

A New Multi-Objective Particle Swarm Optimization Approach to Feature Selection

Hoai Bach Nguyen · Bing Xue · Ivy Liu · Peter Andreae · Mengjie Zhang

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Abstract In classification problems, a large number of features are typically used to describe the problem's instances. However not all of these features are useful for classification. Feature selection is an important preprocessing step to overcome the problem of "curse of dimensionality". Feature selection aims to choose a small number of features to achieve similar or better classification performance than using all features. This paper presents a particle swarm Optimization (PSO) based multi-objective feature selection approach to evolving a set of non-dominated feature subsets which achieve high classification performance. The proposed algorithm uses local search techniques to improve a Pareto front and is compared with a pure multi-objective PSO algorithm, three well known evolutionary multi-objective algorithms and a current state-of-the-art PSO based multi-objective feature selection approach. Their performances are examined on 12 benchmark datasets. The experimental results show that in most cases, the proposed multi-objective algorithm generates better Pareto fronts than all other methods.

Keywords Multi-objective · Feature selection · Classification · Particle Swarm Optimization

1 Introduction

Classification is one of the most important tasks in machine learning and aims to predict the class label of an instance

Hoai Bach Nguyen · Bing Xue · Peter Andreae · Mengjie Zhang
School of Engineering and Computer Science
E-mail: {Hoai.Bach.Nguyen,Bing.Xue,
Peter.Andreae,Mengjie.Zhang}@ecs.vuw.ac.nz

Ivy Liu
School of Mathematics, Statistics and Operation Research
E-mail: Ivy.Liu@msor.vuw.ac.nz
Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

based on the features and their values of the instances. In the learning process, a set of instances, called the training set, is used to train a classification algorithm, which is tested on an unseen dataset, called the test set. In many problems, a large number of features are used to well describe the instances. Unfortunately, due to "the curse of dimensionality" (Gheyas and Smith, 2010), the larger the set of features is, the longer time the training process takes. In addition, many features may contain irrelevant or redundant features, which are not useful for classification. Those features typically lower the quality of the whole feature set (Zhao et al., 2009), because they can conceal or mask the useful information from the relevant features. Feature selection methods (Guyon and Elisseeff, 2003) are used to remove redundant and irrelevant features, which will not only speed up the learning/classification process but may also increase the classification performance over using all features. However, due to the complex interaction between features and the huge search space, it is hard to develop a good feature selection approach.

The main goal of feature selection is to find a small feature subset from a large set of original features that achieves at least as good classification performance as using all features. In feature selection, if there are n original features, then there are 2^n possible subsets. When n is large, an exhaustive search is clearly too slow. Greedy algorithms such as sequential forward selection (Whitney, 1971) and sequential backward selection (Marill and Green, 1963) are much more efficient, but these methods easily get stuck at local optima. Because of the ability of global search to overcome local optima, evolutionary computation (EC) techniques, such as genetic programming (GP) (Neshatian and Zhang, 2009a), genetic algorithm (GAs) (Yuan et al., 1999) and particle swarm optimization (PSO) (Unler and Murat, 2010; Yang et al., 2008), have been applied to solve feature selection problems. Compared with GA and GP, PSO is more prefer-

able because it is simple and easy to implement. In addition, PSO not only uses fewer parameters but also converges more quickly.

Feature selection can be viewed as a multi-objective problem because it needs to simultaneously maximize the classification accuracy and minimize the dimensionality of the selected subset. However, with fewer features being used for classification, the classification accuracy is likely to be decreased. Those two objectives often conflict with each other and the search process needs to consider the trade-off between them. This paper will take the advantages of PSO to develop a multi-objective feature selection approach which can simultaneously achieve both objectives of feature selection problems.

1.1 Goals

The overall goal of this study is to develop a PSO based multi-objective feature selection approach, which can produce a set of non-dominated solutions that specify a small number of features and achieve better classification performance than using all features. To achieve this goal, we develop a new multi-objective PSO (MOPSO) algorithm, called ISRPSO, which uses local search techniques to improve the Pareto front. In addition, the proposed algorithm is also compared with three well known evolutionary multi-objective algorithms including Non dominated sorting genetic algorithm II (NSGAI) (Deb et al., 2000), Strength Pareto evolutionary algorithm 2 (SPEA2) (Zitzler et al., 2001) and Pareto archived evolutionary strategy (PAES) (Knowles and Corne, 1999). Finally the proposed algorithm will then be compared with a state-of-the-art multi-objective PSO algorithm, named CMDPSOFS (Xue et al., 2013). Specifically, we will investigate the following:

- whether the proposed multi-objective PSO algorithm (ISRPSO) evolve a set of non-dominated solutions with a small number of features and better classification performance than using all features.
- whether applying local search can evolve better Pareto front in comparison with a pure multi-objectives PSO.
- whether ISRPSO can evolve a better Pareto front than NSGAI (Deb et al., 2000), SPEA2 (Zitzler et al., 2001) and PAES (Knowles and Corne, 1999) in feature selection problem.
- whether ISRPSO is able to produce a Pareto front of non-dominated solutions, which can outperform a state of the art multi-objective PSO for feature selection, CMDPSOFS (Xue et al., 2013).

1.2 Organization

The remainder of this paper is organized as follows. Section provides background information. In section 3, we propose a novel PSO-based multi-objective feature selection algorithm. Section 4 describes the experimental design, and section 5 presents the experimental results. In section 6, we conclude our work with some possible extensions for future work.

2 Background

2.1 Particle Swarm Optimization (PSO)

In 1995, Kennedy et al. (1995) proposed an evolutionary computation algorithm called Particle Swarm Optimization (PSO), which was developed based on social behaviours. Like other swarm intelligence algorithms, PSO maintained a set of particles, which was also known as a *swarm*. Each particle, which represented a candidate solution, moved around the search space by using its own position and velocity. Particularly, the i^{th} particle's position was a D -dimensional vector, $x_i = (x_{i1}, x_{i2}, \dots, x_{iD})$, where D was the dimensionality of the search space. For each iteration, the positions were updated according to the particle's velocity, which was also represented by a vector, $v_i = (v_{i1}, v_{i2}, \dots, v_{iD})$. In order to avoid skipping good positions due to moving too fast, the particle's velocity was limited by a predefined maximum velocity v_{max} , which meant $-v_{max} \leq v_{id} \leq v_{max}$. In PSO, each particle also recorded the best position discovered by itself, called *pbest*. In addition, the best position discovered by a particle's neighbours and itself was also maintained, which was called *gbest*. According to the two *pbest* and *gbest*, the i^{th} particle moved around the search space by the following updating equations:

$$v_{id}^{t+1} = w * v_{id}^t + c_1 * r_{i1} * (p_{id} - x_{id}^t) + c_2 * r_{i2} * (p_{gd} - x_{id}^t) \quad (1)$$

$$x_{id}^{t+1} = x_{id}^t + v_{id}^{t+1} \quad (2)$$

where t represents the t^{th} iteration, d denotes the d^{th} dimension in the search space, w is a predefined constant inertia weight, c_1 and c_2 are acceleration constants, r_{i1} and r_{i2} are two random values uniformly generated in the interval $[0, 1]$, and p_{id} and p_{gd} represent the position entry of *pbest* and *gbest* in the d^{th} dimension, respectively.

The above description explains how a continuous PSO works. There is still another kind of PSO, called binary PSO (BPSO). In BPSO, the position entries are binary values. There are some potential limitations of the current binary PSO; for example, the update of particle position is based only on the current velocity while in standard PSO, both current velocity and position are used. Although both versions of PSO have been successfully used to solve feature

selection problems (Unler and Murat, 2010; Liu et al., 2011; Chuang et al., 2008; Huang and Dun, 2008), continuous PSO achieves better performance than binary PSO as shown by Xue (Xue et al., 2012a). Therefore, we will develop a multi-objective feature selection approach using continuous PSO.

2.2 Multi-Objective Optimization

2.2.1 Basic Concepts of Multi-Objective Optimization

In many Optimization problems, there is more than one objective that needs to be optimized. Often, the objectives conflict. Multi-objective problems refer to the presence of two or more conflicting objectives. For example, a feature selection problem is a multi-objective problem, in which minimizing both classification error rate and the number of selected features are two conflicting objectives. The conflicting objectives can be expressed in multiple conflicting objective functions, which needs to be maximized or minimized. In mathematical terms, a multi-objective problem can be expressed as in the following formula (as minimization problems):

$$\text{minimize}(f_1(x), f_2(x), \dots, f_k(x)) \quad (3)$$

where x is the vector of variables which describe the problem's solutions, $f_i(x)$ is an objective function of x and the integer $k \geq 2$ is the number of objectives.

In multi-objective problems, the trade off between conflicting objectives is used to measure the quality of a solution. In particular, suppose that y and z are two solutions of a k -objective minimization problems. The solution y is better than z or y dominates z if and only if:

$$\forall i : f_i(y) \leq f_i(z) \text{ and } \exists j : f_j(y) < f_j(z) \quad (4)$$

where $i, j \in 1, 2, 3, \dots, k$. When a solution is not dominated by any other solutions, it is called a non-dominated solution. The set of a non-dominated solution forms a trade-off surface in the objective space, namely *Pareto front*. A multi-objective algorithm is designed to evolve a set of non-dominated solutions.

