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Decomposable Problems, Niching, and Scalability of Multiobjective Estimation of Distribution Algorithms

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Abstract

The paper analyzes the scalability of multiobjective estimation of distribution algorithms (MOEDAs) on a class of boundedly-difficult additively-separable multiobjective optimization problems. The paper illustrates that even if the linkage is correctly identified, massive multimodality of the search problems can easily overwhelm the niching and lead to exponential scale-up. Facetwise models are subsequently used to propose a growth rate of the number of differing substructures between the two objectives to avoid the niching method from being overwhelmed and lead to polynomial scalability of MOEDAs.

1 Introduction

One of the challenging areas in genetic and evolutionary computation that has received increased attention is multiobjective evolutionary algorithms (MOEAs). Several MOEAs have been proposed and applied with significant success to real-world problems [Deb, 2001, Coello Coello, Van Veldhuizen, & Lamont, 2002]. However, studies on the theory and analysis of MOEAs have been limited in part because of the complexity of both the algorithms and the problems. For example, some aspects of problem difficulty and algorithm scalability have been recently studied [Deb, 1999, Chen, 2004].

Recently, there is a growing interest in extending estimation of distribution algorithms (Pelikan, Lobo, & Goldberg, 2002, Larrañaga & Lozano, 2002)—a class of competent genetic algorithms (Goldberg, 1999) that replace traditional variation operators of genetic algorithms (GAs) with probabilistic model building of promising solutions and sampling the model to generate new offspring—to solve multiobjective search problems quickly, reliably, and accurately. Such multiobjective EDAs (MOEDAs) [Bosman & Thierens, 2002b, Khan, Goldberg, & Pelikan, 2002, Ocenasek, 2002, Ahn, 2005] typically combine the model-building and sampling procedures of EDAs with the selection procedure of MOEAs such as the non-dominated sorting GA (NSGA-II) [Deb, Pratap, Agrawal, & Meyarivan, 2002], and a niching method such as sharing or crowding in objective space. MOEDAs have been shown to significantly outperform traditional MOEAs in
efficiently searching and maintaining Pareto-optimal solutions with high probability on boundedly-difficult problems.

However, the scalability of the population size and the number of function evaluations required by EDAs as a function of problem size and the number of Pareto-optimal solutions has been largely ignored. This is the case even though one of the primary motives for designing MOEDAs is to carry over the polynomial (oftentimes sub-quadratic) scalability of EDAs to boundedly-difficult multiobjective search problems. Therefore, we investigate the scalability of EDAs—specifically multiobjective extended compact GA (meCGA) and multiobjective Bayesian optimization algorithm (mBOA) (Khan, Goldberg, & Pelikan, 2002)—on a class of boundedly-difficult additively-separable problems. We demonstrate the even if the sub-structures (or linkages) are correctly identified, massive multimodality of search problems can overwhelm the niching capability and lead to exponential scalability. Using facetwise models we predict the

The paper is organized as follows. We provide a brief background on the MOEAs, particularly NSGA-II, and MOEDAs, specifically, meCGA. The details on the test problems and experimental methodologies are described in section 3. Section 4 presents the scalability results of MOEDAs on a class of boundedly-difficult additively-decomposable multiobjective problems. Subsequently, we demonstrate how massive multimodality of the search problem can overwhelm the niching mechanism and lead to exponential scale-up in section 4.2. In section 4.3, using facetwise models of population-sizing for EDAs and niching methods, we propose a method to predict the growth rate of the number of sub-structures to circumvent the niching from being overwhelmed and lead to polynomial scalability. Finally, we present key conclusions of the study.

2 Background

In this section we briefly review work on multiobjective evolutionary algorithms, specifically NSGA-II. We also outline previous work on multiobjective estimation of distribution algorithms and describe two MOEDAs that we studied.

