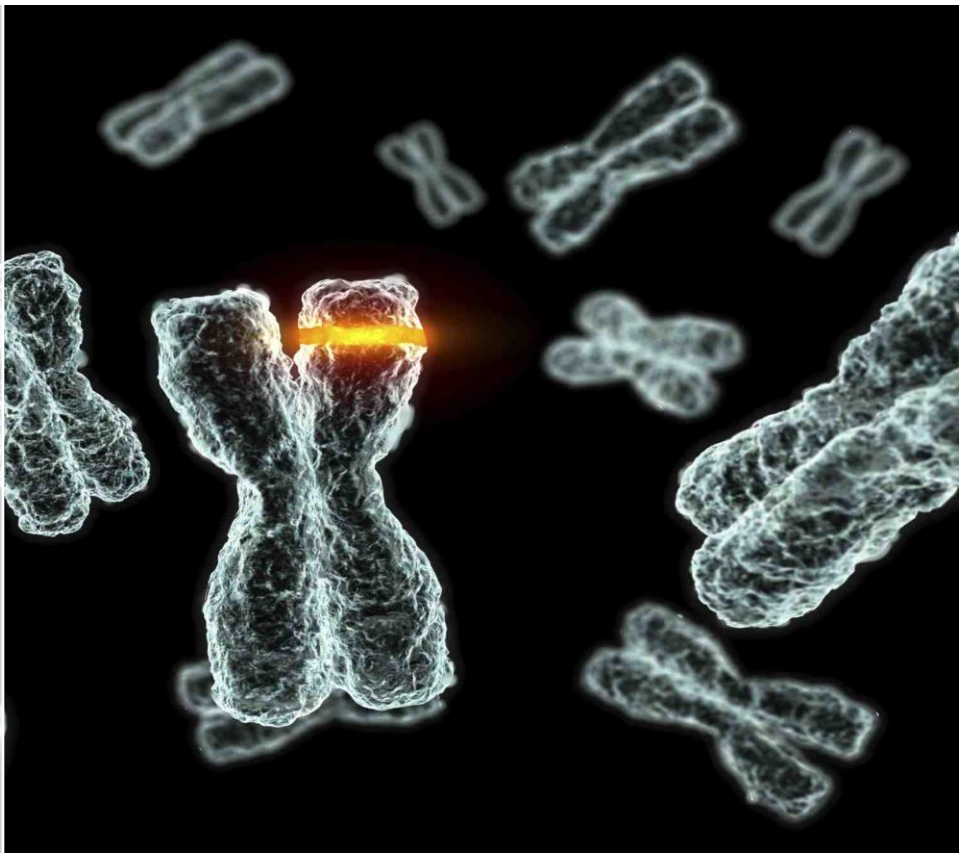
GENETIC ALGORITHMS IN MATERIALS PROCESSING



Under the guidance of

Prof.N.Chakraborti

DEPARTMENT OF METALLURGICAL AND MATERIALS ENGINEERING

&

Prof. P Panighrahi

DEPARTMENT OF MATHEMATICS

INDIAN INSTITUTE OF TECHNOLOGY, KHARAGPUR

Submitted By:

VIKASH KUMAR

05MA2001

DEPARTMENT OF MATHEMATICS

INDIAN INSTITUTE OF TECHNOLOGY, KHARAGPUR

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I am indebted to the Department of Mathematics and Department of Metallurgical & Materials Engineering, IIT Kharagpur for extending help and facilities.

Vikash Kumar
Roll No: 05MA2001

CERTIFICATE

This is to certify that the project entitled **"NEW MULTI-OBJECTIVE GENETIC ALGORITM in Material Processing"** is a bona fide work carried out by Mr. Vikash Kumar (05MA2001) under my supervision and guidance for the 3rd year M. Sc. project in the Department of Metallurgical and Materials Engineering and Department of Mathematics, Indian Institute of Technology, Kharagpur.

Prof.N.Chakraborti
DEPARTMENT OF METALLURGICAL AND MATERIALS ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY, KHARAGPUR

Prof. P Panighrahi
DEPARTMENT OF MATHEMATICS
INDIAN INSTITUTE OF TECHNOLOGY, KHARAGPUR

Submitted By:
VIKASH KUMAR
05MA2001
DEPARTMENT OF MATHEMATICS
INDIAN INSTITUTE OF TECHNOLOGY, KHARAGPUR

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2. Testing NMGA on standard mathematical test functions (ZDT- tests).

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4. Extension of NMGA to a three objective function optimization.

