

Multi-objective evolutionary undersampling algorithm for imbalanced data classification

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Abstract. The classification of imbalanced data is an important topic of research conducted in recent years. One of the commonly used techniques for dealing with this problem is undersampling, aiming to balance the training set by selecting the most important samples of the original set. The selection procedure proposed in this paper is using the multi-objective genetic algorithm NSGA-2, for a search of the optimal subset of the learning set. The paper presents a detailed description of the considered method. Moreover, the proposed algorithm has been compared with a selection of reference algorithms showing promising results.

Keywords: imbalanced data · multi-objective optimization · evolutionary algorithms

1 Introduction

Machine learning applications has an impact on our lives at almost every level, from influencing sources of information, through robotics applications, to medical diagnostics. It is quite easy to observe newcoming challenges such as fake news detection [9]. Regardless of the application, many real-life classification problems are charged with the difficulty of imbalanced class distribution. This topic has been extensively studied, which led to many techniques for dealing with imbalanced data.

Those methods are used to reduce the bias towards the majority class resulting from the *prior* probability of a problem. Most commonly used classification methods are susceptible to any disproportions in the class distribution among training sets. Two main groups of solutions aiming to reduce negative influence coming from class imbalance are (a) data preprocessing methods – being the main topic of this paper, (b) algorithm-level solutions, and (c) hybrid methods, employing mostly ensemble approaches. Solutions described as *preprocessing methods* may be further divided into sample generation methods (*oversampling*), sample selection methods (*undersampling*) or methods combining these two approaches. The purpose of all techniques is to reduce the imbalance ratio between the classes. Generation of new samples may rely on random duplication of existing patterns or the creation of new synthetic representations for the

minority class, such as Synthetic Minority Oversampling Technique (SMOTE) and its modifications [7]. This group of neighborhood-based methods does not include information about the mutual distribution of classes. More sophisticated algorithms such as RBO [8] create a potential function based on the radial function density distribution of classes. As for undersampling techniques, various strategies can be distinguished: Random Undersampling (RUS), NearMiss, or Evolutionary Undersampling (EUS) [6].

The last of the algorithms mentioned above is particularly interesting because of the genetic algorithm (GA) optimization on which it is built on. When dealing with data imbalanced data, the evaluation of created models requires various metrics, especially those that are compromising trade-off between *Sensitivity* and *Specificity* or *Sensitivity* and *Precision*. The multi-objective optimization allows combining those in a way, to create the set of feasible solutions, which are placed on non-dominated *Pareto-optimal front*. To understand this idea, solutions must be considered as points in the solution space (M -dimensional, for M objective functions). At each step algorithm evaluates new solutions, leaving only those which are maximizing all cost functions simultaneously. One way to achieve this is by sorting solutions based on crowding distance [5]. As the final step, provided solutions are placed on the a convex curve, beyond which procedure was not able to find more acceptable solutions.

In most cases, this leads to a situation where user input on the importance of the metrics is required. This can be found as an advantage in real-life problems. However, on most of the benchmark datasets, it is impossible to obtain this information, which forces the selection of one of the solutions from *Pareto-optimal front*. Fortunately, *Multi-criteria Decision Making* (MCDM) techniques can be used for this task, providing a procedural way of selecting the best solution.

The main contribution of this work is the proposal of Multi-objective Evolutionary Undersampling algorithms (MEUS). Experimental studies presented in this paper are comparing proposed algorithm with other undersampling methods.

The rest of the paper is organized as follows. Section 2 provides a detailed description of the proposed algorithm, which consists of a formulation of a multi-objective optimization problem for sample selection and pseudocode presentation of the complete procedure. Section 3 presents the results comparing the proposed algorithm with reference methods. The article concludes in Section 4 where the observations and further directions for the research of this topic are discussed.