2.1 Multiobjective Evolutionary Algorithms (MOEAs)

Unlike traditional search methods genetic and evolutionary algorithms are naturally suited for multiobjective optimization as they can process a number of solutions in parallel and find all or majority of the solutions in the Pareto-optimal front. Based on Goldberg’s (Goldberg, 1989) suggestion of implementing a selection procedure that uses the non-dominance principle, many MOEAs have been proposed (Horn, Nafpliotis, & Goldberg, 1994; Srinivas & Deb, 1995; Fonseca & Fleming, 1993; Deb, Pratap, Agrawal, & Meyarivan, 2002; Zitzler, Laumanns, & Thiele, 2001; Corne, Jerram, Knowles, & Oates, 2001; Van Veldhuizen & Lamont, 2000; Zydallis, Van Veldhuizen, & Lamont, 2001). A detailed survey of various MOEAs is out of the scope of this study and the interested users should refer to (Deb, 2001; Coello Coello, Van Veldhuizen, & Lamont, 2002) and the references therein. Since the selection and niching procedure of NSGA-II are used in the MOEDAs used in this study, we describe them in the following paragraphs.

The selection procedure of NSGA-II consists of three elements:

Non-Dominated sorting: Which sorts assigns domination ranks to individuals in the population based on their multiple objective values. A candidate solution X dominates Y, if X is no worse than Y in all objectives and if X is better than Y in at least one objective. In non-dominated sorting, we start with the set of solutions that are not dominated by any solution in the population and assign them rank 1. Next, solutions that are not dominated by any of the remaining solutions are
assigned rank 2. That is, all solutions with rank 2 are dominated by at least one solution with rank 1, but are not dominated by others in the population. Thus the sorting and ranking process continues by assigning increasing ranks to those solutions that are not dominated by any of the remaining unranked solutions. After non-dominated sorting, we are left with subsets of population with different ranks. Solutions with a given rank are not dominated by solutions that have the same rank or higher and are dominated by at least one solution with a lower rank. Therefore, with respect to Pareto optimality, solutions with lower ranks should be given priority.

**Crowding distance computation:** Apart from finding solutions in the Pareto front, it is also essential to achieve good coverage or spread of solutions in the front. The diversity of solutions in the objective space is usually maintained with a niching mechanism and NSGA-II uses crowding for doing so. Each solution in the population is assigned a crowding distance, which estimates how dense the non-dominated front is in the neighborhood of the solution. Therefore, the higher the crowding distance of the solution, the more diverse the solution is in the non-dominated front. The pseudocode for computing the crowding distance is outlined below:

```pseudocode
crowding_distance_computation(P)
for rank r = 1 to R
  P_r = subset of solutions in P with rank r
  n_r = size(P_r)
  for i = 1 to n_r
    d_c(P_r(i)) = 0
  for j = 1 to M
    Q_r = sort P_r using jth objective, f_j.
    d_c(Q_r(1)) = d_c(Q_r(n_r)) = ∞
    for i = 2 to n_r-1
      dist = Q_r(i+1).f_j - Q_r(i-1).f_j
      d_c(Q_r(i)) = d_c(Q_r(i)) + dist
  return d_c
```

where, P is the population, R is the maximum rank assigned in the population, M is the number of objective, and Q_r(i).f_j is the value of jth objective of the ith individual.

**Individual comparison operator:** NSGA-II uses a custom comparison operator to compare the quality of two solutions and to select the better individual. Both the rank and the crowding distance of the two solutions are used in the comparison operator, a pseudo-code of which is given below. First, the rank of the two individuals are considered and the solution with a lower rank is selected. If the two individuals have the same rank, then the solution with the highest crowding distance is selected.

```pseudocode
compare(X,Y)
if rank(X) < rank(Y) then return X
if rank(X) > rank(Y) then return Y
if rank(X) = rank(Y)
  if d_c(X) > d_c(Y) then return X
  if d_c(X) < d_c(Y) then return Y
  if d_c(X) = d_c(Y)
    then randomly choose either X or Y
```

3
2.2 Multiobjective Estimation of Distribution Algorithms (MOEDA)

Similar to single-objective EDAs (Pelikan, Lobo, & Goldberg, 2002; Larrañaga & Lozano, 2002), multiobjective EDAs replace the variation operators of MOEAs with the probabilistic model building of promising solutions and sampling the model to generate new offspring. Recently, several MOEDAs have been proposed (Bosman & Thierens, 2002b; Khan, Goldberg, & Pelikan, 2002; Ocenasek, 2002; Khan, 2002; Bosman & Thierens, 2002a; Laumanns & Ocenasek, 2002; Ahn, 2005) which have combined variants of the Bayesian optimization algorithm (BOA) (Pelikan, Goldberg, & Cantú-Paz, 2000) and iterated density estimation algorithm (IDEA) (Bosman & Thierens, 1999; Bosman & Thierens, 2000) with the selection and replacement procedures of MOEAs.

