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Algorithm Selection for Machine Learning Classification: An Application of the MELCHIOR Multicriteria Method

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Abstract. This paper aims to select an algorithm for the Machine Learning (ML) classification task. For the proposed analysis, the Multi-criteria Decision Aid (MCDA) *Méthode d'ELimination et de CHoix Includent les relations d'ORdre* (MELCHIOR) method was applied. The experiment considered the following criteria as relevant: Accuracy, sensitivity, and processing time of the algorithms. The data used refers to the intention of buying on the Internet and the purpose is to predict whether the customer will finalize a particular purchase. Among various MCDA techniques available, MELCHIOR was chosen to support the decision-making process because this method provides the evaluation of alternatives without the need to elicit the weights of the criteria. As a result, the Gradient Boosting Decision Tree algorithm has been selected as the most suitable for the ML classification task.

Keywords. Multi-criteria Decision Analysis (MCDA), Machine Learning, Outranking, MELCHIOR.

1. Introduction

The growth of the "data-driven" culture opens space for decision-making and Machine Learning (ML) techniques. The demand for methods and models that generate quality information for academic and professional purposes is growing. The ML grew as a subfield of Artificial Intelligence (AI), developing an important role in research and day-to-day [1].

The classification, a common task of ML, aims to predict binomial or multinomial categorical values. Some examples are product purchase and service cancellation predictions, as well as fraud detection and default risk.

The selection of algorithms in ML can be understood as a problem of multiple alternatives and criteria. Therefore, the purpose in this paper is to explore this possible

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interaction between multicriteria analysis and AI. In this context, the Multicriteria Decision Analysis or Aiding (MCDA) methods aim to help in understanding the decision-making process and choosing alternatives in front of multiple criteria [2,3].

Multicriteria methods consider value judgments and not only technical issues [4], and tend to be increasingly adopted to address the real-world construction problems [5]. These methods have been used to support the decision-making process in several recent complex problems, as presented in [6–12].

Regarding the application of MCDA methods in ML-related problems, the literature presents several cases, such as in the analysis of human decision-making through learning preferences [13]; in a case-clearance procedure for COVID-19 [14]; evaluation of emergency prediction models [15]; supplier performance classification using the Random Forest ML algorithm [16]; selection of classification algorithms for financial risk forecasts [17]; and for propose a new Support Vector Machine (SVM) model based on density weight for binary Class Imbalance Learning CIL problem [18]. Additionally, an improved 2-norm-based density-weighted least squares SVM for binary CIL (IDLSSVM-CIL) is also proposed to increase the training speed of DSVM-CIL.

Given the importance of classification for the success of organizations, the goal of this paper is to select an algorithm for the ML classification task, by applying the *Méthode d'ELimination et de CHoix Incluant les relations d'ORdre* (MELCHIOR) MCDA model.

In this research, the decision-makers (DM) reported a difficulty in evaluating and establishing the weights of the criteria. In these cases, the MELCHIOR method has good adherence, since it provides the evaluation of alternatives without the need to elicit the weights of the criteria, besides not considering interaction between them. Therefore, in this paper we chose to apply this outranking method as a tool to support decision making.

This work is divided into 4 sections besides this introduction. Section 2 discusses the understanding of the problematic situation, with the definition of the criteria and alternatives that make up the proposed case study. Section 3 presents the background of the MELCHIOR method, while section 4 addresses the methodology and the application of the MELCHIOR method to support the decision-making process in the proposed case study. Finally, section 5 concludes this study.

2. Problem Structuring

To help understand the problem, in this article we applied a Problem Structuring Method (PSM) established in the literature – the Soft Systems Methodology (SSM) [19]. Among the most commonly used and consolidated methods in the literature, SSM has been explored in a variety of research fields, as well as serves equally diverse practical interests [20]. According to [19], SSM presents seven stages of application, two of which were addressed in this article for structuring the problem: 1: exploring an unstructured problematic situation; and 2: express it.

In the first stage, the brainstorming technique was used by the authors to demonstrate the group's perceptions about all possible information, without interference or judgment to define the problem. In the second stage, a rich picture was constructed (Figure 1), which has great value as a starting point in the exploratory analysis of the problem [21]. The rich picture is a simple SSM tool, extremely useful for opening the discussion around individual perceptions toward a broad view of the different issues affecting the situation.

They are created freely and unstructured to capture the participants' interpretation of a real situation [19,20].