2.2.2 Evolutionary Multi-objective Algorithms

NAGAI, proposed by Deb et al. (2000), is one of the most popular evolutionary multi-objective algorithms. There are two main ideas introduced in NSGAI: a fast non-dominated sorting technique and a diversity preserving algorithm. The fast nondominated sorting technique is an efficient approach to sorting all parents and offspring into different level of non-dominated solutions. This sorted population is used to

build the parent population for the next generation. The density preserving algorithm estimates the density of solutions based on the crowding distance and uses the estimates to maintain the diversity of the population.

SPEA2 is another popular evolutionary multi-objective algorithm proposed by Zitzler et al. (2001). The most important principle introduced in SPEA2 is the incorporation between the fine-grained fitness assignment strategy, a density estimation technique and an enhanced archive truncation method. In particular, each individual's fitness is the sum of its strength raw fitness and a density estimation. A new population is constructed by selecting non-dominated solutions from both the original solution and the archive. If the number of non-dominated solutions exceeds the population size, the archive truncation method is applied to determine which solutions will be selected. The truncation method bases on the distance between a solution and its k^{th} nearest neighbour.

PAES is an evolutionary multi-objective algorithm proposed by Knowles and Corne (1999). The author argued that PAES is the simplest possible non-trivial algorithm, which is able to generate diverse solutions in the Pareto optimal set. The main idea of PAES is the combination of local search and the usage of an archive of previously found non dominated solutions to identify the approximate dominance rank of the current and candidate solutions.

The success of the Particle Swarm Optimization (PSO) algorithm for a single-objective problem has encouraged researchers to extend PSO to solve multi-objective problems (MOPSO). As explained in the previous section, in PSO for a single objective problem, each particle has exactly one leader *gbest* to update its position. However, in most of current MOPSO algorithms, instead of recording *gbest* for each particle, an *archive set* is used to maintain a set of non-dominated solutions being discovered by the population. Each particle will select a solution from the *archive set* as its *gbest* to update its position. When the final iteration is reached, the archive set represents the final result of the MOPSO algorithm, which forms the *Pareto front*. This work will apply a local search on the archive set to help MOPSO better explore *Pareto front*. Since these algorithms were successfully applied to solve feature selection problems, all these above algorithms will be used as benchmark techniques for the proposed algorithm, which is specifically designed for feature selection.

2.3 Related Work on Feature Selection

2.3.1 Traditional Feature Selection Methods

A basic version of feature selection is feature ranking (Dash and Liu, 1997), where a score is assigned to each feature according to an evaluation criterion. Feature selection can be

performed by selecting the features with the highest scores. However, this type of algorithm ignores the interaction between features. Additionally, the features with the highest scores are usually similar. Therefore, these algorithms tend to selecting redundant features.

Sequential search techniques were also applied to solve feature selection problems. In particular, sequential forward selection (SFS) (Whitney, 1971) and sequential backward selection (SBS) (Marill and Green, 1963) were proposed. At each step of selection process, SFS (or SBS) added (or removes) a feature from an empty (full) feature set. Although these local search techniques achieved better performance than the feature ranking method, they might suffer the “nesting” problem, in which a feature was permanently added or removed from the selected feature set. In order to avoid the nesting effect, Stearns Stearns (1976) proposed a “plus- l -takeaway- r ” method in which SFS was applied l times forward and then SBS was applied for r back tracking steps. However, it was challenge to determine the best values of (l, r) . This problem was addressed by sequential backward floating selection (SBFS) and sequential forward floating selection (SFFS), proposed by Pudil et al. (1994). In SBFS and SFFS, the values (l, r) were dynamically determined rather than being fixed in the “plus- l -takeaway- r ” method.

2.3.2 EC Approaches(Non-PSO) for Feature Selection

EC techniques are well known because of their global search ability. EC algorithms have been applied to feature selection problems, such as GAs (Zhu et al., 2007), GP (Neshatian and Zhang, 2009b). Zhu et al. (2007) proposed a hybrid feature selection approach, which combined both local search and GAs. In this algorithm, a filter method was used to rank features individually. Basing on the ranking information, GAs deleted or added a feature to achieve better fitness value, which was the classification accuracy. The experiments showed that this algorithm outperformed the GAs alone and other algorithms.

Oreski and Oreski (2014) proposed a hybrid genetic algorithm with neural-networks (HGA-NN) to evolve an optimum feature subset. In the initialization step, the feature set was narrowed by different fast filter techniques. So important features, which were selected by the filter approaches, were used to initialise the major part of population. The rest of population was filled randomly. In HGA-NN, an incremental stage was applied to enhance the creation of the initial population, which increased the diversity of the genetic material. The proposed algorithm was evaluated on two real-world credit datasets. The experimental results showed that HGA-NN achieved better classification performance than GA-NN technique proposed by Wang (2005).

Lin et al. (2014) proposed a novel GA-based feature selection approach, in which the prior knowledge about fi-

nancial distress prediction was used to group similar features. After that a filter approach was used to rank all features in the same group and only top-rank features from each group were chosen to participate in the selection process by GAs algorithm. Although the two-step selection approach was efficient, it skipped the interaction between features. Other GA-based feature selection approaches were developed recently to solve real-world problems, such as Chaaraoui and Flórez-Revuelta (2013); Seo et al. (2014); Liang et al. (2015).

Neshatian and Zhang (2009b) proposed a wrapper GP-based approach, which evaluated and ranked feature subset in binary classification tasks. Experiments showed that the proposed methods detected subset of relevant features in different situations, where other methods had difficulties. Bhowan and McCloskey (2015) proposed two GP-based approaches to evolve a set of features, which was used directly in the Watson system, an intelligent open-domain question answering system. The first approach extracted all features, which were used in the best-of-run evolved GP tree. The second approach considers all evolved trees. Particularly, from the set of GP trees, the top N features with the most frequency were chosen as extracting features. Two values of N being used in this paper was 10 and 20. The experiment results showed that, the set of features selecting from the best GP tree only worked well when the number of selected features was small. Meanwhile, selecting top N features from the whole set of trees produces good resulted on both small and large datasets. However, as other ranking features selection algorithms, this algorithm did not consider the interaction between features, especially between redundant features.

2.3.3 PSO-based Feature Selection Methods

Many EC algorithms have been used for feature selection, such as GAs, GP or PSO. PSO is preferable because it is easier to implement and uses fewer parameters than GAs and GP. Wang et al. (2007) proposed a filter PSO-based feature selection algorithm, which applied rough set theory to evaluate feature subset. In the proposed algorithm, the fitness function was the combination of the classification quality of the feature subset calculated by rough set theory and the proportion of the selected features. The experimental results showed that the proposed algorithm could find the optimal solution in a smaller amount of time than a GA using rough sets. Chakraborty and Chakraborty (2013) proposed a filter PSO-based feature selection approach, which used fuzzy set to calculate the fitness value for each particle. Specifically, the membership value of fuzzy set theory was used with more than one thresholds to decide whether or not an instance is consistent according the selected features. The proportion of consistent instances over the total number of

instances was the consistent or fitness measure of the current feature subset. Two PSO based filter feature selection algorithms were proposed in (Cervante et al., 2012), where mutual information and entropy were used in the fitness function to evaluate the relevance and redundancy of the selected feature subset. The experiments showed that the proposed methods significantly reduced the number of features whilst achieved similar or better classification than using all features.

In PSO, premature convergence was a common problem, in which the swarm converged quickly to a local optima. To avoid premature convergence, Chuang et al. (2008) proposed a new *gbest* updating mechanism, which reseted *gbest* elements to zero if it maintained the same value after several iterations. However, the performance of this algorithm was not compared with other PSO based algorithms. Later, Tran et al. (2014) also applied this resetting mechanism cooperating with local searches on *pbest* to simultaneously reduced the number of selected features and improved the classification performance. In addition, the new fitness calculation was proposed, which based on the changed features (selected to not selected or vice-versa). The proposed algorithm achieved smaller feature subset with lower classification error than (Chuang et al., 2008). Another binary PSO based algorithm, which also aimed to avoid premature convergence, was proposed by Bin et al. (2012). At each iteration of this algorithm, the swarm was divided into two groups, named “leaders” and “followers”. The “leaders” had better fitness values. The “followers” updated their positions and velocities based on leaders’ update. The experimental results showed that the proposed update strategy better utilizes the social behaviour phenomenon than the standard binary PSO.

Xue et al. (2014) proposed three new initialization mechanisms, which mimic the sequential feature selection approach. While the small initialization used about 10% of original features to initialize the particles, particles in the large initialization were constructed based on 50% of original features. These two initialization mechanisms were combined in the mixed initialization, which used the small initialization for most of particles and the large initialization for the rest. In addition, three new updating mechanisms for *pbest* and *gbest* were proposed in the paper. The experimental results showed that the new initialization and updating mechanisms led to smaller feature subsets with better classification performance than the standard PSO and two-stage binary PSO algorithm.

