The Machine Learning Algorithm Selection Model: test with multiple datasets

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Abstract: The technological revolution known as Industry 4.0 is permeating and changing the way companies of all sizes manage their processes. The revolution is influencing companies process at all levels, including production, service, and management ones. Not surprisingly, the strong digitalisation currently occurring in the industrial scenario is contributing to the generation of unprecedented quantities of data that companies can exploit for several purposes and scopes. New data analysis approaches, able to exploit the computational power of modern PCs and workstations are being studied by researchers and practitioners to identify patterns and generate knowledge from data. Yet, despite being able to collect increasing quantities of data, many companies still lack the capabilities and competencies to use analytic approaches such as Machine Learning (ML), elaborate data into information and, thus, generate value. A model, namely the Machine Learning Algorithm Selection Model (MLASM), has been proposed to guide the unexperienced users in selecting a set of ML algorithms suitable for their analysis according to the scope of the analysis and the characteristics of the dataset. This paper describes the process used to test the MLASM with several datasets to verify its usefulness and the correctness of its suggestions. In accordance with the results, improvements and updates have been proposed for the MLASM.

Keywords: machine learning; classification; selection framework; data analysis; case study; systematic review

1. Introduction

Among the technologies framed in the industry 4.0 theory, *big data and analytics* is one of the most discussed by researchers and practitioners (Rüßmann et al., 2015). Data collection and elaboration represent some of the most important activities for companies who want to benefit from the digitalization process (Babiceanu and Seker, 2016; Vassakis et al., 2018). Besides data collection, data elaboration emerges as an important matter for companies interested in generating knowledge from data (Marr, 2016).

In terms of analysis approach, Machine Learning (ML), gained attention and popularity among researchers and practitioners for its capability to analyse data and extract patterns useful for knowledge generation (Brynjolfsson and Mitchell, 2017). Results of the analyses may be used to support decision-making on different levels and for different scopes (e.g., maintenance) (Çınar et al., 2020). The availability of historical data is the base for the development of Machine learning because databases of past observations and the automatic association of events and their consequences allow ML to make a very accurate prediction. According to Mishra and Gupta (2017), ML approaches can be categorised into Supervised (labelled input data), Unsupervised (unlabelled input data), and Semi-supervised Learning (both labelled and unlabelled input data). In particular, this paper will discuss the Supervised Learning approaches, postponing the detailed discussion on Unsupervised and Semi-supervised algorithms to the future.

Different algorithms for the analysis are proposed, each one suitable for specific dataset typologies (i.e., labelled or unlabelled), and scopes (e.g., regression, classification, clustering).

Considering the manufacturing domain, maintenance is one of the main areas that can benefit from these types of algorithm (Carvalho et al., 2019). In particular, preventive and predictive maintenance approaches based on health prediction and condition monitoring can significantly benefit from the analysis of equipment data (Aivaliotis et al., 2017; Lin and Tseng, 2005). Determining the condition of in-service equipment can maximise the useful life and reduce unexpected breakdowns reducing at the same time intervention costs (Dinardo et al., 2018; Duffuaa et al., 2020; Higgins et al., 2002).

Sala et al. (2018) proposed an approach for guiding users in selecting a set of ML algorithms suitable for the analysis according to the scope and the characteristics of the dataset. Despite this, the paper by Sala et al. (2018) presents the model only at a theoretical level, delaying its application in a real context to future research. This paper wants to overcome this limitation by presenting the results of a series of applications with multiple datasets also in the scope of improving the model in terms of algorithms classification, selection, and limitations. In particular, the authors firstly approached the validation of the model using maintenance-related datasets, focusing on a specific domain. Following, during the validation activity, the authors decided to expand the list of datasets including new ones pertaining to different fields, also testing the flexibility of the model within different contexts.

The rest of the paper is structured as follows: Section 2 synthetises literature review on the topic. Section 3 summarises the research approach used for the research. Section 4 presents an example of validation and the results achieved. Section 5 discusses the results of the analysis. Section 6 concludes the paper also delineating future research.

2. Theoretical background

Since one of the main application areas of ML is the maintenance domain, a systematic literature review has been performed by the use of the following keywords: *"maintenance", "industry 4.0", "machine learning", "case study"* and related synonyms, and mixing the logic operators "AND" and "OR". More than 130 papers have been identified using the "*article title, abstract, keywords*" search field in SCOPUS, selected as database for the research due to its multidisciplinary coverage (Pirola et al., 2020). The final dataset used for the analysis was composed of conference papers and journal articles. The few results related to book chapters, reviews, notes, and short surveys were discarded.

