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Improved Biogeography-Based Optimization Approach to Secondary Protein Prediction

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***Abstract*--In recent years, many bio-inspired computation algorithms have been proposed to solve constraint problems. Biogeography-Based Optimization (BBO) is one of these newly proposed optimization algorithms. As a new way to solve complicated optimization problems, BBO has a quick convergence. In this paper, we proposed an improved BBO for solving protein structure prediction problems. Comparative experiments with standard BBO and differential evolution algorithm (DE) are also conducted, and the results demonstrate this improved BBO approach performs better in solving these complicated protein prediction problems.**

***Index*--Biogeography-Based Optimization, migration method, Protein Prediction.**

I. Introduction

PROTEIN puts crucial role in biological processes, and thus it has great value to be researched further. There are two main aspects influence the nature of proteins, one is the sequences of amino acids, and the other is the proteins' folding structures [1]. With the breakthrough of DNA project, now scientists can easily obtain the sequence information of proteins. However, compared to the sharp increase in the amount of data of the proteins' sequences, the process of obtaining its structure information through experiments is time consuming. Thus, people have to explore other methods to research the structure of protein, and the technology of protein folding structure prediction is emerged. In the 1950s, Anfinsen proposed that the folding structure of a certain protein is determined entirely by its sequence [2]. This theory provides us with the feasibility of obtaining the protein structure information from its sequence information [3]. However, due to the complex and nonlinear features of this prediction's mathematical model, to predict the structure by this method has been a puzzling problem in computational biology for a long time [4].

In the last several decades, people proposed various evolutionary based optimizations to solve optimization problems with linear or nonlinear constraints in science researching and engineering projects [5]. For example, genetic algorithms (GAs) [6]-[8], particle swarm optimization (PSO) [9]–[10] and differential evolution algorithm (DE) [11]. As a kind of computational tools, these optimization algorithms have powerful efficient to solve complex global optimization problems, including problems like protein structure prediction problems.

Biogeography-based optimization (BBO) [12] is a new bio-inspired computation algorithm aiming to solve global optimization problems. This new algorithm is proposed based on the findings related to biogeography. It uses habitats and its species to represent a group of possible solutions. It optimizes problems by modifying the habitat features according to its immigration rate and emigration rate. This algorithm allows different habitats sharing information with each other in the global range. Compared to genetic algorithm and particle swarm optimization, BBO has the advantage that it requires less parameter [13], is easier to control and converges quickly. It has been applied to solve real problems including optimal power flow (OPF), sensor selection and satellite image classification, etc.

In this paper, we introduce the AB Off-Lattice model in two dimensions [14] in Section II, and the standard BBO algorithm in Section III. Then in Section IV, we optimize the BBO optimization by improving its migration process. We changed its migration method and named this improved BBO as I-BBO. In Section V, comparative experimental results with standard BBO and DE algorithm by using the same mathematical model are given. Our concluding remarks are given in Section VI.

II. Mathematical Model for Protein Structure Prediction

Natural protein forms a thermodynamic system with its environment, and always be in a certain stable structure, which situates the system at the lowest energy level [15]. Based on this thermodynamic theory, some models are proposed to solve the protein structure prediction problem by computing the protein's energy value. AB Off-Lattice Model, which is proposed by Frank H. Stillinger in 1993, is such a widely accepted mathematical model. This model classifies the amino acids into hydrophobicity and hydrophilic types. In this paper, we will apply this model to search for the lowest energy value (the best solution) and obtain the structure information of objective protein sequence.

This model classifies 20 different amino acids into two

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basic sorts based on their hydrophobicity or hydrophilic, and are expressed by A and B respectively. In this model, the angle between two amino acids can get changed in the range from $-\pi$ to π. Generally, this model requires three basic rules:

--First, the bond lengths between two neighboring amino acids are the same.

--Second, each amino acid is simplified as a sphere in specific dimension.

--Third, the bond angle θ_i between two contiguous amino acids is defined as

$$-\pi \le \theta_i < \pi \tag{1}$$

Based on these rules, the structure of a protein, which is composed of N dimension amino acids, is determined by $n-2$ variables: $\theta_2, \theta_3 \ldots \theta_{n-1}$.