Vieira et al. (2013) proposed a new representation for binary PSO, which simultaneously performed feature selection and optimised the SVM kernel parameters. Particularly, each bit string corresponded to an original feature or a kernel parameter, which resulted in the length of the new representation was equal to the total number of features and ker-

nel parameters. Experimental results showed that the proposed algorithm achieved better classification performance than other binary PSO-based feature selection algorithms (Chuang et al., 2008; Lee et al., 2008) and selected smaller feature subsets than GA-based feature selection algorithm (Huang and Wang, 2006). This representation was also applied to continuous encoding (Lin et al., 2008) and a mixture of binary and continuous encoding (Boubezoul and Paris, 2012). Lane et al. (2013) applied statistical clustering, which groups similar features into one cluster. In particular, the proposed method arranged the features in the same cluster together and selected a single feature from each cluster based on the velocity. Lane et al. (2014) further improved his work by applying Gaussian distribution to select multiple features from each cluster. Later, Nguyen et al. (2014) also applied statistical clustering to proposed a new representation, in which each bit string belonged to a certain feature cluster and presented a feature index from the cluster. However, in the new representation a small change of the position might not lead to any different feature subset. Therefore, Nguyen et al. (2015) applied Gaussian distribution to propose a new transformation rule, which could form a smoother fitness landscape than the representation in (Nguyen et al., 2014). An extensive review about EC-based feature selection algorithms was conducted in (Xue et al.).

Feature selection problem can be seen as a multi-objective problem, because its two objective usually conflict with each other. However most of wrapper feature selection approaches used only classification performance as the fitness function (Mohammed et al., 2009; Zhang et al., 2015) or combined the classification accuracy and the number of selected features into a single fitness function (Xue et al., 2012b; Huang and Dun, 2008). Xue et al. (2012a) proposed two multi-objective PSO algorithms for feature selection problems. The first algorithm applied the idea of non-dominated sorting based multi objective genetic algorithm II (NSGAI) into PSO for feature selection. The other algorithm based on the idea of crowding, mutation and dominance (CMDPSOFS) to evolve the Pareto front solutions. According to the experimental results, both algorithms could select a small number of features while achieving better classification performance than using all features. However, the above algorithms did not propose any specific design for feature selection problems. Therefore, this work will propose a new local search technique for MOPSO, which is specifically designed for feature selection problems. The proposed algorithm is then compared with the current state of art multi-objective PSO based algorithm, CMDPSOFS.

3 PSO-Based Multi-Objective Feature Selection

Algorithm: ISRPSO

In this section, we investigate a new approach to feature selection using multi-objective PSO, with two objectives to explore the Pareto front of feature subsets. Initially, standard PSO was proposed to solve single objective problems, in which each particle remembers the best position discovered by its neighbours and itself so far, called *gbest*. In order to develop a multi-objectives PSO algorithm, Li (2003) introduces the idea of an archive set, which is used in NSGA. The archive set contains all non-dominated solutions which have been discovered by the swarm so far. With the archive set, instead of using the individual *gbest* to update velocity, each particle selects an archive member as its *gbest*. Therefore, the whole archive set is guides the swarm through the search space. It is expected that the better archive sets would allow the swarm to construct better solutions, which select a small number of features and maintain or even improve the classification accuracy. In this paper, we investigate a novel PSO-based multi-objective feature selection algorithm (ISRPSO), which uses local search techniques to improve the archive set with a better Pareto front.

3.1 Representation and fitness function for ISRPSO

In this study, a continuous PSO is used to solve feature selection problems. Each particle's position representation is a vector of n real numbers, where n is the total number of features. Each position entry x_i corresponds to the i^{th} feature in the original feature set. The value x_i varies between 0 and 1 and represents the confidence that feature i^{th} should be included in the solution subset. A threshold θ is used to decide whether or not a feature is selected: the i^{th} feature is selected if and only if $\theta < x_i$.

As stated above, each feature selection problem has two objectives: minimising the classification error rate and minimising the number of selected features. These objectives are calculated according to Equations 5 and 6, respectively. Notice that both *ErrorRate* and *FeatureRate* varies in the interval [0,1], which guarantees the fairness between 2 objectives.

$$ErrorRate = \frac{FP + FN}{TP + TN + FP + FN} \quad (5)$$

where TP, TN, FP and FN are true positives, true negatives, false positives and false negatives, respectively.

$$FeatureRate = \frac{\#Selected\ features}{\#All\ features} \quad (6)$$

3.2 Important set concepts from the archive set

Before describing the novel multi-objectives PSO, it is helpful to clearly define some concepts about feature sets being built from the archive set. As mentioned above, the archive set contains all non-dominated solutions, which are not dominated by any other solutions discovered so far. Therefore, the features being selected by these archive members can be considered the important features. These features are contained in one feature set, denoted as S .

Another important concept relates to each individual of the archive set. In particular, a set S_i consists of all features which are selected by the i^{th} archive member. Similarly, a set US_i consists of all features, which selected by all archive members except the i^{th} particle. It can be seen that $S = S_i \cup US_i$ or $US_i = S \setminus S_i$.

Let consider an example. Assume the original feature set contains 5 features, $F = \{f_1, f_2, f_3, f_4, f_5\}$. The archive set contains three members $Archive = \{A_1, A_2, A_3\}$, in which the features selected by each feature are defined as below:

- 1th member (A_1): $S_1 = \{f_1, f_2\}$
- 2nd member (A_2): $S_2 = \{f_1, f_3\}$
- 3rd member (A_3): $S_3 = \{f_2, f_3, f_4\}$

So feature f_5 is not selected by any archive members, which might indicate that f_5 is an irrelevant or a redundant feature. According to the above definition, the set of all features being selected by this archive set is $S = \{f_1, f_2, f_3, f_4\}$. For each archive member, the set US_i is defined as below

- $US_1 = S \setminus S_1 = \{f_3, f_4\}$
- $US_2 = S \setminus S_2 = \{f_2, f_4\}$
- $US_3 = S \setminus S_3 = \{f_1\}$

3.3 Local Search to Improve the Archive Set

As stated above, this work investigates using local search techniques to improve the quality of the archive members, which hopefully results in a better Pareto front. In particular, three operations, including *Inserting* (I), *Swapping* (S), *Removing* (R) are proposed to enhance the archive set. All of these operators use three sets S, S_i, US_i to search around each archive member to find better solutions. These operations are described in the following sections.

3.3.1 Inserting

As mentioned above, for the i^{th} archive member, the set US_i contains all features that are selected by all archive members except the i^{th} members. Since the features being selected by archive members are usually important, it would be possible to improve the classification accuracy of an archive member by adding one feature from the set US_i to the current set of selected features S_i .

The features in each set US_i are sorted according to their single classification accuracy, which is the classification performance when only feature i^{th} is used to perform classification. The better features, which have higher accuracy are in front of the list. After that, each feature in US_i is temporarily added into S_i to form a new feature set, called S'_i . If the accuracy of S'_i is better than the accuracy of S_i , the inserting process stops. The new solution, called SO_{in} , whose selected features are S'_i , is built and passed as an input to the next step (*Removing*). So after the inserting step, the new solution SO_{in} will select at most one feature more than the original archive member, A_i .

Continuing the example from the above section, in which the first archive member A_1 selects $S_1 = \{f_1, f_2\}$ and its $US_1 = \{f_3, f_4\}$. Suppose that $C(\{f_1, f_2, f_3\}) = 0.75$, $C(\{f_1, f_2, f_4\}) = 0.82$, $C(\{f_1, f_2\}) = 0.80$, where $C(\cdot)$ is the classification of a feature set. Also suppose that the single classification accuracy of f_3 is better than f_4 . The inserting process will start with f_3 . At the first step, the “inserting” process will temporarily add feature f_3 to set S_1 , to form a new set $\{f_1, f_2, f_3\}$. However, since $C(\{f_1, f_2, f_3\}) < C(\{f_1, f_2\})$, feature f_3 will be discarded. After that feature f_4 is temporarily added to the set S_1 to form a new feature set, $\{f_1, f_2, f_4\}$. This time, since $C(\{f_1, f_2, f_4\}) > C(\{f_1, f_2\})$, a new solution SO_{in} is created, which uses $\{f_1, f_2, f_4\}$ as its selected features. This solution will be further improved by *Removing* operation, which will be discussed in the next section.

3.3.2 Removing

In the *Inserting* step, at most one feature might be added to the feature selected set of an archive member to form a new solution SO_{in} , which is guaranteed to be similar or better than the archive member in term of classification accuracy. In contrast, *Removing* step tries to improve SO_{in} by removing at most one feature from SO_{in} . The *Removing* process works in the same way as backward selection algorithm. Firstly, all features selected by SO_{in} are sorted according to their single classification accuracy. In the sorted list, the features with less accuracy will be at the top of the list, therefore they are more likely to be removed. After that, each feature from the sorted list will be temporarily removed from the selected set until there is an improvement in terms of the classification accuracy. The new solution, called SO_{re} is built and passed as an input to the next step (*Swapping*). So after the removing step, the new solution SO_{re} will contain at most one feature less than the solution SO_{in} , provided by the *Inserting* step.