5. Application of NMGA to solve new problem in metallurgy and materials systems – The ionic material design problem.

INTRODUCTION

A genetic algorithm is a search technique used in computing to find exact or approximate solutions to optimization and search problems. Genetic algorithms are categorized as global search heuristics. Genetic algorithms are a particular class of evolutionary algorithms (also known as evolutionary computation) that use techniques inspired by evolutionary biology such as inheritance, mutation, selection, and crossover. Genetic algorithms are implemented as a computer simulation in which a population of abstract representations (called chromosomes or the genotype or the genome) of candidate solutions (called individuals, creatures, or phenotypes) to an optimization problem evolves toward better solutions. The evolution usually starts from a population of randomly generated individuals and happens in generations. In each generation, the fitness of every individual in the population is evaluated, multiple individuals are selected from the current population (based on their fitness), and modified (recombined and possibly randomly mutated) to form a new population. The new population is then used in the next iteration of the algorithm. Generally the algorithm terminates when a specified number of cycles are completed or a specified fitness is achieved.

A typical genetic algorithm requires two things to be defined:

1. A genetic representation of the solution domain.
2. A fitness function to evaluate the solution domain.

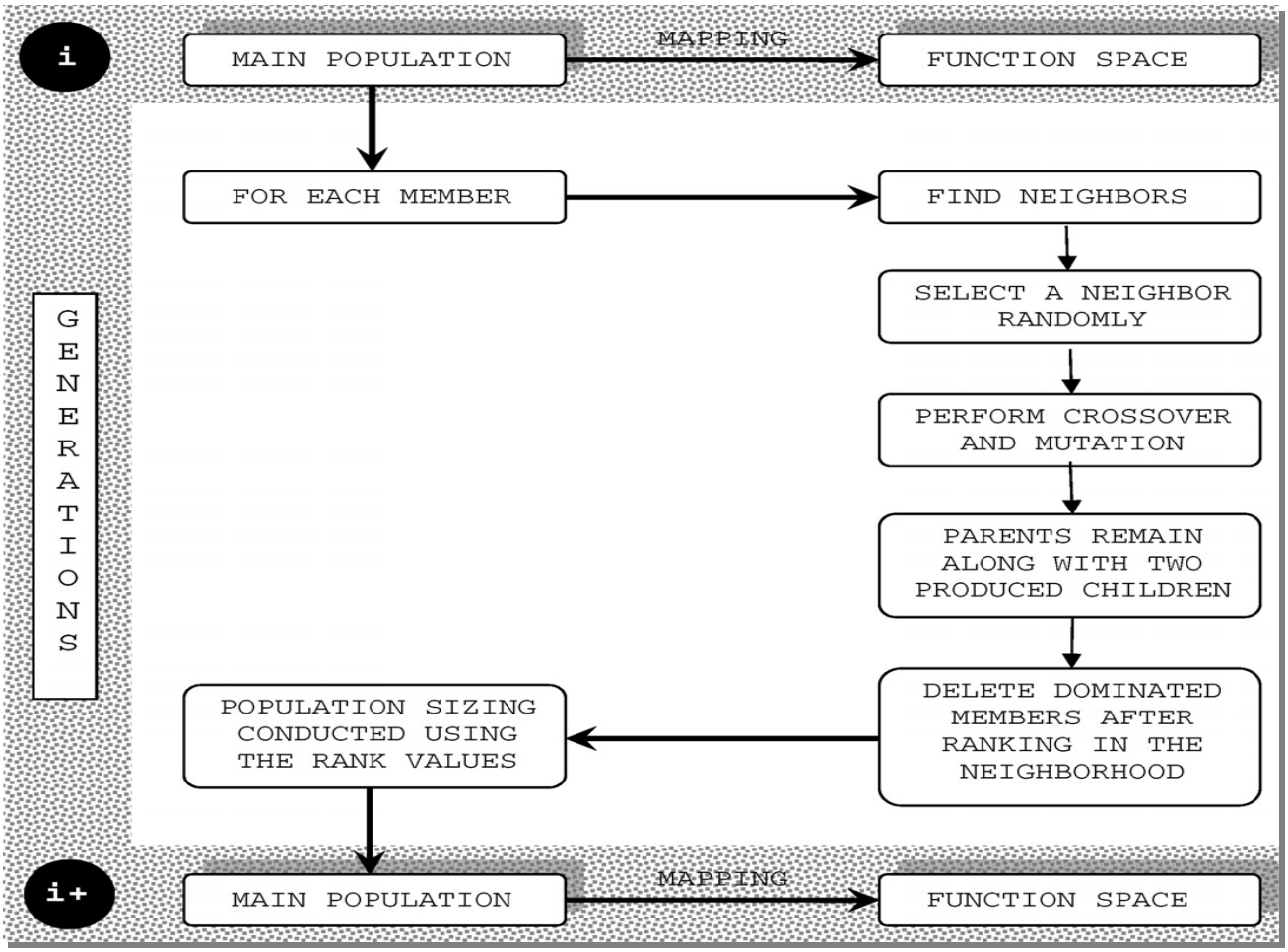
Pseudo code for a Genetic Algorithm.