Information such as the author, the title, the publication year, and the source title were collected and used to cluster and filter the results. By reading the full papers, it has been possible to identify the algorithms used and the context/sector of application. Not surprisingly, case studies related to preventive and predictive maintenance were widely discussed among the datasets.

Furthermore, the analysis allowed to depict frequent application sectors for ML algorithms. Figure 1 shows the evolution of the publications over the years in the considered pool, highlighting a sharp increase in the last three years.

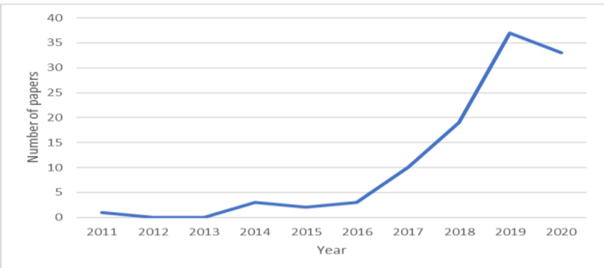

Figure 1: Trend of publications

In addition, Figure 2 shows that the most used machine learning algorithms are: Artificial Neural Networks (ANN), Support Vector Machine (SVM), Decision Tree (DT), Random Forest (RF) and K-Nearest Neighbors (KNN). Among them, ANN show a major predominance in each sector analysed.

In particular, examples of applications extracted from the analysed pool are fault detection of machines, monitoring of the production plants, forecast of unexpected outages, detection and diagnosis of nuclear infrastructure problems, fault detection of medium voltage and wind turbine blade switchgear.

Thus, the use of ML for maintenance purposes has been growing and found application in multiple sectors (Bellinger et al., 2017; Carvalho et al., 2019; Chen et al., 2018; Nalmpantis and Vrakas, 2018). The applicability of ML in each of them is growing and it is easy to understand how the availability of an instrument guiding the selection of ML algorithms for analysis can support its spreading even more. Despite this, the use of an incorrect approach for the analysis could vanish the potentiality of ML and lead to wrong decisions (e.g., maintenance interventions not required due to false-positive results). Hence, it is necessary to provide a link between ML and dataset in such a way that it allows approaching the analysis correctly.

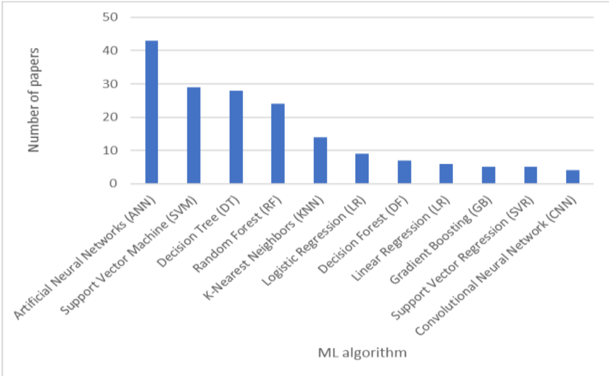

Figure 2: Most frequent algorithms

3. Research approach

3.1 The Machine Learning Algorithm Selection Model (MLASM)

With the main purpose to support unexperienced users dealing with a huge amount of data, Sala et al. (2018) proposed a selection model able to guide the user in selecting a set of machine learning algorithms suitable for the analysis of a dataset according to a set of predefined criteria. Figure 3 clarifies the drivers used to develop the MLASM. The first layer of the framework deals with the approach adopted for the analysis, while the second uses four drivers to match the algorithms with the dataset characteristics. Several algorithms were classified after this framework to create the MLASM. Due to space constraints, an updated version of the MLASM is depicted in Table 4. As it will be explained in the following, Table 4 uses a coloured font to highlight the changes from the original MLSAM presented in (Sala et al., 2018).

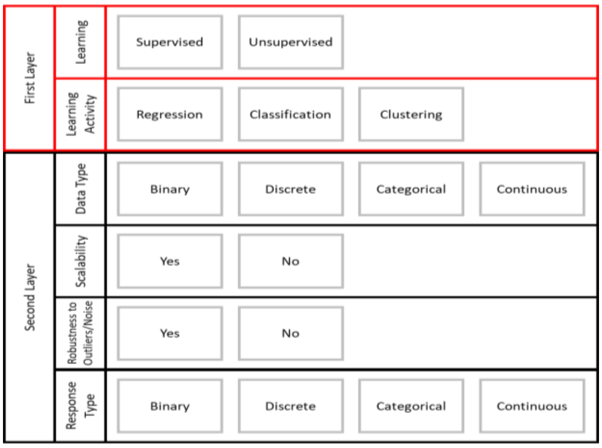

Figure 3: Framework for the Machine Learning Algorithm Selection (Sala et al., 2018)