Khan et al. (Khan, Goldberg, & Pelikan, 2002; Khan, 2002) proposed multiobjective BOA (mBOA) and multiobjective hierarchical BOA (mhBOA) by combining the model building and model sampling procedures of BOA and hierarchical BOA (hBOA) (Pelikan & Goldberg, 2001) with the selection procedure of NSGA-II. They compared the performance of mBOA and mhBOA with those of NSGA-II on a class of boundedly-difficult additively-separable deceptive and hierarchically deceptive functions. Laumanns and Ocenasek (Laumanns & Ocenasek, 2002; Ocenasek, 2002) combined mixed BOA with the replacement procedure of strength Pareto evolutionary algorithm (SPEA2) (Zitzler, Laumanns, & Thiele, 2001) and compared it with NSGA-II and SPEA2 on knapsack problems. Ahn (Ahn, 2005) combined real-coded BOA with selection procedure of NSGA-II with a sharing intensity measure and a modified crowding distance metric.

Bosman and Thierens (Bosman & Thierens, 2002b; Bosman & Thierens, 2002a) combined IDEAs and mixed IDEAs with non-dominated tournament selection and clustering. In contrast to other MOEDAs, they used clustering to split the population into sub-population and separate models were built for each sub-population. They used the clustering procedure primarily to obtain a good model of the selected population, but recently it has been shown that it is one of the essential components in obtaining a scalable MOGA in general, and MOEDA in particular (Pelikan, Sastry, & Goldberg, 2005).

In this study, we use mBOA and the multiobjective extended compact GA and test their scalability on a class of boundedly-difficult problems. The multiobjective extended compact genetic algorithm (meCGA) is similar to mBOA (Khan, Goldberg, & Pelikan, 2002), except that the model building and sampling procedure of BOA is replaced with those of extended compact GA (eCGA) (Harik, 1999). The meCGA is used in this study in part because the simplicity of the probabilistic model and its direct mapping to linkage groups makes it amenable to systematic analysis. The typical steps of meCGA can be outlined as follows:

1. **Initialization**: The population is usually initialized with random individuals. However, other initialization procedures can also be used in a straightforward manner.

2. **Evaluation**: The fitness or the quality-measure of the individuals are computed.

3. **Selection**: As in mBOA, we use the selection procedure of NSGA-II. That is, we first perform the non-dominated sorting, and compute the crowding distance for all the individuals in the population. We then use the individual comparison operator to *bias* the generation of new individuals.

4. **Probabilistic model estimation**: Unlike traditional GAs, however, EDAs assume a particular probabilistic model of the data, or a *class* of allowable models. A *class-selection metric* and a *class-search mechanism* is used to search for an optimum probabilistic model that represents the selected individuals.
Model representation: The probability distribution used in eCGA is a class of probability models known as marginal product models (MPMs). MPMs partition genes into mutually independent groups and specifies marginal probabilities for each linkage group.

Class-Selection metric: To distinguish between better model instances from worse ones, eCGA uses a minimum description length (MDL) metric (Rissanen, 1978). The key concept behind MDL models is that all things being equal, simpler models are better than more complex ones. The MDL metric used in eCGA is a sum of two components:

- **Model complexity** which quantifies the model representation size in terms of number of bits required to store all the marginal probabilities:

  \[ C_m = \log_2(n) \sum_{i=1}^{m} \left( 2^{k_i} - 1 \right). \] (1)

  where \( n \) is the population size, \( m \) is the number of linkage groups, \( k_i \) is the size of the \( i^{th} \) group.

- **Compressed population complexity**, which quantifies the data compression in terms of the entropy of the marginal distribution over all partitions.

  \[ C_p = n \sum_{i=1}^{m} 2^{k_i} \sum_{j=1}^{2^{k_i}} -p_{ij} \log_2(p_{ij}), \] (2)

  where \( p_{ij} \) is the frequency of the \( j^{th} \) gene sequence of the genes belonging to the \( i^{th} \) partition.