2 Algorithms

The proposed algorithm's idea is based on evolutionary undersampling guided for classification measures (EUSCM-MS) [6]. The optimization procedure will target the optimal subset of majority class samples from training set \mathcal{TS} that will maximize the classification measure calculated for the validation set \mathcal{VS} . Both training and validation set are separated from learning set \mathcal{LS} . The learning set

splitting method SPLIT can be treated as a parameter to the algorithm. In this study the stratified split with train-test ratio of 4:1 was used.

The optimization algorithm used by the method proposed in this article is multi-objective version of genetic algorithm - NSGA-2 [4]. The optimization problem that will be considered as a part of proposed method is presented in generalized formulation:

$$\begin{aligned} & \underset{s}{\text{minimize}} && f_i(s) \quad i = 1, 2, \dots, M \\ & \text{subject to} && g(s) = 0 \end{aligned} \quad (1)$$

It is assumed that the solution s is a binary word, for which each bit represents the inclusion of sample from \mathcal{TS} into new training set \mathcal{TS}' . A feasible solution is balancing complete learning set by removing $N_{maj} - N_{min}$ majority samples out from it, which imposes a constraint

$$g(s) = N_{min} - \sum_{i=0}^{i=|s|} s_i. \quad (2)$$

To provide a complete formulation of the algorithm's optimization process it is required to define objective function. As it was already mentioned, the idea behind optimized under-sampling is to maximize the metric for the classifier model ψ trained on \mathcal{TS}' . Evaluation is based on the classifier predictions of \mathcal{VS} , which can be counted into four groups: TP and TN for correct predictions of minority and majority class respectively, FN and FP for error type I and II, respectively.

Considering the preference of each class, some basic metrics describing the ratio of the properly predicted samples to the number of class samples in the validation set can be defined:

True Positive Rate (TPR or *Sensitivity*)

$$TPR = \frac{TP}{TP + FN}, \quad (3)$$

True Negative Rate (TNR or *Specificity*)

$$TNR = \frac{TN}{TN + FP} \quad (4)$$

and Positive Predictive Value (PPV or *Precision*)

$$PPV = \frac{TP}{TP + FP}. \quad (5)$$

However, to give a fair trade-off between those values, geometric mean (Gmean) is often used as a aggregated metric for comparing classifier performance on imbalanced data. There are two known definitions for this metric, one including *Precision*:

$$Gmean = \sqrt{TPR \times PPV} \quad (6)$$

and second considering *Sensitivity*:

$$Gmean_s = \sqrt{TPR \times TNR}. \quad (7)$$

Let $EVALUATE(\mathcal{TS}, \mathcal{VS})$ denote a function which trains classifier using \mathcal{TS} then tests the model using \mathcal{VS} creating a vector of one or more metric values calculated according to aforementioned equations. Results obtained for training set subset \mathcal{TS}' which is based on s will be used to define objective functions $f_i(s)$ of Equation 1.

The output of proposed multi-objective optimization approach, is the set of solution placed on non-dominated *Pareto-optimal front* for defined objective functions. An example of solution space for *Specificity* and *Sensitivity* is presented in Figure 1. The blue dashed curve marks the *Pareto-optimal front*.

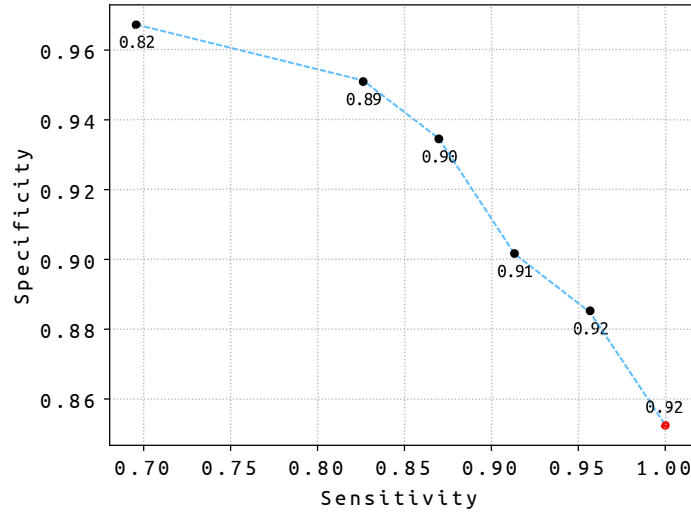


Fig. 1: Example of Pareto-optimal solutions for *Specificity* and *Sensitivity* provided from optimization of training set selection.