1. Choose initial population.
2. Evaluate the fitness of each individual in the population.
3. Repeat
    1. Select best-ranking individuals to reproduce.
    2. Breed new generation through crossover and mutation (genetic operations) and give birth to offspring.
    3. Evaluate the individual fitness's of the offspring.
    4. Replace worst ranked part of population with offspring.
4. Until termination.

NMGA (New Multi-objective Genetic Algorithm)

Several algorithms have been proposed since the pioneering multi-objective algorithm VEGA (Vector Evaluated Genetic Algorithm) that met with a limited success, and the recent algorithms like NSGA II are now being very widely used, our capabilities to extend the evolutionary approaches to some highly complex problems are still somewhat limited. Consequently, even now, an ample opportunity of trying out newer strategies or approaches exists in this area.

The New Multi- Objective Genetic Algorithm (NMGA) is a remarkable effort in this direction. It works on a neighborhood concept in the functional space, utilizes the ideas on weak dominance and ranking and uses its own procedures for population sizing.
The basic algorithm is outlined in the figure given below.



PHASE-1: Develop and implement NMGA.

OBJECTIVE of this phase was to implement the New-Multi-objective Genetic Algorithm (NMGA) using Matlab and analyze its behavior with changing parameters like: mutation and crossover probability, population size, number of iterations and grid size.

The modular and commented code for the algorithm has been developed in MATLAB 7.1. The code was first tested and then analyzed against the changing effect of the parameters viz. **Grid size(ng), No of iterations(no_of_it), Population Size(pop_size), Probability of cross-over(p_crossover), Probability of mutation(p_mutation)** on the Rank-1 solutions.

The performance of Heuristic Crossover with respect to this code is scintillating, hence incorporated here. As far as mutation is concerned, Random mutation is used. Due to complexity of the algorithm, code is developed in modular way. Every function has been defined and developed separately with a systematic transfer of control from one sub-module to the other.

RESULTS:

Analysis of over 120 plots obtained by varying probability of mutation and crossover, grid size, population size and number of generations. Best results were obtained for

- Grid Size=100
- No. of Iterations=500
- Population Size=200
- Crossover Probability=0.8
- Mutation Probability: 0.06

PHASE-2: Testing NMGA against standard ZDT functions.

OBJECTIVE of this phase was to test the algorithm against standard ZDT functions.

Zitzler–Deb–Thiele (ZDT):

Five functions belonging to the Zitzler–Deb–Thiele (ZDT) series of test are the most reliable benchmark for evaluating the multi-objective genetic algorithms. The five functions that are used in this set are quite intricate and they lead to both convex and non-convex Pareto frontiers, which are sometimes discontinuous and often quite cumbersome to get.

Individual functions for heuristic crossover and finding of neighborhood has been developed which apply to all ZDT functions. Further, for each ZDT function, there is a main code which besides the two mentioned above; uses the values obtained from the two objective functions f1 & f2 to finally evaluate Rank-1 members.

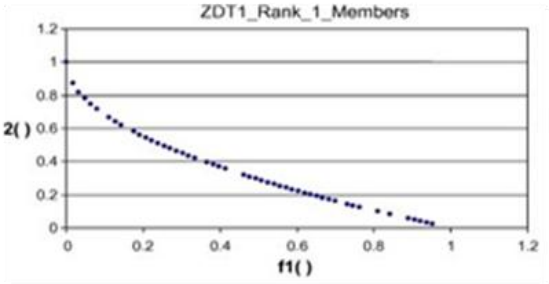
RESULTS:

The algorithm has been successfully tested for all ZDT functions except ZDT-5, because it is a Boolean function defined over bit-strings and we are dealing with a real-coded optimization algorithm. Two of such test results is shown below.

