Grey and black-box modelling based on neural networks and artificial immune systems applied to solid dissolution by rotating disc method

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GENERAL ASPECTS

Modelling and optimizing chemical engineering processes is difficult, especially when the chemical and physical laws governing the system are complex, difficult to implement or partially known.

In this context, the use of alternative approaches that can eliminate these problems is an aspect that can lead to new advances and new methods easy to use by chemical engineers.

This work presents an algorithm developed for modelling and/or optimization. It is based on Clonal Selection (CS) and Artificial Neural Networks (ANN).

SOLID DISSOLUTION

Dissolution of solid in liquid phase is an important step in many processes, such as chemical engineering, nuclear engineering, mineral processing, agriculture, pharmaceuticals, electrochemical processes, environmental protection, and so on…

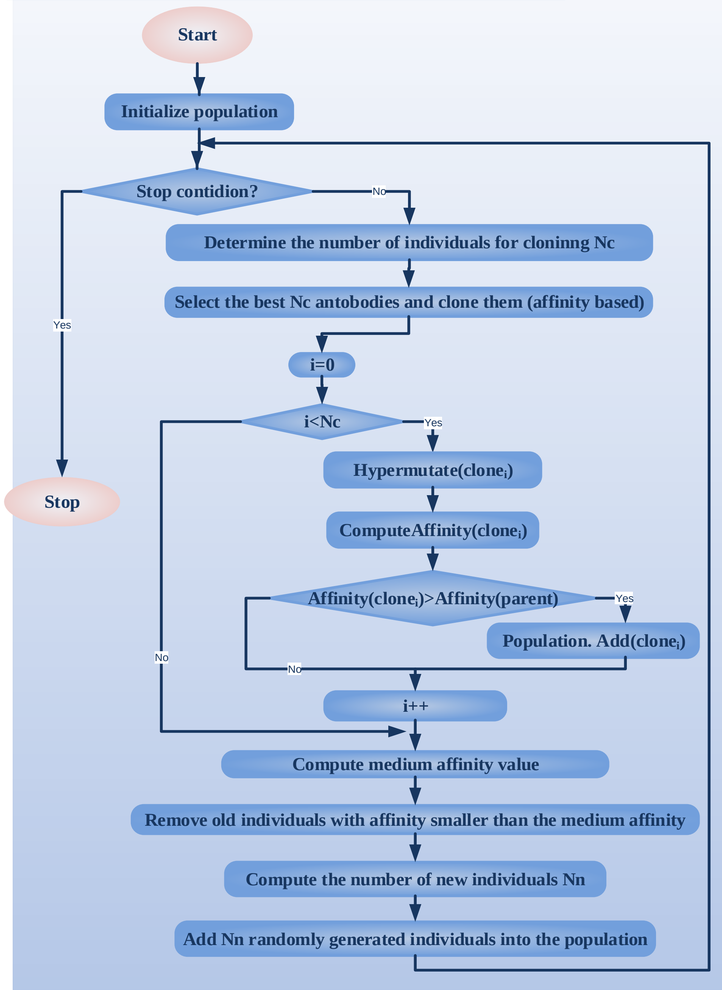
Dissolution of solids in liquids is complex and it is influenced by a number of factors that characterize the properties of solvent, solute, and working conditions.

The process takes place in several successive stages, two of which being the most important: passage of solute molecules from the solid and transfer of separated molecules toward the bulk liquid phase.

The theory of the dissolution by rotating disc method was developed by Levich (1962).

Due to the assumptions considered, the phenomenological model does not always follow the dynamic observed experimentally.

CLONAL SELECTION

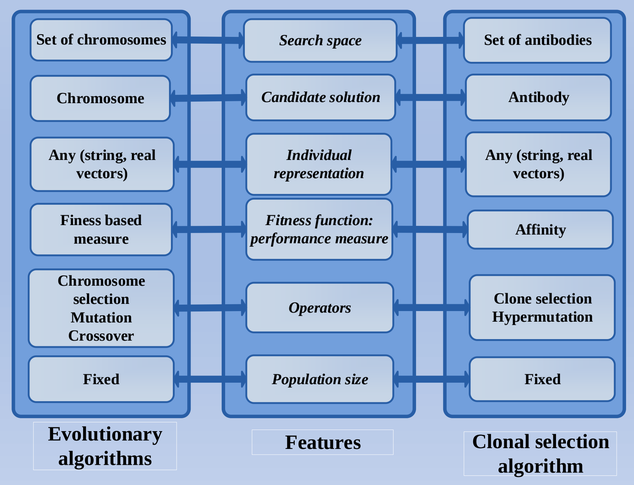


Clonal Selection is an optimization procedure inspired by the response of the vertebrate immune system when attacked by antigens.

Is one of the most known algorithms from the Artificial Immune System group because its theory of inspiration is a fundamental principle of modern immunology.

It has a simple structure and is similar to evolutionary algorithms.