Even if the main purpose of the authors is to address maintenance related data, the MLASM is a flexible framework able to deal with different situations and contexts, not only maintenance. For this reason, multiple open datasets pertaining to different sectors (e.g., manufacturing, finance, households, foods & beverage) were selected to validate the MLASM. Eight datasets were used in input for the analysis: bearings temperature dataset and bearings vibration dataset (Nectoux et al., 2012), iris dataset (Fisher, 1936), banknote dataset (Dua and Graff, 2017), wine quality dataset (Cortez et al., 2009) and housing dataset and concrete (Harrison Jr and Rubinfeld, 1978; Yeh, 1998). From a methodological point of view, the authors decided to focus on the supervised learning approach for this paper, leaving the validation of the MLASM in terms of unsupervised and semi-supervised approaches to a later research. Thus, the validation process has been done for the classification and regression learning activities. Section 3.2 reports the steps followed in the validation process.

3.2 MLASM Validation process

The process adopted for the validation of the MLASM consisted of the following steps:

1) *Pre-processing*: cleaning and re-organisation of the dataset. Often, datasets present missing data or non-useful ones to compute the analysis. If these are not deleted, the analysis may be biased with effects on the reliability of the results on the model accuracy and computational time (Alasadi and Bhaya, 2017). This activity, and the following, were carried out using MATLAB.
2) *Features extraction and selection*: in ML, data are represented in the form of a collection of data elements, also known as features. An analysis of the dataset allows transforming raw data into a set of potentially useful features, which are followingly studied to identify the ones required to conduct the analysis (Addison et al., 2003). This step allows removing features that do not give useful information for the analysis. The features selection contributes to reducing the risk of overlapping and redundancy in the data used for the analysis.
3) *Theoretical selection of ML algorithms using the MLASM*: based on first layer ("Learning type" and "Learning activity") and second layer ("Data Type", "Scalability", "Noise/Outliers", "Response Type") criteria, the ML algorithm suggested by MLASM is identified. In a first phase, maintenance-related datasets were selected and other were added in a second phase to test the MLASM in other contexts.
4) *Train/Test set division*: the dataset is divided into two subsets: training data and testing data (Pawluszek-Filipiak and Borkowski, 2020). During this analysis, the chosen train/test set division was 70/30.
5) *Algorithms application*: After dividing the dataset into train and test sets, all the ML algorithms are applied using MATLAB and its ML toolbox. The ML toolbox features two tools – "Classification Learner" and "Regression Learner" – usable for selecting the ML algorithm and processing the data. In both cases, it is possible to perform supervised machine learning by providing a known set of input data (i.e., observations) and known responses to the data (i.e., labels or classes). The data are used to train an algorithm that generates predictions for the response to new data. Algorithms both suggested and not suggested by the MLASM were selected for the analysis. The scope was to compare the correctness of the suggestions considering the analyses scores.
6) *Performance evaluation*: Concerning classification, the confusion matrix is used. The confusion matrix is a table that allows visualizing the performance of a classification algorithm. Each row of the matrix represents the instances in an actual class while each column represents the instances in a predicted class (or vice versa) (Stehman, 1997). According to Powers (2011), the name derives from the fact that it makes it easy to see if the system confuses two classes (i.e., commonly mislabelling one as another). The effectiveness of the regression is measured using indicators such as the Root Mean Square Error (RMSE).
7) *Comparison of the results*: algorithms that showed the best performance are compared with those theoretically suggested by the MLASM. The comparisons consider the accuracy of the analysis, the prediction speed and the training time required.

4. Validation and results

Due to space constraints, this paper focuses on a single application. It briefly presents the main phases of the research and the results achieved following the application of the algorithms suggested by the MLASM. In particular, a classification problem linked to maintenance will be described in the following.

4.1 Example of the validation of classification learning activity

In the following, a classification activity supported by the MLASM is carried out on a bearing vibration dataset. The dataset is composed of 27,000 observations with seven features belonging to three different types of bearing (i.e., Bearing 1, Bearing 2, Bearing 3). The aim of the ML application in this case is – given the features – the prediction of the bearing class. In particular, the features collected are: Minimum, Kurtosis, Maximum, Energy, Mean, Peak-to-Peak, Root-mean-square and Skewness. According to the MLASM, since the data type is continuous and the response one is discrete, KNN should be one of the most suitable algorithms to be used for the analysis.

