Mapping Molecular Geometry Problems into Pseudo-Boolean Constraints

Priscila M. V. Lima¹, Glaucia C. Pereira², M. Mariela M. Morveli Espinoza², Felipe M. G. França² and Carlile C. Lavor³

¹NCE/Instituto de Matemática, Universidade Federal do Rio de Janeiro - UFRJ, Brazil 
priscila@nce.ufrj.br (contacting author)

²Programa de Engenharia de Sistemas e Computação - COPPE, 
Universidade Federal do Rio de Janeiro - UFRJ, Brazil  
{gpereira,mme,felipe}@cos.ufrj.br

³Departamento de Matemática Aplicada, IMECC, 
Universidade Estadual de Campinas - UNICAMP, Brazil 
clavor@ime.unicamp.br

Keywords: molecular potential energy functions, constraints processing, higher-order Hopfield networks, Boltzmann machines.

Abstract - Predicting the three-dimensional geometry of a molecule is a key issue in, among other important research goals, the discovery of new drugs. This work introduces a novel way to synthesize the potential energy function of a target molecule from which arbitrary partial geometrical information is given. Assuming that the global minimization of the resulting potential energy function provides the three-dimensional structure of the target molecule, a set of pseudo-Boolean constraints is considered here as a way to specify this three-dimensional structure via the inclusion of (i) known information, such as covalent bonding and Van Der Waals iterations, and (ii) observed information, e.g., NMR data, about the molecule. This declarative way of defining the molecular potential energy function proves to be interesting since it becomes possible to deal with diverse, incomplete and/or sparse knowledge about the target molecule. Global optimization of the potential energy function, i.e., the three-dimensional structure of the molecule under investigation, is carried out here by means of higher-order Hopfield networks of stochastic neurons. In previous work, graph coloring and TSP combinatorial problems have been successfully tackled in an analogous way with the help of the SATyrus system, which greatly facilitates the writing of constraints. In the present work, it is shown that any particular molecular potential energy function can be synthesized from a set of constraints expressing the difference between known and observed atomic distances and torsion angles. The precision of the resulting energy function, which can be decided a priori, is dictated by the number of bits representing such distances and angle values.

¹Supported by CNPq and CAPES (Brazil).
References