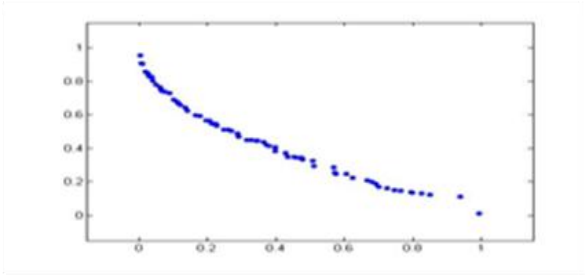
1)

$$\text{ZDT1}: \begin{cases} f_1(x) = x_1 \\ g(x) = 1 + \frac{9}{n-1}\sum_{i=2}^{n} x_i \\ h(f_1, g) = 1 - \sqrt{f_1/g} \end{cases}$$

Expected Plot



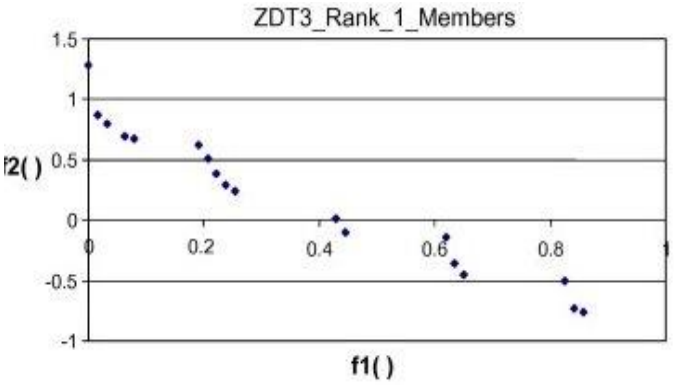
Obtained Plot



2)

$$\text{ZDT3}: \begin{cases} f_1(x) = x_1 \\ g(x) = 1 + \frac{9}{n-1}\sum_{i=2}^{n} x_i \\ h(f_1, g) = 1 - \sqrt{f_1/g} - (f_1/g)\sin(10\pi f_1) \end{cases}$$

Expected Plot



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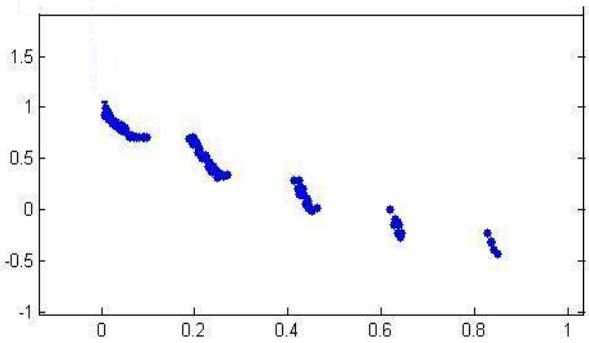


PHASE-3: Performance check against recently solved problems

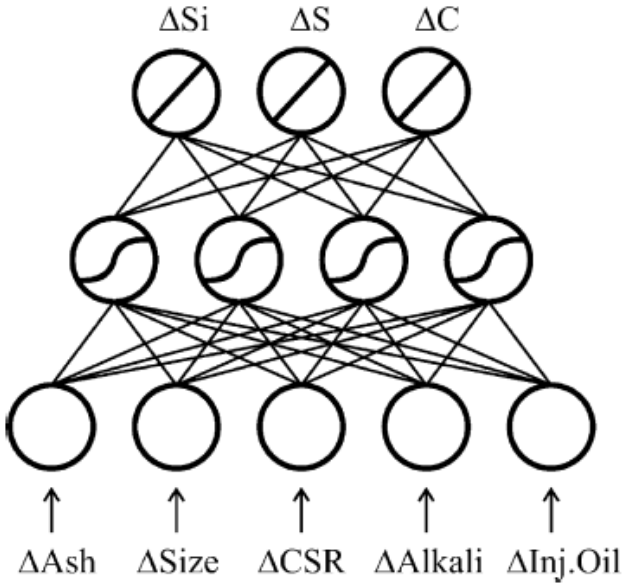
OBJECTIVE of this phase is to test the performance of NMGA against the recently solved Genetic Algorithm based Neural Network problems.

- The blast furnace problem.
- The Spinel system.

a) The blast furnace problem

The process chemistry and the transport phenomena in blast furnaces are highly complex and despite decades of intensive research, a fully reliable analytical model for the blast furnace is yet to emerge. Therefore, data-driven models are of vital importance for throwing light on the complex interrelations between variables in the process. The pig iron, that a blast furnace produces, contains several alloying elements dissolved in it. Among them C, S and Si are three crucial components which need to be controlled efficiently within a specified target. Several input parameters can significantly affect these compositions. In this study, we chose to select five of them, all related to the reductants, i.e., coke and the injected oil, the ash content, size, strength and alkali content of the coke as well as the specific oil injection rate. These five input variables and the concentration of the three alloying elements in the pig iron were assembled into a feed forward neural network. The learning process of the upper part of this neural net was carried out through a linear least square technique, while the lower part was affected by the genetic processes.