It can be observed that the solutions are creating a convex curve, which tends to maximize both metrics. A $Gmean_s$ calculated for the solution is presented near each point. Two far right solutions are maximizing this measure, however only one of them can be selected for creating a final model. For that reason, as a final step of the procedure, *Simple Additive Weighting* (SAW) [12] algorithm is used to select a single solution. As for the discussed example, the chosen solution is marked with red. The complete procedure of MEUS is presented in Algorithm 1.

Algorithm 1 Pseudocode of the proposed MEUS method.

Input: \mathcal{LS} – learning set**Symbols:** \mathcal{TS} – training set \mathcal{TS}_{min} – \mathcal{TS} subset including minority samples \mathcal{TS}_{maj} – \mathcal{TS} subset including majority samples \mathcal{VS} – validation set S – set of solutions found by multi-objective optimization O – set of objective function values for each solution W – scores calculated by SAW s – selected final solution**Output:** \mathcal{TS}' – balanced subset of training set

- 1: $\mathcal{TS}, \mathcal{VS} \leftarrow \text{SPLIT}(\mathcal{LS})$
 - 2: $S, O \leftarrow \text{NSGA-2}(\mathcal{TS}, \mathcal{VS})$
 - 3: $W \leftarrow \text{SAW}(O)$
 - 4: $s = S_i \Leftrightarrow i = \text{argmax}(H)$
 - 5: $\mathcal{TS}' \leftarrow \mathcal{TS}_{min} \cup \{\mathcal{TS}_{maj} \Leftrightarrow s_j = 1\}$
-

3 Experimental Evaluation

This section describes the experimentation setup: implementation of classifiers and selection of datasets used for evaluation. The main motivation for this experimental study is to determine answers for the following questions:

- *RQ1*: Can multi-objective approach improve the method based on single-objective genetic algorithm?
- *RQ2*: Are the algorithms based on evolutionary optimization better than the reference methods?

All the algorithms used in the experiments were evaluated in an experimental environment implemented in Python. Base classifiers are implemented in *sklearn* package [11], undersampling methods in *imblearn* package [10] and optimization algorithms in *pymoo* package [3]. The implementation of the MEUS algorithm proposed in this paper and additional results of experiments are available as additional materials in on-line repository¹. Datasets used for evaluation are collected from the imbalanced category of keel repository [1]. The number of samples per majority and minority class and Imbalance Ratio (IR) are presented in Table 1.

To provide reliable results the experiment protocol used for classifiers validation was 5x2 CV [2] and all the results were tested for statistical significance employing Wilcoxon signed-rank test with the significance level of $\rho < 0.05$. In a series of experiments, MEUS will be used with three combinations of objective functions:

¹ <https://github.com/w4k2/moo-undersampling>

Table 1: Datasets summary

Dataset	N_{maj}	N_{min}	IR
glass1	138	76	1.82
wisconsin	444	239	1.86
pima	500	268	1.87
iris0	100	50	2.00
glass0	144	70	2.06
yeast1	1055	429	2.46
haberman	225	81	2.78
vehicle2	628	218	2.88
vehicle1	629	217	2.90
vehicle3	634	212	2.99
glass-0-1-2-3_vs_4-5-6	163	51	3.20
vehicle0	647	199	3.25
ecoli1	259	77	3.36
newthyroid2	180	35	5.14
new-thyroid1	180	35	5.14
ecoli2	284	52	5.46
segment0	1979	329	6.02
glass6	185	29	6.38
yeast3	1321	163	8.10
ecoli3	301	35	8.60
page-blocks0	4913	559	8.79

- MEUS-SS - *Sensitivity* and *Specificity*,
- MEUS-SP - *Sensitivity* and *Precision*,
- MEUS-SSP - *Sensitivity*, *Specificity* and *Precision*.

