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# Fuzzy Logic vs. Niched Pareto Multiobjective Genetic Algorithm Optimization: Part II: A Simplified Born - Mayer Problem

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## Abstract

A new multiobjective selection procedure for Genetic Algorithms based on the paradigms of fuzzy logic is discussed and compared to the niched Pareto selection procedure. In the example presented here the fuzzy logic procedure optimized the parameters of a series of functions in a more efficient manner than the niched Pareto approach. The main advantage that the fuzzy logic approach has over the niched Pareto approach is that its efficiency is completely independent of the number of objectives being optimized and its efficiency is highest with a comparison set size of 1 whereas the optimal comparison set size for the niched Pareto GA changes with the number of objectives. Furthermore, the fuzzy logic approach accounts for the existence of experimental errors in the values to which a function is being optimized. The functions explored in this work are the derivitives of a simplified Born-Mayer function used in molecular dynamic simulations.

## 1.0 Introduction

### 1.1 Justification For Work

Numerous problems in materials science require the optimization of nonlinear (Fraga, 1996), multiparameter (Duggirala, 1994), multiobjective (Ozyurt, 1996) functions. In addition, many such materials science optimization problems have numerous minimums (or maximums) (Morgan, 1996) where all such points need to be located. Such problems are typified by atomic structure determination of proteins (Bush, 1995), of clusters (Zeiri, 1995), of small molecules (Judson, 1993), of alloys (Sutton, 1994), and of spin glasses (Smith, 1992). Other problems include, potential function parameter optimization (Skinner, 1995), x-ray diffraction pattern recognition (Paszkowicz, 1996), ) curve fitting (Ahonen, 1997; Karr, 1995), and production scheduling (Swinehart, 1996). Unfortunately, such problems are not easily tractable to such methodologies as Newton - Cauchy (Nazareth, 1995) or maximum entropy (Gzyl, 1995) and thus more robust search procedures are needed.

The requirements of an optimization method that can handle the above mentioned conditions are that it (i) account for the fact that there may exist an entire range of feasible solutions and it should determine what that range is, (ii) it must be capable of multiobjective (or attribute) optimization, (iii) it must be able to conduct comparisons solely on the final difference between experiment and theory and thus aim to minimize that difference, and (iv) must obtain reasonable answers in a timely manner that out performs a simple random or Monte Carlo search. At present, the only optimization technique that efficiently attempts to fulfill all of these requirements is the genetic algorithm (GA) (Goldberg, 1989; Holland, 1975, Reardon, 1997).

## 1.2 Generic GA description

Generally speaking, one can formulate any optimization problem into a single standard of measurement - a cost function or a fitness function - that determines the performance of a decision and then recursively improves the performance by selecting from the most feasible of alternatives. For example, the square difference between an experimental quantity, *O*, and its theoretical value *f*(*x*) could define a fitness function such as $(O - f(x))^2$, where *x* represents the independent variable which must be optimized to minimize $(O - f(x))^2$. Traditional deterministic optimization techniques require the use of gradient or higher order statistical analysis of the cost function (Bazaraa, 1979). These methods find optimal solutions exponentially fast. Unfortunately, the solutions are usually locally optimal and insufficient for applied engineering problems (Anderson, 1986).

Darwinian evolution is an intrinsically robust search and optimization procedure. Evolved biota have optimized solutions to complex problems at every level of organization, from the cell up to the population. The problems that biota have solved and continue to improve upon, are typified by chaos, chance, temporality, nonlinearity, and multidimensionality. Such problems have proven to be intractable to deterministic optimization techniques, especially in situations where heuristic solutions are not available.

A GA falls into the much broader category of evolutionary algorithms. These algorithms attempt to simulate the processes of evolved biota in optimization. The essence of such a simulation lies in the expression of a solution to a problem not as a single value but as a string of fundamental building blocks (genes) that can be manipulated in much the same way as an extant species will manipulate its gene pool through selection and mating to produce more optimal offspring for the current environment.

Numerous references are available regarding the formal structure of genetic algorithms and the theoretical foundation of their success (Fogel, 1994; Goldberg, 1989; Chambers, 1995). The specific details of the operators used in this GA study were published previously (Reardon, 1997).

### 1.3.0 Multiobjective Selection Procedures

The simultaneous optimization of multiple objectives or attributes presents a real challenge. Consider a situation in which there are three functions ($f_1(x,y)$, $f_2(x,y)$, and $f_3(x,y)$) whose independent variables $x$ and $y$ need to be optimized. In such a situation the values of $x$ and $y$ that provide an optimal value of $f_1$ may or may not correspond to the optimal values of $f_2$ and $f_3$. Consequently a number of approaches have been adopted to extract a measure of fitness for the multiobjective system as a whole. These methodologies include the least squares approach (Swaragi, 1985), the vector evaluated GA (Schaffer, 1985; Richardson, 1989), and the niched Pareto GA (Horn, 1994; Ritzel, 1994; Reardon, 1997). The pros and cons of each of these multiobjective optimization selection methods were elucidated previously (Reardon, 1997). Generally, the main disadvantages can be described as:

1) Weighting factors have a significant impact on the ability of the GA to optimize all the functions. This is especially true the least squares minimization problems.