A good network should be able to reproduce the data in an acceptable manner. At the same time, it should try to do so with a small number of connections, so that the trained network does not get over-trained. In order to achieve both of these objectives, here we had attempted to simultaneously minimize (i) the training error of the network (E) and (ii) the required number of active connections in the lower part of it (N). The architecture of the lower part of the network and their corresponding weights were



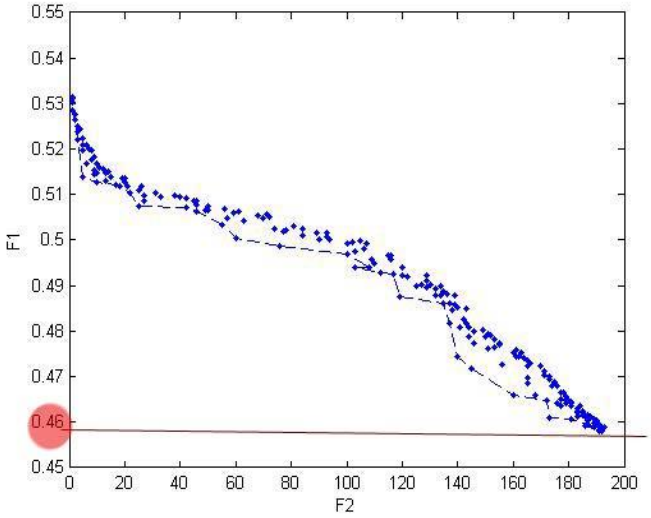
Schematics of the feed forward neural net used

treated as variables influencing the objective functions. These two objectives are however conflicting, in many instances; with smaller number of nodes the training error is expected to rise and vice versa. The trade off situation between them can therefore be represented as a Pareto-front.

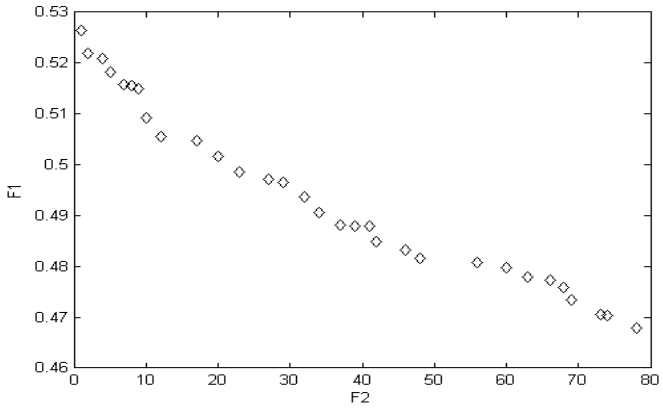
RESULTS:

Following the works of [1] we did a thorough research for improving results. This work uses predator prey model of genetic algorithms in the training process of a feed forward neural network. It was replaced by NMGA and a modified code was developed.

- NMGA based algorithms Pareto front



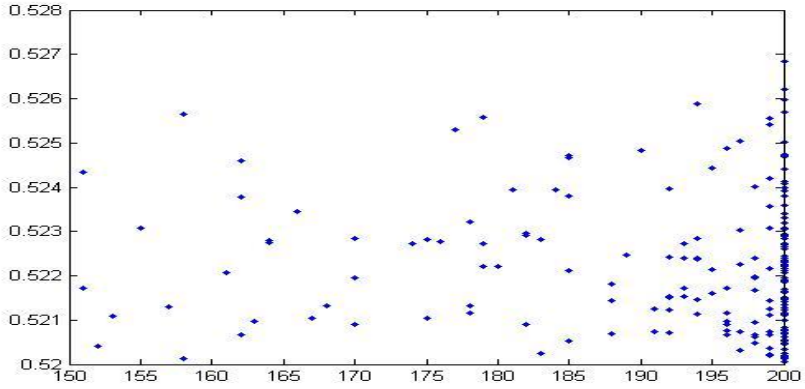
- Predator Prey based algorithms pareto front



