Applying a Hybrid Targeted Estimation of Distribution Algorithm to Feature Selection Problems

Geoffrey Neumann and David Cairns
Computing Science and Mathematics, University of Stirling, Stirling, U.K.

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Abstract: This paper presents the results of applying a hybrid Targeted Estimation of Distribution Algorithm (TEDA) to feature selection problems with 500 to 20,000 features. TEDA uses parent fitness and features to provide a target for the number of features required for classification and can quickly drive down the size of the selected feature set even when the initial feature set is relatively large. TEDA is a hybrid algorithm that transitions between the selection and crossover approaches of a Genetic Algorithm (GA) and those of an Estimation of Distribution Algorithm (EDA) based on the reliability of the estimated probability distribution. Targeting the number of features in this way has two key benefits. Firstly, it enables TEDA to efficiently find good solutions for cases with low signal to noise ratios where the majority of available features are not associated with the given classification task. Secondly, due to the tendency of TEDA to select the smallest promising feature sets, it builds compact classifiers and is able to evaluate populations more quickly than other approaches.

1 INTRODUCTION

Classification problems concern the task of sorting samples, defined by a set of features, into two or more classes. Feature Subset Selection (FSS) is the process by which redundant or unnecessary features are removed from consideration (Dash et al., 1997). Reducing the number of redundant features used is vital as it may improve classification accuracy, allow for faster classification and enable a human expert to focus on the most important features (Saeys et al., 2003) (Inza et al., 2000). We therefore approach the problem of FSS with two objectives: to develop a FSS algorithm that is able to find feature subsets that are as small as possible while also enabling samples to be classified with as great an accuracy as possible.

Evolutionary Algorithms (EAs) have often been applied to FSS problems. An EA is a heuristic technique where a random population of potential solutions is generated and then combined based on a fitness score to produce new solutions. Due to their population based nature they are able to investigate multiple possible sets of features simultaneously.

GAs and EDAs have previously been explored for FSS problems. Inza (Inza et al., 2000) introduced the concept of using EDAs for feature selection. He compared an EDA to both traditional hill climbing approaches (Forward Selection and Recursive Feature Elimination) and GAs and found that an EDA was able to find more effective feature sets than any of the techniques that it was compared against (Inza et al., 2001). Cantu-Paz (Cantu-Paz, 2002) demonstrated that both GAs and EDAs were equally capable of solving FSS problems but that a simple GA was faster at finding good solutions than EDAs.

Many investigations of FSS problems looked at problems with fewer than 100 features. However, many real world problems involve significantly larger feature sets. We therefore explore applying EAs to problems with between 500 and 20,000 features. For these problems the initial number of features is so large that complex EDA approaches are impractical (Inza et al., 2001). Many of these problems are very noisy and only a small proportion of the features are useful (Guyon et al., 2004). For problems which are so noisy that only a tiny proportion of features are useful, driving down the size of the feature set is an important part of the optimization process.

To achieve this objective, techniques such as constraining the number of features and then iteratively removing features to fit within this constraint have been explored (Saeys et al., 2003). This is problematic as it requires previous knowledge of the problem. In this work, we demonstrate a hybrid approach that utilises the advantages of both of EDAs and GAs and is designed to automatically drive down the number of

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features to consider by monitoring chromosome variance across the population.

Targeted EDA (TEDA) predicts the optimal number of features to solve a problem from the number found in high quality solutions. This process is called 'targeting' and was initially developed for Fitness Directed Crossover (FDC) (Godley et al., 2008). Previous work has shown that TEDA is effective at solving 'bang bang control' problems where there is a concept of parameters or features being either 'on' or 'off' and where a key consideration is the total number of variables that are 'on' in a solution (Neumann and Cairns, 2012a; Neumann and Cairns, 2012b).

TEDA transitions over time from initially operating like a GA to operating like an EDA. The transition occurs as the population starts to converge and the probability distribution becomes more reliable. This paper addresses whether TEDA can use this capability to determine the number of features needed to solve a FSS problem and so effectively find both small and accurate feature subsets.

