of abstract observables $\mathcal{V}^\sharp$ and a linear function ϕ from the set $\mathbb{R}^{\mathcal{V}}$ into the set $\mathbb{R}^{\mathcal{V}^\sharp}$ to model this change of variables.*

We say that ϕ induces a forward bisimulation is there exists a function $\mathbb{F}^\sharp$ from the set $\mathbb{R}^{\mathcal{V}^\sharp}$ into itself such that the property $\phi \circ \mathbb{F} = \mathbb{F}^\sharp \circ \phi$ is satisfied.

Question 4 (Forward bisimulation) *Does the function ϕ induce a forward bisimulation ?*
If so, express the corresponding function $\mathbb{F}^\sharp$.

We now investigate about the potential relationships among the concentration of both following configurations:

We say that a pair of configurations induces a backward bisimulation if and only, the concentrations of these configurations remain equal for every solution of the differential semantics that starts in a state when the concentration of these configurations are equal.

Question 5 (Backward bisimulation) *Does this pair of configurations induce a backward bisimulation?*

2 A second variant of the model

We propose to relax the constraints on the phosphorylation of the site on the top. We obtain the second variant of the model which is described in Fig. 2.

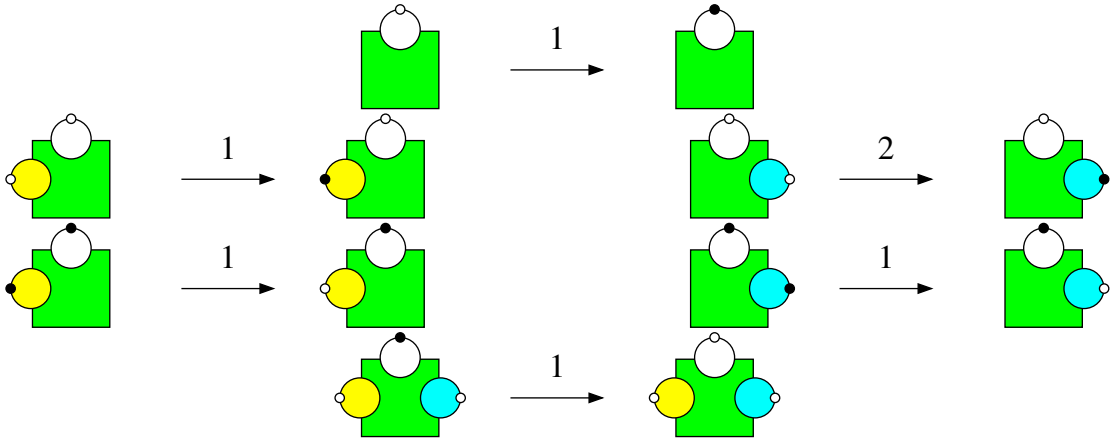

Figure 2: Second variant of the model.

Question 6 *Repeat questions 2, 4, and 5 to the variant of the model that is described in Fig. 2 with the two following configurations of interest:*

3 A third variant of the model

Now, we propose instead to relax the constraints on the dephosphorylation of the site on the top. This third variant is given in Fig. 3.

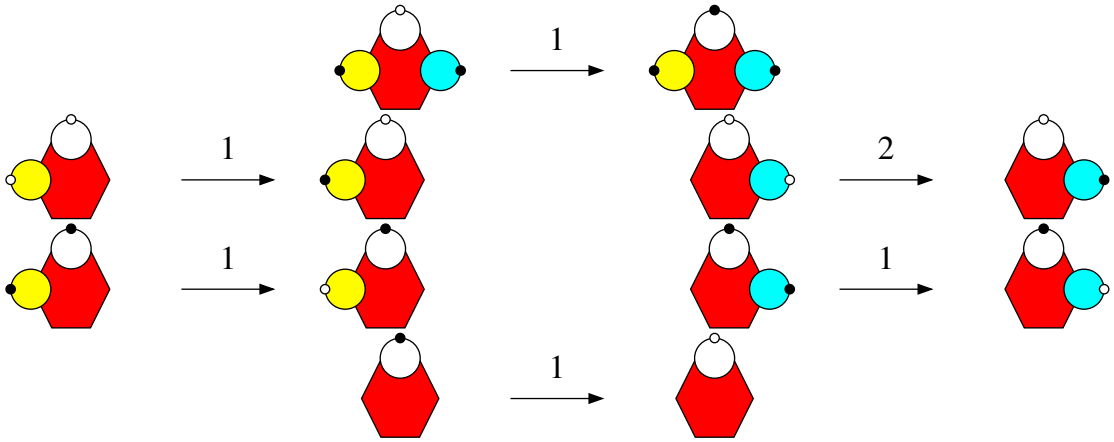

Figure 3: Third case study.

Question 7 *Repeat questions 2, 4, and 5 to the variant of the model that is described in Fig. 3 with the two following configurations of interest:*

4 Wrapping-up

Question 8 *Propose some sufficient conditions over the rules of a model to ensure that some contextual symmetries induce a forward bisimulation?*

Question 9 *Propose some sufficient conditions over the rules of a model to ensure that some contextual symmetries induce a backward bisimulation?*