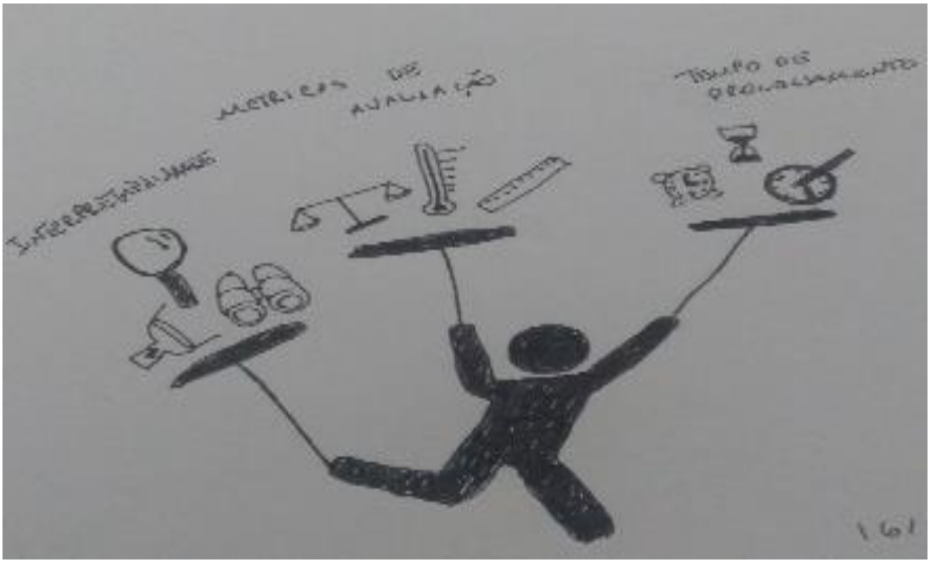

Figure 1. Rich Picture.

The purpose of the case study is to choose a classifier algorithm to predict whether the individual on the internet will finalize the purchase (positive class) or not (negative class). The rich picture portrays the attempt to balance the criteria in choosing the algorithm. Regarding the quantitative criteria, while evaluation metrics reflect the algorithm's effectiveness, processing time is a measure of performance. The metrics of evaluation accuracy and sensitivity are based on the confusion matrix (Table 1).

Table 1. Confusion matrix.

	Positive	**Negative**
Predicted Positive	True Positive (TP)	False Positive (FP)
Predicted Negative	False Negative (FN)	True Positive (TP)

Accuracy measure assertiveness when predicting positive class and its formula is TP/(TP+FP). Sensitivity, on the other hand, can achieve and classify positive scans, its formula is TP/(TP+FN). For the processing time, the average time of 3 runs was considered. In addition, the following algorithms were considered as alternatives:

- K-nearest neighbor (KNN), which aims to find the nearest Neighbor K of a new sample and perform the prediction based on them;
- Support Vector Machine (SVM), which works to find the hyperplane that best separates the training base, maximizing the distance between the hyperplane and the points closest to it, in order to avoid wrong classifications of new samples;
- Random Forest (RF): a set of decision trees built into data samples; and
- Gradient Boosting Decision Tree (GBM): which performs sequential training, developing new models from previous model errors.

3. The MELCHIOR method

For the establishment of preference relationships, the MELCHIOR method, proposed by [22], establishes three fundamental situations of comparison between alternatives:

I – Weak Preference (q): There are clear and positive reasons that do not imply a strict preference in favor of one (well defined) of the two actions, but these reasons are insufficient to assume a strict preference in favor of another, or the indifference between them [23];

II - Strict preference (p): There are clear and positive reasons that justify a significant preference in favor of one (well defined) of the two actions;

III – Veto (v): Limit defined for each criterion that sets a value for the difference $g_j(b)$-$g_j(a)$ (difference in relation to criterion j and discordant of the aSb statement), from which the proposition aSb will not be accepted [24].

In the MELCHIOR method, the basic information is a family F of pseudocriteria, that is, criteria g_j with indifference threshold q_j and a preference threshold p_j ($p_j > q_j \geq 0$) in such a way that, $\forall j \varepsilon J$ and $\forall a, b \varepsilon A$ [25]:

- *a* is strictly preferable to *b* (aP_jb) in relation to g_j if $g_j(a) > g_j(b + p_j[g_j(b)]$;
- *a* is weakly preferable to *b* (aQ_jb) in relation to g_j if $g_j(b) + p_j[g_j(b)] \geq g_j(a) > g_j(b) + q_j[g_j(b)]$;
- *a* and *b* are indifferent (aI_jb) if there is no strict or weak preference between them.

