

Machine learning methods for model classification: A comparative study

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ABSTRACT

In the quest to reuse modeling artifacts, academics and industry have proposed several model repositories over the last decade. Different storage and indexing techniques have been conceived to facilitate searching capabilities to help users find reusable artifacts that might fit the situation at hand. In this respect, machine learning (ML) techniques have been proposed to categorize and group large sets of modeling artifacts automatically. This paper reports the results of a comparative study of different ML classification techniques employed to automatically label models stored in model repositories. We have built a framework to systematically compare different ML models (feed-forward neural networks, graph neural networks, k -nearest neighbors, support vector machines, etc.) with varying model encodings (TF-IDF, word embeddings, graphs and paths). We apply this framework to two datasets of about 5,000 Ecore and 5,000 UML models. We show that specific ML models and encodings perform better than others depending on the characteristics of the available datasets (e.g., the presence of duplicates) and on the goals to be achieved.

CCS CONCEPTS

• **Software and its engineering** → **Model-driven software engineering**; • **Computing methodologies** → **Machine learning**.

KEYWORDS

Model classification, Model-Driven Engineering, Machine learning

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1 INTRODUCTION

In recent years, the use of Artificial Intelligence (AI) and Machine Learning (ML) techniques to solve Model-Driven Engineering (MDE) problems has begun to gain traction. This is an active line of work intended to explore the application of ML to enhance several MDE-related scenarios, as testified by the increasing research corpus [9]. For instance, feed-forward neural networks have been used to label metamodels stored in model repositories automatically [29]. An LSTM architecture is used to perform model transformation by example [10]. A graph neural network assesses realistic model generators [25]. Model assistants based on providing recommendations are starting to be built using different techniques [15, 36].

Common obstacles which need to be addressed when applying ML-based projects for dealing with MDE problems are twofold: *i*) understand the typical steps that need to be performed to employ ML algorithms; *ii*) determine the best combination of ML model and representation (i.e., the encoding of software models for their consumption by ML algorithms) for the problem at hand. Unfortunately, this topic is not yet well understood and has not been explored in depth. By considering these shortcomings, this paper overviews the typical process that needs to be followed to apply ML projects in MDE. Subsequently, a concrete instance of the presented methodology is presented to systematically compare several ML methods and representations used to support the model classification task. The goal is to determine the pros and cons of each method and derive a set of applicable lessons. To this end, we will consider the model classification problem using `MODELSET` [21] as the target dataset. Over it, we will run and compare different classification algorithms. Thus, the paper makes the following contributions:

- Overview of a typical workflow that needs to be followed when applying ML models for MDE problems. The paper itself serves as a guide for MDE experts who want to apply ML techniques to understand the different types of models available and how to map software models to the input representations expected by these ML models;
- A methodology instantiating the overviewed process to automatically evaluate the suitability of different ML models to address a particular problem in MDE;
- A framework implementing the proposed methodology for the task of model classification, in which several ML models are systematically compared.

Organization. Section 2 presents the related work and some background about ML and MDE. Section 3 describes our methodology to perform the comparison of ML methods, while Sect. 4 describes in detail the models and encodings used. Section 5 describes the experimental setup and Sect. 6 presents the results of the experiments and a critical discussion. Finally, Section 7 concludes the paper and highlights possible future directions.

2 BACKGROUND AND RELATED WORK

This section presents an overview of recent applications of ML to address MDE problems (Sect. 2.1) and describes a typical workflow to apply ML (Sect. 2.2), which is adapted for the sake of the software model classification problem as presented in Section 3.

2.1 Machine Learning in MDE

Machine learning is a branch of artificial intelligence that encompasses techniques to make computers learn from data. Depending on the shape of the data, ML techniques can be classified as supervised and unsupervised learning. In *supervised learning* the data includes the labels, and the ML algorithm has to learn a mapping function between the input data and the target labels. If this function is real-valued, then a *regression* problem is faced. Whereas, if this function is discrete, we have a *classification problem*. In contrast, in *unsupervised learning* the data is not labelled, and the system tries to identify patterns by itself. A typical task is clustering, in which the system identifies groups of similar examples according to some criteria and similarity functions.

Machine Learning algorithms have been successfully employed to face different issues in MDE [4, 18]. For example, in [12, 17] ML techniques were used to automatically infer model transformation rules from sets of source and target models. In [13], the authors discussed about the *cognification* of Model-Driven Software Engineering. The goal is to boost the performance of a process with the utilization of knowledge. The cognification concept is referred not only to artificial intelligence but also includes a combination of past and current human intelligence.

Breuker [8] reviews the main modeling languages used in machine learning to explore model-driven big data analytics. The result is a conceptualization of a DSML. Such a DSML can support code generation from a visual representation of probabilistic models.

ML-Quadrat [27] is a research project conceived to improve ThingML, an open-source modeling tool for IoT/CPS. The authors integrate ML concepts into ThingML at modeling and code generation levels.