We begin this paper with a discussion of the background to this research area, introducing existing FSS and classification techniques. We then introduce TEDA in Section 2.1. The final three sections are used for explaining our methodology (Section 3), presenting our results (Section 4), and exploring any conclusions drawn (Section 5).

2 BACKGROUND

A typical classification problem will involve constructing a classifier based on samples in a training set where the class that a given sample belongs to is already known. New samples are then classified based on the information extracted from the training set.

Popular approaches include K Nearest Neighbour (KNN) (Keller et al., 1985) and Support Vector Machines (SVM). In KNN the k individuals in the training set that are most similar to the new sample are used to determine the new sample's class. SVM is a classification technique where two classes are distinguished by determining the hyperplane that separates the instances of each class by the greatest margin.

Feature Subset Selection (FSS) involves the identification of the minimum number of features that will most accurately classify a given set of samples. As there are 2^n possible subsets of a feature set of length n an exhaustive search is not possible and so various search heuristics have been developed (Dash et al., 1997). Techniques can be divided into filter and wrapper methods (Lai et al., 2006). Filters build feature sets by calculating the capacity of features to separate classes whereas wrappers use the final classifier to assess complete feature sets. Wrapper methods can be more powerful than filter methods because they consider multiple features at once and yet they tend to be more computationally expensive (Guyon et al., 2004). This paper focusses on wrapper methods.

Some state of the art methods include Forward Selection (FS) and Recursive Feature Elimination (RFE) (Lai et al., 2006). In Forward Selection the most informative feature is selected to begin with. After this a greedy search is carried out and the second most informative feature is added. This process is repeated until a feature set of size L, a pre-specified limit, is reached. In Reverse Feature Elimination an SVM initially attempts to carry out classification using the entire feature set. The SVM assigns a weight to each feature and the least useful features are eliminated. Both of these techniques suffer from a similar disadvantage. In FS, a selected feature cannot later be eliminated and in RFE an eliminated feature cannot later be selected (Pudil et al., 1994). This prevents the techniques from carrying out further exploration once a solution has been discovered.

2.1 Evolutionary Algorithms

GAs. In GAs, new solutions are generated by exchanging genetic information between two fit solutions via a crossover process. The two most common crossover operators are one-point crossover and uniform crossover. In *One Point Crossover* a single index is selected within the genome to be the position where the parents are to be crossed over. A new child will be produced that combines the genes taken from before the index in one parent with the genes taken from after the index in the other parent. In *Uniform Crossover*, a separate decision is made for each individual gene as to which parent it should be selected from.

In Fitness Directed Crossover (Godley et al., 2008) two parent individuals, Q_1 and Q_2, are selected and used as follows to derive a target number of interventions, I_T:

function GETTARGETNUMOFFEATURES(Q_1,Q_2)
  I_1 = NumberOfFeaturesIn(Q_1)
  F_1 = NormalisedFitness(Q_1)
  I_2 = NumberOfFeaturesIn(Q_2)
  F_2 = NormalisedFitness(Q_2)
  I_f = NumberOfFeatures(Fittest(Q_1,Q_2))
  if *MinimisationProblem* **then** $t \leftarrow 0$
  else $t \leftarrow 1$
  return $I_t \leftarrow I_f + (2t-1)(I_1 - I_2)(F_1 - F_2)$

The effect of this process is that if the fitter parent has more interventions than the less fit parent then I_T will be greater than the number in the fitter parent and

vice versa. The level of overshoot is determined by the difference in fitness between the two parents.

Once I_T has been determined, we need to choose which particular interventions to set. We start by placing all interventions set in both parent solutions in the set S_{dup} and all interventions set in only one parent in the set S_{single}. Interventions are then selected randomly from S_{dup} until either I_T interventions have been set or S_{dup} is empty. If more interventions are needed then interventions will be selected randomly from S_{single} until it is empty or I_T has been reached.

