On initial population generation in feature subset selection

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Abstract

Performance of evolutionary algorithms depends on many factors such as population size, number of generations, crossover or mutation probability, etc. Generating the initial population is one of the important steps in evolutionary algorithms. A poor initial population may unnecessarily increase the number of searches or it may cause the algorithm to converge at local optima. In this study, we aim to find a promising method for generating the initial population, in the Feature Subset Selection (FSS) domain. FSS is not considered as an expert system by itself, yet it constitutes a significant step in many expert systems. It eliminates redundancy in data, which decreases training time and improves solution quality. To achieve our goal, we compare a total of five different initial population generation methods; Information Gain Ranking (IGR), greedy approach and three types of random approaches. We evaluate these methods using a specialized Teaching Learning Based Optimization searching algorithm (MTLBO-MD), and three supervised learning classifiers: Logistic Regression, Support Vector Machines, and Extreme Learning Machine. In our experiments, we employ 12 publicly available datasets, mostly obtained from the well-known UCI Machine Learning Repository. According to their feature sizes and instance counts, we manually classify these datasets as small, medium, or large-sized. Experimental results indicate that all tested methods achieve similar solutions on small-sized datasets. For medium-sized and large-sized datasets, however, the IGR method provides a better starting point in terms of execution time and learning performance. Finally, when compared with other studies in literature, the IGR method proves to be a viable option for initial population generation.

Keywords: Feature subset selection, Initial population, Multiobjective optimization

1. Introduction and Background

With advances in technology and the effects of globalization, electronic devices get cheaper and cheaper. As of today, technology has spread among users having various types of demographics and it has been an indispensable part of our lives. As a result, 2.5 quintillion bytes of data had been created every day in 2012 and this volume increases massively

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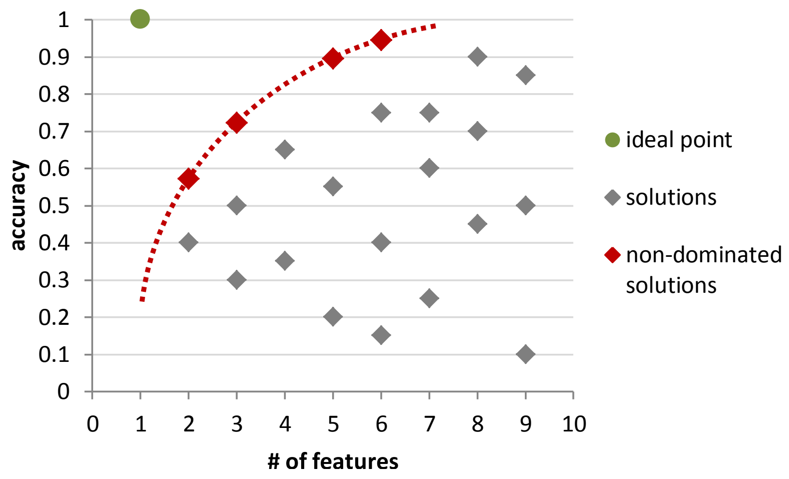

Figure 1: Non-dominated solutions fitting to a pareto curve in a multiobjective FSS problem (Deniz et al., 2017).

every passing minute (BBC, March 2014). It is not feasible to analyze this amount of data by manual processing, hence, we need to utilize machine learning techniques to do it automatically. However, building an efficient and accurate machine learning models is not a straightforward process. Also, training a machine learning model requires analyzing every single feature of every single instance. Therefore, removing redundant and/or irrelevant features from data could be beneficial in terms of computation time and learning performance. Feature Subset Selection (FSS) has been a preferable tool to achieve this goal (Guyon & Elisseeff, 2003).

FSS is the process that tries to remove redundant and/or irrelevant features from data. Since these features may not be clear initially, the utilization of such searching algorithms for finding the features that represent the data best is crucial. In this study, we use the MTLBO-MD searching algorithm to find the best feature subset. MTLBO-MD is a multiobjective teaching learning based optimization algorithm, proposed in our previous study (Kiziloz et al., 2018). Detailed information on the MTLBO-MD algorithm is given in subsection 2.1. We need a multiobjective search algorithm since there are two objectives in this problem domain, namely, decreasing number of features and increasing classification performance (accuracy). In a multiobjective optimization environment, different solutions may dominate each other in different objectives, hence, there may exist a solution set rather than only one solution (Horn et al., 1994). Figure 1 shows a sample of non-dominated solutions in a hypothetical problem.

Evolutionary based algorithms are utilized in many combinatorial and optimization problems and they require an initial population to begin their search. Traditionally, this initial population is set randomly (Michalewicz, 1996). However, poor selection of initial population may lead to getting stuck in local optima rather than finding the global optimum (Toğan & Daloğlu, 2008). Also, choosing the initial population wisely could possibly lead to faster convergence to the global optimum. For this reason, we investigate the effects of using different initial population generation methods in FSS domain. Our main motivation is to analyze empirical results and find a promising initial population generation method in this domain.

There are many studies proposing different strategies to generate an initial population in evolutionary algorithms. Maaranen et al. (2007) show that the initial population may have a considerable effect on the objective function in continuous optimization problems. They test different initial population seeds and conclude that smarter initial populations may decrease computation time or may bring out better solutions. Similarly, Karci (2004) proposes a method to initialize the population for continuous global optimization problems. The study emphasizes that the initial population should be evenly distributed for not getting stuck in local optima. Three benchmark problems having many dimensions were used in their experiments and it is seen that their method finds near-optimal solutions. Besides, Diaz-Gomez & Hougen (2007) propose five different (two gene-level, two chromosome-level, and one population-level) metrics to evaluate population diversity. However, they do not compare these metrics with empirical results.

Studies investigating the initial population for well-known optimization problems also exist. Hill (1999) proposes a heuristic for generating the initial population for two-dimensional knapsack problems, which performs better than the traditional methods according to their experiments. Similarly, Escobar et al. (2011) propose a constructive heuristic algorithm to generate the initial population for transmission expansion planning problem. They use real data in their experiments and their algorithm gives better results than random initialization. In addition, Jorapur et al. (2016) proposes a population initialization algorithm for the job shop scheduling problem. Their algorithm uses random job based initialization after a simple job based representation and obtains better results than mere random based one. Moreover, Deng et al. (2015) propose a k-means based initial population generation algorithm for the travelling salesman problem. Experimental results indicate high performance improvement as compared to generating an initial population in a random or greedy fashion. Meanwhile, setting the initial population in k-means clustering is also very important since it may affect the clustering result dramatically. Zhou et al. (2018) propose a method, called SeedClust, which generates the best chromosome for automatic k-means clustering by applying an adaptive genetic algorithm. Experiment results show that SeedClust is an effective method for finding an effective initial population.

Up to our best knowledge, the effects of the initial population have not been investigated thoroughly in the FSS domain. On the other hand, all mentioned studies state, with empirical results on different problem domains, that initial population should be selected wisely, rather than being generated randomly. Wise selection methods refer to statistical or greedy approaches, both of which are included in our tests.