Class-Search method: In eCGA, both the structure and the parameters of the model are searched and optimized to best fit the data. While the probabilities are learnt based on the variable instantiations in the population of selected individuals, a greedy-search heuristic is used to find an optimal or near-optimal probabilistic model. The search method starts by treating each decision variable as independent. The probabilistic model in this case is a vector of probabilities, representing the proportion of individuals among the selected individuals having a value ‘1’ (or alternatively ‘0’) for each variable. The model-search method continues by merging two partitions that yields greatest improvement in the model-metric score. The subset merges are continued until no more improvement in the metric value is possible.

5. Offspring creation: New individuals are created by sampling the probabilistic model. The offspring population are generated by randomly generating subsets from the current individuals according to the probabilities of the subsets as calculated in the probabilistic model.

6. Replacement: We use two replacement techniques in this study: (1) Restricted tournament replacement (RTS) (Harik, 1995) in which offspring replaces the closest individual among \( w \) individuals randomly selected from the parent population, only if the offspring is better than the closest parent. (2) Elitist replacement used in NSGA-II, in which the parent and offspring population are combined. The domination ranks and crowding distances are computed on the combined population. Individuals with increasing ranks are gradually added starting from those with the lowest rank into the new population till its size reaches to \( n \). However, if it is not possible to add all the solutions belonging to a particular rank without increasing the population size to greater than \( n \), then individuals with greater crowding distances are preferred.

7. Repeat steps 2–6 until one or more termination criteria are met.
3 Experiments

As mentioned earlier, one of the purposes of this study is to investigate the scalability of MOEDAs, particularly meCGA and mBOA, on a class of boundedly-difficult multiobjective problems. In this section, we describe the test functions used to test the scalability and the methodology used in obtaining the empirical results.

3.1 Test Problems

Our approach in verifying the performance of sub-structural niching is to consider bounding adversarial problems that exploit one or more dimensions of problem difficulty (Goldberg, 2002). Particularly, we are interested in problems where building-block identification is critical for the GA success. Additionally, the problem solver (eCGA) should not have any knowledge of the building-block structure of the test problem, but should be known to researchers for verification purposes.

One such class of problems is the m-k deceptive trap problem, which consists of additively separable deceptive functions (Ackley, 1987; Goldberg, 1987; Deb & Goldberg, 1992). Deceptive functions are designed to thwart the very mechanism of selectorecombinative search by punishing any localized hillclimbing and requiring mixing of whole building blocks at or above the order of deception. Using such adversarially designed functions is a stiff test—in some sense the stiffest test—of algorithm performance. The idea is that if an algorithm can beat an adversarially designed test function, it can solve other problems that are equally hard or easier than the adversarial function.

In this study, we use a class of test problems with two objectives: (1) m-k deceptive trap, and (2) m-k deceptive inverse trap. String positions are first divided into disjoint subsets or partitions of $k$ bits each. The $k$-bit trap and inverse trap are defined as follows:

\[
\text{trap}_k(u) = \begin{cases} 
1 & \text{if } u = k \\
(1 - d) \left[1 - \frac{u}{k-1}\right] & \text{otherwise}
\end{cases},
\]

\[
\text{invtrap}_k(u) = \begin{cases} 
1 & \text{if } u = 0 \\
(1 - d) \left[\frac{u}{k-1}\right] & \text{otherwise}
\end{cases},
\]

where $u$ is the number of 1s in the input string of $k$ bits, and $d$ is the signal difference. Here, we use $k = 3, 4, \text{ and } 5$, and $d = 0.9, 0.75, \text{ and } 0.8$ respectively.

The m-k trap and inverse trap functions have conflicting objectives. Any solution that sets the bits in each partition either to 0s or 1s is Pareto optimal and thus there are a total of $2^m$ solutions in the Pareto-optimal front with $m + 1$ distinct points in the objective space. We investigate the scalability of MOEAs and consider the population size and number of function evaluations required to maintain at least one copy of all the representative Pareto-optimal solutions.

To illustrate, how additively decomposable problems with conflicting objectives can overwhelm the niching mechanism used in MOEAs—irrespective of linkage adaptation capabilities of the evolutionary algorithm—and lead to exponential scalability, we consider a problem where linkage learning is not required. Specifically, we consider the OneMax-ZeroMax problem which is similar to bicriteria OneMax problem used by Chen for developing facetwise models of population sizing and convergence time (Chen, 2004). In OneMax-ZeroMax problem, the task is to maximize two objectives, one which is the sum of all the bits with value 1, and the other is the sum of all the bits.
with value 0:

\[
f_{\text{OneMax}}(X) = \sum_{i=1}^{\ell} x_i,
\]

\[
f_{\text{ZeroMax}}(X) = \sum_{i=1}^{\ell} (1 - x_i),
\]

where \( \ell \) is the problem size, and \( x_i \) is the value of the \( i^{\text{th}} \) bit of a candidate solution \( X \).

