An Algebraic Approach for Inferring and Using Symmetries in Rule-based Models

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Abstract

Symmetries arise naturally in rule-based models, and under various forms. Besides automorphisms between site graphs, which are usually built within the semantics, symmetries can take the form of pairs of sites having the same capabilities of interactions, of some protein variants behaving exactly the same way, or of some linear, planar, or 3D molecular complexes which could be seen modulo permutations of their axis and/or mirror-image symmetries.

In this paper, we propose a unifying handling of symmetries in Kappa. We follow an algebraic approach, that is based on the single pushout semantics of Kappa. We model classes of symmetries as finite groups of transformations between site graphs, which are compatible with the notion of embedding (that is to say that it is always possible to restrict a symmetry that is applied with the image of an embedding to the domain of this embedding) and we provide some assumptions that ensure that symmetries are compatible with pushouts. Then, we characterise when a set of rules is symmetric with respect to a group of symmetries and, in such a case, we give sufficient conditions so that this group of symmetries induces a forward bisimulation and/or a backward bisimulation over the population semantics.

Keywords: Rule-based models, symmetries, category theory, group actions, bisimulations

1 Introduction

Symmetries play an important role in rule-based modelling. One simple example is the case of symmetric sites, that is to say when two sites in a protein have exactly the same capabilities of interaction. Symmetric sites can be handled with in various ways according to the choice of modelling language. Some languages propose syntactic solutions to describe them explicitly. In BNGL [1] a site can occur several times in the interface of an agent. In the Formal Cell Machinery Language [7] and in React(C) [20], one can use hyper-edges to connect several sites of the same kind

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with a given agent. In Kappa [13], there is no direct means to specify that two sites are symmetric in the core language, but it is possible in higher level front ends such as Meta-Kappa [10]. Models in Meta-Kappa can then be macro-processed into proper Kappa models, by enumerating the concrete instances of symmetric rules. Another approach consists in detecting which sites are symmetric by inspecting the rules, and in lumping [2,16] the states of the model accordingly [6], by the means of back and forth (both forward and backward) bisimulations [3]. As a consequence, symmetric models enjoy nice statistical properties: (i) if for each pair (q, q') of symmetric states, the system has the same probability (we assume for the sake of simplicity that q and q' have no non trivial automorphism) to be in the state q as in the state q' at a given time t, then, it is also the case for any time t' such that $t' \geq t$. (ii) otherwise, if there exists a state that can be reached by each other state in the system, any two symmetric states q and q' will have the same probability to occur at the limit when time goes to the infinity. Moreover, the bisimulations that are induced by symmetries are particular in the sense that they are induced by a partitioning of the variables (of the systems) and can also be used to lump the ODE semantics of Kappa [4].

Symmetries between sites are not the only kind of symmetries: there are many other kinds. For instance, we can consider the sites of an agent as a list of ordered loci on a ring, seen modulo circular permutations. Another example is the case of rigid structures. In such structures, the sites of agents should not be permuted independently: we should only consider as symmetries the transformations in which the sites of each pair of agents that have the same type and that are in the same connected component are reordered by the same permutation. This former kind of symmetry is especially useful in the case of macro-molecules, self-assembly models, and diffusion models. For instance, in the population migration model that is described in [19], ants are moving on a landscape that is encoded as a grid of agents linked by some specified sites named 'north', 'west', 'south', and 'east'. These sites encode the orientation of the landscape: a rotation of the landscape can be modelled by applying the same circular permutation to the four direction sites of all the agents of the grid. To the best of our knowledge, there is no tool to describe such symmetries in any rule-based language.

In this paper, we propose an algebraic framework for describing symmetries among site-graphs. This framework is abstract enough so that all the kinds of symmetries that we have mentioned so far can be dealt with in a uniform setting. Indeed, circular permutations and homogeneous symmetries (in which the same permutation is applied with the sites of all the agents of a given connected component) can easily be defined as subgroups of another (simpler) group of symmetries. Then, we show that our notion of symmetry is compatible with the single pushout construction, which we use as a foundation of the operational semantics of Kappa [8]. We give sufficient conditions for a model to be symmetric with respect to a given group of symmetries, and give extra-assumptions so that these symmetries induce forward bisimulations or even back and forth bisimulations over the Markov chain that is induced by this model.