The main contribution of this study is to investigate the effects of using different initial population generation methods in FSS domain. For this reason, we compare five different methods (traditional methods along with our proposed methods) using various datasets and analyze their effectiveness with empirical results. FSS is generally not the main functionality of an expert system, yet, applying it to remove redundant data becomes a crucial step as

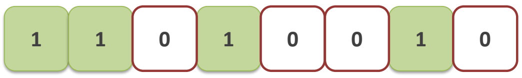

Figure 2: Chromosome structure (1 indicates selected features, 0 otherwise).

dataset sizes grow larger. Moreover, it should be applied without compromising efficiency. We expect our study to help researchers apply FSS with higher accuracy using less resources when building an expert system.

The rest of the manuscript is organized as follows. In Section 2, our model is introduced with the following subsections: population selection, initial population generation methods, and applied machine learning techniques. Experimental results and discussion are given in Section 3. Finally, concluding remarks and possible future works are shared in the last section, Section 4.

2. Model

In this section, we introduce the model used in our study. First, we describe the population selection algorithm, MTLBO-MD, in detail. Then, we give the initial population generation methods used. Finally, we briefly mention the machine learning techniques used for evaluating individuals.

2.1. Individual description and population selection

Finding the best population in a multiobjective environment is not a straightforward process since an improvement in one objective may worsen other objectives. In a previous study (Kiziloz et al., 2018), we proposed a promising algorithm, called Multiobjective Teaching Learning Based Optimization with Minimum Distance (MTLBO-MD), to overcome this problem. For FSS domain, we define a chromosome as given in Figure 2. Here, a chromosome consists of 1s and 0s, indicating whether its corresponding feature in the dataset is selected or not, respectively.

In a multiobjective domain, an individual in the population dominates another one if and only if it gives better result in at least one of the objectives while all other objectives give the same result. If two individuals can not dominate each other, then they are called non-dominated to each other. MTLBO-MD consists of two phases: the teacher phase and learner phase (see Figure 3). In teacher phase, all non-dominated individuals are found and the one that is closest to the ideal point is chosen as the teacher while the other individuals are set as students. The ideal point in feature subset selection domain is the point where the *number of features* $= 1$ and *accuracy* $= 1.0$, i.e. being able to classify perfectly using only one feature. After the teacher is selected, a crossover is applied between the teacher and all students, separately. We keep both old and new individuals (students) in the possible population set. Teacher phase of the algorithm ends with this operation and the learner phase begins. In the learner phase, a crossover is applied to two random students for

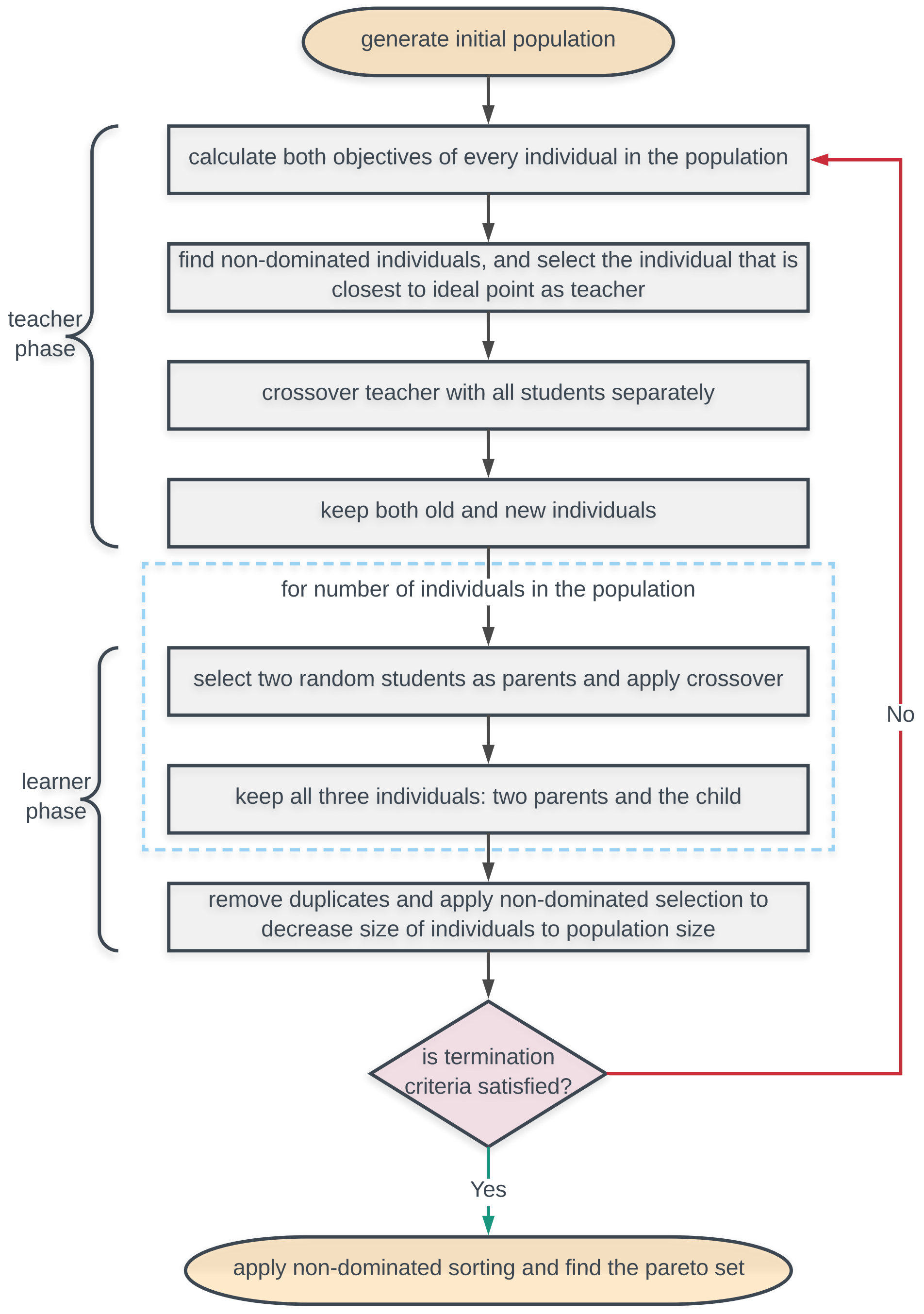
generate initial population
teacher phase
calculate both objectives of every individual in the population
find non-dominated individuals, and select the individual that is closest to ideal point as teacher
crossover teacher with all students separately
keep both old and new individuals
for number of individuals in the population
learner phase
select two random students as parents and apply crossover
keep all three individuals: two parents and the child
remove duplicates and apply non-dominated selection to decrease size of individuals to population size
is termination criteria satisfied?
No
Yes
apply non-dominated sorting and find the pareto set

Figure 3: MTLBO with Minimum Distance (MTLBO-MD).

the number of population size. Meanwhile, all new individuals are added to the possible population set. When the crossover is complete, first, duplicate individuals in the possible population set are removed and the number of individuals is decreased to population size via non-dominated sorting. For this purpose, individuals are divided into fronts (i.e. the first front includes all non-dominated solutions, the second front includes solutions that are only dominated by first front solutions and are non-dominated to each other, etc.). The population is filled by selecting from these fronts in order. Crowding distance method is used to select individuals constituting a front if only a part of that front is needed to fill the population. When the teacher and learner phase run for the specified number of generations, the algorithm terminates after finding the pareto set.