Continuing the example from the above section, the *Inserting* process provides $SO_{in} = \{f_1, f_2, f_4\}$ as an input to the *Removing* process. Suppose that $C(f_2) < C(f_1) < C(f_4)$. After sorting features according to their classifica-

tion accuracy, the order of removing features is $f_2 \rightarrow f_1 \rightarrow f_4$. Suppose that $C(\{f_1, f_4\}) = 0.80$, $C(\{f_2, f_4\}) = 0.85$, and $C(\{f_1, f_2\}) = 0.75$. Firstly, f_2 is temporarily removed from SO_{in} , which results in a feature set $\{f_1, f_4\}$. However, since $C(\{f_1, f_4\}) = 0.80 < C(\{f_1, f_2, f_4\}) = 0.82$, feature f_2 restored. Next feature f_1 is temporarily removed from SO_{in} , which produces another feature set, $\{f_2, f_4\}$. This time, as $C(\{f_2, f_4\}) = 0.85 > C(\{f_1, f_2, f_4\}) = 0.82$, a new solution SO_{re} is created, which uses $\{f_2, f_4\}$ as its selected features. This solution will be improved in the last operation called *Swapping*, which will be discussed in the following section.

3.3.3 Swapping

Compared with *Inserting* and *Removing* operations, *Swapping* is a bit more complicated. For each solution, this operation acts on both the selected set S_i and unselected set US_i . In addition, instead of adding or removing features from the solution, this operation tries to find out better solutions by swapping between features in S_i and US_i . In other word, this operation will temporarily replace one feature from S_i by one feature from US_i .

Firstly, all features in S_i are sorted according to their single classification accuracy in ascending order, so the worst feature is more likely to be replaced. In contrast, all features in US_i are sorted in descending order, therefore the feature with better single classification performance will have more chance to be added. For each feature u in US_i , this process will try to replace with a feature in S_i . Once feature u finds a suitable feature s in S_i , which means the classification accuracy is improved when s is replaced by u , the replacing process for u is stopped. After that the swapping process will continue with the feature after feature u in US_i .

Continuing the example from the above section to explain for this operation, $\{f_2, f_4\}$, the new solution SO_{re} is fed into *Swapping* process. Its selected and unselected set are $S_{re} = \{f_2, f_4\}$ and $US_{re} = \{f_1, f_3\}$. Suppose that $C(f_1) < C(f_3)$ and $C(f_2) > C(f_4)$, the above two sets are sorted as following $S_{re} = \{f_4, f_2\}$ and $US_{re} = \{f_3, f_1\}$. The *Swapping* operation starts with the first element of the set US_{re} , which is feature f_3 . Firstly, f_3 will try to swap with the worst feature in the set S_{re} , which is feature f_4 . Suppose that $C(\{f_3, f_2\}) > C(\{f_4, f_2\})$, then f_3 immediately replaces f_4 to create a better solution SO_{s1} , which selects the following feature $\{f_3, f_2\}$. Note that the selected set is updated, which is $S_{s1} = \{f_3, f_2\}$. The *Swapping* processes will continue until all features in the unselected set US_{re} have been considered.

3.3.4 Overall ISRPSO Algorithm

Algorithm 1 shows the pseudo-code of ISRPSO. In order to determine a leader, ISRPSO maintains a set of non-dominated

Algorithm 1 : Pseudo-code of ISRPSO

```

1: begin
2: divide Dataset into a Training set and a Test set;
3: initialize the swarm;
4: evaluate two objectives values for each particle;
5: add non-dominated solutions into Archive set;
6: while Maximum iterations is not reached do
7:   if iteration is divided by 5 then  $\triangleright$  improve the Archive set
   for each 5 iterations
8:     for each solution i in the Archive do
9:        $(SO_{in}, S_{in}, US_{in}) = \text{Inserting}(A_i, S_i, US_i)$ 
10:       $(SO_{re}, S_{re}, US_{re}) = \text{Removing}(SO_{in}, S_{in}, US_{in})$ 
11:       $(SO_{sw}, S_{sw}, US_{sw}) = \text{Swapping}(SO_{re}, S_{re}, US_{re})$ 
12:      if  $SO_{sw}$  is not dominated by any archive members
      then
13:        insert  $SO_{sw}$  into Archive set
14:      end if
15:    end for
16:  end if
17:  for each particle i in the swarm do
18:    select a leader (gbest) from Archive set for each particle
    by using a binary tournament selection based on the objectives
    distance;
19:    update the velocity and the position of particle i;
20:    evaluate two objective values for each particles;
21:    update the pbest for each particle;
22:    if the  $i^{th}$  particle is not dominated by any archive members
    then
23:      insert  $i^{th}$  particle into Archive set;
24:    end if
25:  end for
26: end while
27: calculate the testing classification error rate of the solutions in
Archive set on the test set;
28: return the solutions in Archive;
29: return the training and test classification error rates of the solutions
in Archive; end

```

solutions being discovered so far. A *gbest* for a particle is selected from the *Archive* set according to their objective distance and a binary tournament selection. Specifically, the binary tournament selection is used to select two solutions from the *Archive* set, and the closest solution (to the particle) in the objective space is chosen as the *gbest*. The maximum size of the *Archive* set is set as the number of particles in the swarm.

The local search, which aims to improve the solutions in *Archive* set, is performed every 5 iterations. Particularly, three operations are used to improve the solution quality of the *Archive* set. For each *Archive* member, the *inserting* operation tries to add one more feature into the member's feature set to create a new solution, called SO_{in} . If adding one feature improves the classification accuracy of the current *Archive* member, then SO_{in} is built based on the new feature set. Otherwise, SO_{in} is exactly the same as the current *Archive* member. After that, the solution SO_{in} is further improved by the *removing* operation. On the contrary,

removing operation tries to delete at most one feature from SO_{in} , which results in similar (no feature is deleted) or higher classification accuracy. Once more, the output of *removing* operation, SO_{re} , is improved by the *swapping* operation. Instead of removing or inserting features, this operation finds a better solution by swapping between features selected by current solution (SO_{re}) and features which are selected by the other *Archive* members. So the *swapping* operation might produce a new solution, SO_{sw} , which has the same number of selected features but achieves better accuracy than SO_{re} . A new position is built based on the feature set SO_{sw} . In the new position, all position entries corresponding to features from SO_{sw} are set to 1 and all other entries are set to 0. Finally, if the new solution is not dominated by any *Archive* member, it will be inserted into the *Archive* set. In addition, all solutions, which are dominated by the new solution, will be removed from the *Archive* set.

With these three operations, it is expected that at least the final improved solution SO_{sw} will not be dominated by any *Archive* members. In a good case, SO_{sw} might even dominate some *Archive* members. Therefore this local search technique either maintains the diversity of the swarm or even improves the Pareto front by creating a better solution. Currently, since the classification accuracy is used to compare between two solutions, it is quite expensive to perform this local search. Therefore, the solutions within the *Archive* set are improved by these three operations for every 5 iterations.

4 Design of Experiments

The proposed multi-objectives PSO based algorithm is examined and compared with a pure multi-objective PSO algorithm (MOPSO), three well-known evolutionary multi-objectives algorithms (NSGAI, SPEA2 and PAES) and a state-of-the-art PSO-based multi-objectives feature selection algorithm (CMDPSOFS). The comparison is performed on twelve datasets shown in Table 1, which were selected from the UCI machine learning repository (Asuncion and Newman, 2007). These datasets have different numbers of features, classes and instances. For each dataset, all instances are randomly divided into a training set and a test set, which contains 70% and 30% of the instances, respectively.

All the algorithms are wrapper approaches, which use K-nearest neighbour (KNN) as their classification/learning algorithms where $K=5$. In recent literature Xue et al. (2015), the generality of wrapper feature selection approaches is discussed. The experiment results show that feature subsets, which are selected by wrappers using simple classification algorithms like KNN, can be general to other classification algorithms. Therefore, in this work, only KNN is used as a classification algorithm to select features and to test the performance of selected feature subset. Another reason using KNN instead of other classifier algorithms, like SVM and

Dataset	#Features	#Classes	#Instances
Wine	13	3	178
Australian	14	2	178
Vehicle	18	4	846
German	24	2	1000
Ionosphere	34	2	351
Lung Cancer	56	3	32
Sonar	60	2	208
Movementlibras	90	15	360
Hillvalley	100	2	606
Musk1	166	2	476
Madelon	500	2	4400
Isolet5	617	2	1559

Table 1: Datasets.

DT, is to make the evaluation process faster in this wrapper approach. During the training process, each particle, which represents a set of selected features, is evaluated by using 10-fold cross-validation. After the training process, the selected features are evaluated on the test set to obtain the testing classification error rate. For each dataset, all of the algorithms have been conducted for 50 independent runs.

In all of the PSO-based algorithms, the fully connected topology is used. The parameters are set as follows (Van Den Bergh, 2006): $w = 0.7298$, $c_1 = c_2 = 1.49618$, $v_{max} = 6.0$. The population size is 30 and the maximum number of iterations is 100. The threshold θ is set as 0.6.

In NSGAI (Deb et al., 2000), SPEA2 (Zitzler et al., 2001) and PAES (Knowles and Corne, 1999), the representation of each individual is the same as the GA-based feature selection algorithms (Chakraborty, 2002; Hamdani et al., 2007), where each individual is a n -bit binary string and n is the number of available features. Each bit in the representation corresponds to a feature in the original feature set. If a bit value is “1” then the corresponding feature is selected. Otherwise the bit with value “0” indicates that the corresponding feature is not selected. In these algorithms, a bit-flip mutation operator is applied and a single point crossover operator is used in NSGAI and SPEA2. The mutation rate is $\frac{1}{n}$, where n is the number of features in the original set and the crossover rate is 0.9. In these algorithms, the number of individuals is 30 and the number of generations is 100. Therefore, the total number of evaluations is 3000.