2) Second, the presence of a square, is often necessary to properly define the fitness function as a minimization problem, however, this results in a loss of information that could otherwise be used by the GA.

3) In the vector evaluate GA, bias occurs against middling individuals that represent an adequate compromise between competing objective functions.

4) In the niched Pareto method, as the number of objectives being optimized goes up, the likelihood that one randomly selected member dominates another goes down. Thus, the likelihood that a member is selected due to actual fitness superiority rather than simple niche counting is dependent on the number of objectives.

5) Finally, another important point to consider in many engineering problems is that optimization of a function towards an experimentally derived value should in principle account for some degree of error in the experiment. All of the multi-objective optimization procedures described above assume that the value one is optimizing towards is an absolute. Furthermore, the above procedures do not allow the user to make adjustments for the fact that some objectives may be known experimentally to a high degree of accuracy while others will be known to a lower degree.

These drawbacks reveal a need for a revision to the niched Pareto procedure. The revision proposed in this work involves a rudimentary application of fuzzy logic as a selection method.

### 1.4 Fuzzy Logic Selection Methodology

Multiobjective optimization using fuzzy logic (Bandemer, 1995; Sakawa, 1997; Sanchez, 1997), as presented here, is fundamentally a hybrid of the least squares selection method and the niched Pareto selection method. The whole procedure can be summarized in two steps. First, a single fitness value that incorporates the values of all the objectives is calculated using fuzzy rules. Second, as in the Pareto selection procedure, two randomly selected members are compared to a comparison set. If one member has a fuzzy fitness value that dominates the set and the other does not then the dominating member is selected. Otherwise, continuously updated phenotypic niching is incorporated.

The key to the fuzzy logic approach lies in the definition of the fitness function and its corresponding fuzzy rules:

$$F = \frac{1}{N}\sum_{i=1}^{N} f'\left(f_i\right) \qquad \text{Eq. 1}$$

which is essentially an average over the *N* objectives in question. *f'* is a fuzzy logic rule set that scales the objective, $f_i$, according to how far away it is from the experimentally optimal solution. A typical fuzzy set would have the form:

$$\text{if } f_i \le \left(O_i - E_i\right) \rightarrow f'\left(f_i\right) = \left(\frac{S_{\min}}{f_{i\min} - \left(O_i - E_i\right)}\right)\left(f_i - \left(O_i - E_i\right)\right) \qquad \text{Eq. 2a}$$

$$\text{if } \left(O_i - E_i\right) \le f_i \le \left(O_i + E_i\right) \rightarrow f'\left(f_i\right) = 0 \qquad \text{Eq. 2b}$$

$$\text{if } f_i \ge \left(O_i + E_i\right) \rightarrow f'\left(f_i\right) = \left(\frac{-S_{\max}}{\left(O_i + E_i\right) - f_{i\max}}\right)\left(f_i - \left(O_i + E_i\right)\right) \qquad \text{Eq. 2c}$$

where $O_i$ is the *i*th experimental value that the *i*th function, $f_i$, is being optimized towards, $E_i$ is the error or accepted uncertainty in $O_i$, $S_{min(max)}$ is a scaling parameter for values below(above) the accepted value, $f_{imin(imax)}$ is the smallest (largest) value of all the ith objectives in the population. Figure 1 is a graphic representation of the above functions.

Defining a multiobjective fitness function in such a way has a number of practical advantages. First, experimental uncertainty in the values to which a function are being optimized can be accounted for since all the calculated values within a certain range have the same fitness. Second, values less than or greater than the optimal value will each have their own distinct fitness and thus the GA will in effect have more information with which to optimize. Third, as will be shown explicitly in this report, the ability of the GA to select a member will not be influenced by the number of objectives as is the case in the niched Pareto method. Fourth, while one could argue that $S_{max}$ and $S_{min}$ are user defined parameters, their net influence on the final optimization procedure is not as great or as unpredictable as that of the weighting factors in the sum of least squares approach since it is a relatively simple matter to set $S_{max}$ and $S_{min}$ to the same values for all objectives.

A fifth idiosyncrasy of this procedure is that the fuzzy fitness is a function of the least optimal members of a population ($f_{imax}$, $f_{imin}$). Thus, the fitness of a particular member in one generation will not necessarily be equivalent to its fitness in a subsequent generation. The ramifications of such a dynamic defination of fitness will be not be discussed here but in subsequent papers.