We used crossover and mutation operators in the generation of new chromosomes. Half uniform crossover is implemented for the crossover part, and bit-flip mutation is implemented for the mutation part. In half uniform crossover, one new chromosome, namely child chromosome, is generated by using two existing chromosomes, namely parent chromosomes. Feature genes of the parent chromosomes are compared, and the same ones are kept in the child chromosome. If a feature gene is different in the parents, then one of them is randomly chosen and transferred to the child chromosome. Mutation, on the other hand, operates on a single chromosome. It inverts one of the feature genes randomly and generates a new chromosome. We set the mutation probability to 0.02 in our implementation.

2.2. Initial population generation methods

We initially designed four different initial population generation methods, as described below. The fifth method, SR, is introduced as a post hoc study after obtaining initial test results.

Random (Rnd): In this method, initial population is generated in a complete random fashion.

Distinct Random (DR): Rather than complete randomness, we wanted to add a heuristic into random population generation and investigate its effects. For this purpose, we randomly generated individuals that is 10 times the population size and selected the most distinct individuals among them as the initial population. Here, we use the Hamming Distance, i.e. the number of different features, as distinctness metric between two chromosomes.

Information Gain Ranking (IGR): In this method, we utilized a filter based feature selection approach, information gain (Quinlan, 1986), to find the most promising features in our dataset. Then we generate the initial population as follows: the first individual is the chromosome having only the most promising feature selected, the second individual is the chromosome having the most two promising features selected, and so on. We continue to generate individuals in this fashion until population size is met.

Greedy (Gr): Finally, we utilized a greedy approach, sequential forward selection, to generate the initial population. For this purpose, we evaluate all chromosomes having only one feature selected, and pick the feature with the highest accuracy value. We add the individual having this picked feature selected into our initial population. Then, for the second individual, we fix the picked feature as selected and evaluate all possible chromosomes having two features selected. Now, we pick the features achieving the highest accuracy value, and add this individual into the initial population. Search for the third individual is similar, picked two features are fixed as selected, and all chromosomes having three individuals are evaluated. This iteration continues until population size is met. The main difference of this method from others is its requirement to evaluate many chromosomes for generating the initial population. This method evaluates many possibilities and could be considered as an extreme case, yet, its solutions are valuable for evaluating the performances of other methods.

Small Random (SR): In Rnd and DR, the initial population is deployed in a totally random fashion, giving it a small chance to find the global optima in small population size and number of generations. Accordingly, we introduced the SR method as a smarter option for random based initial population generation methods. In this method, the first individual is the chromosome having only one randomly selected feature. This individual is added to the initial population. The second individual is the chromosome having two features: the first one is the selected feature for the first individual, the second one is randomly selected. After adding this individual into the initial population, the third individual is generated similarly: the first two features selected from the second individual, the third feature is selected randomly. Iteration continues until population size is met.

2.3. Applied machine learning techniques

We used Logistic Regression (LR), Support Vector Machines (SVM) and Extreme Learning Machine (ELM) to evaluate solution sets obtained by MTLBO-MD algorithm. LR uses a probabilistic model to perform classification, SVM tries to maximize the distance between different classes, and ELM utilizes the power of neural networks.

Logistic Regression: LR analyzes the similarity of the data points to estimate the occurrence probability of an event. Once this probability is calculated, it decides on the occurrence result and performs classification accordingly. We used a Matlab function, *glmfit*, for LR classification.

Support Vector Machines: SVM constructs a line between different classes by maximizing the distance between the line and closest data points to the line. We used a Matlab function, *fitcsvm*, for SVM classification. We chose kernel type as linear and set normalization parameter to *True*. Other than these, default parameters of the built-in function are used.

Extreme Learning Machine: ELM is a feedforward neural network consisting of a single hidden layer. ELM does not need tuning which distinguishes it from other neural networks. Consequently, the training time of ELM is less than other traditional neural networks. We used an ELM library, developed by Huang et al. (2011), for ELM classification. We set the activation function as sigmoidal and node count to 20 in the hidden layer.

3. Experimental Results

In this section, we describe our experimental environment, problem instances, and obtained results. We carried out the experiments on a computer with AMD Ryzen 7 1800X

Table 1: Specification of the datasets used in the experiments.

Dataset	**Problem ID**	**Number of features**	**Actual number of classes**	**Number of instances**	**Class proportions**
Covertype	CT	54	7	$581,012$	43% - 57%
Mushrooms	MR	22	2	8124	48% - 52%
Spambase	SB	57	2	4601	39% - 61%
Nursery	NU	8	5	$12,960$	50% - 50%
Connect-4 Opening	C4	42	3	$67,557$	27% - 73%
Waveform	WF	40	3	5000	50% - 50%
Financial	FI	93	2	$17,108$	3% - 97%
Pima Indian Diabetes	PM	8	2	768	35% - 65%
Breast Cancer	BC	9	2	699	35% - 65%
Ionosphere	IO	34	2	351	36% - 64%
Wisconsin Breast Cancer	WBC	30	2	569	37% - 63%
Musk (Version 2)	MU	168	2	6598	15% - 85%

Eight-Core Processor with a 3.6 GHz clock rate and 16 GB of main memory. We used MATLAB 2015a for evaluating individual accuracy, and Java for remaining parts.

In our study, we used 12 datasets, 11 of which are obtained from the University of California UCI Machine Learning Repository (Dua & Graff, 2017). One remaining dataset, *Financial*, is retrieved from a study by Pacheco et al. (2009). Detailed information on datasets is given in Table 1. Most of the datasets used in this study have two actual classes. In different cases, datasets are reduced to two classes with the selection of the classes having most instances. Categorical values in datasets are converted to numerical values by arbitrary coding of symbols, in the preprocessing phase of the study.

In supervised learning, classification accuracy mainly relies on how well training data represents actual data. To eliminate any bias towards one class, the data is generally split into k-partitions and each partition is used for testing in separate turns, while all remaining partitions are used for training. This methodology is called k-fold cross-validation. However, some of our datasets have a high amount of instances (the number of instances increases up to $581,012$) and application of k-fold cross-validation on these datasets would consume an enormous amount of time. For this reason, we first reduced the instance sizes of the CT, NU, WF, and FI datasets to $10,000$, with respect to their original class proportions, and then applied 5-fold cross-validation on all datasets. A validation set is not used in the experiments.