EDAs. Estimation of Distribution Algorithms use a set of relatively fit solutions to build a probability model indicating how likely it is that a given gene has a particular value. They sample this model to produce new solutions that are centred around the derived probability distribution. Univariate EDAs treat every gene as independent whereas multivariate approaches also model interdependencies between genes. Multivariate EDAs are essential in many problems where genes are highly interrelated but they have the disadvantage that, as the number of interactions increases, there is a substantial increase in computational effort required to model these interdependencies (Larranaga and Lozano., 2002).

A common univariate EDA is the Univariate Marginal Distribution Algorithm (UMDA) (Muhlenbein and Paass, 1996). For a binary problem, Equation 1 shows how UMDA calculates the marginal probability, ρ_i, that the gene at index i is set.

$$\rho_i = \frac{1}{|B|} \sum_{x \varepsilon B, x_i = 1} 1 \tag{1}$$

$$\rho_i = \frac{1}{\sum_{x \varepsilon B} f_x} \sum_{x \varepsilon B, x_i = 1} f_x \tag{2}$$

Here B is a subset of fit solutions selected from the current population. ρ_i is the proportion of members of B in which x_i is true. Alternatively, we can weight the probability based on the normalised fitness f of each solution where x_i is true, as shown in Equation 2. Once the probabilities for each gene being set have been calculated, new solutions are generated by sampling this distribution according to probability ρ_i.

Hybrid Algorithms. TEDA falls into the category of hybrid algorithms that use both GAs and EDAs. These approaches are useful as neither EDAs nor GAs perform better than the other approach on all problems. On some problems EDAs become trapped in local optima while on other problems they produce faster convergence than GAs. It can be difficult to predict whether an EDA or a GA will perform better for a particular problem (Pena et al., 2004). Pena developed a hybrid called GA-EDA (Pena et al., 2004) that generates two populations, one through an EDA and one through a GA.

TEDA. The main principle behind TEDA is that it should use feature targeting in a similar manner to FDC and that it should transition from behaving like a GA before the population has converged to behaving like an EDA after it has converged. Specifically, the pre-convergence behaviour of TEDA should match that of FDC as this proved effective when using the targeting principle. This transitioning process is important as dictating exactly how many features solutions should have risks causing a loss of diversity in the population that can lead to premature convergence (Larranaga and Lozano., 2002).

TEDA is described in detail in Algorithm 1. The process of producing each new generation begins with selecting a 'breeding pool', B of size b. Targeting is carried out with the fittest and least fit individuals in B. Equation 2 is then used to build a model from B and this is used to create b new solutions, each with I_T features set. This is repeated until a new population has been produced.

The TEDA transitioning process controls whether TEDA behaves like an EDA or a GA by managing the size of two sets - the 'selection pool' S and the breeding pool B. S consists of the fittest s solutions in the population and B consists of the parents that are used to build the probability model. B is selected from S using tournament selection.

The sizes of B and S are limited to between b_{min} and b_{max} and between s_{min} and s_{max} respectively. To begin with s is equal to s_{max} where s_{max} is set to the size of the whole population. B will initially contain b_{min} parents where b_{min} is 2. In this initial configuration, TEDA operates as a standard GA, selecting 2 parents for breeding from the whole population with tournament selection. The crossover mechanism is equivalent to that used by FDC.

The probability that a new parent should be added is based on a measure of overlap between two candidate parents:

function GETOVERLAP(B_1, B_2)
  $\bar{f}_1 \leftarrow$ all features in B_1
  $\bar{f}_2 \leftarrow$ all features in B_2
  return size($f_1 \cap f_2$) / size($f_1 \cup f_2$)

B_1 and B_2 are the last two parents to be added to B. Initially they will be the first two parents in the pool. If a parent is added according to this rule, the process is repeated until a parent fails the probability test above or b_{max} is reached.