### 3.2 Methodology

We tested the scalability of the following MOEAs: (1) Univariate marginal distribution algorithm (UMDA) ([Mühlenbein & Paß, 1996]), (2) NSGA-II with two-point crossover and bit-flip mutation, (3) meCGA, and (4) mhBOA. For each recombination operator, both elitist replacement of NSGA-II and restricted tournament replacement were used.

For all test problems and algorithms, different problem sizes were examined to study scalability. For each problem type, problem size, and algorithm, a bisection method was used to determine a minimum population size to allocate at least one individual to each representative solution in the Pareto front. As mentioned earlier, for the test problems we consider in this study, for an \( \ell \)-bit problem—where \( \ell = m \cdot k \)—there are \( 2^m \) Pareto-optimal solutions with \( m + 1 \) distinct objective value pairs. In this study, we investigate the population size required to (1) find at least one copy of all the \( 2^m \) Pareto-optimal solution, and (2) find at least one copy of the \( m + 1 \) distinct points in the Pareto-optimal front. That is, we consider Pareto-optimal solutions with the same values of both objectives to be equivalent.

The probability of maintaining at least one copy of all the representative Pareto-optimal solutions at a given population size is computed by averaging 10–30 independent MOEA runs. The minimum population size required to maintain at least one copy of all the representative solutions in the Pareto front are averaged over 10-30 independent bisection runs. Therefore, the results for each problem type, problem size, and algorithm correspond to 100–900 independent GA runs. The number of generations for UMDA, meCGA, and mhBOA was bounded by \( 5\ell \), whereas the runs with NSGA-II were given at most \( 10\ell \) or \( 20\ell \) generations because of their slower convergence.

### 4 Results

We described the test problems and the experimental methodology used in testing the scalability of MOEDAs in the previous section. In this section we present the scalability results, followed by a demonstration of how multiobjective problems with conflicting sub-substructures can overwhelm the niching mechanism and lead to exponential scale-up. Finally, we use facetwise models of population sizing as dictated by model building, decision making, and supply ([Sastry & Goldberg, 2004][Pelikan, Sastry, & Goldberg, 2003]), and niching ([Mahfoud, 1994]) to estimate the growth rate of conflicting sub-structures that circumvents the niching method from being overwhelmed and leads to polynomial scalability.

#### 4.1 Scalability of MOEDAs

We measure the algorithm performance in terms of minimum number of function evaluations required to find and maintain at least one copy of all the representative Pareto-optimal solutions.
Figure 1: Scalability of meCGA with Crowding and with RTS for the m-3 deceptive trap and inverse trap with the problem size. Here, we plot the minimum number of function evaluations required to search and maintain at least one copy of (a) all the $2^m$ solutions in the Pareto-optimal front, and (b) only the $m + 1$ solutions in the Pareto-optimal front with different objective-value pairs. Here, we treat the genotypically (and phenotypically) different Pareto-optimal solution with same values in both objectives to be equivalent.

Even though we have tried m-k deceptive trap and inverse trap functions for $k = 3, 4$, and 5, for brevity, we only show results for $k = 3$ in this paper. However, we note that the results for other values of $k$ are qualitatively similar and those for $k = 3$ are representative of the behavior of the MOEAs.

Figure 1(a), shows the scalability of meCGA with the problem size for m-3 deceptive trap and inverse trap problem. We plot the minimum number of function evaluations required to allocate at least one copy of all the solutions in the Pareto-optimal front. As shown in the figure, all algorithms scale-up exponentially. The scale-up does not improve even if we restricted the requirement to finding only those $m + 1$ Pareto-optimal solutions with different objective-value pairs as shown in Figure 1(b). That is, even if we consider genotypically (and phenotypically) distinct solutions that have the same value in both objectives to be equivalent, all the algorithms scale exponentially. This is despite the linkage information being identified correctly by meCGA and mhBOA and tight linkage assumption for NSGA-II. Additionally, the scalability does not improve if the niching or speciation is performed in the objective space (as in NSGA-II) or in the variable space (as in restricted tournament selection).