In an evolutionary algorithm, especially in MTLBO-MD, population size and number of generations are two main factors that affect the quality of the results. In our previous study (Deniz et al., 2017), we discovered with experimental results that, selecting population size as 40 and the number of generations as 60 could lead to finding good enough solutions in an acceptable amount of time. However, we opted to halve both values since we are only analyzing the effects of initial population generation methods in this study. This choice would limit the exploration and exploitation capability of the MTLBO-MD algorithm, and hence, initial population generation would become more important. As a result, population size and the number of generations are selected as 20 and 30, respectively.

Table 2: Maximum accuracy, number of features at maximum accuracy, and execution time values for each initial population generation method and machine learning technique.

Dataset (Feature size)	**Method**	**Max. accuracy**			**# of features at max. accuracy**			**Exec. time (sec.)**		
		LR	**SVM**	**ELM**	**LR**	**SVM**	**ELM**	**LR**	**SVM**	**ELM**
CT (54)	Rnd	0.775	0.778	0.685	10	14	8	1341.9	20170.5	251.6
	Gr	0.779	0.776	0.666	10	7	2	927.5	16932.8	385.8
	IGR	0.772	0.773	0.655	8	6	3	86.6	6727.1	59.3
	DR	0.777	0.776	0.586	11	11	10	590.5	13769.8	135.0
	SR	0.751	0.621	0.673	3	3	4	79.3	592.7	35.7
MR (22)	Rnd	0.938	0.958	0.981	3	8	4	113.0	3621.5	83.5
	Gr	0.955	0.952	0.990	9	6	2	294.0	2875.4	113.7
	IGR	0.950	0.957	0.989	6	8	3	44.6	5703.3	18.4
	DR	0.945	0.950	0.990	8	6	4	87.4	3758.7	51.5
	SR	0.938	0.956	0.947	4	6	4	23.8	4481.5	20.7
SB (57)	Rnd	0.917	0.919	0.882	15	15	14	138.0	4561.8	135.5
	Gr	0.922	0.922	0.889	14	15	8	146.8	2748.6	220.2
	IGR	0.900	0.906	0.882	8	13	7	28.9	978.5	26.3
	DR	0.915	0.910	0.887	18	25	12	121.8	3719.0	63.8
	SR	0.869	0.854	0.818	13	13	8	34.1	2410.0	33.3
NU (8)	Rnd	1.000	1.000	1.000	1	1	1	34.4	168.4	31.0
	Gr	1.000	1.000	1.000	1	1	1	40.4	104.5	30.9
	IGR	1.000	1.000	1.000	1	1	1	20.0	43.0	8.7
	DR	1.000	1.000	1.000	1	1	1	29.0	443.5	27.4
	SR	1.000	1.000	1.000	2	2	2	13.9	210.0	10.8
C4 (42)	Rnd	0.805	0.797	0.792	21	11	9	308.3	15743.8	225.4
	Gr	0.818	0.728	0.798	16	1	14	188.1	4872.9	522.6
	IGR	0.806	0.813	0.793	13	17	11	46.2	10347.2	124.8
	DR	0.813	0.803	0.791	17	16	11	156.5	12621.0	160.6
	SR	0.744	0.738	0.759	11	5	7	74.6	1206.8	86.2
WF (40)	Rnd	0.923	0.924	0.904	9	14	7	47.4	2314.4	74.7
	Gr	0.924	0.926	0.902	9	9	7	47.5	2392.2	125.7
	IGR	0.925	0.929	0.903	10	11	6	18.4	790.2	11.6
	DR	0.922	0.926	0.906	13	14	6	24.0	2283.7	33.7
	SR	0.900	0.893	0.871	9	6	4	15.3	497.4	12.2
FI (93)	Rnd	0.966	0.966	0.966	8	11	15	2566.8	71212.4	203.2
	Gr	0.966	0.966	0.966	1	1	1	547.5	23589.3	672.0
	IGR	0.966	0.966	0.966	1	1	1	71.2	302.8	28.2
	DR	0.966	0.966	0.966	14	15	10	2209.0	76677.8	119.8
	SR	0.966	0.966	0.966	1	1	1	45.1	615.9	30.9
PM (8)	Rnd	0.773	0.776	0.727	5	6	1	2.9	23.0	7.1
	Gr	0.777	0.776	0.741	6	6	1	2.4	23.7	5.5
	IGR	0.773	0.776	0.746	5	6	1	4.6	12.3	3.5
	DR	0.777	0.773	0.720	6	3	1	2.9	19.7	6.3
	SR	0.771	0.773	0.714	4	3	4	3.5	7.9	2.7
BC (9)	Rnd	0.969	0.971	0.966	4	5	4	2.6	12.4	6.8
	Gr	0.967	0.971	0.966	5	5	3	3.6	11.6	6.1
	IGR	0.967	0.971	0.970	5	5	3	1.8	4.1	3.2
	DR	0.969	0.971	0.967	3	5	3	3.3	8.7	5.9
	SR	0.966	0.969	0.969	4	6	4	1.2	6.2	2.4
IO (34)	Rnd	0.900	0.906	0.917	6	12	5	40.7	89.8	26.6
	Gr	0.906	0.912	0.917	8	7	3	114.0	77.6	35.2
	IGR	0.858	0.877	0.923	6	5	3	4.3	28.8	6.9
	DR	0.895	0.915	0.926	10	12	4	20.0	53.5	12.1

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Table 2 – continued from previous page

Dataset (Feature size)	Method	Max. accuracy			# of features at max. accuracy			Exec. time (sec.)		
		LR	**SVM**	**ELM**	**LR**	**SVM**	**ELM**	**LR**	**SVM**	**ELM**
	SR	0.895	0.877	0.915	7	9	3	14.2	33.8	5.5
WBC (30)	Rnd	0.979	0.981	0.954	7	10	7	17.0	74.4	32.9
	Gr	0.981	0.984	0.930	6	9	3	15.7	76.5	27.9
	IGR	0.979	0.975	0.928	6	5	3	4.6	14.9	7.2
	DR	0.974	0.979	0.960	5	7	5	13.1	32.3	21.7
	SR	0.979	0.984	0.947	6	9	5	6.6	33.6	7.3
MU (168)	Rnd	0.938	0.944	0.866	72	69	37	880.8	55579.0	293.3
	Gr	0.910	0.921	0.890	11	10	9	354.8	20854.9	978.8
	IGR	0.920	0.920	0.880	10	16	5	25.6	3306.1	40.9
	DR	0.941	0.943	0.867	64	50	30	628.6	43691.9	180.7
	SR	0.868	0.896	0.870	6	7	5	19.1	1687.3	39.4

Accuracy results of the non-dominated solutions, execution times and the number of features for each initial generation method and machine learning technique are summarized in Table 2. Complete results (all the non-dominated solutions separated by datasets) are provided in the supplementary document.

