Evolutionary Computation in Bioinformatics: A Review

Sankar K. Pal, *Fellow, IEEE*, Sanghamitra Bandyopadhyay, *Senior Member, IEEE*, and Shubhra Sankar Ray

Abstract—This paper provides an overview of the application of evolutionary algorithms in certain bioinformatics tasks. Different tasks such as gene sequence analysis, gene mapping, deoxyribonucleic acid (DNA) fragment assembly, gene finding, microarray analysis, gene regulatory network analysis, phylogenetic trees, structure prediction and analysis of DNA, ribonucleic acid and protein, and molecular docking with ligand design are, first of all, described along with their basic features. The relevance of using evolutionary algorithms to these problems is then mentioned. These are followed by different approaches, along with their merits, for addressing some of the aforesaid tasks. Finally, some limitations of the current research activity are provided. An extensive bibliography is included.

Index Terms—Biocomputing, data mining, evolutionary algorithm, molecular biology, soft computing.

I. INTRODUCTION

OVER the past few decades, major advances in the field of molecular biology, coupled with advances in genomic technologies, have led to an explosive growth in the biological information generated by the scientific community. This deluge of genomic information has, in turn, led to an absolute requirement for computerized databases to store, organize, and index the data, and for specialized tools to view and analyze the data.

Bioinformatics can be viewed as *the use of computational methods to make biological discoveries* [1]. It is an interdisciplinary field involving biology, computer science, mathematics, and statistics to analyze biological sequence data, genome content and arrangement, and to predict the function and structure of macromolecules. The ultimate goal of the field is to enable the discovery of new biological insights as well as to create a global perspective from which unifying principles in biology can be derived [2]. There are three important subdisciplines within bioinformatics.

1) Development of new algorithms and models to assess different relationships among the members of a large biological data set in a way that allows researchers to access existing information, and to submit new information as they are produced.

2) Analysis and interpretation of various types of data including nucleotide and amino acid sequences, protein domains, and protein structures.

3) Development and implementation of tools that enable efficient access and management of different types of information.

Recently, evolutionary algorithms (EAs), a class of randomized search and optimization techniques guided by the principles of evolution and natural genetics, have been gaining the attention of researchers for solving bioinformatics problems. Genetic algorithms (GAs) [3]–[9] evolutionary strategies (ES), and genetic programming (GP) are the major components of EAs. Of these, GAs are the most widely used. GAs are efficient, adaptive, and robust search processes, producing near optimal solutions, and have a large amount of implicit parallelism. Data analysis tools used earlier in bioinformatics were mainly based on statistical techniques such as regression and estimation. The role of GAs in bioinformatics gained significance with the need to handle large data sets in biology in a robust and computationally efficient manner.

This paper provides a survey of the various evolutionary-algorithm-based techniques that have been developed over the past few years for different bioinformatics tasks. First, we describe the basic concepts of bioinformatics along with their biological basis. Methodology for applying GAs to bioinformatics tasks is also mentioned in Section II. In Section III, various bioinformatics tasks and different evolutionary algorithms based methods available to address the bioinformatics tasks are explained. Finally, conclusions and some future research directions are presented in Section IV.

II. BASIC CONCEPTS IN BIOINFORMATICS AND RELEVANCE OF EVOLUTIONARY ALGORITHMS

First, we introduce the basic biological concepts required to understand the various problems in bioinformatics, and then we describe the relevance of EAs in bioinformatics with particular emphasis on their application of GAs.

A. Basic Units of Cell Biology and Bioinformatics Tasks

Deoxyribonucleic acid (DNA) and proteins are biological macromolecules built as long linear chains of chemical components. A DNA strand consists of a large sequence of nucleotides, or bases. For example there are more than three billion bases in human DNA sequences. DNA plays a fundamental role in different biochemical processes of living organisms in two respects. First, it contains the templates for the synthesis of proteins, which are essential molecules for any organism [10]. The second role in which DNA is essential to life is as a medium to transmit hereditary information (namely, the building plans for