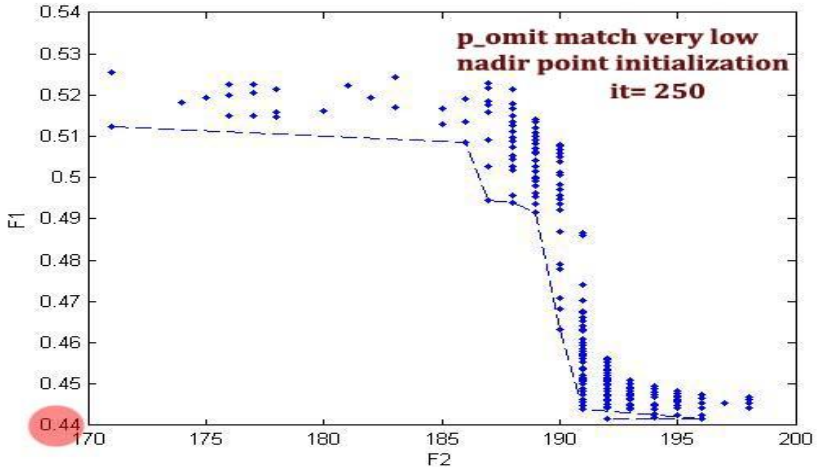
As before we did several variables change for analyzing the behavior of the neural NMGA code and settled in for the parameters as now. P_omit Match has been identified as the key parameter influencing the direction of development of the population. Nadir point initialization

of the starting population was able to solve the problem of localized development and provided with a new improved convergence point.

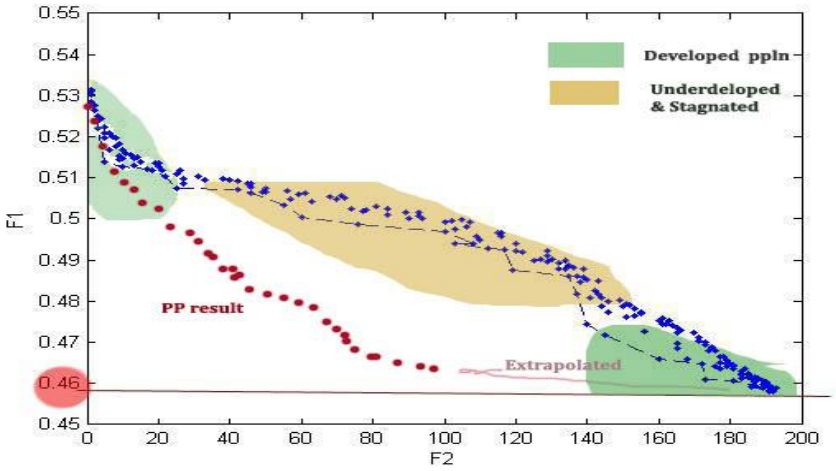
- Initial population



- Unconverged front



- Comparison plot



b) The Spinel System

To further test the algorithm and its efficacy we applied it to another data set of a Spinel Nitride system. Nitride spinels are typically characterized by their unique AB_2N^4 structure containing a divalent cation A, a trivalent cation B, and an anion N. Numerous such species may exist as metals, semiconductors or semimetals leading to their extensive usage in diverse scientific and engineering fields. Experimental and theoretical data on the physical or material properties of nitride spinels are however severely limited for coming up with a data driven, generic description for their material properties. The results from a recent study [1] were used . The study employed state of the art soft computing tools like Genetic Algorithms, Data Mining and the Neural Networks. The paucity of the available data was circumvented in this work with a data mining strategy, important inputs were identified through an evolving neural net, and finally, the best possible tradeoffs between the bulk moduli and the relative stabilization energies of the nitride spinels were identified by constructing the Pareto-frontiers between them through a Genetic Algorithms based multi-objective optimization strategy.
We used the identified important inputs from the above study and tested it on the predator-prey based neural net as well as NMGA based neural net and results were comparable.

The spinel phase has a unique AB_2X_4 structure containing a divalent cation A, a trivalent cation B, and an anion X (=O, S, Se, or Te). Altering the combination of cations expands their usage to diverse scientific and engineering fields for electrical, magnetic, or mechanical purposes. Although there have been various studies on the spinel structure, systematic studies of parameters for nitride spinels AB_2N_4 are precious few. The reason is that the new spinel phase of cubic Si_3N_4 with anion valence of -3 was discovered at approximately 15GPa of pressure and high temperature exceeding 2000K within the last few years and 6-fold bonding for Si in a spinel structure is not usual from the viewpoint of crystal chemistry. Since then, nitride based spinels indeed have become fascinating examples of the synergy between structure and properties that correlate fundamental issues ranging from electronic structure to crystal chemistry for high temperature and super hard materials. As a result of many efforts, γ-Ge_3N_4 from the IVA based nitride spinels has been also synthesized in the lab. Since the study of spinel nitrides are still in the early stage, experimental and theoretical data on the physical or material properties of nitride spinels are severely limited to come up with a data driven, generic description for such properties.