When a new parent is added, s is decreased (un-

til it reaches s_{min}). The result is that as the level of variance within the population decreases, the selection pressure increases. We recommend that b_{min} and s_{max} should be equal in value. If this is the case then TEDA will eventually use the fittest b individuals in the population to build a probability model, and therefore behave like an EDA.

This method of transitioning is an improvement on the method described in earlier work on TEDA (Neumann and Cairns, 2012b), (Neumann and Cairns, 2012a) whereby the variation was measured from a large sample of the population and this was used to control convergence. By introducing the probabilistic element we have helped to ensure a smoother transitioning process.

All methods use genome similarity between solutions to measure population diversity. This should be a more reliable indicator than using the variance in fitness across the population. Previous work (Neumann and Cairns, 2012b) has shown that for some problems the fitness function is volatile, leading to situations where a sharp drop in fitness variance may not necessarily mean that the population has converged and the probability distributions can be relied upon.

Algorithm 1: TEDA Pseudocode.

```
function EVOLVE
    P_0 ← InitialisePopulation()
    s ← s_max                          ▷ normally s_max = popSize
    for g = 0 → generations do
        ∀P_{g_i} ∈ P_g AssessFitness(P_{g_i})
        P_{g+1} ← Elite(P_g)
        while |P_{g+1}| < popSize do
            B ← GetBreedingPool(l, b, P_g)
            I_T ← GetTargetNumOfFeatures
            (fittest(B), leastFit(B))
            ρ⃗ ← BuildUMDAProbabilityModel(B)
            S_all ← ∀i ∈ ρ where ρ_i = 1
            S_some ← ∀i ∈ ρ where 0 < ρ_i < 1
            for b times do
                I ← Mutate(Breed(S_all, S_some, ρ⃗, I_T))
                P_{g+1} ← P_{g+1} ∪ I
function GETBREEDINGPOOL
    S ← bestSelection(s)
    b ← b_min                          ▷ normally b_min = 2
    B_1, B_2 ← tournamentSelectionFromSet(S)
    p ← getOverlap(B_b, B_{b-1})
    while random(1) < p do
        b ← b + 1
        s ← s − 1
        S ← bestSelection(s)
        B_b ← tournamentSelectionFromSet(S)
        if b = b_max then p ← 0
        else p ← getOverlap(B_b, B_{b-1})
    return B
function BREED(S_all, S_some, ρ⃗, I_T)
    A ← {}                             ▷ Make new individual
    while I_t > 0 and S_all ≠ {} do
        r ← random feature ∈ S_all
        A ← A ∪ r
        I_t ← I_t − 1
        remove S_{all_r} from S_all
    while I_t > 0 and S_some ≠ {} do
        r ← random feature ∈ S_some
        if ρ_r > random(1.0) then
            A ← A ∪ r
            I_t ← I_t − 1
            remove S_{some_r} from S_some
    return A
```

3 EXPERIMENTAL METHOD

In the results that follow we compare the performance of TEDA and FDC against both a standard EDA using UMDA and a standard GA using one point crossover, previously shown to be effective at FSS problems (Cantu-Paz, 2002). *UMDA1* is a configuration of UMDA that uses parameters common in literature. As such it does not use mutation and builds a probability model using equation 1 from a breeding pool consisting of the top 50% of the population. *UMDA2* is a configuration of UMDA with parameters that match those used in TEDA. As such it uses the same mutation rate as used in TEDA and builds a probability model using equation 2 from a breeding pool consisting of the top 10% of the population.

The datasets used, detailed in Table 1, are binary classification problems from the NIPS 2003 feature selection challenge (Guyon et al., 2004). The only preprocessing and data formatting steps applied to the datasets are those described in (Guyon et al., 2004). Madelon is an artificial dataset designed to feature a high level of interdependency between features, and so by using it we are able to demonstrate how well TEDA performs in a highly multivariate environment. In Dexter and Madelon the number of positive samples is equal to the number of negative samples whereas in Arcene 56% of samples are negative (Frank and Asuncion, 2010). The datasets are therefore relatively balanced, and so a simple accuracy score is used to assess how successful the classifiers that we use are.