Rather than discussing all 12 datasets separately, we categorize our existing datasets into three clusters as small-, medium-, and large-sized datasets, in order to make comparisons easier. For this purpose, we sorted all the datasets by their number of features in ascending order. Categorizing PM, NU, and BC as small-sized datasets was straightforward due to their small number of features (up to 9). For deciding on where to split the medium- and large-sized datasets, the increment in the number of features from 42 (C4) to 54 (CT) stands out at first glance. However, the huge difference in the number of instances between WF (5000) to C4 (67,557) is also remarkable, and C4 resembles CT (581,012) more on this aspect. As a result, even though the number of features between WF and C4 differentiates by only 2, we decided to categorize WF as a medium-sized dataset, and C4 as a large-sized dataset, due to their number of instances. Hence, we obtain the clusters as specified below:

- small-sized datasets: PM, NU, and BC
- medium-sized datasets: MR, WBC, IO, and WF
- large-sized datasets: C4, CT, SB, FI, and MU

We would like to note that our categorization is not a representative of a universal categorization considering enormous datasets used in other domains such as text mining or bioinformatics. We categorize some of our datasets as large since they are larger than the others in this study only.

Obtained results indicate that, on the small-sized datasets, all methods can decrease the number of features with similar accuracy values. The execution time of IGR is less than other methods in most cases. For medium-sized datasets, it is clear that Gr performs well in

Table 3: Mean and standard deviation of the dataset accuracies with LR classification.

Dataset	**Rnd**	**Gr**	**IGR**	**DR**	**SR**
CT	0.741 ± 0.064	0.768 ± 0.012	0.762 ± 0.011	0.771 ± 0.006	0.716 ± 0.070
MR	0.807 ± 0.169	0.904 ± 0.070	0.859 ± 0.147	0.900 ± 0.073	0.831 ± 0.128
SB	0.896 ± 0.022	0.897 ± 0.022	0.854 ± 0.052	0.900 ± 0.017	0.826 ± 0.076
NU	1.000 ± 0.000	1.000 ± 0.000	1.000 ± 0.000	1.000 ± 0.000	0.807 ± 0.272
C4	0.794 ± 0.012	0.787 ± 0.024	0.782 ± 0.021	0.788 ± 0.025	0.739 ± 0.005
WF	0.904 ± 0.022	0.893 ± 0.040	0.905 ± 0.024	0.912 ± 0.014	0.837 ± 0.126
FI	0.966 ± 0.000	0.966 ± 0.000	0.966 ± 0.000	0.953 ± 0.018	0.966 ± 0.000
PM	0.765 ± 0.011	0.767 ± 0.011	0.765 ± 0.011	0.767 ± 0.011	0.737 ± 0.052
BC	0.954 ± 0.018	0.955 ± 0.016	0.955 ± 0.016	0.950 ± 0.021	0.939 ± 0.043
IO	0.844 ± 0.086	0.896 ± 0.008	0.840 ± 0.015	0.838 ± 0.092	0.835 ± 0.089
WBC	0.920 ± 0.115	0.964 ± 0.024	0.967 ± 0.014	0.956 ± 0.026	0.921 ± 0.105
MU	0.930 ± 0.004	0.891 ± 0.022	0.896 ± 0.027	0.935 ± 0.004	0.856 ± 0.009

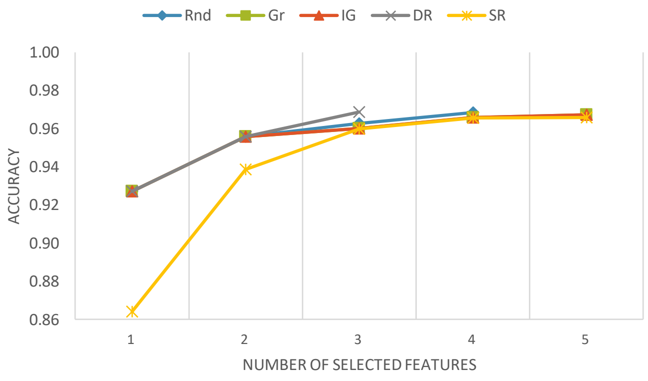
terms of both minimizing the number of features and maximizing accuracy. Rnd and IGR compete with each other, and both dominate DR. Similar to small-sized datasets, execution times of IGR are much less than the execution times of the others. The result for the large-sized datasets is interesting. Both Rnd and DR are outperformed by Gr and IGR in terms of minimizing the number of features. Among Gr and IGR, Gr achieves more diverse non-dominated solutions than IGR does. Again, IGR is the fastest method among all of them. Also, results show that SR can reduce the number of features well, yet, it struggles to find high accuracy values in most cases.

This analysis shows us that, Rnd and DR are competitive initial population generation methods in small-sized datasets, however, they tend to get stuck in local optima as datasets grow larger. This outcome could be triggered by the number of selected features in the initial population. Gr and IGR algorithms begin selecting the number of features from 1, up to population size in the initial population. This is actually a good starting point considering that one of the objectives is reducing the number of features. In medium- and large-sized datasets, Rnd and DR can only achieve high accuracy values with a higher number of features than other methods (Gr, IGR, and SR).

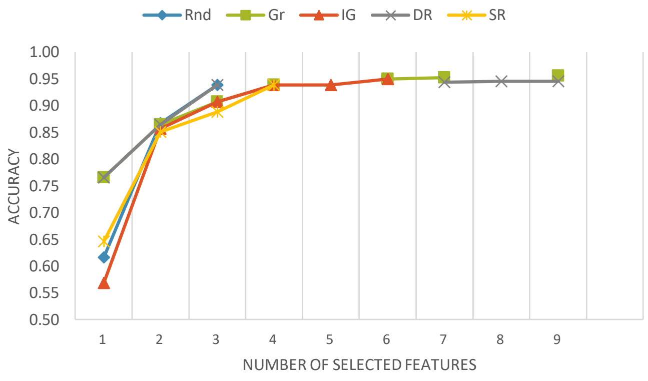
To carry out a more complete comparison, we give mean and standard deviation of the accuracy values of datasets for all initial population generation methods when LR is applied, in Table 3. Moreover, Figure 4 presents the non-dominated solution sets of each initial population generation method on three selected datasets when LR is applied.

To provide more robust analysis, we enhance the comparison results with statistical tests. We use Friedman's Test to test differences of accuracy, the number of features and execution time between initial population generation methods, which indicates a significant difference in every comparison. A post hoc Wilcoxon signed-rank test with Bonferroni Correction is employed for pairwise comparison, with setting the significance level at $p < 0.01$, and the results are presented in Table 4.

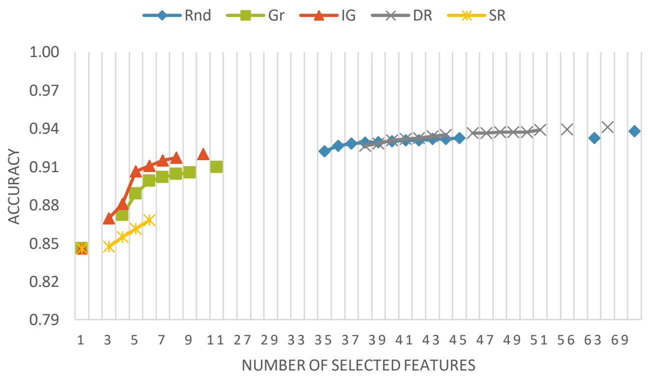
Statistical tests indicate no significant difference between initial population generation methods in terms of maximizing accuracy. The only exception is the SR method, which per-



(a) Non-dominated solutions on BC dataset evaluated by LR.