The energy value function of AB Off-Lattice Model is defined as

$$\Phi = \sum_{i=2}^{n-1} V_1(\theta_i) + \sum_{i=1}^{n-2} \sum_{j=i+2}^{n} V_2(r_{ij}, \xi_i, \xi_j) \tag{2}$$

where V_1 represents the energy of the backbone, it is only determined by the sequence of amino acids. V_2 represents the energy between the amino acids which are not contiguous and is determined by not only the sequence of amino acids, but also the distance between each couple of amino acids. V_1 and V_2 are given by the following equations

$$V_1(\theta_i) = \frac{1}{4}(1 - \cos\theta_i) \tag{3}$$

$$V_2(r_{ij}, \xi_i, \xi_j) = 4\left(r_{ij}^{-12} - C(\xi_i, \xi_j) r_{ij}^{-6}\right) \tag{4}$$

The notation ξ_i represents the category of the amino acid. When the amino acid is hydrophobic, $\xi_i = 1$, on the contrary, when the amino acid is hydrophilic, $\xi_i = -1$. The notation r_{ij} is the Euclidean distance between amino acid i and amino acid j, which can be computed by Eq. (5)

$$r_{ij} = \left\{ \left[1 + \sum_{k=i+1}^{j-1} \cos\left[\sum_{l=i+1}^{k} \theta_l \right] \right]^2 + \left[\sum_{k=i+1}^{j-1} \sin\left[\sum_{l=i+1}^{k} \theta_l \right] \right]^2 \right\}^{1/2} \tag{5}$$

The coefficient $C(\xi_i, \xi_j)$ is computed by

$$C(\xi_i, \xi_j) = \frac{1}{8}(1 + \xi_i + \xi_j + 5\xi_i\xi_j) \tag{6}$$

When the amino acids pair is AA, $C(\xi_i, \xi_j) = 1$, when it is BB, $C(\xi_i, \xi_j) = 0.5$, and when it is AB, $C(\xi_i, \xi_j) = -0.5$.

Applying this model for protein structure prediction in two dimensions, what we need to do is to find a group of applicable value θ_i $(i = 2,\ldots,n-1)$, reaching the minimum of the energy function. And then, we obtain the structure information from the bond angles θ_i. Then the problem is simplified to search for the constraint minimum of objective function

$$\min_{\theta_i \in (-\pi, \pi)} \Phi(\theta_2, \ldots, \theta_{n-1}) \tag{7}$$

III. BIOGEOGRAPHY-BASED OPTIMIZATION

Biogeography-based optimization has been developed based on the research of biogeography. Its mathematical model describes the process of the generation, extinction and migration of species.

The potential solutions of a certain global optimization problem are considered to be a group of habitats. Each habitat has its amount of species, and different habitats usually have different amount of species. It uses the habitat suitability index (HSI), which is depended on many features of a habitat, to measure the quality of this habitat, that is, the quality of the solution. A higher HSI express a better solution of the problem. HSI is related to the immigration rate and emigration rate of the habitat. Habitats with high HSI are suitable for survival, the number of species tend to be the maximum of environment carrying capacity. Thus, these habitats have low immigration rates and high emigration rates. In opposite, habitats with low HSI have high immigration rates and low emigration rates. They have more opportunities to accept a lot of new features from other habitats, especially from the habitats with high HSI, to evolve them. This mechanism makes BBO can realize global information sharing, and has a strong ability to deal with the problem in parallel process. In addition, BBO model includes the mutation operate to avoid the local optimum and resist premature convergence, includes the elitism to avoid the algorithm degeneration phenomena.

A. Migration

In this paper, we apply the linear migration model in standard BBO to calculate immigration rate λ_s and emigration rate μ_s, they are evaluated by Eq. (8) and (9).

$$\lambda_s = I\left(1 - \frac{S}{S_{\max}}\right) \tag{8}$$

$$\mu_s = \frac{ES}{S_{\max}} \tag{9}$$

where I denotes the maximum of immigration rate, E is the maximum of emigration rate, S_{max} is the maximum species count among all the habitats, and S is the species count in present habitat. Each habitat has its own λ_s and μ_s according to its species count. In the process of migration based on the probability of immigration and emigration, a feature H_i from a habitat is replaced by another feature H_j from a different habitat. It can be expressed as

$$H_i \leftarrow H_j \tag{10}$$

B. Mutation

Define P_s to be the probability of species count. The probability of a certain habitat owning S species count is P_s. It satisfies the following formula.