Table 1: Datasets.

Name	Domain	Type	Feat.
Arcene	Mass Spectrometry	Dense	10000
Dexter	Text classification	Sparse	20000
Madelon	Artificial	Dense	500

The basis for the fitness function is the accuracy, calculated as the percentage of samples in the test set that are correctly classified. A penalty is subtracted

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from this to reflect the fact that smaller numbers of features are preferable. Given an accuracy value of a, a feature set of size l and a penalty of p, the fitness function f is calculated as $f = a - lp$. LIBSVM, A Support Vector Machine produced by (Chang and Lin, 2011) is used as the classifier with all parameters kept at their default values.

All algorithms were tested using the parameters given in Table 2, where n is the maximum number of features for each problem. The same mutation technique was applied to every algorithm. For each solution mutation is attempted a number of times equal to the current size of the feature set, each time with a probability of 0.05. Then, where mutation occurs, with a 0.5 probability a feature currently not used will be picked at random and added to the feature set, otherwise a feature will be picked at random and removed from the feature set.

Table 2: Evolutionary Parameters.

Parameter	Value
Population Size	100
Crossover Probability (for GAs)	1
Mutation Probability	0.05
Generations	100
Replacement Method	Generational
Tournament Size	5
Elitism	1
Penalty(p)	$10/n$
TEDA: s_{min} and b_{max}	10
TEDA: s_{max}	100
TEDA: b_{min}	2

For each algorithm, every individual in the starting population was initialised by first choosing a size k between 1 and n. Features are then chosen at random until k features have been selected.

4 RESULTS

The following section shows the results for each of the three problems. For each problem three graphs are provided, showing the following metrics:

- The accuracy achieved by the fittest individual in the population on the y axis against the number of generations on the x axis. Accuracy is given as the percentage of correctly classified test samples.
- The number of features used by the fittest individual in the population on the y axis against the number of fitness evaluations on the x axis.
- The accuracy achieved by the fittest individual in the population on the y axis against time on the x axis. This is the mean of the times that each solution in the population took to complete the classification task. This is important as classification can be time consuming for large problems that use a lot of features.

Each test was run 50 times and the value plotted is the median of the 50 runs with first and third quartiles given by the variance bars. The median was judged to be more reliable than the mean due to the fact that the variance in accuracy and feature set sizes do not follow a normal distribution. From the data in the accuracy over time graphs we also present, in table 3, the length of time that each algorithm took to reach a given accuracy level. Kruskal Wallis (KW) analysis (Siegel and Jr., 1988) was carried out on these results. TEDA was compared to each of the other approaches and where it offers an improvement that is statistically significant with a confidence level of at least 0.05 the result is marked with an asterisk.

Classification Task: Dexter. The results for the *Dexter* classification problem are shown in figures 1 to 3. The results in figure 1 show that TEDA is consistently able to find better solutions than any of the other techniques up until at least the 50th generation. UMDA1 performs worse than any other technique throughout the test.

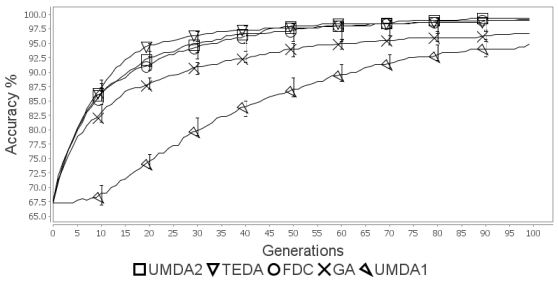

Figure 1: Dexter - Accuracy vs Generations.

The graph in figure 2 indicates that algorithms that are most effective at finding accurate feature sets also tend to be more effective at finding smaller feature sets. The exception is FDC, which finds feature sets that are of an accuracy similar to those found by UMDA2 but tend be smaller.