Therefore, the exponential scale-up is not due to incorrect linkage identification and mixing (Goldberg, Thierens, & Deb, 1993; Thierens & Goldberg, 1993; Thierens, 1999), but because the niching mechanism gets quickly overwhelmed due to the exponential growth in the number of Pareto-optimal solutions. Furthermore, the distribution of the $2^m$ solutions in the Pareto-optimal front is not uniform. There are exponentially as many solutions in the middle of the front than at the edges (see table 1). That is, there is only one solution—a binary string with all 0s and all 1s—at each extreme of the Pareto-optimal front. In contrast, there are $\binom{m}{m/2} \approx O(e^m)$ genotypically different solutions in the middle of the Pareto-optimal front with same values in both objectives.
Table 1: Distribution of genotypically and phenotypically different solutions in the Pareto-optimal front with same values in both objectives. $n_{1, BBs}$ refers to the number of $k$-bit partitions (sub-structures) with 1s and $n_{0, BBs}$ is the number of $k$-bit partitions with 0s.

![Image of Table 1]

Figure 2: Probability of finding and maintaining different solutions on the Pareto-optimal for the 10-3 deceptive trap and inverse trap problem as a function of population size.

This highly non-linear distribution of solutions in the Pareto-front has two effects on the niching mechanisms used in MOEAs in general, and MOEDAs in particular:

- Since the extremes of the Pareto-optimal front (maximizing most partitions or sub-structures with respect to one particular objective) has exponentially smaller representatives than in the middle, it takes exponentially longer time, or exponentially larger population size (Goldberg, 2002; Thierens, 1999) to search and maintain the solutions at the extremes of the Pareto-optimal front. When the population size is fixed, the probability of maintaining a solution in the middle of the Pareto-optimal front is higher than doing so in extremes of the front, as shown in figure 2.

- Since there are multiple points that are genotypically and phenotypically different, but lie on the same point on the Pareto-optimal front (the solutions have same values in both objectives), some of them vanish over time due to drift. The drift affects both the solutions in the middle and the near extremes of Pareto-optimal front.
Problem size, \( l \)

Number of function evaluations, \( n_{fe} \)

NSGA-II: \( O(2^{1.03m}) \)

UMDA + RTS: \( O(2^{0.92m}) \)

Figure 3: Scalability of NSGA-II and UMDA on the OneMax-ZeroMax problem. Both algorithms with two different niching methods scale-up exponentially with the problem size.

4.2 Overwhelming the Niching Method

To better illustrate how sub-structure competition in all the partitions of a decomposable problem can lead to niching overwhelm, we use the OneMax-ZeroMax problem. We specifically choose the OneMax-ZeroMax problem to isolate the effect of linkage identification or lack thereof from those of the niching methods on the scalability of the MOEAs. Unlike the m-k deceptive trap and inverse trap function, linkage identification is not necessary for the OneMax-ZeroMax problem. Furthermore, both OneMax and ZeroMax problems are GA-easy problems which a simple selectorecombinative GA with uniform crossover and tournament selection can solve in linear time. In contrast, MOEAs scale-up exponentially in solving OneMax and ZeroMax as shown in figure 3.

The results clearly indicate how the niching methods—both those that work in parameter space (RTS) and those that work in objective space (Crowding)—get overwhelmed due to exponentially large number of solutions in the Pareto-optimal front. Additionally, the results also show that even if the requirement is relaxed by treating all the different points that lie on the same point in the Pareto-optimal front to be equivalent, the scale-up does not improve. Finally, the results suggest that in decomposable problems, if all or majority of the sub-structures compete in the two objectives, then the niching method fails to maintain good coverage, leading to exponential scale-up.

4.3 Circumventing the Burden on the Niching Method

The results in the previous two sections clearly indicate that MOEDAs with either RTS or crowding mechanism of NSGA-II scale-up exponentially with problem size. We also demonstrated that the exponential scalability is due to the niching method being overwhelmed because of exponentially large number of solutions in the Pareto-optimal front. One way to circumvent the niching method from being overwhelmed is to control the growth rate of the number of sub-structures that compete in the two objectives, \( m_d \). That is, for a problem with \( m \) sub-structures, the two objectives compete in only \( m_d \) sub-structures and share the same \( m - m_d \) sub-structures. Since the total number of
Pareto-optimal solutions, \( n_{opt} = 2^m_d \), by controlling the number of competing sub-structures, we implicitly control the total number of Pareto-optimal solutions.