$$\dot{P}_s = \begin{cases} (\lambda_s + \mu_s)P_s + \mu_{s+1}P_{s+1} & S = 0 \\ (\lambda_s + \mu_s)P_s + \lambda_{s-1}P_{s-1} + \mu_{s+1}P_{s+1} & 1 \le S \le S_{\max} - 1 \\ (\lambda_s + \mu_s)P_s + \lambda_{s-1}P_{s-1} & S = S_{\max} \end{cases} \tag{11}$$

The mutation rate value is defined as

$$m_i = m_{\max}\left(1 - \frac{P_i}{P_{\max}}\right) \quad (12)$$

where m_{max} is the maximum of mutation rate ranging from 0 to 1. It is usually suitable to be set as 0.005. P_i is the species count probability of habitat i, and P_{max} is the maximum of the species count probability of all the habitats.

C. Elitism

We add elitism to suppress the phenomenon of degeneration in iterations of the algorithm. In each generation, the best solution in present is compared with the best solution in the whole history. If the present solution is better than the history solution, it replaces the latter to be the new best solution in history. In the opposite situation, it will be replaced by the latter. This operation ensures that the best solution in the whole history is always involved in iterations to optimize the solution continually.

D. Improvement on migration of BBO

We propose a new approach to enhance the global searching capacity of BBO. We improved the process of migration, and call this improved model I-BBO.

In real world, one migration process among habitats is not simply related to only two habitats, but determined by all habitats nearby. Because the species amount is limited, a habitat with a high immigration can affect the immigrating process of nearby habitats. This phenomenon can be summarized that the migration process is determined by several habitats in an area. Inspired by this, in I-BBO, instead of simply replace a feature H_i by another feature H_j from a different habitat, we create a new migration method. The original feature in the habitat is H_j, we select N different features $H_{j1}, H_{j2}, \ldots, H_{jn}$ from N different habitats according to their emigration rates. Then we mix H_i and $H_{j1}, H_{j2}, \ldots, H_{jn}$ with coefficient $\alpha, \beta_1, \beta_2, \ldots, \beta_n$. In this paper, we choose N to be three and use the same coefficient β. This migration model is defined as

$$H_i \leftarrow \alpha H_i + \beta\left(H_{j1} + H_{j2} + H_{j3}\right) \quad (13)$$

where α and β are real numbers as weight parameters. Feature H_{j1}, H_{j2} and H_{j3} are all select based on emigration rate and immigration rate equally, thus the same value β for these three features is reasonable. Parameters α and β can be determined by different approaches according to different optimization problems to be suitable. The result of the AB Off-Lattice model using this improved migration method demonstrate I-BBO can often obtain better solutions than standard BBO, and have advantage in the ability of escaping from the local optimum.

IV. I-BBO Algorithm Approach to Protein Structure Prediction Problem

A. I-BBO Used for Protein Structure Prediction Problem

The algorithm has been encoded in Matlab language and implemented on a PC with 4 GB of RAM using Windows 7. The parameters in the prediction experiment were set to be the following values: $I = 1$, $E = 1$, $m_{max} = 0.005$, Maximum species count = 30, Habitat counts = 30, Maximum iteration cycles = 1000, elitism number = 2, $\alpha = 1$, $\beta = 1$.

To avoid the potential solution being out of boundaries, we added the below step in Table II after each migration.

B. Standard BBO and DE Tested for Comparing

In standard BBO, parameters were set the same as that in I-BBO. We also compute the AB Off-Lattice model using the DE algorithm. We chose DE because it is a typical mature algorithm with few parameters to be selected and it performs well in many optimization problems. Besides, scholars have made researches on blending DE and BBO. They finally obtained better optimization results compared with single BBO approach [16].