In the MELCHIOR method no weight is assigned to the criteria. A binary relationship M in F is defined in such a way that g_iMg_j means that "criterion g_j is as important as criterion g_j" [25].

In order to obtain the comprehensive outranking relationship aSb, Leclercq [22] proposed a particular form of analysis, in which the criteria for and against the outranking relationship are evaluated to verify agreement if there is no situation of disagreement. That is, no criterion g_j of F exists such that $g_j(b) > g_j(a) + v_j$, where v_j is a veto threshold for criterion g_j (absence of disagreement).

In this method, a criterion $g_j \varepsilon F$ is said to be in favor of the aSb outranking if one of the following situations are verified:

- aP_jb (strict marginal preference of *a* in relation to *b*) (1st condition);
- aP_jb or aQ_jb (strict or weak marginal preference of *a* in relation to *b*) (2nd condition);
- $g_j(a) > g_j(b)$ (3rd condition).

A criterion $g_j \varepsilon F$ is said to be against the aSb outranking relationship if one of the following situations are verified:

- bP_ja (strict marginal preference of *b* over *a*) (1st condition);
- bP_ja or bQ_ja (strict or weak marginal preference of *b* over *a*) (2nd condition);
- $g_j(b) > g_j(a)$ (3rd condition).

The analysis of agreement of the outranking relationship aSb, for a, b ε A, is made verifying whether the family of G criteria in favor of this relationship "masks" the family of h criteria that are against the relationship aSb [25]. These subsets of criteria are compared only using the binary relationship M in F. It is said that a subset G of criteria "masks" a subset H of criteria ($G, H \subset F$, $F \cap G = \emptyset$) if, for each criterion g_i of H, there is a criterion g_j of G such that:

- g_jMg_i (1st condition); or
- g_jMg_i or not (g_iMg_j)(2nd condition).

Where the same criterion g_j of G is allowed to mask at most one criterion of H. Leclercq [22] explains that by choosing two appropriate combinations of the above conditions, the first being more rigorous than the second, and verifying the agreement and absence of disagreement, a strong or weak outranking relationship can be constructed respectively (Table 2).

Table 2. Establishment of outranking relationships.

Relationship	Conditions
aP_j^+b	If $g_j(a) > g_j(b) + p_j$
aQ_j^+b	If $g_j(a) > g_j(b) + p_j$ and $g_j(a) > g_j(b) + q_j$
aI_j^+b	If $g_j(a) > g_j(b) + q_j$ and $g_j(a) > g_j(b)$
aE_jb	If $g_j(a) = g_j(b)$
aP_j^-b	If bP_j^+a
aQ_j^-b	If bQ_j^+a
aI_j^-b	If bI_j^+a

For the establishment of strong and weak outranking relationships between alternatives, Leclercq [22] defines:

I) Strong outranking (S_F): For an alternative *a* to present a strong overcoming relationship over *b*, necessarily:

- There are no criteria for which *b* is strictly preferable to *a*;

- Criterion i for which *b* is weakly preferable to *a* must be masked by more important criteria for which A enjoys strict preference.

II) Weak outranking (S_f): For an alternative *a* to present a weak outranking over *b*, it is necessary that the criteria i for which *b* has the advantage must be masked by criteria j at least as important in favor of *a*.

Finally, it is emphasized that, when applying the MELCHIOR method, no possibility of interaction between criteria is considered, since the outranking relationships are constructed by analyzing, one by one, the criteria for and against the relation aSb [25].

4. Case Study

The proposal is to use the MELCHIOR method to select a classifier to predict whether or not the individual will make an online purchase. The data contains information about the date, access behavior, and characteristics of the individual. The database used is part of the UCI Machine Learning repository and has 12,330 observations, 18 attributes and approximately 16% of the data are related to consumers who have completed the purchase. So, it is an unbalanced base.

At first, the sets of alternatives and criteria for structuring the problem were inserted: K-nearest neighbor (KNN), Support Vector Machine (SVM), Random Forest (RF) and Gradient Boosting Decision Tree (GBM) as alternatives, as well as accuracy, sensitivity, and processing time as criteria. Table 3 shows the performances of alternatives in the light of the established criteria, as well as the strict (p), weak (q) and veto (v) preference thresholds, established together with specialists in ML.

Table 3. Performance Matrix.