**3.0 A Simplified Born - Mayer Function**

The Born - Mayer function is a standard function often used to model the atomic interaction of ionic materials such as NaCl. It has the form:

$$\Phi = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1 \\ j\neq i}}^{N}\left(\frac{z_j z_i}{r_{ij}} + A_{ij}\exp\left(\left(\sigma_i + \sigma_j - r_{ij}\right)d_{ij}\right)\right) \qquad \text{Eq. 3}$$

where $r$ is the distance between two atoms $i$ and $j$, $z$ is the charge of an ion, $\sigma$ is the radius, $N$ is the total number of atoms in the system, and the fitting parameters $A$ and $d$ are the pre-exponential and hardness parameters respectively. The empirical nature of this function requires that $A$, $d$ and often the $\sigma$'s be optimized to give the proper crystal energy, pressure, elastic moduli, and thermal expansion coefficients. To complicate matters, most materials are not purely ionic and may require the addition of empirical terms to account for covalence. Thus, a routine is needed that can effectively optimize the empirical parameters of functions like these as the need for simulations of new materials comes about.

A quantitative study of the GA's ability to optimize such functions will begin with a simplified version of the above equation:

$$f_1 = -r^{-1} + A\exp((\sigma - r)d). \qquad \text{Eq. 4}$$

If $A$=4, σ=0.4 and $d$=4, then *f1* would have a minimum at $r$ = 1.1489 and the value of *f1* and its higher order derivates with respect to r at $r$ = 1.1489 can easily be determined. By treating *f1* and each of its derivatives with respect to r as objectives, a quantitative study of the GA's ability to find the appropriate values of $A$, σ and $d$ can be made as a function of the number of objectives utilized. From a pragmatic standpoint, this example is useful for the determination of the statefuction of a material. The objective values and the associated 'errors,' which are set arbitrarily, of the nine functions to which the GA must optimize $A$, σ, and $d$ are: $f_1$=-0.6703±0.0670, $f_2$=-0.04251±0.00425, $f_3$=1.8816±0.1000, $f_4$=-9.3580±0.1000, $f_5$=39.217±0.1000, $f_6$=-152.65±1.0000, $f_7$=546.81±1.0000, $f_8$=-1617.0 ±10.000 and $f_9$=24670.±100.00.

This study will look at the effect of the number of objectives and size of the comparison set on the efficiency of the niched Pareto and the fuzzy logic selection methods to find the correct values of $A$, σ, and $d$. The search ranges are arbitrarily set to $0.1<A<9.0$, $0.1<\sigma<1.0$ and $0.1<d<9.0$. Table I lists the parameters used in the niched Pareto GA and Table II lists the additional parameters used in the fuzzy logic GA.

### 3.1 Procedure

The procedure involves two steps. First, the effects of comparison set size and number of objectives on the number of Pareto selections and niche selections will be determined for both the niched Pareto selection procedure and the fuzzy logic procedure. This determination involves calculating the average number of selection types in the first generation of 50 independent optimizations. Based on this data an optimum comparison set size will be determined and used by the respective selection procedures to optimize the three variables in question. The goal of this second step is to determine if the fuzzy logic procedure can find the optimum variable values in a more efficient manner than the niched Pareto procedure.

### 3.2 Results And Discussion

### 3.3 The Effects Of Comparison Set Size And Number Of Objectives.

Figure 2 shows the average number (over 50 individual optimization runs) of members of the population Pareto selected (one member is nondominated by the comparison set while the other member is dominated) vs. comparison set size for the niched Pareto GA after the first generation. This graph clearly shows a maximum in the number of Pareto selections vs. comparison set size that shifts to higher comparison set sizes with the number of objectives. Furthermore, the number of Pareto selections tends to increase as the number of objectives increases. This trend is sensible since as the number of objectives increases the likelihood that a comparison set member can dominate another member from the population decreases.

Figure 3 shows the number of members selected through niching because both members were nondominated by the comparison set. As the size of the comparison set increases, the likelihood that the set dominates the members increases. Likewise, as the number of objectives increases the likelihood that the comparison set dominates the members decreases.

Figure 4 shows the number of niche selections due to both members being dominated by the comparison set. Again, as the comparison set size increases there is an increase in the probability that the comparison set will dominate both members but as the number of objectives increases there is a decrease in the probability that the comparison set will dominate both members.

The competing effects of the comparison set size and the number of objectives on the selection procedure results in the shifting comparison set maximum in the number of members Pareto selected. This presents a genuine limitation to the niched Pareto selection procedure since in most engineering optimizations there is no a priori knowledge of the optimal comparison set size and it has been shown by others that the comparison set size can have a dramatic effect on the net optimization efficiency.

Figure 5 shows the same type of data as in figures 2, 3 and 4 but for the fuzzy logic selection procedure. As Figure 5 indicates, there is no apparent dependence of the selection procedure on the number of objectives. Instead, the selection procedure is only a function of the comparison set size where there is a distinct decrease in the number of members that are Pareto selected or niche selected due to both members being nondominated as the comparison set size increases.

