Evolutionary optimization /modeling methods and their applications in materials (including oxides) design

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Abstract

Evolutionary computation relates to a family of nature inspired algorithms that draw inspiration from biological systems, attempt to mimic some natural phenomena and use them for systems that are actually far apart from natural biology. They are now ubiquitous in the areas of materials design, modeling and optimization and this series of lectures will attempt to provide a comprehensive overview of these strategies with a special reference to the oxide materials.

Lecture 1

Here the basic background information of the evolutionary algorithms will be provided. The focus will be on the single objective evolutionary algorithms. The discussions will involve the prominent strategies like genetic algorithms, differential evolution, particle swarm optimization, ant colony optimization, artificial immune algorithm etc.

Lecture 2

Here the notion of evolutionary multi-objective optimization and Pareto optimality will be introduced. It will be explained how evolutionary multi-objective algorithms can create intelligent data-driven models from the noisy date and also optimize them. In this context, three of the algorithms from the research group of this lecturer, EvoNN (Evolutionary Neural Net), BioGP (Bi-objective Genetic Programming) and EvoDN2 (Evolutionary Deep Learning), will be introduced and their machine learning and optimization capabilities will be elaborated.

Lecture 3

In recent years, numerous studies have been conducted for the oxide materials using the evolutionary concepts. This lecture will provide an overview of some of the state of the art studies in this area and also elaborate the scope and the

expected directions of future research for studying the oxides using evolutionary algorithms.