The growth-rate of the competing sub-structures should be such that the effect of model accuracy, decision making, and sub-structure supply on the population sizing is dominant over the effect of niching on the population size. The effect of model accuracy, decision making and sub-structure supply on the population sizing of EDAs is given by \( \text{Pelikan, Sastry, & Goldberg, 2003, Sastry & Goldberg, 2004} \):

\[
 n_{eda} \propto c_1 \cdot 2^k \cdot m \log m. \tag{7}
\]

The effect of niching method on the population-sizing of GAs was modeled by Mahfoud \( \text{Mahfoud, 1994} \) and is reproduced below:

\[
 n_{niching} \propto \frac{\log \left( \left( 1 - \gamma^{1/t} \right) / n_{opt} \right)}{\log \left( (n_{opt} - 1) / n_{opt} \right)} \approx c_2 \cdot 2^m_d, \tag{8}
\]

where \( t \) is the number of generations we need to maintain all the niches. While Mahfoud derived the population-sizing estimate for fitness-sharing method, it is generally applicable to other niching methods and MOEAs as well \( \text{Reed, 2002, Khan, 2002} \).

To circumvent the niching method from being overwhelmed we require \( n_{eda} \geq n_{niching} \). That is,

\[
 c_2 \cdot 2^m_d \geq c_1 \cdot 2^k \cdot m \log m. \tag{9}
\]

The above equation can be approximated \(^1\) to obtain a conservative estimate of the maximum number of competing sub-structures that circumvent the niching mechanism from being overwhelmed is given by:

\[
 m_d \approx k + \log_2(m). \tag{10}
\]

The above growth rate is compared to empirical results for different values of \( k \) as a function of total number of sub-structures in the problem and the results are shown in figure 5. As shown in figure 5 the results indicate that once the growth-rate of competing sub-structures are controlled, the MOEDAs scale-up polynomially with the problem size, even on the OneMax-ZeroMax problem.

5 Summary and Conclusions

In this paper, we studied the scalability of multiobjective estimation of distribution algorithms (MOEDAs), specifically multiobjective extended compact genetic algorithm (meCGA) and multi-objective hierarchical Bayesian optimization algorithm (mhBOA), on a class of boundedly-difficult additively separable problems. We observed that even when the linkages were correctly identified, the MOEDAs scaled-up exponentially with problem size due to failure in the niching mechanisms. We demonstrated that even if the linkage is correctly identified, massive multimodality of the search problems can easily overwhelm the nichers and lead to exponential scale-up. That is, in decomposable problems, if majority or all the sub-structures compete in different objectives, then the number of Pareto-optimal solutions increase exponentially. This exponential increase overwhelms the nichers and causes significant problems in maintaining a good coverage of the Pareto-optimal front. Finally, using facetwise models that incorporate the combined effects of model accuracy, decision making, and sub-structure supply, and the effect of niching on the population sizing, we proposed a growth rate of maximum number of sub-structures that can compete in the two objectives to circumvent...

\(^1\)we neglect the \( \log_2 \left( \frac{c_1 \log m}{c_2} \right) \) term.
Figure 4: The growth rate of number of sub-structures that compete in the two objectives for different values of $k$ as a function of total number of sub-structures.

\[ d_k = 1, 3, 4, 5 \]

Figure 5: The scalability of meCGA with the crowding mechanism of NSGA-II and RTS niching for both OneMax-ZeroMax and m-3 deceptive trap and inverse trap problems. The growth rate of number of sub-structures that compete in the two objectives for a given problem size is controlled as given by equation 10.
the failure of the niching method. Once the growth-rate of the number of Pareto-optimal solutions are controlled, the MOEDAs scale-up polynomially with the problem size.

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Number of building blocks, \( m \)

Number of function evaluations, \( n_{fe} \)

- meCGA + Crowding: \( O(m^{4.03}) \)
- meCGA + RTS: \( O(m^{3.91}) \)
Number of building blocks, $m$

Number of function evaluations, $n_{fe}$

- meCGA + Crowding: $O(m^{5.96})$
- meCGA + RTS: $O(m^{5.46})$
Probability of finding the optima

$n = 50$

$n = 100$

$n = 250$