Exclusion of Symmetries in Search – A Spin-off from Bioinformatics Research

Rolf Backofen

Ludwig-Maximilians-Universität München, Institut für Informatik,
Oettingenstr. 67, D-80538 München (Germany),
Email: backofen@informatik.uni-muenchen.de

Exclusion of symmetry is a long-standing problem in automated deduction as well as in constraint-based search. Several approaches have been proposed, which usually try to restrict the problem in a way that only one solution of the equivalence class (with respect to the symmetries) is found. To our knowledge, in all previously proposed approaches, this element is fixed in advance and does not depend on the search strategy. This has the drawback that the search strategy might interfere with the symmetry exclusion.

We considered the problem of lattice protein folding (a mathematical simplification of the real protein folding problem, albeit still NP-hard), where we were faced with a different situation. Here, the symmetries are well-known (geometric symmetries: translations, rotations and reflections), but it was not known how to exclude these symmetries efficiently. The standard approaches could not be applied since they restricted the search strategy.

Therefore, we introduced a new method for dynamically excluding symmetries in during search. The method is not restricted to a specific problem but can be applied to arbitrary symmetries (where our emphasis is not to detect automatically symmetries but to excluded known symmetries). Our method is based on the notion of symmetric constraints, which are used in our modification of a general constraint based search algorithm. The method does not influence the search strategy. Furthermore, it can be used with either the full set of symmetries, or with an subset of all symmetries.

We will show how to apply the method in the special case of geometric symmetries (rotations and reflections) and permutation symmetries. Furthermore, we give results from practical applications, and compare our system with systems proposed in the literature.