In DE, Maximum of iteration is set to be 1000, the same as that in BBO and I-BBO. In each generation, DE algorithm firstly finds the best solution S_{best} in present, and then it selects four different individuals S_i (i = 1, 2, 3, 4)randomly. Then generate the offspring S_{new} by Eq. (14).

$$S_{new} = S_{best} + F_1\left(S_1 - S_2\right) + F_2\left(S_3 - S_4\right) \quad (14)$$

In this work, we set F_1 and F_2 to be 0.3.

V. Experimental results

We test the prediction model using standard BBO, I-BBO and DE algorithm. The parameters adopted are the same as those descried in the previous section. For each test, we run the optimization independently for 25 times to get average results. Each run is computed for1000 iterations.

Table III shows the performance comparison on the same sequences for BBO, I-BBO and DE algorithms. The results show that the precisions of all these three algorithms decline when the dimension increases. I-BBO performs much better than standard BBO in most sequences, it can get a lower energy (means a better solution) and from the averages of 25 independent tests we can know that it is usually more stabilized. When comparing with DE algorithm based on the best result and the mean result, we can get the findings that DE can usually get a lower energy than I-BBO in short sequences in 3 or 4 dimensions, except for sequences ABBA, BABB, and BBBB. In these three short sequences, I-BBO gets lower energy in the mean results. In the long sequences, however, I-BBO can usually obtain better results than both DE and standard BBO. The characters overstriking in Table III are the results that I-BBO performs at least not worse than both standard BBO and DE algorithm.

TABLE I
IMPROVED BIOGEOGRAPHY-BASED OPTIMIZATION

Initialize the parameters of I-BBO, including maximum of species count S max, maximum of immigration rate I and emigration rate E, maximum of mutation Mu max, weighting parameters α,β.
Initialize a group of habitats, which corresponds a group of potential solutions.
While the halting criterion is not satisfied
Do
  Compute the immigration rate, emigration rate and species probability of each habitat.
  For each habitat (A possible solution)
    For each habitat feature (Angles between every two amino acids)
      Determine whether to modify habitat feature Hi based on immigration rate.
      If H_i is selected
        Select habitat feature H_{j1}, H_{j2} and H_{j3} from different habitats for modification of H I based on emigration rate.
        $H_i \leftarrow \alpha H_i + \beta(H_{j1} + H_{j2} + H_{j3})$
      End If
      Determine whether to mutate Hi based on mutation rate
      If Hi is selected
        Replace Hi based on mutation rules.
      End If
    Next For
  Next For
  Compute HIS values for every habitat H.
End While

TABLE II
ALGORITHM TO KEEP THE HABITATS IN BOUNDARY

For each habitat
  For each habitat feature H_i
    While H_i is below lower boundary
      $H_i=H_i+2\pi$
    End While
    While H_i is above upper boundary
      $H_i=H_i-2\pi$
    End While
  Next For
Next For

Figs. 1- 4 show the performance of these three algorithms in four different sequences visually.

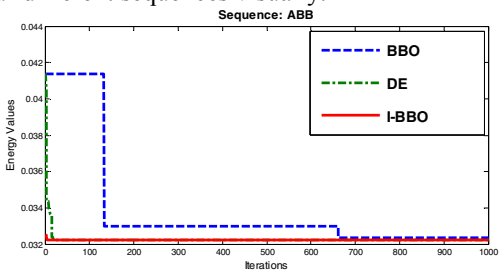

Fig. 1. The sequence of the protein is ABB

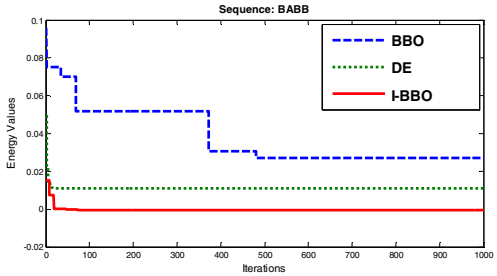

Fig. 2. The sequence of the protein is BABB.

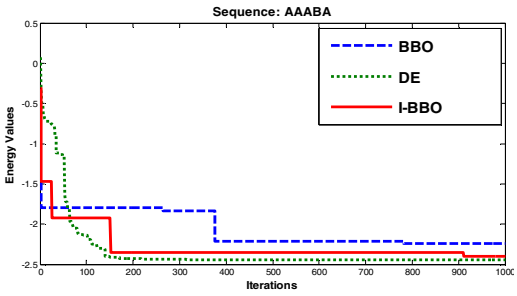

Fig. 3. The sequence of the protein is AAABA.