The proposed method will be compared with other reference approaches: *Random Undersampling* (RUS), *NearMiss* (NM), evolutionary undersampling guided for *Gmean* (EUS-GM), evolutionary undersampling guided for *Gmean_s* (EUS-GMS) and finally with the original unbalanced learning set (None).

To provide a wide range of experiments, all undersampling methods were combined with three different base classifiers: *Classification and Regression Trees* (CART), *Naive Bayes Classifier* (GNB), *k-Nearest Neighbors Classifier* (KNN).

Both MEUS and EUS approaches are based on GA approach for optimization. In case of each preprocessing method, optimization algorithm is sharing the same parameters characteristic for evolutionary approach:

- **Population**
The population is constructed from 50 individuals (solutions) at each epoch. The initial population is guaranteed to meet the balancing constraint.
- **Mutation**
The mutation is implemented as a bit-flip operation on two opposite bits in solution. This approach guarantees that the new individual will repre-

sent a feasible solution. All experiments were carried out with a mutation probability of 25%.

– **Crossing**

For the crossing procedure, two parents are paired randomly. First, a new individual is created from bit-wise AND operation between both parents. The created solution is not guaranteed to be feasible, but the sum of bits will always be lower or equal the designated value. To repair this individual, random '0' bits are flipped until a solution is feasible. All experiments were carried with the crossing probability of 25%.

– **Termination**

The algorithm is guaranteed to stop after 10000 iterations. However, it can finish faster if after 20 epochs best solution was not improved by the tolerance limit. The tolerance limit is higher for multi-objective optimization (0.0025) than for single-objective (0.0001) which is justified by algorithm-specific behavior.

4 Results

The comparison of preprocessing methods combined with CART base classifier is presented in Table 2. Results are provided as an average of $Gmean_s$ scores obtained in the experiment. Also, the presented table shows the result for the non-parametrical Wilcoxon paired test (fold-wise) listed below each result, denoting reference method to which the score was better and the null hypothesis was rejected.

It can be observed that in most cases, all methods achieve a better result than NM and the classifier trained on the dataset without preprocessing, with an exception of *glass-0-1-2-3_vs_4-5-6* where basic CART was better than other models, and significantly better than proposed MEUS-SS method. It should be also noticed, that in almost every case, optimization based methods were better than RUS except for *ecoli3* dataset. The most interesting aspect observed in the presented results is the relationship between single-objective optimization algorithms and multi-objective optimization algorithms. The only case in which it is possible to indicate a statistically significant advantage of multi-objective optimization is the set *glass1* for which MEUS-SP was better than EUS-GMS. In conclusion to *RQ1*, based on the considered example it cannot be unequivocally stated that multi-objective optimization gives better results than single-objective optimization.

It is particularly interesting that, contrary to what could have been expected, the precision-based optimization (EUS-GM, MEUS-SP, MEUS-SSP) in some cases gives better results for the $Gmean_s$ which does not include this metric. One possible explanation for this phenomenon is that the *Precision* grows with the decreasing number of predictions made for the minority class, thus favoring the majority class's predictions. In that case, it should also increase the *Sensitivity*. It is worth noticing that only the training set is balanced. Therefore the imbalance still remains in the validation set. As a result, *Precision* may turn out to be a better optimization criterion than *Sensitivity*.