Figure 6 shows the evolution of the population of parameters $A$, $\sigma$, and $d$ as a function of generation for the 2 objective niched Pareto GA and fuzzy logic GA. The niched Pareto GA used a comparison set size of 5 and the fuzzy logic GA used a comparison set size of 1 which corresponds to the maximums in Pareto selection as shown in figures 2 and 5. This data is typical of all 2 objective runs in that the fuzzy logic GA optimized the parameters to the correct values (4.0, 0.4, 4.0) in a more efficient manner than the niched Pareto GA. The fuzzy logic GA optimized the parameters within 45 generations and found the correct general area within the search space where the values were most optimal. The niched Pareto GA did converge in a few number of generations but towards incorrect areas in the search space.

Figure 7 shows the evolution of the population of parameters *A*, σ, and *d* as a function of generation for the 4 objective niched Pareto GA and fuzzy logic GA. The niched Pareto GA used a comparison set size of 5 and the fuzzy logic GA used a comparison set size of 1. Both the niched Pareto GA and the fuzzy logic GA optimized the parameters to the correct general area but the fuzzy logic GA did so in 50 generations as opposed to the 75 generations needed for the niched Pareto GA. Inspection of the equations being optimized shows that as the number of objectives increases the *d* parameter becomes more influential. Thus, the *d* parameter is typically optimized in a quicker fashion and the *A* and σ parameters become more difficult to optimize.

Figure 8 shows the evolution of the population of parameters *A*, σ, and *d* as a function of generation for the 9 objective niched Pareto GA and fuzzy logic GA. Again the fuzzy logic GA is performing more efficiently than the niched Pareto GA. The fuzzy logic GA optimizes the *d* parameter within 40 generations as opposed to the 50 generations of the niched Pareto GA. The niched Pareto GA could not optimize towards the optimal σ value but the fuzzy logic GA could. Both GAs had trouble optimizing the *A* parameter but this should not be surprising since the *A* parameter does not have a large influence on the final values of the 9 objective functions.

The apparent efficiency of the fuzzy logic GA over the niched Pareto GA can most likely be attributed to three inherent idiosyncrasies of the fuzzy logic method. First is the use of real differences between the experimental and calculated values as opposed to the absolute or squared differences used in the niched Pareto GA.

Second is the use of error bars in the fuzzy logic optimization which effectively broadens the optimal area in search space. Of course, if the error bars are too large then niching becomes the dominate selection methodology and real optimization does not occur.

The third aspect that potentially offered greater efficiency was the rescaling of fitness using $S_{max}$ and $S_{min}$ and the maximum and minimum objective values.

### 3.4 Conclusions

Multiobjective optimization is a challenging aspect of modern day engineering and the use of evolutionary techniques such as the niched Pareto GA have greatly facilitated many optimization problems. However, there remains room for improvement. One limitation addressed in this report was the fact that the efficiency of the niched Pareto GA is greatly effected by the number of objectives. Overcoming this limitation resulted in the use of fuzzy logic to help define a new measure of fitness. As shown here, the efficiency of the fuzzy logic selection criteria is not influenced by the number of objectives and tends to be more efficient at optimizing the parameters of the functions in question.

Additionally, the fuzzy logic GA has two distinct advantages that make it ideal for multiobjective engineering problems. First, it allows for the use of error bars when optimizing a function towards an experimentally derived value. This point is important when considering that every engineering problem has built into it some degree of error. The second point is that the fuzzy logic GA does not require the use of squares or absolute values in the difference between the experimental and calculated values. Thus, using this procedure, the GA now has the ability to determine whether a value is too high or too low and to use that information to enhance the efficiency of optimization.

### Tables

Table I. Parameters used in the niched Pareto GA

| | |
|---|---|
| $p_c$ | 0.9 |
| $p_m$ | 0.01 |
| Populations size ` | 200 |
| comparison set sizes | 1, 10 , 20 |
| Niching scale | 0.01 |
| range of *A* | 0.1 to 9.0 |
| range of $\sigma$ | 0.1 to 1.0 |
| range of *d* | 0.1 to 9.0 |

| | |
|---|---|
| chromosome length | 14bits/variable * 3 variables = 42 bits |
| generations | 200 |

Table II. Additional parameters used for the fuzzy logic selection criteria:

| | |
|---|---|
| Fuzzy scaling: $S_{min}$,$S_{max}$ | 1.0,1.0 |

**Figures**

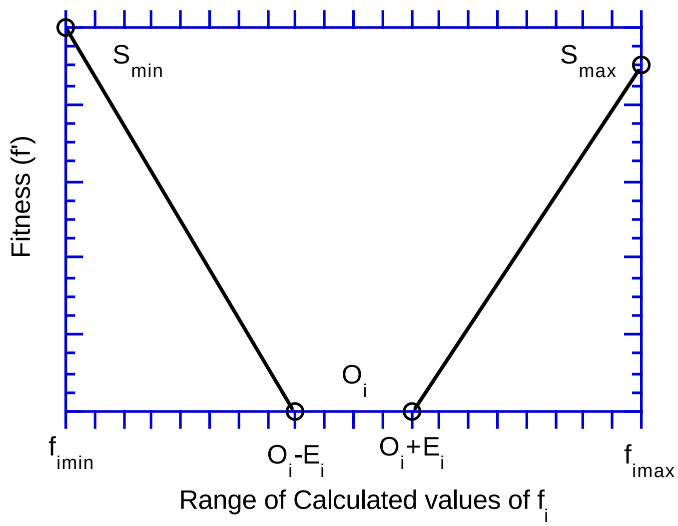


Figure 1) The fuzzy logic fitness as a function of one of the objective values of the *i*th member of a population.