When we compare performance against time (figure 3) rather than against number of evaluations, the margin of difference between TEDA and UMDA2, the GA and UMDA1 is greater. This is because the feature sets that TEDA finds are smaller and so quicker to evaluate. Classification with these smaller feature sets is completed in less time.

It is interesting that it appears that this problem is unsuitable for a conventional EDA. It might be the

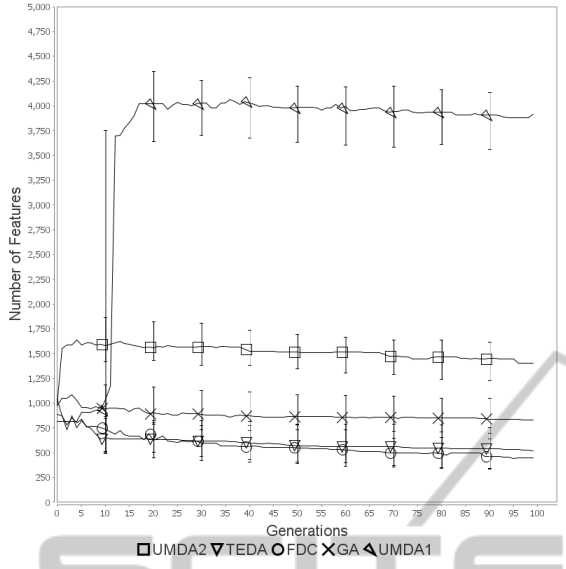

Figure 2: Dexter - Features vs Generations.

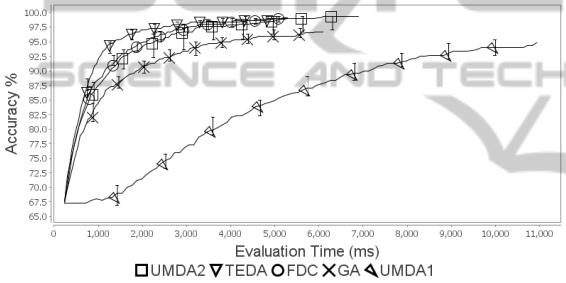

Figure 3: Dexter - Accuracy vs Classification Time.

case that in problems where effective feature sets are small, fit solutions can only be found once the size of the explored feature set has been substantially reduced. Due to the high level of noise in Dexter, determining a useful probability distribution model for a large set of candidate features of which only a few are valid can be difficult.

In the initial population it is possible that some small feature sets are generated by chance. Due to the feature penalty, these are likely to have a better fitness compared to other solutions in the population. In a conventional EDA the large breeding pool may obscure these solutions as they will have little effect on the probability distribution. A GA may select such solutions as one of its two parents and when it does so it is likely to produce a smaller child solution. Whilst GAs might by chance produce new solutions of the same size as these small solutions, TEDA and FDC do this explicitly and drive beyond the size of these solutions to find even smaller feature sets.

UMDA2, which uses a smaller breeding pool and mutation like a GA, is able to overcome the noise that affects UMDA1 while taking advantage of the ability of EDAs to exploit patterns within the population and so proves very effective. This advantage that EDAs demonstrate explains why TEDA outperforms FDC.

Classification Task: Arcene. The accuracies obtained by selecting features for the Arcene classification task are shown in figure 4. From these results, it can be seen that FDC and TEDA both find better solutions early on than the other approaches. UMDA2 starts to perform slightly better than these approaches from around generation 25 onwards but for the first 10 generations it is completely unable to improve upon the fittest individual in the initial population. UMDA1 is only able to start improving after about generation 70. The GA is also slower at finding good solutions than TEDA and FDC, even though it is more effective early on than UMDA.

By looking at the number of features used (figure 5) we can see that for both UMDAs the fittest solution in the initial population has a median size of 75 and that for a period of time both techniques are unable to improve upon this. This is considerably smaller than the maximum feature set size of 10,000 features. We can assume that the sizes of solutions in the initial population is evenly distributed across the range 1 to 10,000. Small individuals would be effectively invisible to the probability model.

