学位論文の要旨

学位論文題目：The Research of Evolutionary Computation in Medical and Engineering Applications

（進化計算の医学・工学への応用に関する研究）

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Optimization problems widely exist now in human living, scientific research, and industry. With their development, the complexity of optimization problems exponentially increases. Meanwhile, traditional exact methods are unable to provide satisfactory solutions due to their non-linearity and non-convexity. Then, evolutionary computation inspired by natural biology is proposed to handle the problems. It includes different algorithms such as genetic algorithm (GA), particle swarm optimization (PSO), gravitational search algorithm (GSA), and differential evolution (DE), and has been successfully used to solve real-world applications (e.g., medical and engineering applications). However, these applications are usually non-linearity, non-differentiable, and multi-peaks resulting in evolutionary algorithms still suffering from the issues of low performance, local optima, and premature convergence. Researchers balance between the exploitation and exploration of algorithms to improve their performance via new operator factors, self-adaptive parameters, and new learning schemes. In this thesis, I propose evolutionary algorithms to solve real-world problems (medical and engineering applications). I proposed a many-objective algorithm to solve protein structure prediction problem. I also proposed an improved genetic learning particle swarm optimizer to optimize wind farm layout optimization problems. These are introduced as follows.

(1) Protein structure prediction (PSP) problems are a major biocomputing challenge, owing to its scientific intrinsic that assists researchers to understand the relationship between amino acid sequences and protein structures, and to study the function of proteins. Although computational resources increased substantially over the last decade, a complete solution to PSP problems by computational methods has not yet been obtained. Using only one energy function is insufficient to characterize proteins because of their complexity. Diverse protein energy functions and evolutionary computation algorithms have been extensively studied to assist in the prediction of protein structures in different ways. Such algorithms are able to provide a better protein with less computational resources requirement than deep learning methods. For the first time, this study proposes a many-objective protein structure prediction (MaOPSP) problem with four types of objectives to alleviate the impact of imprecise energy

functions for predicting protein structures. A many-objective evolutionary algorithm (MaOEA) is utilized to solve MaOPSP. The proposed method is compared with existing methods by examining thirty-four proteins. An analysis of the objectives demonstrates that our generated conformations are more reasonable than those generated by single/multi-objective optimization methods. Experimental results indicate that solving a PSP problem as an MaOPSP problem with four objectives yields better protein structure predictions, in terms of both accuracy and efficiency.

(2) The wind farm layout optimization (WFLO) problem optimizes the location of wind turbines in a wind farm to reduce the wake effect and improve maximum power generation. Traditional mathematical methods cannot provide a satisfactory solution for a wind farm due to the high complexity of the problem. Therefore, mete-heuristic algorithms have been used to optimize it. Genetic algorithms (GA) have been widely used and obtained success in WFLO problems. However, GA still suffers from the issues of insufficient optimization efficiency. In this study, a genetic learning particle swarm optimization with an adaptive strategy, termed AGPSO, is proposed to optimize WFLO problems. The strategy adaptively adjusts the location of the worst turbine to improve the conversion efficiency of a wind farm. Four wind scenarios, including single wind speed with single wind direction, single wind speed with uniform multiple wind directions, single wind speed with nonuniform multiple directions, and multiple wind speeds with multiple wind directions, are utilized to verify the effectiveness of AGPSO and the effect of different wind scenarios for it. Twelve constraints and three different scales are used to further verify the robustness of AGPSO and the effect of wind turbine location on WFLO problems. Extensive experimental results demonstrate that AGPSO performs significantly better than other eight state-of-the-art competitors in terms of conversion efficiency under different wind farms, wind scenarios, and constraints.

The thesis is organized as follows. Chapter 1 describes a many-objective protein structure prediction problem and proposes a many-objective algorithm to solve it. Chapter 2 presents an adaptive replacement strategy-incorporated particle swarm optimizer for WFLO problems.

【学位論文審査結果の要旨】（雷　振宇）

当博士学位論文審査委員会は，標記の博士学位申請論文を詳細に査読した。本博士論文と従来の論文との類似性指標は9%であり，剽窃等の問題がないことを確認した。また論文公聴会を令和5年1月27日(金曜日)に公開で開催し，詳細な質疑応答を行って論文の審査を行った。以下に審査結果の要旨を示す。

本論文では、実世界の問題（医療や工学への応用）を解決するための進化的アルゴリズムを提案する。具体的には、タンパク質構造予測問題に対する多目的アルゴリズムを提案した。また、風力発電所のレイアウト最適化問題を解決するために、改良型遺伝的学習粒子群最適化装置を提案した。

タンパク質構造予測に関して,本研究では不正確なエネルギー関数の影響を緩和するために、4種類の目的関数を持つ多目的タンパク質構造予測(Many-Objective Protein Structure Prediction (MaOPSP)) 問題を提案した。MaOPSP問題を解くために、多目的進化アルゴリズム(Many-Objective Evolutionary Algorihtm (MaOEA))を用いた。提案手法を34種類の既知のタンパク質の構造予測に適用し、既存の予測手法と比較した。目的別解析の結果、我々のアルゴリズムによって予測された立体構造は、単一/多目的最適化手法によって予測されたものよりも実際の構造に対して整合性が高いことが示された。この結果は、PSP問題を4つの目的を持つMaOPSP問題として解く方法が、精度と効率の両面において優れたタンパク質構造予測をもたらすことを示している。

次に、発電所のレイアウト最適化(Wind Farm Layout Optimization (WFLO)) 問題を最適化するために、適応的な戦略を持つ遺伝的学習粒子群最適化（Genetic Learning Particle Swarm Optimization with An Adaptive Strategy (AGPSO)）を提案した。この戦略は、風力発電所の変換効率を向上させるために、最悪のタービンの位置を適応的に調整するものである。風向が単一である単一風速、風向が均一である単一風速、風向が不均一である単一風速、風向が複数である複数風速の4つの風シナリオを利用し、提案したアルゴリズムの有効性と風シナリオの違いの影響を検証した。さらに、12 種類の制約条件と3種類のスケールを用いて、AGPSOの頑健性とWFLO問題における風力発電機の位置の影響を検証した。広範な実験結果により、異なる風力発電所、風力シナリオ、制約条件のもとで、AGPSOが他の8つの最先端競争相手よりも変換効率の面で著しく優れていることが実証された。

当博士論文審査委員会は、研究内容及び研究成果を慎重に吟味した結果，本博士学位申請論文が博士の学位を授与することに十分に値するものと認め，合格と判断した。