(b) Non-dominated solutions on MR dataset evaluated by LR.



(c) Non-dominated solutions on MU dataset evaluated by LR.

Figure 4: Non-dominated solutions evaluated by LR on three datasets (one to represent each small, medium and large-sized datasets) using five different initial population generation methods.

Table 4: Results of post hoc pairwise Wilcoxon signed-rank test with Bonferroni Correction (significance level set to $p < 0.01$). Friedman's test results for each group are given in parantheses under each machine learning technique. Significant differences are presented in **bold**.

(a) Accuracy

	LR ($\chi^2(4) = 19.705$, $p = 0.001$)				**SVM** ($\chi^2(4) = 23.280$, $p < 0.001$)				**ELM** ($\chi^2(4) = 17.745$, $p = 0.001$)			
	Rnd	**Gr**	**IGR**	**DR**	**Rnd**	**Gr**	**IGR**	**DR**	**Rnd**	**Gr**	**IGR**	**DR**
Gr	Z=-1.173 p=0.241	-	-	-	Z=-0.700 p=0.484	-	-	-	Z=-0.714 p=0.475	-	-	-
IGR	Z=-0.296 p=0.767	Z=-1.304 p=0.192	-	-	Z=-0.841 p=0.400	Z=-0.070 p=0.944	-	-	Z=-0.204 p=0.838	Z=-0.771 p=0.441	-	-
DR	Z=-1.023 p=0.306	Z=-0.459 p=0.646	Z=-1.201 p=0.230	-	Z=-0.210 p=0.833	Z=-0.663 p=0.507	Z=-1.020 p=0.308	-	Z=-0.306 p=0.760	Z=-0.889 p=0.374	Z=-0.631 p=0.528	-
SR	Z=-2.490 p=0.013	**Z=-2.934 p=0.003**	**Z=-2.941 p=0.003**	**Z=-2.824 p=0.005**	**Z=-2.934 p=0.003**	**Z=-2.847 p=0.004**	**Z=-2.936 p=0.003**	**Z=-2.934 p=0.003**	**Z=-2.934 p=0.003**	**Z=-2.845 p=0.004**	**Z=-2.667 p=0.008**	Z=-2.401 p=0.016

(b) Number of features

	LR ($\chi^2(4) = 12.905$, $p = 0.012$)				**SVM** ($\chi^2(4) = 11.752$, $p = 0.019$)				**ELM** ($\chi^2(4) = 20.451$, $p < 0.001$)			
	Rnd	**Gr**	**IGR**	**DR**	**Rnd**	**Gr**	**IGR**	**DR**	**Rnd**	**Gr**	**IGR**	**DR**
Gr	Z=-1.424 p=0.154	-	-	-	**Z=-2.666 p=0.008**	-	-	-	**Z=-2.805 p=0.005**	-	-	-
IGR	Z=-1.836 p=0.066	Z=-1.943 p=0.052	-	-	Z=-2.310 p=0.021	Z=-0.140 p=0.889	-	-	**Z=-2.670 p=0.008**	Z=-0.511 p=0.610	-	-
DR	Z=-1.782 p=0.075	Z=-2.497 p=0.013	**Z=-2.599 p=0.009**	-	Z=-1.274 p=0.203	Z=-2.310 p=0.021	Z=-2.293 p=0.022	-	Z=-1.367 p=0.172	**Z=-2.666 p=0.008**	**Z=-2.670 p=0.008**	-
SR	Z=-1.929 p=0.054	Z=-2.253 p=0.024	Z=-1.252 p=0.211	**Z=-2.669 p=.008**	**Z=-2.825 p=0.005**	Z=-1.067 p=0.286	Z=-1.156 p=0.248	Z=-2.224 p=0.026	Z=-2.395 p=0.017	Z=-0.045 p=0.964	Z=-0.939 p=0.348	Z=-1.993 p=0.046

(c) Execution time

	LR ($\chi^2(4) = 28.533$, $p < 0.001$)				**SVM** ($\chi^2(4) = 20.867$, $p < 0.001$)				**ELM** ($\chi^2(4) = 42.200$, $p < 0.001$)			
	Rnd	**Gr**	**IGR**	**DR**	**Rnd**	**Gr**	**IGR**	**DR**	**Rnd**	**Gr**	**IGR**	**DR**
Gr	Z=-0.628 p=0.530	-	-	-	Z=-2.275 p=0.023	-	-	-	Z=-2.275 p=0.023	-	-	-
IGR	**Z=-2.903 p=0.004**	**Z=-2.903 p=0.004**	-	-	Z=-2.510 p=0.012	Z=-1.726 p=0.084	-	-	**Z=-3.059 p=0.002**	**Z=-3.059 p=0.002**	-	-
DR	**Z=-2.903 p=0.004**	Z=-1.177 p=0.239	**Z=-2.903 p=0.004**	-	Z=-1.255 p=0.209	Z=-1.177 p=0.239	Z=-2.510 p=0.012	-	**Z=-3.059 p=0.002**	**Z=-2.903 p=0.004**	**Z=-3.059 p=0.002**	-
SR	**Z=-2.981 p=0.003**	**Z=-2.981 p=0.003**	Z=-0.784 p=0.433	**Z=-2.981 p=0.003**	Z=-2.275 p=0.023	Z=-2.118 p=0.034	Z=-0.784 p=0.433	Z=-2.510 p=0.012	**Z=-3.059 p=0.002**	**Z=-3.059 p=0.002**	Z=-0.157 p=0.875	**Z=-3.059 p=0.002**

forms worse than all others, in almost all cases. In the comparison of the number of features: IGR and SR methods perform better than DR for LR; Gr and SR perform better than Rnd for SVM; Gr and IGR perform better than Rnd and DR for ELM. Moreover, the difference is only marginally insignificant in 6 cases ($p < 0.025$). We conclude that Gr, IGR and SR perform better than Rnd and DR in terms of reducing the number of features. Next, we compare execution times of the initial population generation methods. Results indicate that IGR and SR methods execute faster than Rnd, Gr and DR methods, in general. SVM, at