Evolutionary Computation In Bioinformatics

Franz Rothlauf

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Evolutionary Computation in Bioinformatics Gary B. Fogel,David W. Corne,2002-09-27 Bioinformatics has never been as popular as it is today The genomics revolution is generating so much data in such rapid succession that it has become difficult for biologists to decipher In particular there are many problems in biology that are too large to solve with standard methods Researchers in evolutionary computation EC have turned their attention to these problems They understand the power of EC to rapidly search very large and complex spaces and return reasonable solutions While these researchers are increasingly interested in problems from the biological sciences EC and its problem solving capabilities are generally not yet understood or applied in the biology community This book offers a definitive resource to bridge the computer science and biology communities Gary Fogel and David Corne well known representatives of these fields introduce biology and bioinformatics to computer scientists and evolutionary computation to biologists and computer scientists unfamiliar with these techniques The fourteen chapters that follow are written by leading computer scientists and biologists who examine successful applications of evolutionary computation to various problems in the biological sciences Describes applications of EC to bioinformatics in a wide variety of areas including DNA sequencing protein folding gene and protein classification drug targeting drug design data mining of biological databases and biodata visualization Offers industrial and academic researchers in computer science biology and bioinformatics an important resource for applying evolutionary computation Includes a detailed appendix of biological data resources **Evolutionary Computation In Bioinformatics** Evaluationary Computation In Bioinformatics,2003-01-01 Evolutionary Computation for Modeling and Optimization Daniel Ashlock,2005-12-15 Concentrates on developing intuition about evolutionary computation and problem solving skills and tool sets Lots of applications and test problems including a biotechnology chapter **Evolutionary Computation in Gene Regulatory Network Research** Hitoshi Iba,Nasimul Noman,2016-02-23 Introducing a handbook for gene regulatory network research using evolutionary computation with applications for computer scientists computational and system biologists This book is a step by step guideline for research in gene regulatory networks GRN using evolutionary computation EC The book is organized into four parts that deliver materials in a way equally attractive for a reader with training in computation or biology Each of these sections authored by well known researchers and experienced practitioners provides the relevant materials for the interested readers The first part of this book contains an introductory background to the field The second part presents the EC approaches for analysis and reconstruction of GRN from gene expression data The third part of this book covers the contemporary advancements in the automatic construction of gene regulatory and reaction networks and gives direction and guidelines for future research Finally the last part of this book focuses on applications of GRNs with EC in other fields such as design engineering and robotics Provides a reference for current and future research in gene regulatory networks GRN using evolutionary computation EC Covers sub domains of GRN research using EC such as

expression profile analysis reverse engineering GRN evolution applications Contains useful contents for courses in gene regulatory networks systems biology computational biology and synthetic biology Delivers state of the art research in genetic algorithms genetic programming and swarm intelligence Evolutionary Computation in Gene Regulatory Network Research is a reference for researchers and professionals in computer science systems biology and bioinformatics as well as upper undergraduate graduate and postgraduate students Hitoshi Iba is a Professor in the Department of Information and Communication Engineering Graduate School of Information Science and Technology at the University of Tokyo Toyko Japan He is an Associate Editor of the IEEE Transactions on Evolutionary Computation and the journal of Genetic Programming and Evolvable Machines Nasimul Noman is a lecturer in the School of Electrical Engineering and Computer Science at the University of Newcastle NSW Australia From 2002 to 2012 he was a faculty member at the University of Dhaka Bangladesh Noman is an Editor of the BioMed Research International journal His research interests include computational biology synthetic biology and bioinformatics **Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics** Clara Pizzuti,Marylyn D. Ritchie,Mario Giacobini,2010-04-03 This book constitutes the refereed proceedings of the 7th European Conference on Evolutionary Computation Machine Learning and Data Mining in Bioinformatics EvoBIO 2010 held in Istanbul Turkey in April 2010 co located with the Evo 2010 events This 15 revised full papers were carefully reviewed and selected from 40 submissions EvoBIO is the premiere European event for those interested in the interface between evolutionary computation machine learning data mining bioinformatics and computational biology Topics addressed by the papers include biomarker discovery cell simulation and modeling ecological modeling fluxomics gene networks biotechnology metabolomics microarray analysis phylogenetics protein interactions proteomics sequence analysis and alignment and systems biology **Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics** Clara Pizzuti,Marylyn D. Ritchie,Mario Giacobini,2009-04-10 This book constitutes the refereed proceedings of the 7th European Conference on Evolutionary Computation Machine Learning and Data Mining in Bioinformatics EvoBIO 2009 held in T bingen Germany in April 2009 colocated with the Evo 2009 events The 17 revised full papers were carefully reviewed and selected from 44 submissions EvoBio is the premiere European event for experts in computer science meeting with experts in bioinformatics and the biological sciences all interested in the interface between evolutionary computation machine learning data mining bioinformatics and computational biology Topics addressed by the papers include biomarker discovery cell simulation and modeling ecological modeling uxomics gene networks biotechnology metabolomics microarray analysis phylogenetics protein interactions proteomics sequence analysis and alignment as well as systems biology **Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics** Leonardo Vanneschi,William S. Bush,Mario Giacobini,2013-02-26 This book constitutes the refereed proceedings of the 11th European Conference on Evolutionary Computation Machine Learning and Data Mining in Bioinformatics EvoBIO 2013 held in Vienna Austria in April