Following the validation process steps (Section 3.2), the dataset was divided into train and test set. Particularly, the train set was represented by 70% of the dataset while the test one the 30%. Using the MATLAB Classification Learner tool, it has been possible to test multiple algorithms. Analysing the output of the analysis, it is possible to notice that:

- In the first case - using the K-Nearest Neighbors - the reached accuracy is around 88% with very high precision in prediction of bearings 1 and a slight inaccuracy for both bearings 2 and 3.

- In the second case - using the Decision Trees - the reached accuracy is around 87.40% with results for each bearing very similar than using SVM. In particular, it is more precise in providing for bearings 3 and less for bearings 2.

Table 1 summarizes the results in terms of accuracy (Acc.), total misclassification cost (Penalty), prediction speed (Prediction), and training time (Training). According to Table 1, the most accurate algorithm was the KNN with an accuracy equal to 88% and total misclassification cost equal to 773. However, the faster was the Decision Trees with a prediction speed equal to 96000 obs/sec and a training time equal to 3.28 sec. Thus, a trade-off between accuracy and speed seems exists. The final decision depends on the priorities of the analyst and the user, who can choose whether to focus on the training speed and processing or on the accuracy depending on the necessities and constraints.

Table 1: ML algorithm results for classification activity of bearing vibration dataset

Algorithm	Acc.	Penalty	Prediction speed	Training speed
K-Nearest Neighbors	0,885	773	3000 obs/sec	26,66 sec
Decision Trees	0,832	812	96000 obs/sec	3,28 sec
SVM Classification	0,881	774	5700 obs/sec	48,44 sec

4.2 Validation results

Validation results are divided based on the learning activity tested and are reported in two tables, one for classification (Table 2) and the other for regression (Table 3) problems For each dataset, the tables show the algorithm suggested by the MLASM, the top performing algorithm, and clarify if the MLASM suggestion is correct. As it is possible to notice from Table 2, in all cases the MLASM was able to suggest the algorithm correctly:

- For the *bearings temperature* dataset, the MLASM suggested the suitable algorithm.
- For the *bearings vibration* dataset, the best algorithms in terms of accuracy are both SVM and KNN. However, the Decision Tree resulted the faster one.
- For the *wine quality* dataset, the best accuracy and prediction speed is given by SVM Classification, as suggested by the MLASM.
- For the *iris* dataset, the best accuracy is given by both the Decision Trees and the SVM classification even if the first one is faster.
- For the *banknote* dataset, the best accuracy is given by KNN but the faster resulted to be the SVM.

On the other hand – in the regression problem (Table 3) – the MLASM suggested, in most cases, a suitable algorithm:

- In the case of *bearings temperature* dataset, the best algorithms are two. The Linear Regression is a little more accurate if compared to the Regression Tree, but the latter is a slightly faster than the first one. It has to be mentioned that Linear Regression was not among the algorithms originally suggested by the MLASM because it was not present in the model.
- For the *housing* dataset, the Regression Tree is more accurate than the others. It is also faster at predicting each observation but slightly slower in the training phase.
- Concerning the *concrete* dataset, the SVM algorithm is the best in terms of accuracy even if turns out to be slightly slower than the Regression Tree.

Table 2: Results for the classification problem.

Dataset	MLASM	Top performing	Correct
Bearings temperature	Decision Trees	Decision Trees	Yes
Bearings vibration	K-Nearest Neighbors SVM Classification	K-Nearest Neighbors	Yes
Wine quality	Decision Trees SVM Classification K-Nearest Neighbors	SVM Classification	Yes
Iris	Decision Trees SVM Classification K-Nearest Neighbors	Decision Trees SVM Classification	Yes
Banknote	Decision Trees SVM Classification K-Nearest Neighbors	K-Nearest Neighbors	Yes

Table 3: Results for the regression problem.

Dataset	MLASM	Top performing	Correct
Bearings temperature	Regression Trees	Regression Trees	Yes
	SVM Regression	Linear Regression	No
Housing	Regression Trees SVM Regression	Regression Trees	Yes
Concreate	Regression Trees SVM Regression	SVM Regression	Yes