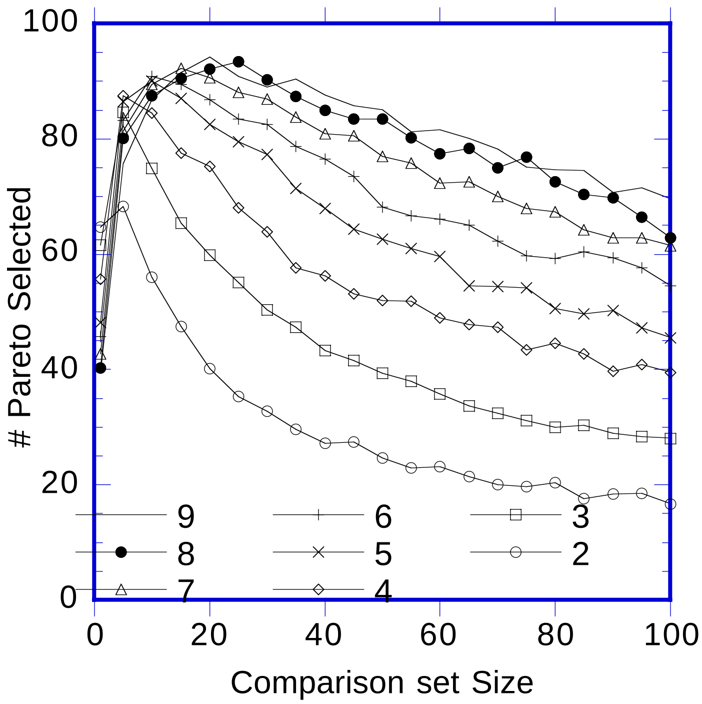


Figure 2) Number Pareto selected vs. comparison set size for the niched Pareto GA

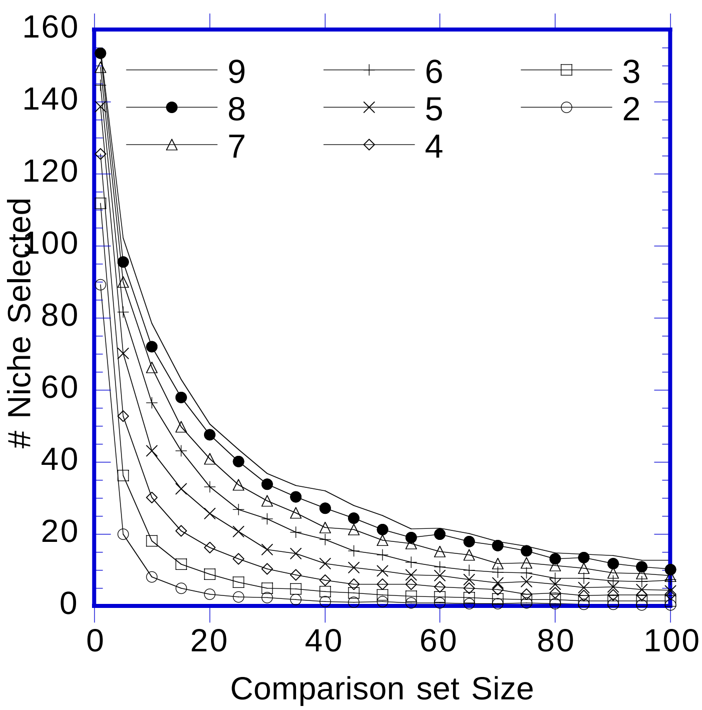


Figure 3) Number niche selected due to each member nondominated by the comparison set vs. comparison set size for the niched Pareto GA