5 Results and Discussion

For each dataset, five multi-objectives algorithms, ISRPSO, CMDPSOFS, NSGAI, SPEA2, PAES and CMDPSOFS are conducted for 50 independent runs. After each run, a set of non-dominated solutions are obtained. In order to compare these algorithms, firstly all 50 archive sets are combined together to create an union set. In this union set, the classification error rate of feature subsets, which share the same

number of features, are “averaged”. A set of “average” solutions is obtained by using the average classification error rate and the corresponding number of features. This average set is called the “average” *Pareto front*. The meaning of *average Pareto front* is the estimation of classification error when the number of features is predefined. In addition, for each dataset, all non-dominated solutions are selected from the union set to create a set of “best” solutions, called “best” set.

Firstly ISRPSO is compared with a pure multi-objective PSO algorithm to illustrate how the local search can improve the Pareto front. This comparison on the training and test sets are shown in Figure 1 and 2 respectively. Meanwhile, Figure 3 and 4 show the comparison between ISRPSO and NSGAI, SPEA2, PAES on the training and test sets respectively. Finally, ISRPSO is compared with the state of art multi-objective PSO based feature selection, CMDPSOFS (Xue et al., 2013). In particular, the classification error on training set between ISRPSO and CMDPSOFS are shown in the Figure 5, while Figure 6 indicates these algorithms’ classification performance on the test set. In these figures, “-Ave” stands for the “average” *Pareto front* resulted from the 50 independent runs. “-Best” represents the non-dominated solutions (“best” set) of all multi-objectives algorithms. In each figure, the top line means the dataset name followed by the total number of features and the classification error rate achieved by using all features.

5.1 Comparison Between ISRPSO and Using All Features

According to Figure 2, in all cases, ISR-Ave includes three or more feature subsets, which select a smaller number of features and achieve a lower classification error rate than using all features.

As can be seen in Figure 2, ISR-Best includes two or more solutions, which select a small number of features while still achieve lower classification error rate than using all features. On all datasets, ISRPSO evolves at least one feature set, which only selects less than 10% of the total number of features but achieves better classification performance than using all features. Specially, on Madelon dataset, despite of selection only 5 out of 500 features, ISRPSO still can achieve around 10.05% better than using all features.

The results suggest that ISRPSO with three operations applied on the *Archive* set can effectively explore the Pareto front, which can select a small number of features and achieve better classification accuracy than using all features.

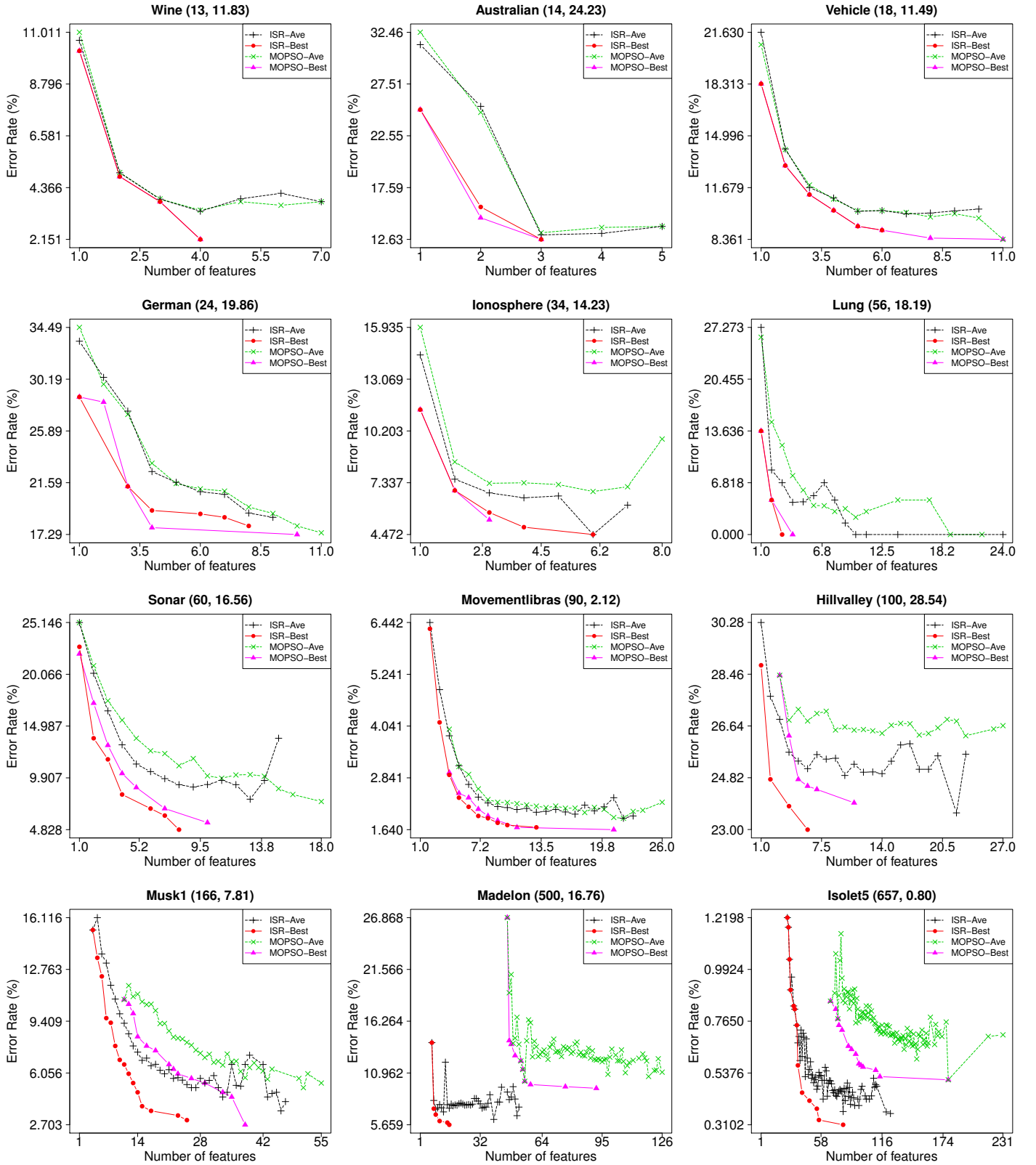


Fig. 1: Comparison between IRPSO and MOPSO on the training set.

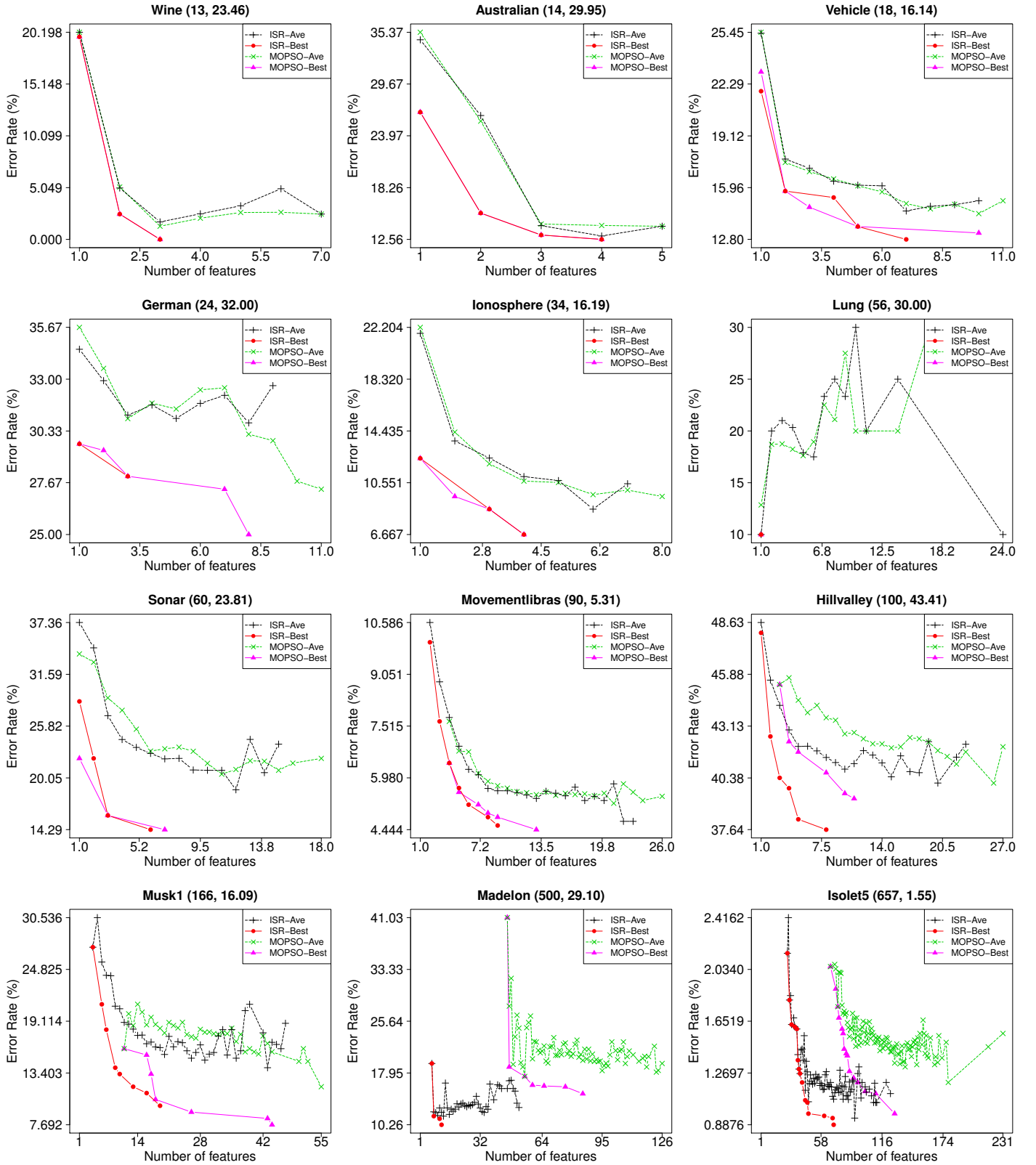


Fig. 2: Comparison between ISRPSO and MOPSO on the test set.