Table 2: $Gmean_s$ results for CART base classifier

Preprocessing	NONE ¹	EUS-GMS ²	EUS-GM ³	MEUS-SS ⁴	MEUS-SP ⁵	MEUS-SSP ⁶	NM ⁷	RUS ⁸
Dataset								
<i>ecoli1</i>	0.813	0.865 1, 7	0.852	0.853 1, 7	0.868 1, 7	0.864 1, 7	0.798	0.867 1, 7
<i>ecoli2</i>	0.833 7	0.849 7	0.860 7	0.850 7	0.842 7	0.838 7	0.738	0.833 7
<i>ecoli3</i>	0.725 7	0.797 1, 7	0.800 1, 7	0.780 7	0.781 1, 7	0.815 1, 7	0.490	0.832 1, 7
<i>glass-0-1-2-3_vs_4-5-6</i>	0.901 4	0.867	0.880	0.874	0.876	0.870	0.899	0.899
<i>glass0</i>	0.776 7	0.781 7	0.784 7	0.792 7	0.790 7	0.804 7	0.707	0.760
<i>glass1</i>	0.712 7	0.692 7	0.720 7	0.742 2, 7	0.727 7	0.722 7	0.627	0.725 7
<i>glass6</i>	0.864	0.888 8	0.882	0.887 8	0.877	0.891 8	0.870	0.856
<i>haberman</i>	0.531	0.577 1	0.595 1	0.580 1	0.604 1	0.591 1	0.577 1	0.580
<i>iris0</i>	1.000	0.998	0.998	1.000	1.000	1.000	1.000	1.000
<i>new-thyroid1</i>	0.927	0.925	0.925	0.936	0.931	0.936	0.934	0.921
<i>newthyroid2</i>	0.896	0.931	0.933	0.956 1, 7	0.952 1, 7	0.956 1, 7	0.886	0.923
<i>page-blocks0</i>	0.896 7	0.936 1, 7	0.938 1, 7, 8	0.932 1, 7	0.935 1, 7	0.938 1, 7, 8	0.854	0.926 1, 7
<i>pima</i>	0.651	0.674	0.676	0.679	0.680	0.679	0.666	0.664
<i>segment0</i>	0.980 7	0.984 7	0.982 7	0.984 7	0.986 7	0.983 7	0.885	0.981 7
<i>vehicle0</i>	0.900	0.916	0.920	0.917	0.915	0.921	0.840	0.906
<i>vehicle1</i>	0.641	0.717 1, 7	0.717 1, 7	0.705 1, 7	0.713 1, 7	0.706 1, 7	0.634	0.703 1, 7
<i>vehicle2</i>	0.926	0.928	0.935 8	0.930	0.941 1, 7, 8	0.937	0.921	0.928
<i>vehicle3</i>	0.639	0.709 1, 7	0.715 1, 7, 8	0.708 1, 7	0.710 1, 7	0.702 1, 7	0.602	0.696 1, 7
<i>wisconsin</i>	0.938	0.949 1, 7, 8	0.947 7, 8	0.948 7, 8	0.947 7	0.947 7, 8	0.934	0.937
<i>yeast1</i>	0.606 7	0.661 1, 7	0.657 1, 7	0.651 1, 7	0.658 1, 7	0.667 1, 4, 7	0.567	0.643 1, 7

Table 3 shows the results for the mean rankings for all tested methods to provide a more general comparison of all methods. The Wilcoxon test results are provided below each of the presented values as in the case of the previously discussed results. It is not possible to clearly state that evolutionary undersampling can benefit from multi-objective optimization. However, it can be observed that in the case of CART and GNB, MEUS-SSP achieves the best results. An interesting relationship occurs in the case of KNN for $Gmean_s$, where EUS-GMS turned out to be the best preprocessing method. However, there is also a statistical relationship between a given method and MEUS-SSP. Also, the only metric for which the evolutionary method managed to achieve a better result than the RUS was *Precision*, which had no significant impact on $Gmean$.