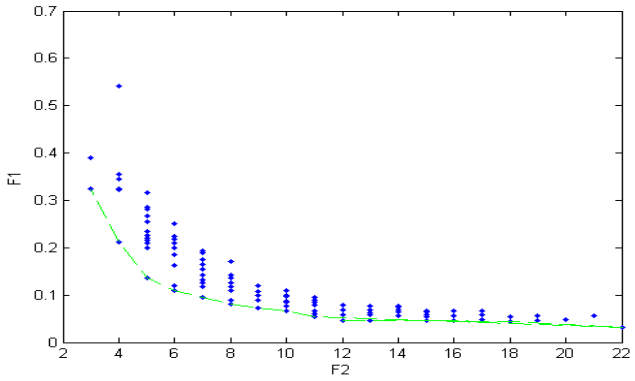
Numerous such species may exist as metals, semiconductors or semimetals leading to their extensive usage in diverse scientific and engineering fields. Experimental and theoretical data on the physical or material properties of nitride spinels are however severely limited for coming up with a data driven, generic description for their material properties. Previous studies have attempted to establish methodology for handling such sparse data where the various features of some of the state of the art soft computing tools like the Genetic Algorithms, Data Mining and the Neural Networks are used in tandem to construct some generic predictive models, in

principle applicable to the nitride spinel structures at large, irrespective of their electronic characteristics. The paucity of the available data was circumvented in this work with a data mining strategy, important inputs were identified through an evolving neural net, and finally, the best possible tradeoffs between the bulk moduli and the relative stabilization energies of the nitride spinels were identified by constructing the Pareto-frontiers between them through a Genetic Algorithms based multi-objective optimization strategy.

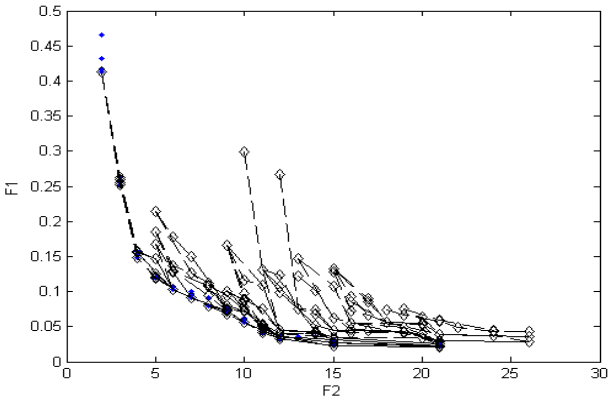
We attempted to get similar results as in [1] using a NMGA based neural network.

RESULTS:

We used the data set from this problem as a practice problem. On running the code we saw that we had wonderful results correlating to those in literature.



NMGA based Pareto front

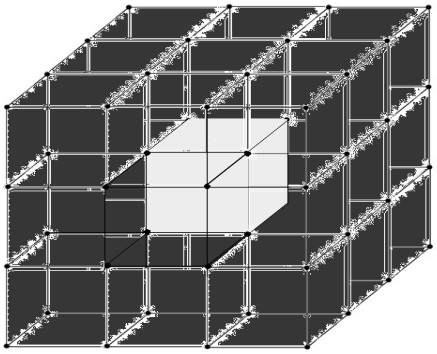


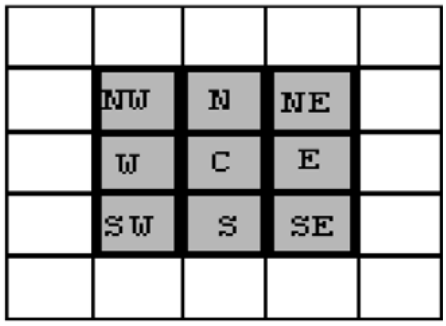
Predator Prey based Pareto front

PHASE-4: Extend NMGA to three objection function optimization

We further extended the algorithm for optimizing three objective functions instead of two. For this the following changes were done:

1. The functional space was changed into a 3-D grid from a 2-D matrix.
2. The concept of Moore's neighborhood was extended to 3 dimensions.





3. Neighborhood in 3-D space. The white cell is the center while the red cells represent the neighborhood of the yellow cell.

PHASE-5: The Ionic Material Design Problem.

Our present work deals with the design of ionic materials as an "inverse problem" where we determine suitable inter-ionic distance to arrive at the desired properties. Specifically, we design ionic materials with high fracture toughness, low density and high thermodynamic stability. Fracture toughness of the material is determined through molecular dynamics simulations, and the three conflicting objectives are optimized using multi-objective Genetic Algorithms. Two typical lattice systems, namely the NaCl (B1) structure and CsCl (B2) structure, are studied. The inter-ionic potential is modeled by a combination of Buckingham and Coulomb potentials which represent the electron orbital repulsion and unlike ion attraction respectively. Attempt has been made to develop a general framework for the design of ionic materials by Genetic Algorithms.