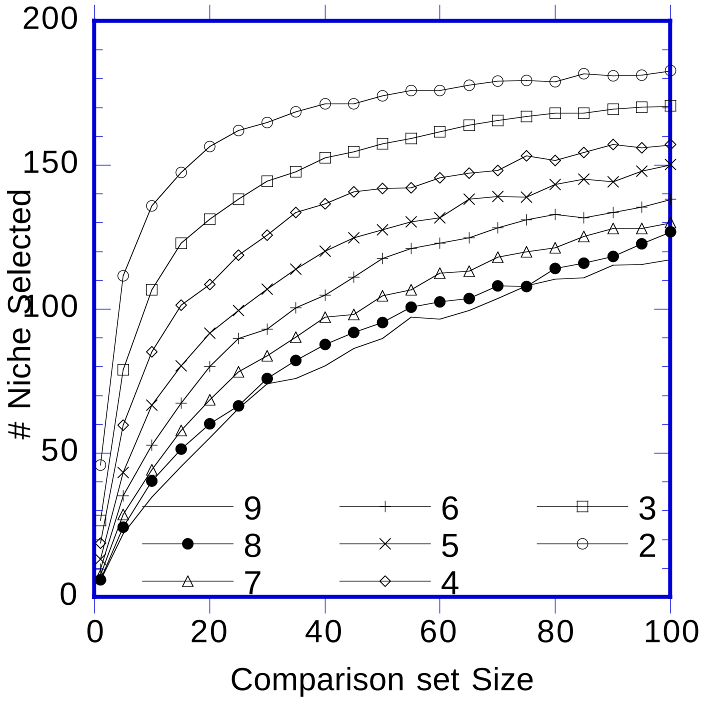


Figure 4) Number niche selected due to each member dominated by the comparison set vs. comparison set size for the niched Pareto GA

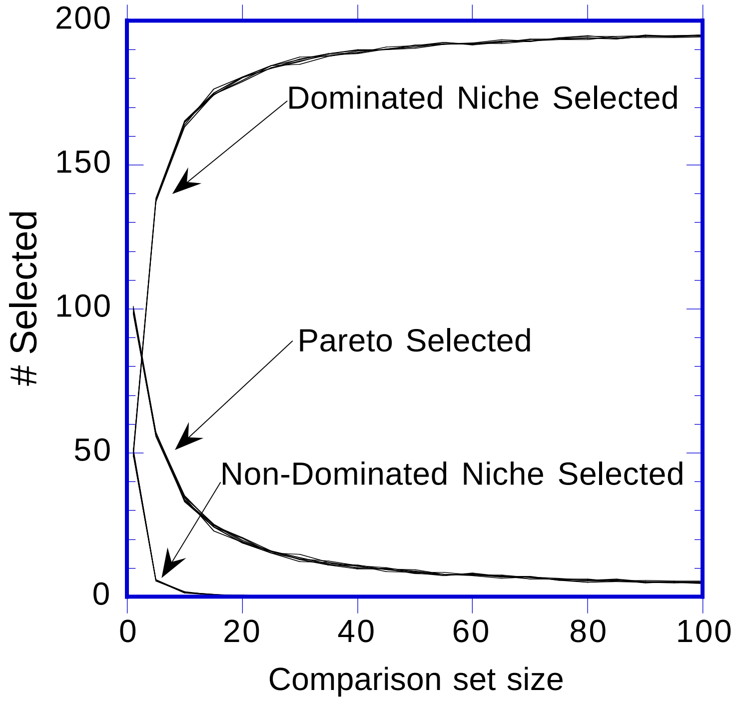


Figure 5) Number of Pareto selections, nondominated niche selection, and dominated niche selections for the fuzzy logic selection procedure.