Table 3: Ranking Results

Preprocessing	NONE ¹	EUS-GMS ²	EUS-GM ³	MEUS-SS ⁴	MEUS-SP ⁵	MEUS-SSP ⁶	NM ⁷	RUS ⁸
CART								
Sensitivity	1.275	5.125 1	5.450 1	5.025 1, 7	5.100 1	4.600 1	3.850 1	5.575 1, 7
Specificity	7.825 2, 3, 4, 5 5, 6, 7, 8	3.725 7, 8	4.650 2, 7, 8	4.500 7, 8	4.850 2, 7, 8	6.225 2, 3, 4, 5 7, 8	1.950	2.275 7
Precision	7.725 2, 3, 4, 5 6, 7, 8	3.600 7, 8	4.700 2, 7, 8	4.525 7, 8	4.975 2, 7, 8	6.325 2, 3, 4, 5 7, 8	1.925	2.225 7
G-mean _s	2.675 7	4.800 1, 7	5.400 1, 7	5.575 1, 7, 8	5.925 1, 7, 8	6.075 1, 2, 7, 8	2.025	3.525 1, 7
G-mean	4.275 7	4.250 7, 8	5.200 2, 7, 8	4.775 7, 8	5.575 2, 7, 8	6.375 1, 2, 4, 7 8	2.275	3.275 7
GNB								
Sensitivity	4.200 7	5.125 6, 7	5.200 6, 7	5.075 6, 7	5.575 6, 7	3.625 7	2.375	4.825 1, 7
Specificity	4.625	4.275 7, 8	4.325 8	4.800 7, 8	4.450 8	6.575 2, 3, 4, 5 7, 8	3.875	3.075
Precision	4.475 7, 8	4.575 7, 8	4.675 7, 8	4.950 7, 8	4.850 7, 8	6.675 1, 2, 3, 4 5, 7, 8	2.725	3.075 7
G-mean _s	3.275 7	5.375 1, 7, 8	4.825 1, 7, 8	6.100 1, 3, 7, 8	5.600 1, 7, 8	5.575 1, 7, 8	2.275	2.975 7
G-mean	4.025 7	4.925 1, 7, 8	5.375 1, 7, 8	4.950 1, 7, 8	5.400 1, 7, 8	5.325 1, 7, 8	2.575	3.425 7
KNN								
Sensitivity	1.025	6.375 1, 4, 5, 6 7	5.700 1, 4, 5, 7	4.375 1, 7	4.525 1, 7	4.700 1, 7	2.775 1	6.525 1, 3, 4, 5 6, 7
Specificity	7.725 2, 3, 4, 5 6, 7, 8	3.725 8	3.225 8	4.525 2, 3, 8	4.775 2, 3, 8	4.925 2, 3, 8	4.425	2.675
Precision	7.700 2, 3, 4, 5 6, 7, 8	4.075 8	3.525 8	4.500 3, 8	4.750 3, 8	4.975 3, 8	3.600	2.875
G-mean _s	2.725	5.825 1, 3, 4, 5 7	4.925 1, 7	4.900 1, 7	5.050 1, 7	4.975 1, 7	2.375	5.225 1, 7
G-mean	4.675 7	5.175 7	4.175 7	4.550 7	4.900 7	5.175 7	2.675	4.675 7

In the results for GNB as base classifier a significant advantage of the proposed methods over the reference ones can be observed. It is also worth paying attention to the high MEUS-SSP result for *Specificity* and *Precision*, but very low *Sensitivity*, also noticeable for CART.

Based on the conducted experiments *RQ2* can be answered. The proposed undersampling methods based on evolutionary optimization are in many cases outperforming reference algorithms. Same as it was observed before, it cannot be unequivocally stated that multi-objective optimization gives better results than single-objective optimization because of statistical analysis, however it can

be also observed that the proposed multi-objective approach is improving the ranking results.

5 Conclusions

A series of experiments showed that the proposed method achieves very good results for the metrics used to evaluate the classifiers. There is also a noticeable statistical relationship between the single-objective and multi-objective approaches.

One of the advantages of the proposed methods, which was not discussed in results evaluation, is that it creates many acceptable Pareto-optimal solutions. Under benchmark circumstances, it is necessary to choose one solution using the SAW method. However, it could be possible to obtain information from the expert in which optimized metric she/he is interested in, particularly in a real-life application. It should also be noticed that the metrics used in this study were limited to the basic ones. The expert can define his/her own set of metrics for which the solutions will be optimized or provide weights from MCDM.

In the perspective of further research, the parameters of GA should be optimized for best performance. Moreover, the definition of fitness function could be extended to static analysis of the set, e.g., some overlapping regions or statistical analysis metrics.

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