It works with a population of potential solutions that are evolved until a stop criterion is reached.



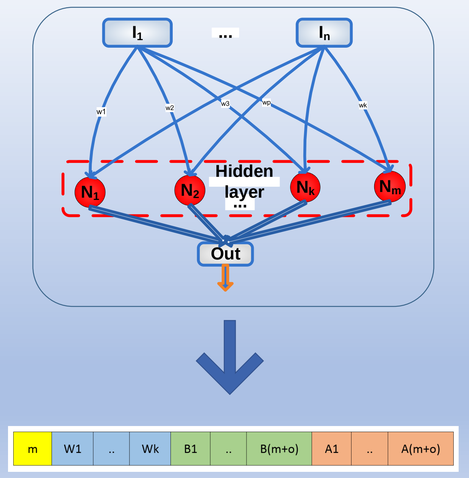
CS-NN

The potential solutions of CS are encoded ANNs (feed forward multilayer perceptrons).

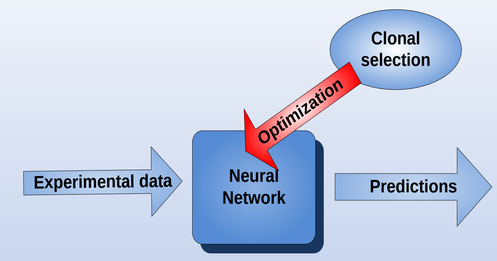
A direct encoding is used to transform the ANN parameters -phenotype- to a structure that can be evolved by CS -genotype-.

The affinity function is based on MSE:

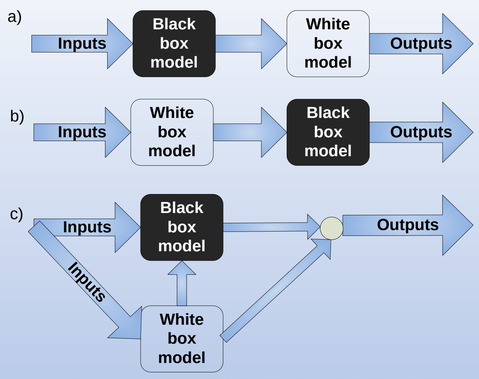
$$affinity = \frac{1}{low + MSE_{training} + MSE_{validation}}$$



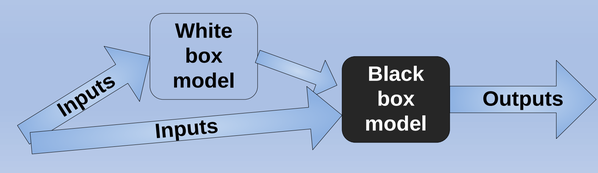
GREY AND BLACK BOX



Black box modelling using CS-NN algorithm



Grey box approaches: a) Serial I, b) Serial II, c) Parallel

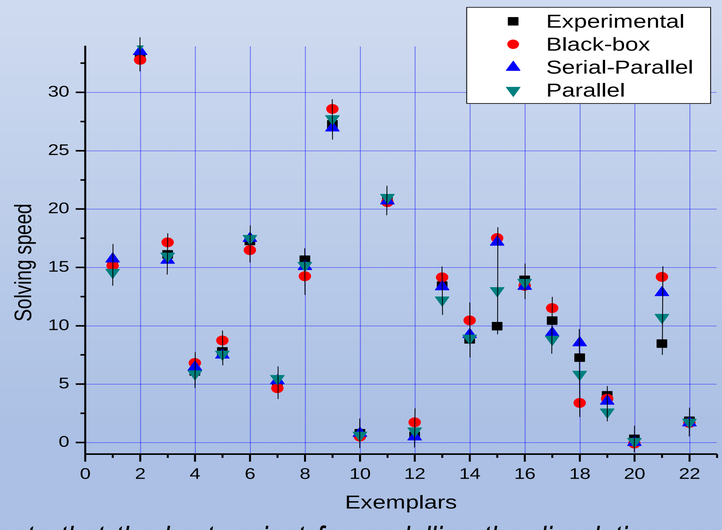


Serial-Parallel grey box approach

RESULTS

CS was initially developed to work as an optimizer for neural network model (black box), the simulation results indicating that the best results were obtained with a network structure of 20 neurons in the hidden layer, 40 individuals in the population and 1500 iteration. The same CS settings were used for grey box modelling.

Approach	PRE train	PRE validation	PRE test
Phenomenological	31.641	14.61	37.407
Black-box	8.162	18.189	25.122
Serial	24.529	8.399	30.637
Serial-Parallel	6.357	9.068	11.189
Parallel	7.092	24.521	12.617



The results indicate that the best variant for modelling the dissolution process is represented by Serial-Parallel, in the testing phase an 11% percent error being obtained. This error is much lower compared with the phenomenological model and consequently, it can replace it in various optimization procedures.