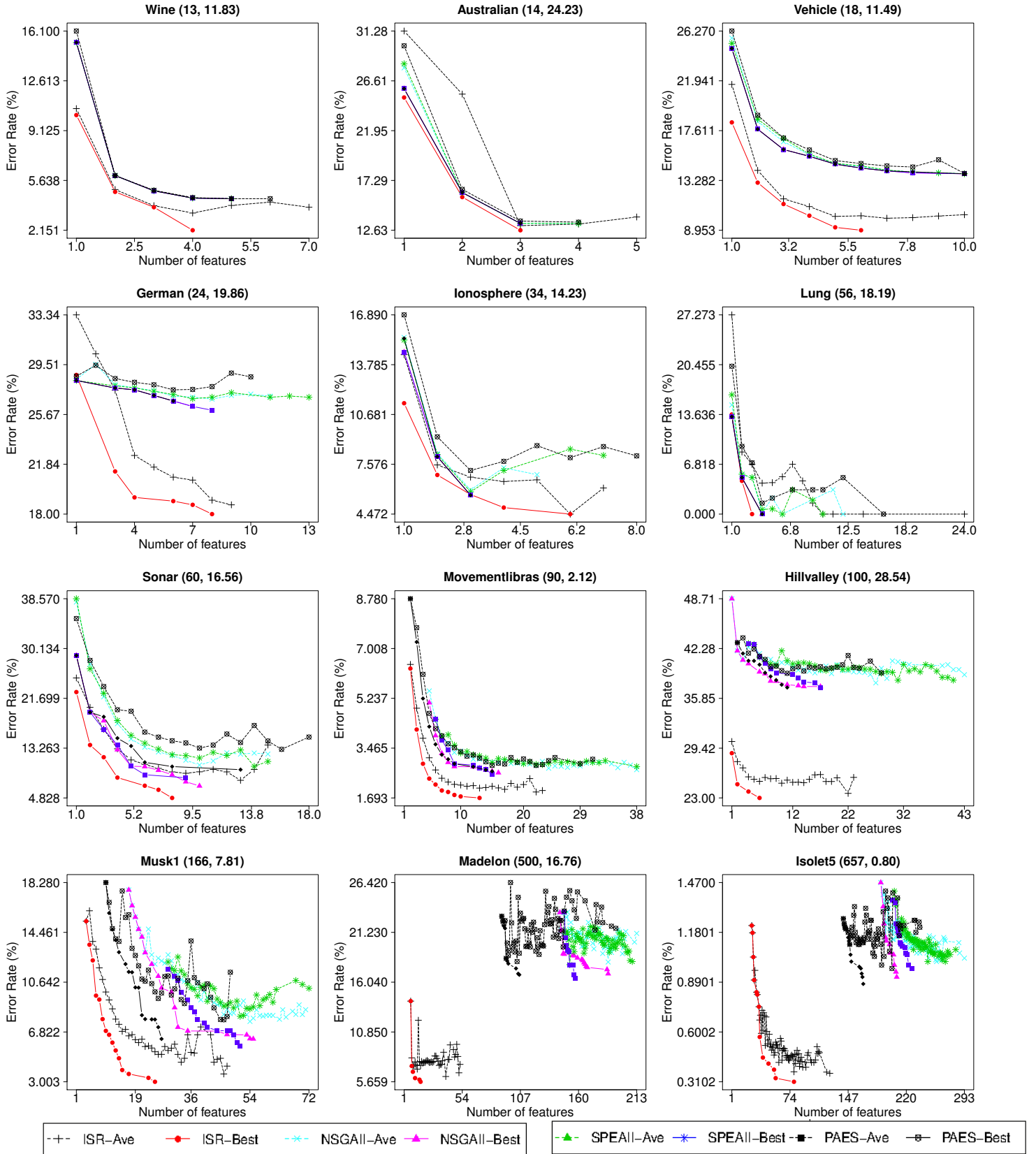


Fig. 3: Comparisons between NSGAIL, SPEA2, PAES and ISRPSO on the training set.

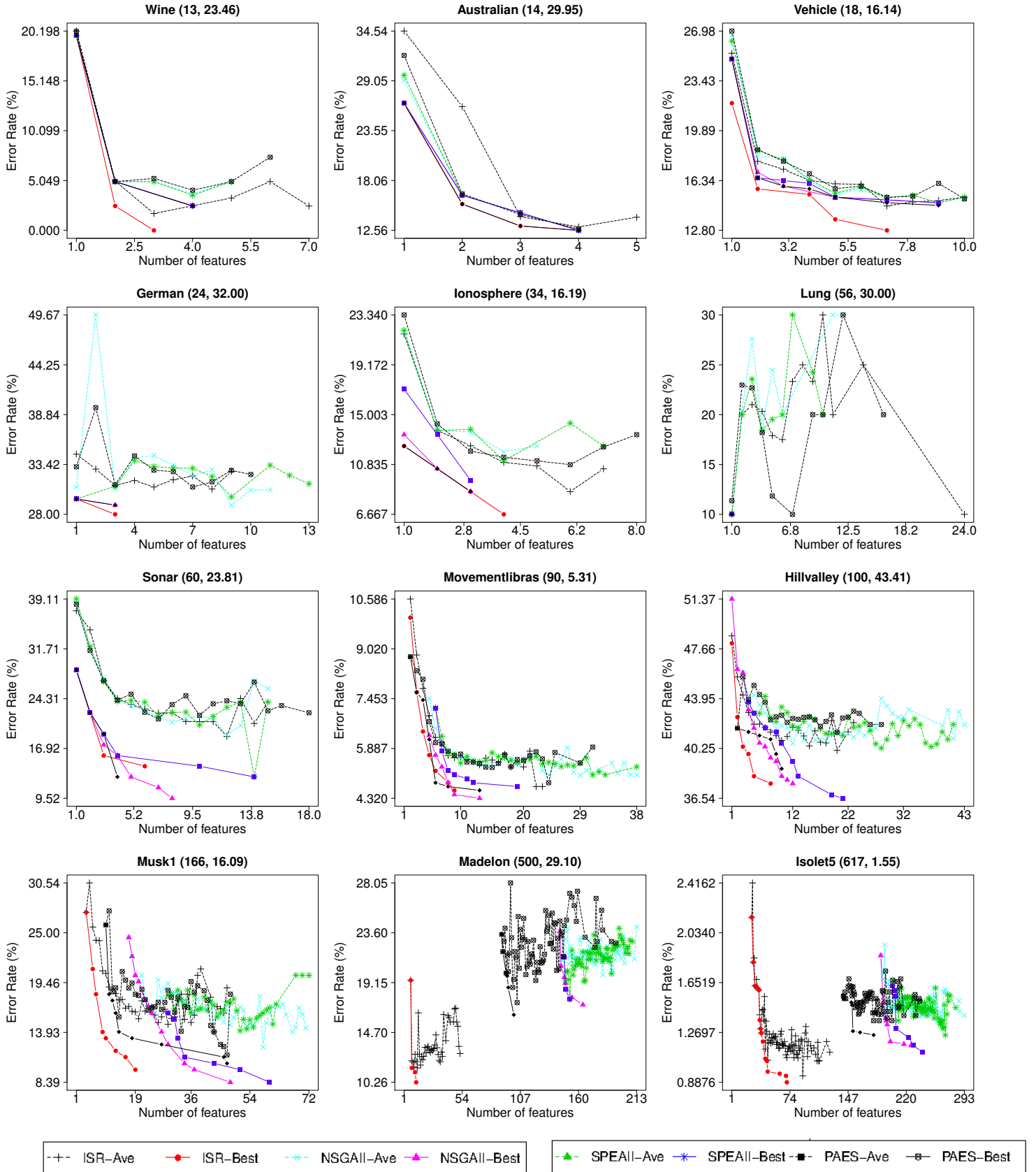


Fig. 4: Comparisons between NSGAII, SPEA2, PAES and ISRPso on the test set.