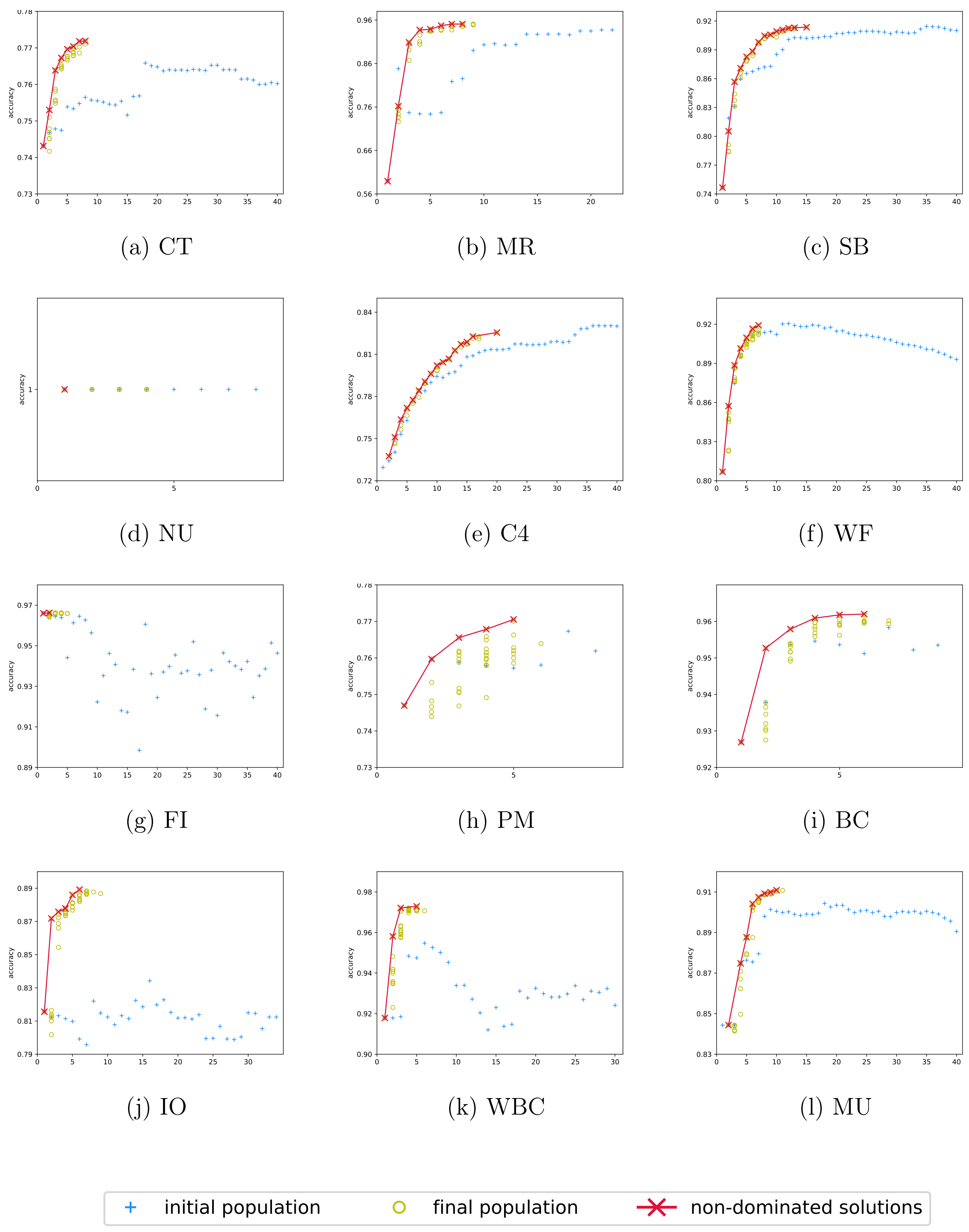


Figure 5: Initial population and final population distributions of the MTLBO-MD + IGR (population size=40, number of generations=60).

Table 5: Training and test set sizes of datasets for comparison with previous studies.

	CT	MR	SB	NU	C4	WF	FI	PM	BC	IO	WBC	MU
Training set	600	1300	600	400	1200	400	1000	268	199	101	169	400
Test set	200	200	200	200	200	200	200	200	100	50	80	200

first glance, seems like an exceptional case with no significant differences between methods. However, even though pairwise differences in SVM is not significant, Friedman's test indicates a significant difference between initial population generation methods. Furthermore, the difference between IGR and Rnd, IGR and DR, and, SR and DR is only marginally insignificant, with a p-value of 0.012.

Analyzing the results, it is clear that SR cannot perform well in terms of accuracy. Among the remaining 4 initial population generation methods, Gr and IGR perform better than Rnd and DR, in terms of minimizing the number of features. As a final comparison to decide between Gr and IGR, we see that the execution time of IGR is better than the execution time of Gr. From these results, we conclude that the IGR method achieves good enough solutions in a timely manner, standing as a promising method for initial population generation. We also present the performances of initial and final populations for each dataset in Figure 5, when the IGR method is employed.

Finally, we compare the results of the IGR initial population generation method with results obtained from our previous studies, where MTLBO-MD (Kiziloz et al., 2018) and NSGA-II (Deniz et al., 2017) were used as metaheuristics with LR as the classifier and the initial population was generated randomly. However, in those studies, population size and number of generations were twice as much (population size was 40 and the number of generations was 60). Also, they used another method for splitting data into training and test sets, similar to other studies in the literature (Pacheco et al., 2009; Unler & Murat, 2010). Briefly, for each dataset, they calculated instance proportion per class, and randomly selected instances from classes with respect to their proportion to fill up the training set sizes given in Table 5. Then, they randomly selected instances, apart from those existing in the training set, for the test set. Hence, we mimicked this methodology for all datasets prior to the study and generated 10 training set and 10 test set per each training set (a total of 100 test sets). Similar to those studies, we increased the population size to 40 and the number of generations to 60, reran our tests of IGR method with LR selected as the classifier. Comparison results for all 12 datasets are given in Table 6. IGR produces close enough solutions to randomly initialized MTLBO-MD and NSGA-II algorithms. Numerically, out of 73 available comparisons (a row in the table, where MTLBO-MD + IGR method may be compared with at least one other method in terms of accuracy value, is considered as an available comparison), IGR can find the maximum accuracy value in 36 occasions. It finds a solution with up to 0.005 decrease in maximum accuracy in 60 occasions. Moreover, it requires less amount of time to execute in medium and large-sized datasets.

Possible limitations to the study could be specified as follows. The most important drawback is the specific domain we evaluate our results on, namely FSS. FSS is an important step for building an expert system, yet it is not considered as one by itself. Hence, we do not directly evaluate its effect on a real expert system. Secondly, the selected crossover and mutation operators have their own working schemes, which may affect the outcome of the study. Likewise, other types of search algorithms could lead to different results.

4. Conclusion

Machine learning applications may suffer from high dimensional data. As the number of redundant and/or irrelevant features in a dataset increase, learning time and accuracy are affected badly. Feature Subset Selection (FSS) is an important tool for dimension reduction, and evolutionary based heuristic algorithms are utilized for this purpose. These algorithms require an initial population to begin their search, and initial population selection may affect the final solution.

