Cellular Evolutionary Algorithms for Solving Protein Folding Problem

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Abstract:
Proteins are vital components of living cells. A number of diseases such as Alzheimer's, Cystic fibrosis and Mad Cow diseases are shown to result from malfunctioning of proteins. Protein folding problem is the process of predicting the optimal 3D molecular structure of a protein, or tertiary structure, which is an indication of its proper function. An enhancement over Cellular Genetic Algorithm (CGA) and Cellular Estimation of Distribution Algorithm (CEDA) was made to minimize the energy of proteins indicating how far it is from its optimal 3D structure. Energy was calculated using the Empirical Conformational Energy Program for Peptides (ECEPP) package. Experiments were performed on the Met-enkephalin protein. The enhanced algorithms reached energy of -10.1 and -10.78 for CGA and CEDGA surpassing the Elitism-based compact Genetic Algorithm and Breeder Genetic Algorithm which didn't reach this energy but reached -7.378, and Breeder Genetic Algorithm (BGA) which reached -3. Results show that the proposed two algorithms "CGA and CEDA" are better than DGA, BGA, and EcGA and a computational alternative to costly laboratory methods and an efficient means for solving organic docking problems.

Keywords: Estimation of distribution algorithm, elitism-based compact genetic algorithm, persistent elitist compact genetic algorithm, Cellular Estimation of Distribution Algorithm, Cellular Genetic Algorithm

Published In:
Egyptian Computer Science journal, ISSN-1110-2586, vol.34 No.1 January 2010.

References:


Abstract:
Proteins are vital components of living cells. A number of diseases such as Alzheimer’s, Cystic fibrosis and Mad Cow diseases are shown to result from malfunctioning of proteins. From the formulation of the protein folding problem, the angles that describe the protein structure in 3D are strongly inter-related and dependent. This is strongly tackled in Estimation of Distribution Algorithms (EDAs) and consequently the enhanced algorithm that model the interactions between chromosomes in terms of a probability distribution vector. Thus, the Elitism-Based Compact Genetic algorithm moves progressively towards the optimal interacting angles 3D structure, by generating individuals conforming with higher fitness probability distribution individuals.

Keywords:
Estimation of distribution algorithm, elitism-based compact genetic algorithm, persistent elitist compact genetic algorithm, non-persistent elitist compact genetic algorithm

Published In:
Journal of Computer Science 4 (7): 527-531, 2008, ISSN 1549-3636

References:


Author:

1. **Name:** Yosr Eman Abdelrahman Mohamed

2. **Work experience:**

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<th>Dates</th>
<th>Occupation or position held</th>
<th>Main activities and responsibilities</th>
<th>Name and address of employer</th>
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<tr>
<td>[ Sep. 2009 - Now]</td>
<td>Lecturer Assistant</td>
<td>Teaching architectural subjects such as: Computer Algorithms, Computer Organization, Artificial Intelligence, Assembly Language, Data Structures, Operating Systems, Software Engineering.</td>
<td>Department of Computer Science, Faculty of Computers and Information, Fayoum University, Egypt.</td>
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3. **Postgraduate Education:**

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<tr>
<td>[April. 2008 – April. 2009]</td>
<td>[Master in Bioinformatics &quot; Cellular Meta-heuristics in bioinformatics &quot;]</td>
<td>Primary objective was to try different Cellular Algorithms like &quot;Cellular Genetic Algorithm and Cellular Estimation of Distribution” that could be used in solving different types of problems like Protein Folding Problem and DNA Fragmentation problem.</td>
<td>Faculty of computers and information, Cairo University, Cairo, Egypt.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Master degree in bioinformatics, Excellent grade. Title of the thesis: &quot;Cellular Meta-heuristics in bioinformatics”</td>
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4. **Publications**

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<td>[Jul. 2008]</td>
<td>Solving Protein Folding Problem using Elitism-Based Compact Genetic Algorithm</td>
<td></td>
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