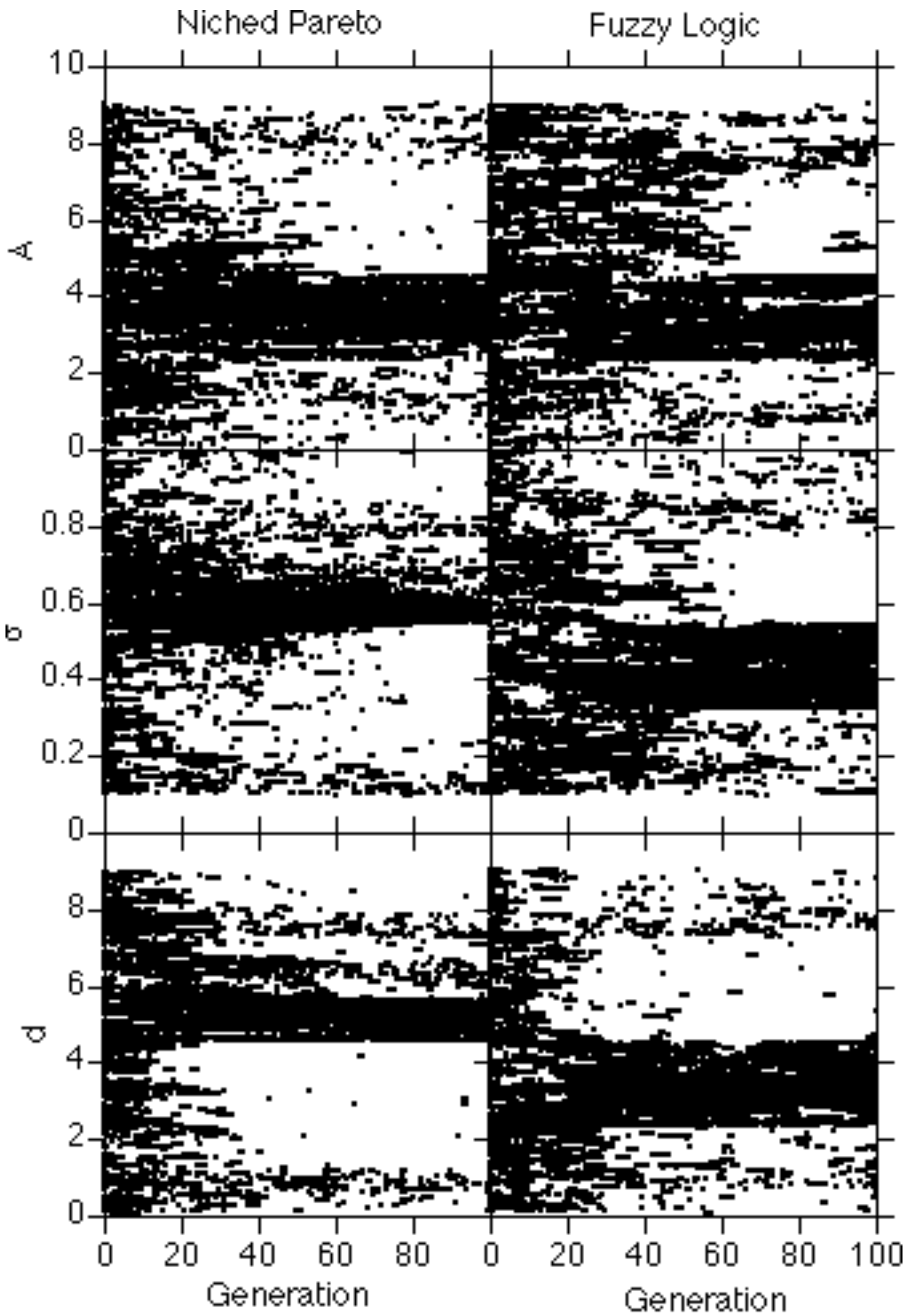


Figure 6) The evolution of the population of parameters *A*, σ, and *d* as a function of generation for the 2 objective niched Pareto GA and fuzzy logic GA.