2013 colocated with the Evo 2013 events EuroGP EvoCOP EvoMUSART and EvoApplications The 10 revised full papers presented together with 9 poster papers were carefully reviewed and selected from numerous submissions The papers cover a wide range of topics in the field of biological data analysis and computational biology They address important problems in biology from the molecular and genomic dimension to the individual and population level often drawing inspiration from biological systems in oder to produce solutions to biological problems Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics Mario Giacobini,Leonardo Vanneschi,William S. Bush,2012-03-28 This book constitutes the refereed proceedings of the 10th European Conference on Evolutionary Computation Machine Learning and Data Mining in Bioinformatics EvoBIO 2012 held in M laga Spain in April 2012 co located with the Evo 2012 events The 15 revised full papers presented together with 8 poster papers were carefully reviewed and selected from numerous submissions Computational Biology is a wide and varied discipline incorporating aspects of statistical analysis data structure and algorithm design machine learning and mathematical modeling toward the processing and improved understanding of biological data Experimentalists now routinely generate new information on such a massive scale that the techniques of computer science are needed to establish any meaningful result As a consequence biologists now face the challenges of algorithmic complexity and tractability and combinatorial explosion when conducting even basic analyses **Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics** Elena Marchiori,2007-04-02 This book constitutes the refereed proceedings of the 5th European Conference on Evolutionary Computation Machine Learning and Data Mining in Bioinformatics EvoBIO 2007 held in Valencia Spain April 2007 Coverage brings together experts in computer science with experts in bioinformatics and the biological sciences It presents contributions on fundamental and theoretical issues along with papers dealing with different applications areas **Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics** Clara Pizzuti,Marylyn D. Ritchie,Mario Giacobini,2011-04-27 This book constitutes the refereed proceedings of the 9th European Conference on Evolutionary Computation Machine Learning and Data Mining in Bioinformatics EvoBIO 2011 held in Torino Italy in April 2011 co located with the Evo 2011 events The 12 revised full papers presented together with 7 poster papers were carefully reviewed and selected from numerous submissions All papers included topics of interest such as biomarker discovery cell simulation and modeling ecological modeling fluxomics gene networks biotechnology metabolomics microarray analysis phylogenetics protein interactions proteomics sequence analysis and alignment and systems biology Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics Elena Marchiori,Jason H. Moore,2008-04-03 Coverage in this proceedings volume includes biomarker discovery cell simulation and modeling ecological modeling gene networks biotechnology microarray analysis protein interactions proteomics sequence analysis and alignment and systems biology **Frontiers of Evolutionary Computation** Anil Menon,2004-02-29 The articles feature a mixture of informal discussion interspersed with formal statements thus providing

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including evolutionary algorithms EAs The main motivation for applying EAs to KDD tasks is that they are robust and adaptive search methods which perform a global search in the space of candidate solutions for instance rules or another form of knowledge representation **Theoretical Aspects of Evolutionary Computing** Leila Kallel,Bart Naudts,Alex Rogers,2001-05-08 This book is the first in the field to provide extensive entry level tutorials to the theory of Evolutionary Computing covering the main approaches to understanding the dynamics of Evolutionary Algorithms It combines this with recent previously unpublished research papers based on the material of the tutorials The outcome is a book which is self contained to a large degree attractive both to graduate students and researchers from other fields who want to get acquainted with the theory of Evolutionary Computing and to active researchers in the field who can use this book as a reference and a source of recent results *Applications of Evolutionary Computing* Günther R. Raidl,Stefano Cagnoni,Jürgen Branke,David W. Corne,Rolf Drechsler,Yaochu Jin,Colin G. Johnson,Penousal Machado,Elena Marchiori,Franz Rothlauf,George D. Smith,Giovanni Squillero,2004-03-09 Evolutionary Computation EC deals with problem solving optimization and machine learning techniques inspired by principles of natural evolution and netics Just from this basic de nition it is clear that one of the main features of theresearchcommunityinvolvedinthestudyofitstheoryandinitsapplications is multidisciplinarity For this reason EC has been able to draw the attention of an ever increasing number of researchers and practitioners in several elds In its 6 year long activity EvoNet the European Network of Excellence in Evolutionary Computing has been the natural reference and incubator for that multifaceted community EvoNet has provided logistic and material support for thosewhowerealreadyinvolvedinECbut inthe rstplace ithashadacritical role in favoring the signi cant growth of the EC community and its interactions with longer established ones The main instrument that has made this possible has been the series of events rst organized in 1998 that have spanned over both theoretical and practical aspects of EC Ever since 1999 the present format in which the EvoWorkshops a collection of workshops on the most application oriented aspects of EC act as satellites of a core event has proven to be very successful and very representative of the multi disciplinarity of EC Up to 2003 the core was represented by EuroGP the main European event dedicated to Genetic Programming EuroGP has been joined as the main event in 2004 by EvoCOP formerly part of EvoWorkshops which has become the European Conference on Evolutionary Computation in Combinatorial Optimization

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