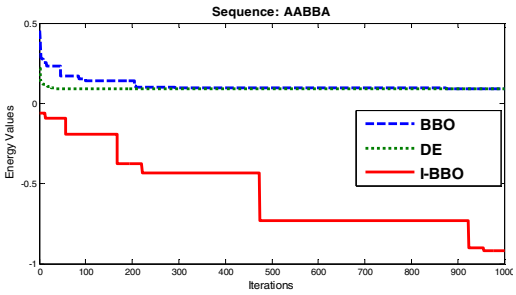

Fig. 4. The sequence of the protein is AABBA.

From Figs 1-4, it is obvious that our proposed I-BBO can converge much quicker than the basic DE algorithm.

VI. CONCLUSIONS

In this paper, we apply an improved biogeography-based optimization algorithm to solve the problem of protein structure prediction. A new migration method is adopted to improve the basic BBO algorithm, and the experimental results of protein structure prediction based on 2D AB Off-Lattice model show that:

1) BBO is a bio-inspired computation algorithm with potential in solving constrained linear and nonlinear problems.

2) I-BBO with an improved migration strategy performs more effectively than basic BBO in precision and the ability of escaping local optimum.

3) I-BBO performs a little worse than DE algorithm in the ability of searching the best solutions, but seems to be more effective to avoid the local optimum solutions. Thus it still has high probability to obtain good solutions. When solving relatively long sequences with more dimensions, I-BBO performs much better.

4) As new global optimization algorithms, either standard BBO or I-BBO that is proposed in this paper still has potential to be better optimized to adapt to more real problems.

Protein structure prediction problem is a challenging direction. Our future work will focus on the optimization of this newly proposed BBO algorithm by referring to the advanced intelligent algorithms, such as PSO, GA, and so on [17]-[18]. We will also conduct further research on different prediction models to get better structure prediction results and make it more conform to the real situation of protein.

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TABLE III
PROTEIN STRUCTURE PREDICTION RESULT OBTAINED BY BBO, I-BBO AND DE ALGORITHMS