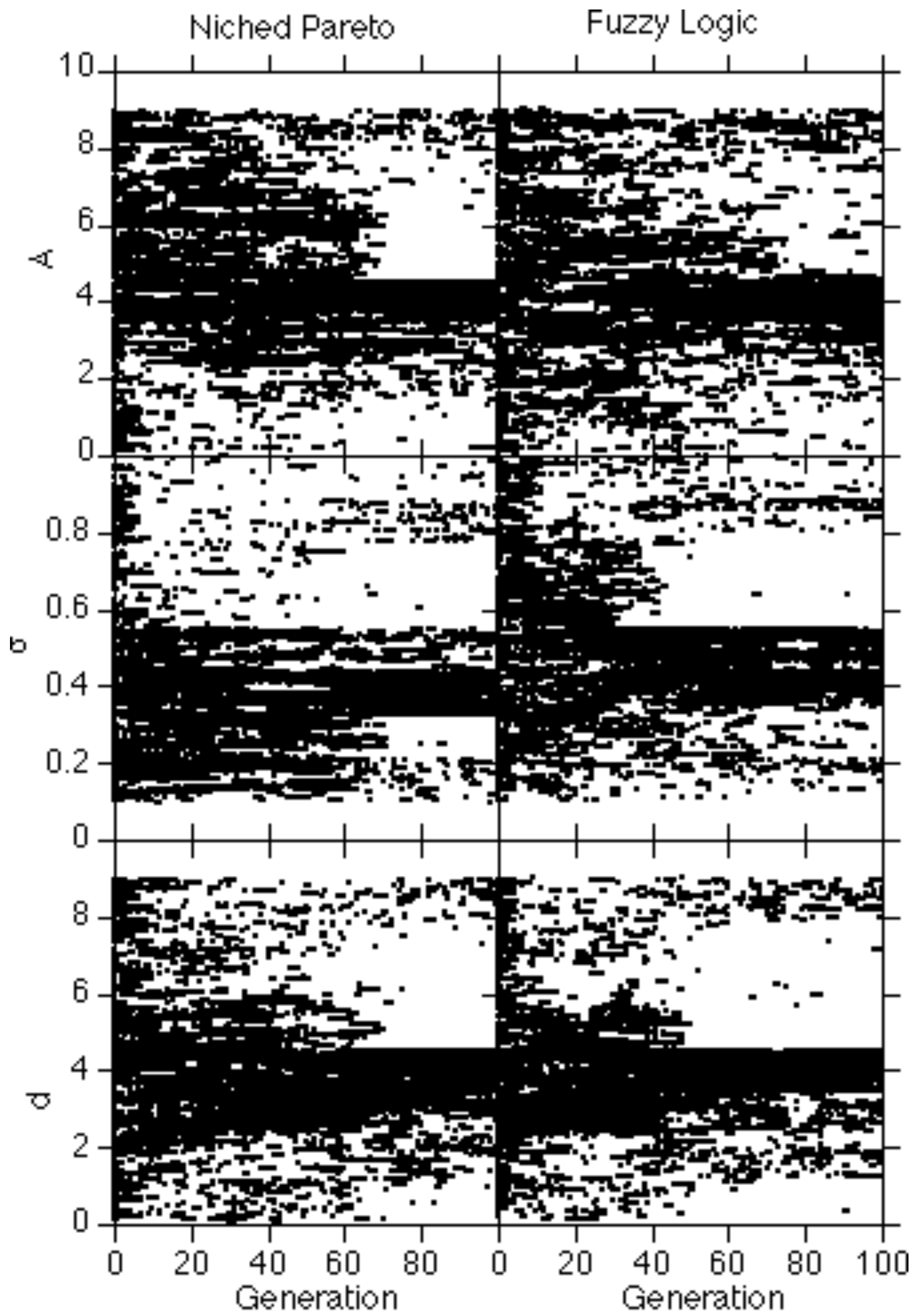


Figure 7) The evolution of the population of parameters *A*, σ, and *d* as a function of generation for the 4 objective niched Pareto GA and fuzzy logic GA.

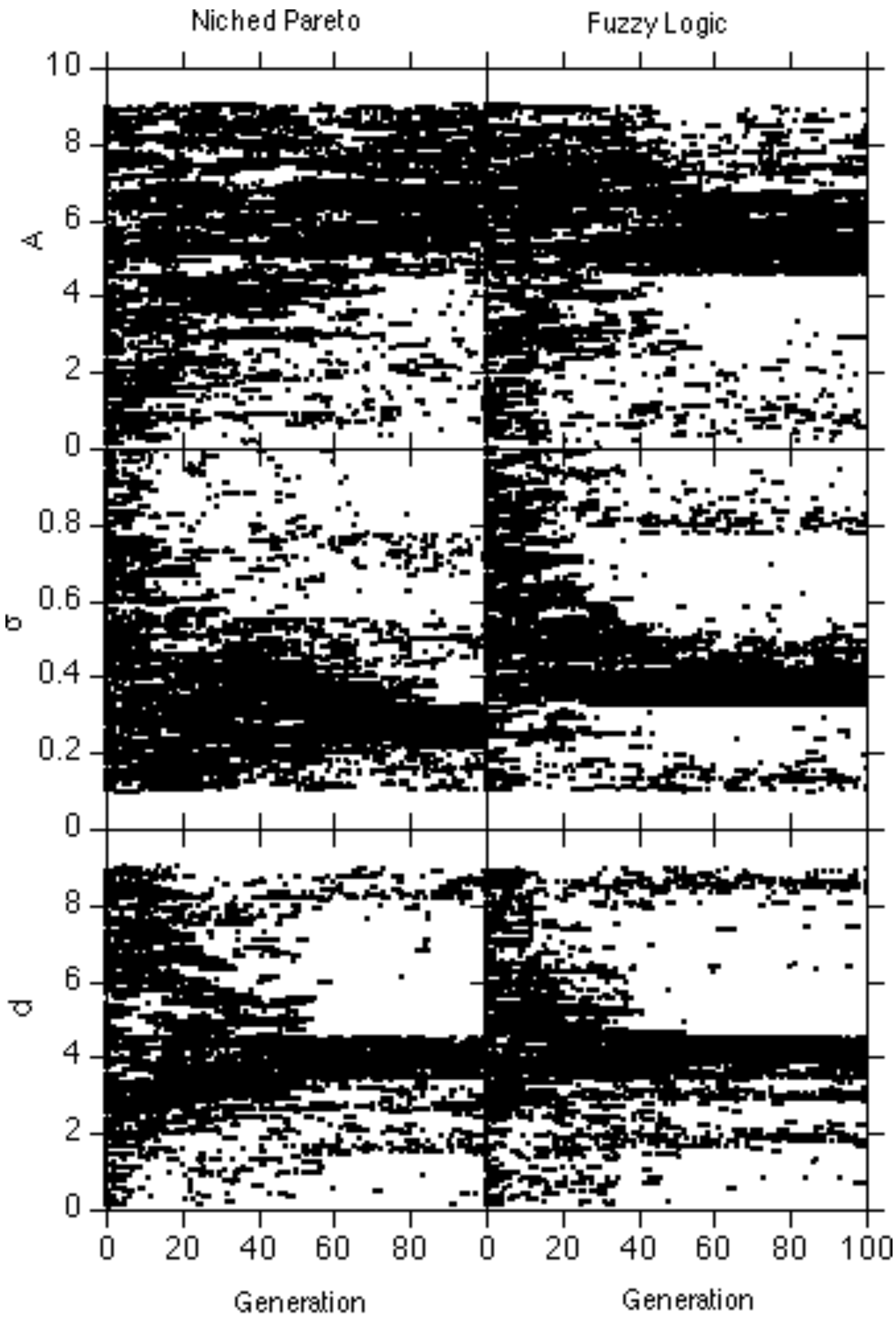


Figure 8) The evolution of the population of parameters *A*, σ, and *d* as a function of generation for the 9 objective niched Pareto GA and fuzzy logic GA.

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