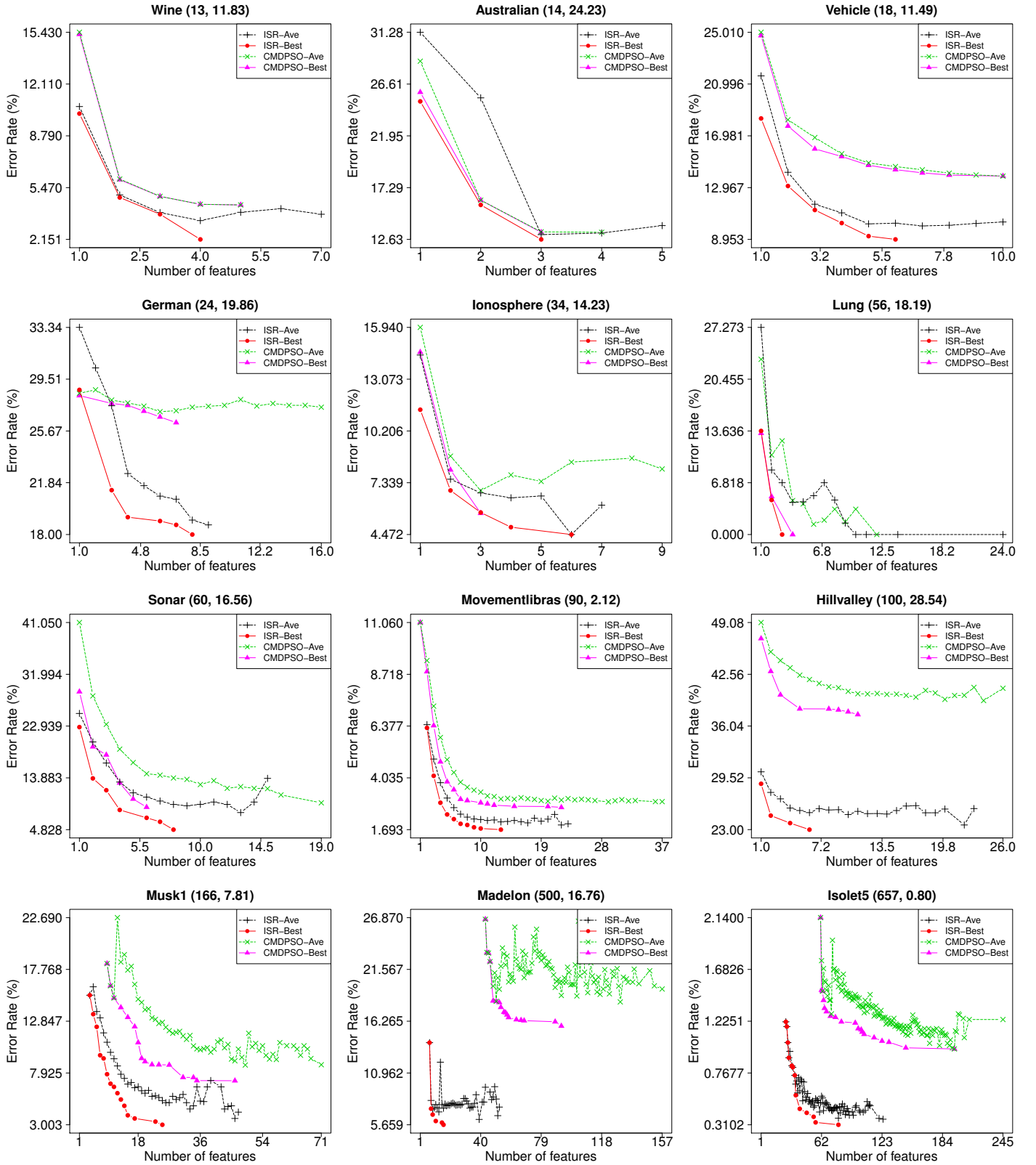


Fig. 5: Comparison between ISRPSO and CMDPSOFS on the training set.

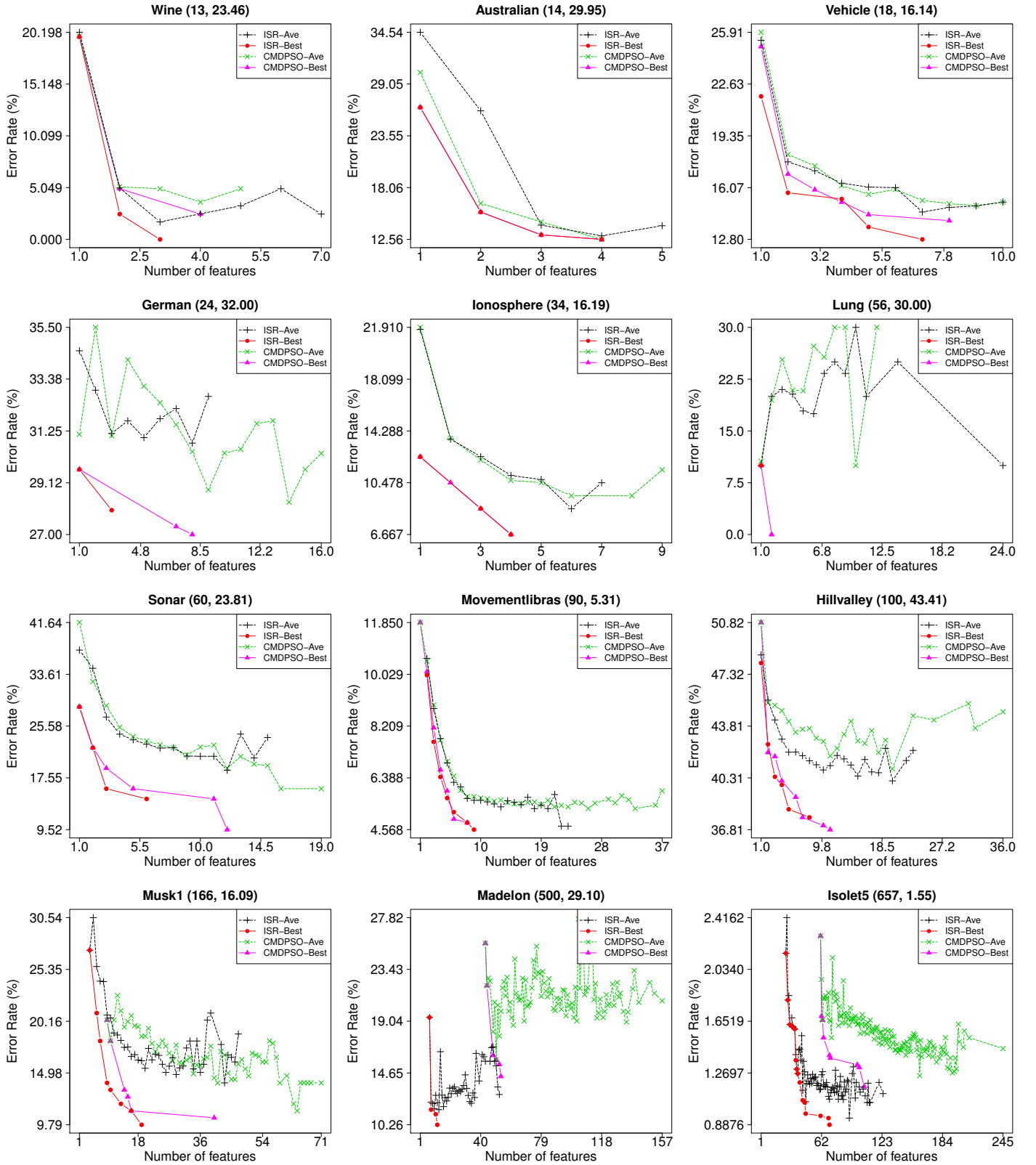


Fig. 6: Comparison between ISRPSo and CMDPSOFS on the test set.

5.2 Comparison Between ISRPSO and a pure multi-objective PSO (MOPSO)

In order to test the effect of the local search applied in ISRPSO, ISRPSO is compared with a pure multi-objective PSO algorithm (MOPSO) for feature selection. The comparisons on the training and the test set are shown in Figures 1 and 2 respectively.

As can be seen from two figures, on the first 6 datasets in which the number of features is quite small, the Pareto fronts evolved by these two algorithms are similar. It is clear that on small datasets, MOPSO is able to effectively explore the search space to produce an optimal or near optimal Pareto front without any additional help. However, the big differences between these two algorithms occur on the other 6 datasets, which have larger number of features than the first 6 datasets. As can be seen from two Figures 1 and 2, in both training and test set, ISRPSO outperforms MOPSO in terms of the number of selected features as well as the classification performance. For example, in the Hillvalley dataset, even selecting the same number of features, ISRPSO always achieves 2-3% better classification accuracy than MOPSO. Similarly, in the Musk1 dataset, ISRPSO only selects around 7 features to achieve the same performance as 20 features selected by MOPSO. The biggest difference can be seen in the Madelon dataset. ISRPSO selects only 10 features but still achieves 5% better performance than 90 features selected by MOPSO. Similarly, in the Isolet5 dataset, ISRPSO is able to evolve at least 3 solutions with very low classification error, which can not be achieved by MOPSO even when a large number of features are selected.

