Chapter 12

Data-Driven Bi-Objective Genetic Algorithms EvoNN and BioGP and Their Applications in Metallurgical and Materials Domain

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ABSTRACT

Data-driven modeling and optimization are now of utmost importance in computational materials research. This chapter presents the operational details of two recent algorithms EvoNN (Evolutionary Neural net) and BioGP (Bi-objective Genetic Programming) which are particularly suitable for modeling and optimization tasks pertinent to noisy data. In both the approaches a tradeoff between the accuracy and complexity of the candidate models are sought, ultimately leading to some optimum tradeoffs. These novel strategies are tailor-made for constructing models of right complexity, excluding the non-essential inputs. They are constructed to implement the notion of Pareto-optimality using a predator-prey type genetic algorithm, providing the user with a set of optimum models, out of which an appropriate one can be easily picked up by applying some external criteria, if necessary. Several materials related problems have been solved using these algorithms in recent times and a couple of typical examples are briefly presented in this chapter.

INTRODUCTION

This chapter deals with two recent algorithms Evolutionary Neural Net (EvoNN) and Bi-objective Genetic Programming (BioGP) and their applications in metallurgical and materials problems. The EvoNN and BioGP algorithms were developed and proposed by the present author and his collaborators a few years ago (Pettersson et al. 2007; Mondal et al. 2011; Giri et al. 2013a, 2013b). Since then, these algorithms

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have been applied successfully to numerous materials related problems (Bhattacharya et al. 2009; Rajak et al. 2009, 2011; Bansal et al. 2013, Jha et al. 2014). Both the algorithms share certain common features, which in general terms, could be listed as:

- They are suitable for creating data-driven meta-models out of highly non-linear and/or noisy data.
- They use multi-objective genetic algorithm over other paradigms, namely neural network and genetic programming, to generate a set of optimum models; while using a particular model remains the Decision Maker's (DM) prerogative.
- They are geared to work out an optimum tradeoff between the accuracy and complexity of the model and tend to eliminate incorporation of any superfluous noise in the process.

In recent times the present author has written two other book chapters (Chakraborti 2013, Chakraborti 2014) detailing these algorithms beside a number of journal articles involving their applications. Therefore only the basic features of these algorithms will be presented here and the emphasis will be more on their mode of usage. The source codes of both the algorithms are open and coded in Matlab™ and are available free of cost from the author of this chapter for any non-commercial academic usage. The details of their various features from a user's point of view will be presented in this chapter, along with some pertinent applications.

EvoNN AND BioGP IN A NUTSHELL

The essential features of both the algorithms are presented below:

The Essentials of EvoNN

For any given system, EvoNN tends to create an optimum set of neural network-based models that would tend to eliminate any random noise present in the data, prune any superfluous input avoiding any tendencies to either overfit or underfit (Collet 2007). To achieve this, the EvoNN algorithm deals with a population of neural nets with flexible architecture, allows custom made crossover and mutation processes in the lower part of the network, and being a hybrid algorithm, applies a Linear least Square (LLSQ)

Figure 1. The training strategy in EvoNN