Alternatives	Accuracy	Sensitivity	Processing time (s)
KNN	39.6	19.8	4.5
SVM	71.5	34.6	7.5
RF	67.2	62.6	5.2
GBM	66.3	61	4.7

q	10	13	0.5
p	20	20	1
v	40	50	4

We emphasize that Accuracy and Sensitivity are maximizing criteria, while processing time, minimization. After defining the alternatives, criteria, preference thresholds and veto, the MELCHIOR method can be applied. Table 4 illustrates the outranking relationships, based on [22]:

Table 4. Establishment of outranking relationships.

Pairwise evaluation	Accuracy	Sensitivity	Processing time (s)	Relationship
KNN/SVM	P^-	Q^-	P^+	SVM S_f KNN
KNN/RF	P^-	P^-	Q^+	RF S_F KNN
KNN/GBM	P^-	P^-	I	GBM S_F KNN
SVM/RF	I	P^-	P^-	RF S_F SVM
SVM/GBM	I	P^-	P^-	GBM S_F SVM
RF/GBM	I	I	Q-	GBM S_f RF

Where S_F represents strong outranking and S_f illustrates a weak outranking between alternatives. Thus, with the relationships established between the alternatives, it is possible to generate an outranking graph (Figure 2).

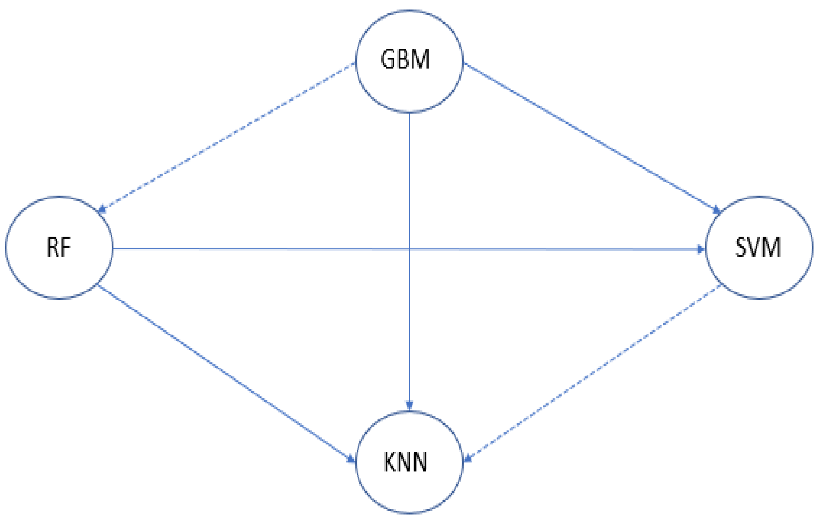

Figure 2. Graph representing the outranking relationships between the alternatives.

The origin of the edges represents the alternative that outranks, while the target, the overqualified. Dotted arrows depict weak outranking relationships (S_f), while continuous ones symbolize strong relationships (S_F). Analyzing the graph, we obtain the final outranking ratio, according to [22]:

- GBM } RF } SVM } KNN.

We emphasize that, in this research, the same symbols (}) used by [22] were applied to represent the outranking relationships, that is, the relation GBM } RF means that the first alternative outranks the second one.

In view of the above, the GBM can be considered as the most indicated alternative to be selected as an algorithm for the ML classification task. Analyzing the reasons that justify this choice, it is observed that the GBM and RF alternatives present good performances in all the analyzed criteria, with relationships of indifference in the criteria accuracy and sensitivity.

We observe that the criterion that defined the choice of GBM was the processing time, defining the weak outranking relationship between the two best alternatives in favor of the GBM algorithm.

5. Conclusions

The ML classification task contributes to the prediction and understanding of results in various sectors. The MELCHIOR method effectively supported the decision to choose a classifier algorithm. The chosen alternative, Gradient Boosting Decision Tree, was selected as the most indicated algorithm, and its result was justified by a good performance in all evaluated criteria, which provides credibility to the result achieved.

The application of the MELCHIOR method occurred in a context in which the decision-makers claimed great difficulty in eliciting the weights of the criteria, which justifies the option for a multicriteria method that does not present interactions and that allows the analysis of alternatives without assigning weights to the criteria.

In view of the above, it was clear that the methodology presented in this paper can be used to solve problems of various types, considering that it presents a simple, flexible, reliable and fast methodology. Future work could address comparative analyses or hybrid modeling of the MELCHIOR method with other MCDA tools to support high-level decision-making on tactical, operational, strategic, and political level issues.

As a limitation of this study, we highlight that, among different types of LM algorithms, only four were evaluated. Future research could address more ranking models, as well as a greater number of criteria for analyzing systems..

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