Sequence	I-BBO			BBO			DE		
	Best	Mean	Worst	Best	Mean	Worst	Best	Mean	Worst
AAA	-0.658205	**-0.658204**	**-0.658201**	-0.658205	-0.654918	-0.637089	-0.658205	-0.658205	-0.658205
AAB	**0.0322266**	**0.0322266**	0.0322267	0.0322266	0.0323676	0.0332627	0.0322266	0.0322266	0.0322266
ABA	**-0.658205**	**-0.658204**	-0.658204	-0.658205	-0.654865	-0.629185	-0.658205	-0.658205	-0.658205
ABB	**0.0322266**	**0.0322266**	**0.0322266**	0.0322266	0.0322739	0.0326634	0.0322266	0.0322266	0.0322266
BAB	-0.030273	**-0.030273**	**-0.030273**	-0.030273	-0.030201	-0.029759	-0.030273	-0.030273	-0.030273
BBB	-0.030273	**-0.030273**	**-0.030273**	-0.030273	-0.030116	-0.028454	-0.030273	-0.030273	-0.030273
AAAA	-1.67623	**-1.67407**	**-1.66703**	-1.67626	-1.59369	-1.43142	-1.67633	-1.67633	-1.67633
AAAB	**-0.585264**	**-0.584861**	**-0.582416**	-0.585203	-0.574684	-0.517678	-0.585273	-0.585273	-0.585273
AABA	-1.45095	**-1.44594**	**-1.42529**	-1.45069	-1.19036	-0.536077	-1.45098	-1.45098	-1.45098
AABB	**0.0672133**	0.0672961	**0.0674981**	0.0672191	0.0672191	0.0685846	0.0672041	0.0672041	0.0672041
ABAB	-0.649344	**-0.64897**	**-0.647997**	-0.64936	-0.64133	-0.581846	-0.649375	-0.649375	-0.649375
ABBA	**-0.359883**	**-0.340772**	**-0.027891**	-0.034693	0.0415988	0.0608892	-0.036171	0.0437505	0.0589737
ABBB	**0.0047067**	**0.0047428**	**0.0048845**	0.0047121	0.0049233	0.0055111	0.0047041	0.0047041	0.0047041
BAAB	**0.0617174**	**0.0617848**	**0.0620139**	0.0617181	0.0620713	0.0638108	0.0617172	0.0617172	0.0617172
BABB	-0.0007768	**-0.0007195**	**-0.0004045**	-0.000778	0.0010915	0.0128108	-0.000783	0.0015899	0.011081
BBBB	**-0.139732**	**-0.139375**	**-0.138556**	-0.139183	-0.101974	-0.060141	-0.139738	-0.096923	-0.063283
AAAAA	**-2.83801**	**-2.74761**	**-2.6741**	-2.81753	-2.43693	-1.85307	-2.84828	-2.77785	-2.60608
AAAAB	-1.58695	**-1.56029**	**-1.43495**	-1.58883	-1.43181	-1.15798	-1.58944	-1.53557	-1.4772
AAABA	**-2.43388**	**-2.32423**	**-2.10196**	-2.41291	-1.98232	-0.75505	-2.44493	-2.40095	-2.33499
AAABB	-0.546235	**-0.542692**	**-0.534961**	-0.54627	-0.541966	-0.532244	-0.546878	-0.546878	-0.546878
AABAA	**-2.52376**	**-2.43498**	**-2.27053**	-2.49042	-1.917	-0.569261	-2.5317	-2.53169	-2.53168
AABAB	-1.33959	**-1.32056**	**-1.28554**	-1.34726	-1.11748	-0.425707	-1.34774	-1.34627	-1.34306
AABBA	**-0.925277**	**-0.82497**	**-0.627264**	-0.905484	-0.059237	0.0949816	-0.926621	-0.151725	0.0929749
AABBB	0.0401862	0.0411605	0.0433465	0.0401852	0.0406419	0.0416867	0.0401702	0.0401702	0.0401702
ABAAB	**-1.37377**	**-1.34947**	**-1.29935**	-1.37302	-1.13822	-0.370248	-1.37647	-1.37647	-1.37647
ABABA	**-2.2195**	**-2.10812**	**-1.85662**	-2.21507	-1.86425	-1.18745	-2.2202	-2.2202	-2.22019
ABABB	-0.616121	**-0.613087**	**-0.604571**	-0.616718	-0.609813	-0.58719	-0.616795	-0.615122	-0.595882
ABBAB	-0.0036184	**0.0145747**	**0.0275231**	0.0043039	0.0289875	0.0650924	-0.0056451	0.0251689	0.0264528
ABBBA	**-0.395263**	**-0.345089**	**-0.251206**	-0.18532	0.0230795	0.0404773	-0.39804	-0.135991	0.0387054
ABBBB	**-0.0651591**	**-0.0574868**	**-0.0414973**	-0.0650415	-0.0303851	-0.0093792	-0.0659612	-0.0409847	-0.0137165
BAAAB	-0.520613	**-0.516347**	**-0.507642**	-0.520988	-0.512573	-0.487777	-0.521076	-0.521076	-0.521076
BAABB	0.0963302	0.097517	0.103351	0.0962163	0.0966784	0.0981387	0.0962067	0.0962067	0.0962067
BABAB	-0.647495	**-0.644109**	**-0.633758**	-0.647823	-0.642811	-0.630535	-0.648025	-0.648025	-0.648025
BABBB	**-0.182494**	**-0.157731**	**-0.0976296**	-0.176268	-0.0507278	-0.0265388	-0.182657	-0.0502991	-0.0287933
BBABB	**-0.239185**	**-0.224346**	**-0.193279**	-0.226549	-0.0881531	0.182805	-0.240204	-0.11136	0.0282197
BBBBB	**-0.451625**	**-0.434865**	**-0.395186**	-0.450891	-0.332608	-0.0958679	-0.452663	-0.340031	-0.0967803

Protein structure prediction result obtained by standard BBO, I-BBO and DE algorithms over 25 independent runs with 1000 iterations in every run. The table shows the best, mean and worst values. The sequences of protein are expressed by A and B according to their hydrophobicity and hydrophilic.