Modeling Metal Protein Complexes from Experimental Extended X-ray Absorption Fine-Structure using Evolutionary Algorithms

Collin Price

Department of Computer Science

Submitted in partial fulfillment
of the requirements for the degree of

Master of Science

Faculty of Mathematics and Science, Brock University
St. Catharines, Ontario

To Martin.

Abstract

Experimental Extended X-ray Absorption Fine Structure (EXAFS) spectra carry information about the chemical structure of metal protein complexes. However, predicting the structure of such complexes from EXAFS spectra is not a simple task. Currently methods such as Monte Carlo Optimization or simulated annealing are used in structure refinement of EXAFS. These methods have proved somewhat successful in structure refinement but have not been successful in finding the global minima. Evolutionary algorithms have had success in overcoming local minima issues in other domains. We propose the use of three different approaches to better predict the structure of metal protein complexes: genetic algorithm (GA), particle swarm optimization (PSO), and differential evolution (DE).

Preface

The Sirius Cybernetics Corporation is "a bunch of mindless jerks who'll be the first against the wall when the revolution comes." An edition of the Encyclopaedia Galactica that had the good fortune to fall through a time warp from a thousand years in the future defined the Sirius Cybernetics Corporation as "a bunch of mindless jerks who were the first against the wall when the revolution came." Note: We would welcome applications from anyone interested in taking over the post of robotics correspondent.

Acknowledgements

Thank you to the number 42.

R.J.H

Contents

List of Tables

List of Figures

Chapter 1

Introduction

Thirty million generations of philosophers have debated the definition of intelligence. The most popular definition appears in the Sirius Cybernetics Corporation android manuals:

Intelligence is the ability to reconcile totally contradictory situations without going completely bonkers. For example, having a stomach ache and not having a stomach ache at the same time, holding a hole without the doughnut, having good luck and bad luck simultaneously, or seeing a real estate agent waive his fee.

Chapter 2

Conclusion

The answer to this is very simple. It was a joke. It had to be a number, an ordinary, smallish number, and I chose that one. Binary representations, base thirteen, Tibetan monks are all complete nonsense. I sat at my desk, stared into the garden and thought '42 will do'. I typed it out. End of story.

Bibliography

Appendix A

Martin's Programming Lanuage

It is very easy to be blinded to the essential uselessness of them by the sense of achievement you get from getting them to work at all

In other words - and this is the rock solid principle on which the whole of the Corporation's Galaxy-wide success is founded - their fundamental design flaws are completely hidden by their superficial design flaws.