

Evolutionary Algorithms for Biological Science

MSU Genetic Algorithms Research and Applications Group the GARAGe (<http://garage.cse.msu.edu>)

MSU's Genetic Algorithms Research and Applications Group ("GARAGe") performs research in evolutionary computation, and has established collaborations with a variety of researchers from the life sciences. The group, co-directed by Bill Punch and Erik Goodman, is jointly administered in Computer Science and the Case Center for Computer-Aided Engineering and Manufacturing in the College of Engineering. We have worked on a number of joint projects involving the use of genetic algorithms, genetic programming or other evolutionary computational techniques as applied to biological problems. We can divide these applications into two general categories:

- Data mining, the discovery of regularities in large volumes of data for the subsequent identification of new biological knowledge.
- Conformational exploration, searching biological and other constrained structures for optimal configurations.

Data Mining

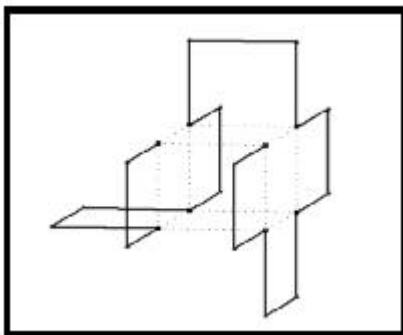
Evolutionary computation methods have been widely applied to discovering rules or regularities in noise-laden biological data, both separately and in conjunction with other techniques including neural nets and/or fuzzy logic. Projects we have collaborated on include:

- Ongoing collaboration with Dr. Leslie Kuhn's laboratory (in Biochemistry) for classification of water molecules' role in docking
- Classification of soil microbial samples as to their environment (rhizosphere, non-rhizosphere and other environments), based on Biolog plate test results (with the Center for Microbial Ecology)
- Feature extraction and feature selection in thyroid deficiency data using masking genetic algorithms.
- Improving management of prostate cancer patients through better prediction of outcomes (with Henry Ford Health Systems, Detroit)

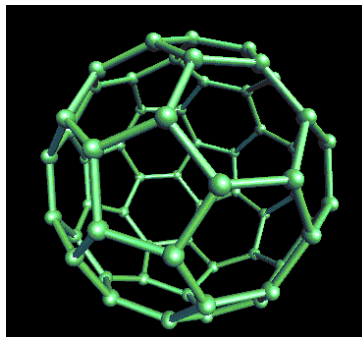
Conformational Search

A number of researchers have used Evolutionary Computational techniques to search for optimal configurations in areas such as protein conformation, molecular configuration and design applications. Collaborations include:

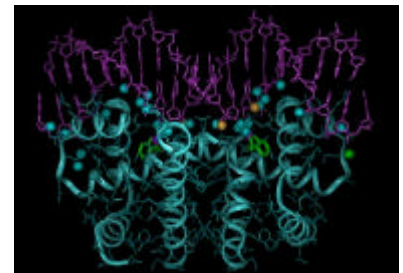
- Search for tertiary structure of a protein from its primary sequence. This has include simpler problems such as "lattice" models and presently more ambitious models (in Leslie Kuhn's lab) for tertiary structures from secondary structures (such as helices and sheets).
- Optimal configurations of molecules for the creation of structures such as buckyballs or ferro-fluids.



Lattice model of a minimal looped cube using simple "amino acids"



Bucky Ball, a "minimal" configuration of 60 carbon atoms



Model of water molecules for trp repressor, including ligand