Table 4: The updated Machine Learning Algorithm Selection Model

ML Algorithm	First layer		Second layer			
	Learning Type	Learning Activity	Data Type	Scalability	Robustness to Noise/Outliers	Response Type
Logit	Supervised	Classification	Binary	Yes	Yes	Binary
Multinomial Logit	Supervised	Classification	Discrete – Categorical	Yes	Yes	Categorical
Decision Trees	Supervised	Classification	Binary - Discrete – Categorical – Continuous	No	Yes	Binary – Discrete - Categorical
SVM Classification	Supervised	Classification	Binary – Discrete – Continuous	Yes	No	Binary - Discrete
K-Nearest Neighbour	Supervised	Classification	Binary – Discrete – Continuous	No	No	Binary - Categorical
Neural Networks	Supervised	Classification	Binary - Discrete - Categorical	Yes	Yes	Binary - Categorical
Linear Regression	Supervised	Regression	Continuous	Yes	No	Continuous
Regression Trees	Supervised	Regression	Discrete - Categorical - Continuous	No	Yes	Categorical- Continuous
SVM Regression	Supervised	Regression	Discrete - Continuous	Yes	No	Discrete - Continuous
K-Nearest Neighbour	Supervised	Regression	Discrete - Continuous	No	No	Categorical
Neural Networks	Supervised	Regression	Binary - Discrete - Categorical - Continuous	Yes	Yes	Categorical - Continuous
k-Mean	Unsupervised	Clustering	Continuous	Yes	No	Continuous - Categorical
k-Medoids (PAM)	Unsupervised	Clustering	Continuous	Yes	Yes	Categorical
FCM (Fuzzy C-Means)	Unsupervised	Clustering	Continuous	Yes	No	Categorical
BIRCH	Unsupervised	Clustering	Continuous	Yes	Yes	Discrete
CURE	Unsupervised	Clustering	Continuous	Yes	Yes	Discrete
ROCK	Unsupervised	Clustering	Continuous	No	Yes	Discrete

5. Discussion

The application discussed in Section 4 allowed to depict how the validation of the MLASM has been approached. The analysis discussed in the previous section is only one of the multiple analyses carried out during the validation process. The results allowed to identify strengths and weaknesses of the MLASM.

First, the MLASM allows to identify suitable algorithms able to sustain the dataset analysis in many of the considered cases. Recalling the scope of the MLASM, the idea underneath the development was to support unexperienced users providing them a method to select one or more suitable algorithms for the analysis. Thus, the aim is not to identify the best algorithm, but rather to avoid the selection of unsuitable ones. From the results, it is possible to conclude that the MLASM can support the user in the selection of an appropriate set of algorithms to perform data analyses.

On the other hand, as anticipated in the introduction section, the validation process allowed to identify some of the limits of the MLASM and cope with them adding new information such as the identification of some characteristics for the dataset (e.g., in the original version the "continuous" type data type for some algorithms was not considered) or the introduction of a new algorithm like the Linear Regression algorithm. Adding new characteristics to guide the dataset selection could improve the MLASM reliability and guide the user in a sounder selection. The modifications and additions to the MLASM, result of the tests conducted with various datasets, as exemplified in section 4, are highlighted in red in Table 4.

These limits were addressed during the development of the paper. Other important aspects that the MLASM is not currently considering are related to the "interpretability" problem, which deals with the easiness of interpretation of the results and computations that led to the final result.

The possibility to show and provide examples could even ease the following application of the algorithm since the user would have something to rely on to carry out the analysis.

6. Conclusions

Industry 4.0 programs are revolutionising the way companies manage processes and make decisions. The unprecedented data availability is opening the path towards an increased adoption of data-driven approaches to decisions-making. Always more frequently, researchers and practitioners are relying on ML approaches to extract information from their datasets. Because of the high availability of ML algorithms available in literature, it is difficult for newcomers to devise which algorithm use for their analysis.

The aim of this work was to test the MLASM presented in (Sala et al., 2018) by using it to select a set of algorithms suitable for the analysis of eight datasets. Analysing the results, it is possible to affirm that this study has shown how the use of MLASM to select ML algorithms applied in different areas led to favourable results. The MLASM (Sala et al., 2018) suggests in the correct way the choice of ML algorithms for each case presented. However, a few changes – concerning the classification and the regression – were required.

As it can be noticed from Table 4, the analysis allowed to add one option to the "Data Type" driver for some algorithms – *Continuous type*.

Regarding the regression learning activity, the *linear regression* algorithm, which was not present in the previous version of Table 1 but resulted to be the most accurate one of the regression cases analysed, was added.

The empirical analysis allowed to identify differences in terms of accuracy, prediction speed, and training speed for the various ML algorithm. This allowed to introduce the topic of the users' priority, which guide them in selecting a more accurate algorithm over one able to process dataset in a shortest time.

This work is not free from limitations. To make it more consistent more tests with other algorithms and datasets should be run. For instance, at the current stage, the MLASM has been tested only with supervised learning problems, additional analyses should be executed considering the unsupervised learning problem. Also, additional studies related to the supervised learning problem should be done.

The current MLASM could be additionally updated, considering other kind of inputs (e.g., the interpretability of the algorithms' output) or adding real analysis examples to facilitate the understating of each algorithm potential application.

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