In this study, we aim to improve the performance of an expert system, by improving the performance of an intermediate step, FSS. To improve the FSS performance, we propose selecting its initial population wisely. For this reason, we compare five initial population selection methods, namely Random (Rnd), Distinct Random (DR), Information Gain Ranking (IGR), Greedy (Gr), and Small Random (SR). We use the MTLBO-MD heuristic algorithm and three machine learning techniques, namely Logistic Regression, Support Vector Machines, and Extreme Learning Machine, for evaluating the performance of the solutions. In our experiments, we utilize a total of 12 publicly available datasets, most of which are

Table 6: Multiobjective comparison of the IGR method with previous studies.

(a) C4

F. size	**MTLBO MD + IGR**	**MTLBO MD + Rnd**	**NSGA II + Rnd**
1	-	0.729	-
2	0.737	0.746	-
3	0.751	0.755	-
4	0.764	0.764	0.765
5	0.772	0.772	0.772
6	0.778	0.777	0.778
7	0.784	0.784	0.785
8	0.791	0.791	0.791
9	0.796	0.796	0.796
10	0.802	0.797	0.800
11	0.804	0.799	0.802
12	0.807	0.799	0.807
13	0.813	-	0.810
14	0.817	-	0.812
15	0.819	-	0.815
16	0.823	0.805	0.819
17	-	-	0.821
19	-	-	0.822
20	0.826	-	0.822
22	-	-	0.825
23	-	-	0.826
24	-	-	0.826
Time	502.6	431.6	1197.6

(b) SB

F. size	**MTLBO MD + IGR**	**MTLBO MD + Rnd**	**NSGA II + Rnd**
1	0.747	0.782	-
2	0.805	0.835	0.835
3	0.857	0.857	0.857
4	0.871	0.871	0.871
5	0.883	0.879	0.883
6	0.888	0.891	0.890
7	0.898	0.896	0.902
8	0.905	0.905	0.906
9	0.906	0.910	0.910
10	0.909	0.911	0.914
11	0.911	0.913	0.915
12	0.913	-	0.916
13	0.913	0.915	0.917
14	-	-	0.919
15	0.914	-	0.919
16	-	-	0.920
17	-	-	0.920
18	-	-	0.920
Time	372.1	426.1	1171.8

(c) MU

F. size	**MTLBO MD + IGR**	**MTLBO MD + Rnd**	**NSGA II + Rnd**
2	0.844	-	-
4	0.875	-	-
5	0.888	-	-
6	0.904	-	-
7	0.907	-	-
8	0.909	-	-
9	0.910	-	-
10	0.911	-	-
21	-	0.907	-
22	-	0.910	-
23	-	0.912	-
24	-	0.914	-
25	-	0.916	-
26	-	0.917	-
27	-	0.918	-
28	-	0.919	-
Time	76.9	931.2	-

(d) CT

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.743	0.743	0.743
2	0.753	0.753	0.753
3	0.764	0.764	0.764
4	0.767	0.767	0.767
5	0.770	0.770	0.770
6	0.770	0.772	0.772
7	0.772	0.773	0.772
8	0.772	0.773	0.773
9	-	0.774	0.774
10	-	-	0.774
13	-	-	0.774
14	-	-	0.775
Time	170.4	548.7	964.4

(e) WF

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.807	0.789	0.868
2	0.857	0.868	0.893
3	0.889	0.893	0.902
4	0.901	0.902	0.915
5	0.910	0.915	0.917
6	0.917	0.917	0.919
7	0.919	0.919	0.921
8	-	0.921	0.922
9	-	0.922	0.923
10	-	0.923	0.923
Time	47.9	88.8	176.6

(f) MR

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.589	0.763	0.750
2	0.762	0.905	0.867
3	0.909	0.937	0.937
4	0.937	0.940	0.937
5	0.939	0.949	0.945
6	0.947	0.950	0.946
7	0.951	-	-
8	0.951	-	0.946
9	-	-	0.949
Time	211.3	158.8	303.9

(g) IO

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.816	0.816	-
2	0.872	0.872	0.872
3	0.876	0.876	0.876
4	0.878	0.882	0.878
5	0.886	0.886	0.886
6	0.889	0.886	0.889
7	-	0.887	-
8	-	0.890	-
Time	85.1	131.6	239.6

(h) BC

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.927	0.927	0.927
2	0.953	0.953	0.953
3	0.958	0.963	0.963
4	0.961	0.963	0.963
5	0.962	0.963	0.963
6	0.962	-	-
Time	11.1	7.2	12.4

(i) PM

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.747	0.747	0.747
2	0.760	0.760	0.760
3	0.766	0.766	0.766
4	0.768	0.768	0.768
5	0.771	0.771	0.770
Time	4.8	4.9	5.9

(j) WBC

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.918	0.920	0.920
2	0.958	0.961	0.961
3	0.972	0.971	0.972
4	-	0.975	0.975
5	0.973	-	-
Time	35.5	54.1	89.2

(k) FI

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	0.966	0.966	0.966
2	0.966	-	-
3	-	0.967	0.966
Time	115.8	702.8	2721.7

(l) NU

F. size	MTLBO MD + IGR	MTLBO MD + Rnd	NSGA II + Rnd
1	1.000	1.000	1.000
Time	22.0	12.5	17.5

obtained from the UCI Machine Learning Repository.

Experimental results indicate that all initial population generation methods can find good enough solutions in a timely manner when dataset size is small. As dataset size grows larger, random based methods get stuck in local optima and cannot compete with Gr and IGR. Among these two algorithms, Gr achieves slightly better results than IGR. On the other hand, the execution time of Gr is enormous as compared to the IGR method. Additionally, the IGR method is compared with two other algorithms in literature having random initializations. The obtained results show that the IGR method can achieve comparable solutions with smaller execution time. As a result, we suggest using IGR as the initial population generation method for FSS, for small, medium and large-sized datasets.

The main strength of the proposed method is its simplicity. Information Gain is a well-known algorithm, and its implementation in our method is straightforward. On the other hand, this method is not readily available in many existing frameworks, hence an additional step is required for its implementation.

The main contribution of this study can be summarized as follows. Even though the importance of initial population generation is theoretically well-known, initializing the population randomly is still the common approach. We analyze five different initial population generation methods with empirical results to emphasize the subject and find the most promising method. Our experiment results clearly show that generating the initial population wisely improves the overall performance, for all dataset sizes.

Possible future work for this study can be implementing different types of initial population generation methods, such as a hybrid method that combines information gain, greedy approach and/or randomness. Also, other existing methodological settings can be tested. For example, different searching algorithms such as NSGA-II or PSO may be used instead of MTLBO-MD. Similarly, different types of crossover and mutator operators exist in the literature. We used half uniform crossover and bit-flip mutation, respectively, and it could be interesting to see whether the obtained results generalize over all operators. Moreover, in this study, we verified the importance of generating the initial population wisely, for the FSS domain. Wise initial population generation approaches for other problem domains, such as bin packing, graph coloring, travelling salesman, etc., can also be investigated. Finally, initial population generation methods can be implemented specifically to different dataset types such as image, text, etc.

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