It would appear that the situation is the same for both *Arcene* and *Dexter*. Initial high levels of noise mean that until an algorithm starts to explore smaller solutions all solutions are equally ineffective. A GA might by chance select a small solution and breed a new, similarly sized solution but TEDA accelerates this process by making it explicit.

As with *Dexter*, figure 6 shows that these small solutions can be classified more efficiently than larger solutions and so, when plotted against time, we see that TEDA and FDC have almost completed a 100 generation run before UMDA and the GA start to discover effective solutions.

Classification Task: Madelon. The results for the Madelon classification task are shown in figures 7 to 9. In the Madelon problem both TEDA and UMDA2 find good feature sets quicker than the other techniques but UMDA1 eventually overtakes both techniques. Both FDC and the GA are less effective.

A traditional EDA is more effective at this problem than the other problems possibly because the need to dramatically reduce the size of feature set does not apply in this case. The feature set size is considerably smaller and there is less noise, so feature sets that use a large proportion of the available features can be very effective. Figure 8 confirms this, showing no steep declines or sudden drops in feature

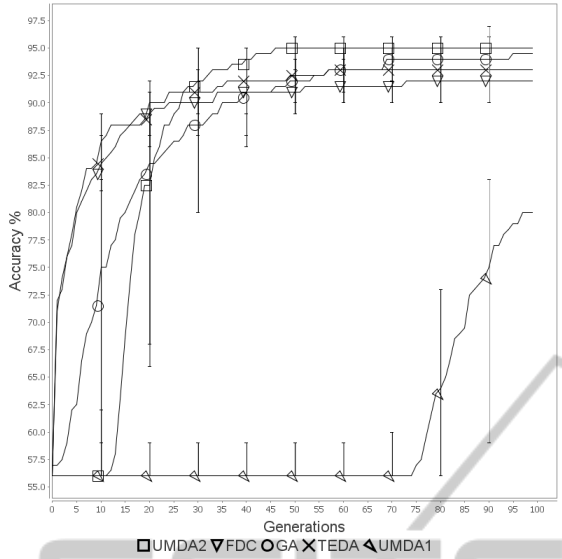

Figure 4: Arcene - Accuracy vs Generations.

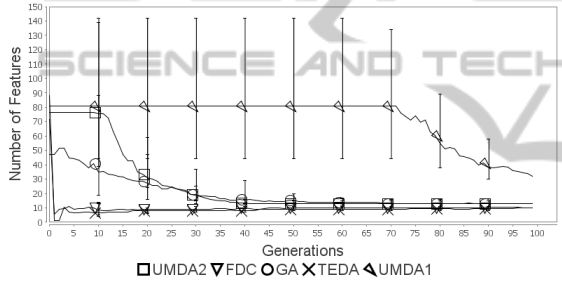

Figure 5: Arcene - Features vs Generations.

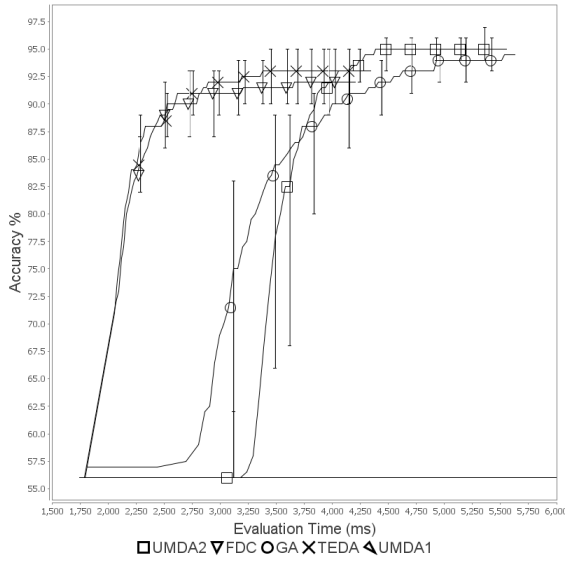

Figure 6: Arcene - Accuracy vs Classification Time.