The newly developed NMGA code for 3 function optimization is currently being used to optimize the above mentioned objectives and the results are being compared with a well known algorithm NSGA-II . Potentially a material this way could find extensive applications as electrode materials which are subjected to cracking and subsequent stress related failure.

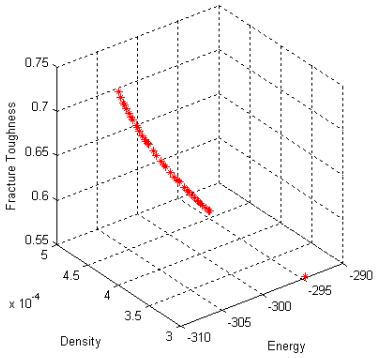
The problem is formulated as:

- Maximization of fracture toughness
- Maximization of volume (for a given mass). This is the same as maximizing the lightness and minimizing the density.
- Minimization of energy of the system to make it thermodynamically stable.

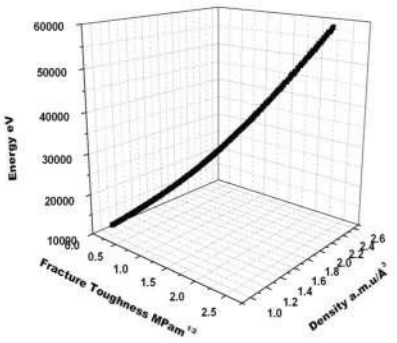
In an endeavor to design materials with the desired fracture toughness and density with higher stabilization energy work is going on to consider the all crystal structures belonging to the NaCl and CsCl-type crystal system. The mass ratio of the anion and cation being the variables covering the variety of crystal systems will be our variable of interest.

RESULTS:

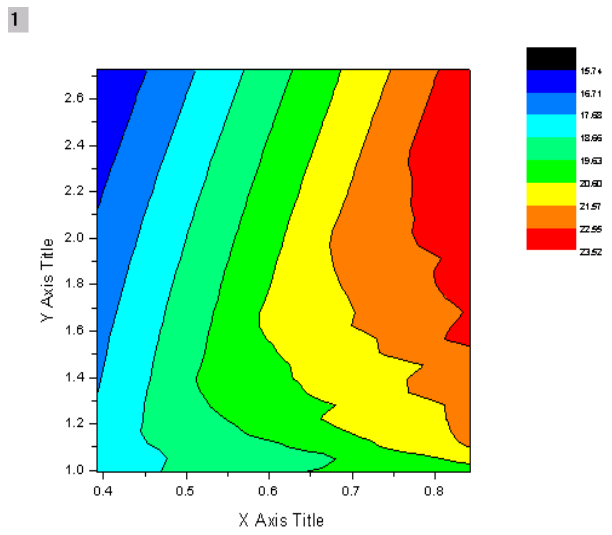
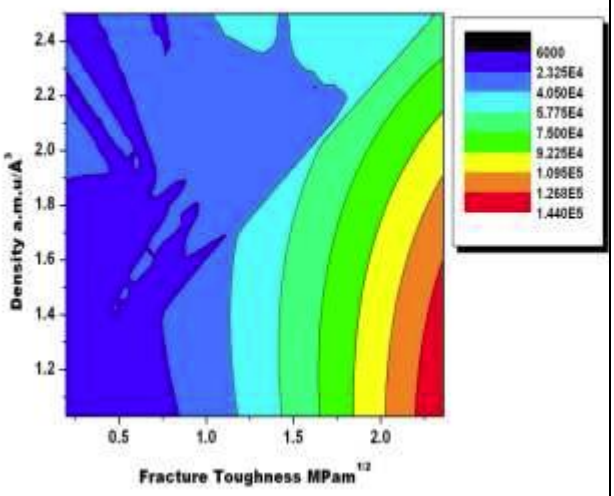
The work is in progress. One of the intermediate plots is shown below.



Plot obtained



Expected Plot

	
Plot obtained	Expected Plot

Further work:

1. Test the newly developed 3 objective NMGA code .
2. Use the code to plot the pareto-front and compare the result with NSGA-II. Initially, only r (inter-ionic separation) is treated as a variable and the results are compared for a fixed m1/m2 ratio.
3. Implement the functionality to vary the m1/m2 ratio and then generate the pareto-front and compare the results with NSGA-II .

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4. **R Sreevathsan1, B Bhattachary, N Chakraborti , Designing of Ionic Materials through Multi- Objective Genetic Algorithms , Article in press**

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