The larger number of features, the more complicated the search space. Therefore, in the datasets with a large number of features, MOPSO tends to stuck at local optima. In these cases, applying local search techniques in MOPSO will help the particle to exploit better solutions, which results in a better Pareto front. Specifically, three proposed operations try to improve the classification performance of each archive member while maintain or even reduce the number of selected features by using the set of promising features. The idea is by improving the archive set, the whole swarm will be guided to better positions. The experimental results show that the proposed local search technique is helpful for MOPSO to better exploit the Pareto front.

5.3 Comparison Between ISRPSO and NSGAII, SPEA2, PAES

In order to test the performance of ISRPSO, it is compared with three popular evolutionary multi-objective algorithms, namely, NSGAII, SPEA2 and PAES. Comparisons between ISRPSO, NSGAII, SPEA2 and PAES on training and test set are shown in Figure 3 and 4 respectively.

According to Figure 3, on the training set, in most cases, the average Pareto fronts evolved by ISRPSO are much better than the other multi-objective algorithms. Similarly, ISRPSO's best Pareto fronts provide better solutions than NSGAII, SPEA2 and PAES. Particularly, on the small datasets (the first six dataset in tables 1), the ISRPSO's Pareto fronts are quite similar to other algorithms' Pareto front, except in Vehicle dataset, ISRPSO's accuracy is about 9% better than other algorithms' accuracy while they selects the same number of features. On the other big dataset, ISRPSO's Pareto fronts are significantly better than NSGAII and SPEA2. With the same number of selected features, ISRPSO's accuracy is about 2%-15% better than the best accuracy of NSGAII, SPEA2 and PAES. Especially, on large dataset like Madelon and Isolet5, ISRPSO is able to find out solutions with a very small number of feature, which can not be found by either NSGAII, SPEA2 or PAES. In addition, on Madelon dataset, the worst solution of ISRPSO significantly dominates the best solution of NSGA, SPEA2 and PAES algorithms.

As can be seen in Figure 4, in most cases, ISRPSO's Pareto front is similar or better than other multi-objective algorithms. Particularly, ISRPSO usually selects a smaller number of features to achieve the same accuracy with NSGA, SPEA or PAES. However, in the first nine small datasets, sometimes ISRPSO sacrifices the classification accuracy to select a small number of features. For example, in Hillvalley dataset, ISRPSO can not find out the solution which achieves higher classification performance than the best solution of PAES. On the other datasets (big datasets), ISRPSO's Pareto front is significantly better than the other three algorithms. For example, in the Isolet5 dataset, the lowest classification error achieved by ISRPSO is 0.88% with 74 selected features. Meanwhile the lowest classification achieved by NSGAII is 1.2%, which requires more than 220. In addition, on the Madelon dataset, the lowest classification accuracy, achieved by ISRPSO, is 80.5% with only 2 selected features. Meanwhile, 80.5% is also the best performance that NSGAII can achieve but NSGAII needs to select a large feature set, which contains more than 160 features.

The results in Figure 3 and 4 suggest that ISRPSO can effectively improve the Pareto front. In most cases, ISRPSO outperforms NSGAII, SPEA2 and PAES in both objectives. However, on Hillvalley dataset, ISRPSO sacrifices the classification accuracy to achieve smaller number of features. The reason is that the proposed algorithm lacks of exploration ability. Since the local search operations aim to add or remove at most one feature from the current feature set, the operations can only find out the better subset which are close to the current position but better performance than the current feature set. Therefore, the positions, which correspond to a much higher number of features than the current solution, are too far and hard to be discovered by the local search operations. However, with the same number of selected fea-

tures, the local search operations ensure that the better feature combination will be discovered. Therefore, ISRPSO usually achieves better performance than other multi-objective algorithms when the same number of features are selected.

5.4 Comparison Between ISRPSO and CMDPSOFS

Figure 5 indicates the performance of ISRPSO and CMDPSOFS on the training set. As can be seen from Figure 5, on all datasets, ISRPSO selects a smaller number of features and still achieve better classification performance than CMDPSOFS. With the same number of selected features, ISRPSO outperforms CMDPSOFS in terms of classification accuracy. For example, in the Hillvalley, with 7 selected features, ISRPSO's performance is about 14% better than CMDPSOFS's classification accuracy. In most cases, the ISRPSO's average Pareto front is even better than the best Pareto front involved by CMDPSOFS. In Madelon dataset, despite of selecting only 5 features, ISRPSO still achieves better performance than the performance of 100 features selected by CMDPSOFS. In order to achieve same classification accuracy as ISRPSO, CMDPSOFS usually needs to select much more feature than ISRPSO. For example in Movementlibras dataset, CMDPSOFS selects from 2 to 8 times more features than ISRPSO.

Figure 6 shows the differences between ISRPSO and CMDPSOFS on the test set. In the first ten datasets, the average pareto fronts of ISRPSO and CMDPSOFS are similar in terms of classification accuracy but ISRPSO usually selects smaller number of features than CMDPSOFS. Similarly, on the first ten datasets, ISRPSO's best pareto fronts are almost identical to the best pareto fronts from CMDPSOFS. Although, in the best pareto fronts, ISRPSO still selects slightly smaller number of features than CMDPSOFS. However, on some datasets like Sonar or German, ISRPSO can not find out the solution which selects large number of features but achieves low classification rate. Once more, ISRPSO sacrifices the classification accuracy to select a small number of features. On the other big datasets, namely Madelon and Isolet5, ISRPSO outperforms CMDPSOFS in terms of the number of selected features and the classification performance. For example, in Madelon dataset, in order to achieve 19% classification error rate, ISRPSO selects only 5 features while CMDPSOFS needs to select more than 40 features. In Isolet5, with 63 selected features, ISRPSO's classification error rate is 0.88% which is much smaller than CMDPSOFS's error rate (1.3%).

The results in Figures 5 and 6 shows that in most cases ISRPSO evolves similar or better pareto front than CMDPSOFS. Specially, in the datasets with large number of features, ISRPSO significantly outperforms CMDPSOFS in term of classification accuracy and number of selected features. This result illustrates that for a complicated search space

(high dimension) the proposed local search technique, which is specifically designed for feature selection, provides a better support than crossover and mutation operators being used in CMDPSOFS. Particularly, CMDPSOFS uses a general mutation operator on the whole swarm to improve both global and local search abilities of the algorithm. However, the mutation operator in CMDPSOFS is not specifically designed for feature selection problems. In our algorithm, the local search technique uses the sequential forward/backward idea to add/remove feature from the current feature set. In addition, the local search technique also uses a good feature set (all features selected by the archive set) to improve the current feature, which is likely to be faster and more effective than using all features, like in CMDPSOFS. Furthermore, our local search concentrates on improving the quality of the archive set rather than the whole swarm like CMDPSOFS. The reason is a good archive set is expected to guide the whole swarm to discover better feature subsets and evolve a more optimal Pareto front. However, the improvement over CMDPSOFS made by ISRPSO on the training set is much better than on the test set, which might be a result of overfitting problem.

6 Conclusions and Future Work

The goal of this study was to develop a PSO based multi-objective feature selection approach to evolving a set of non-dominated feature subsets and achieving a high classification performance. The algorithm ISRPSO was proposed to simultaneously minimise the number of features and the classification error rate. In ISRPSO, three operations, namely *inserting*, *removing* and *swapping* are applied on each archive member to better explore the Pareto front. The experiments on 12 datasets show that ISRPSO successfully evolved a set of non-dominated solutions, which reduce the number of features and achieve better classification performance than using all features. In comparison with a pure multi-objective PSO (MOSPO), ISRPSO usually evolves better Pareto front especially on the datasets with a large number of features, which indicates that the proposed local search is useful for feature selection problems. Furthermore, the results show that ISRPSO outperformed three well-known evolutionary multi-objective algorithms (NSGAI, SPEA2, PAES) in terms of both classification accuracy and the number of selected features. Compared with CMDPSOFS, ISRPSO achieves similar or better classification accuracy while selects smaller number of features. Especially, for the data sets with a large number of features, ISRPSO significantly outperformed all other algorithms.

However, there are some potential limitations of ISRPSO. Firstly, overfitting is one of ISRPSO's problem. As can be seen from the results, sometimes the significant improvement made by ISRPSO on the training set does not lead to

a significant improvement in the test set. Therefore, in the future, we will further develop ISRPSO to improve its generalization. In addition, for some datasets, ISRPSO seems to sacrifice the classification accuracy to select a small number of features. It is necessary to further balance between these two objectives for ISRPSO, which is left for future work. In addition, as can be seen from the experimental results, both genetic operators such as crossover, mutation and three local search operators helps MOSPO to better explore the Pareto front. Therefore, the combination between these two ideas might even better support MOPSO, which will be investigated in the future. Additionally, ISRPSO is not tested with high-dimensional datasets mainly because of the expensive computation cost of wrapper approaches. In the future, it would be interesting to reduce the computation cost of ISRPSO so that it can be extended to deal with high-dimensional datasets such as gene datasets. Although the experimental results show that ISRPSO could evolve a good Pareto front, the computation complexity of the algorithm is not analysed in detail due to the variation in the fitness evaluation process of feature selection problems. Investigating the complexity of a feature selection algorithm is still an open issue, which is left for future work.

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