set size as seen in the other problems. TEDA and FDC show the greatest reduction in the size of feature set and UMDA1 shows the least reduction as with the

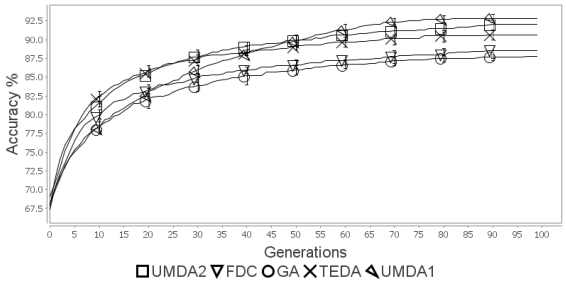

Figure 7: Madelon - Accuracy vs Generations.

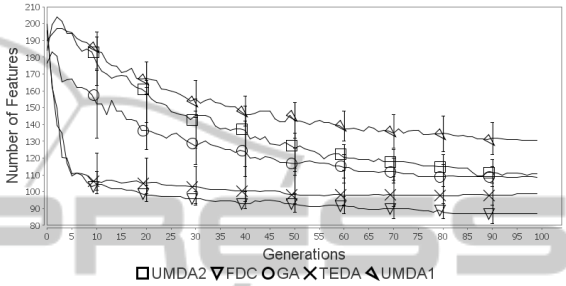

Figure 8: Madelon - Features vs Generations.

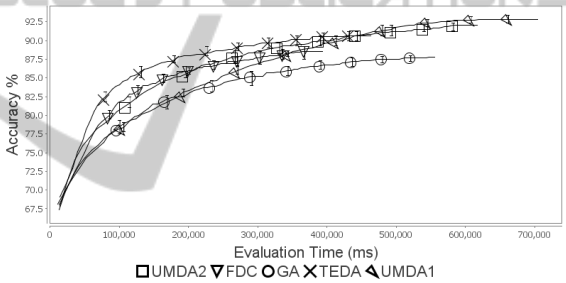

Figure 9: Madelon - Accuracy vs Classification Time.

other problems. Despite not reducing the feature set size as fast or as far as for the other problems, plotted against time (figure 9), TEDA is still able to find good solutions earlier than the other techniques.

5 CONCLUSIONS

In this work we have shown the benefits of applying TEDA to feature selection problems. We have tested TEDA on three FSS problems from literature and in all three cases it was able to find feature sets that were both small and accurate in comparably quicker time and less effort than standard EDAs and GAs. The speed with which TEDA finds these small solutions enables it to complete fitness function evaluations at a faster rate than comparable algorithms. TEDA is therefore a suitable algorithm for problems that have a large number of features and where fitness function evaluations are time consuming.

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Table 3: Seconds to Reach Accuracy Level.

Dexter					
Acc.	TEDA	UMDA2	FDC	GA	UMDA1
70.0	0.29	0.3	0.31	0.34	1.65*
76.0	0.4	0.43	0.43	0.54*	2.73*
82.0	0.6	0.63	0.65	0.82*	4.02*
88.0	0.81	1.1*	0.92*	1.46*	6.16*
Arcene					
70.0	2.06	3.44*	2.07	3.03*	26.42*
74.0	2.08	3.49*	2.11	3.11*	26.53*
78.0	2.12	3.49*	2.16	3.27*	26.68*
82.0	2.18	3.58*	2.21	3.38*	-
86.0	2.28	3.69*	2.35	3.63*	-
Madelon					
70.0	23.54	24.79	24.02	23.52	30.67
74.0	39.98	35.74	50.0	52.19*	50.01*
78.0	52.43	67.28*	69.27	92.89*	96.97*
82.0	74.17	123.1*	106.58*	168.88*	175.93*
86.0	136.32	210.82*	200.73*	343.32*	270.93*

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