In [25], the authors use Graph Neural Networks (GNNs) to characterize realistic model generators by mapping this problem to a binary classification problem. The analysis and classification of model repositories have been addressed also from a clustering perspective. Hierarchical clustering is applied in [6] to organize a collection of metamodels and provide meaningful visualizations of them. Similarly, in [7] the models handled by the MDEForge tool are organized by employing hierarchical clustering. The topic of model encoding for clustering has also been addressed in [5].

AURORA [28, 29] is a tool that exploits a feed-forward neural network to classify metamodels. The authors proved the tool's capability to classify Ecore models with considerable precision.

In a similar vein, a convolutional neural network (CNN) is used to build the MEMOCNN metamodel classifier [30]. The idea is to transform metamodels into special 2D images that the CNN can process. However, both AURORA and MEMOCNN may be biased due to the small size of the dataset (555 Ecore metamodels) and the presence of duplicates. Another issue of the current state-of-the-art in ML applied to MDE is that it typically targets Ecore metamodels. Therefore, we also use UML models in this work, which allows us to contrast the results for the same task applied to Ecore metamodels.

The authors in [14] propose the application of graph kernels to MDE. In this context, Di Rocco et al. [15] proposes MORGAN, a tool based on graph kernels to support the completion of both models and metamodels. The tool is conceived to recommend structural features to complete the models under construction. In particular, MORGAN can recommend classes, fields, and methods within a model class, metaclasses, and structural features like attributes and references.

Burgeño et al. [11] proposed a NLP-based architecture for the completion of software models. The core of their proposal is to use two word embedding models (e.g., GloVe [31], word2vec [26], etc), one trained with general knowledge and the other with contextual knowledge. Both models are interpolated to perform the recommendations.

Altogether, there is a trend to apply ML algorithms to address MDE problems. However, there is currently a gap regarding the knowledge about which ML models and representations are best suited for each type of MDE problem. This work attempts to address this shortcoming for the problem of model classification.

2.2 Common Machine Learning workflow

The application of ML techniques encompasses the execution of a common workflow [2] consisting of typical tasks as shown in Fig. 1 and discussed below.

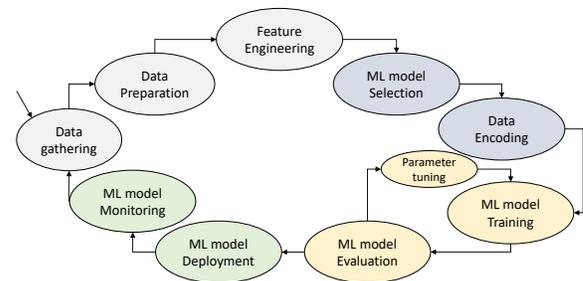


Figure 1: Overview of a common workflow for ML.

Data gathering: Identifying data sources relevant to the problem at hand is the first step in a ML project. The size and quality of the considered data are among the peculiar characteristics affecting the final results. Once data sources are identified, data is fetched and typically archived locally for subsequent manipulations.

Data preparation: A key aspect is to ensure that data is in a suitable condition to be used. In this phase, clearing and pre-processing operations are performed to fix issues like missing values, duplication, contradictions, and outlier values. Such a phase is of paramount

importance because if the ML application being developed is based on inaccurate data, the corresponding quality will not be as wanted.

Feature engineering: In this phase, the properties of the subjects under investigation are extracted from raw data. For instance, if we want to predict the population growth in a specific geographical area, we could discard attributes like hair color or height, but select attributes like salary and unemployment rates.

ML model selection: Several machine learning algorithms might be suitable for the available data. By relying on previous experiences or similar applications already developed, candidate ML algorithms are selected. It is important to remark that this is an iterative process that encompasses conducting different experiments to evaluate how the chosen algorithms perform with the available data with the final goal of identifying the best configuration.

Data encoding: Depending on the previously selected ML algorithm, prepared data must be encoded accordingly. For instance, if the chosen ML algorithm is based on a graph-based similarity, it is necessary to encode data as graphs.

ML model training: This is the process of feeding the selected ML algorithm with the prepared and encoded data. In the case of supervised learning, training data consist of input values and one or more target variables (labels). The goal is to train the algorithm so that in case values that are not in the training data are given as input, expected output values are produced. In the case of unsupervised learning, the goal is determining patterns in the data, e.g., to automatically organize input items in clusters (i.e., groups of objects that are similar with respect to some similarity function).

ML model evaluation: In this phase, the trained model is evaluated against a testing dataset. Values not in the training data are given as input to assess the model's accuracy. The produced values are compared with the expected ones, organized in a purposely prepared ground truth. A number of evaluation metrics can be used to assess the accuracy of the model under analysis, including precision, recall, and success rate. If the obtained results are not satisfactory, there are different ways to intervene, including fine-tuning the parameters of the considered model, or moving back to the process, e.g., to improve the encoding of the data, select a different ML algorithm, or even refine or change the data under disposal.

ML model deployment: The trained model, which is satisfactory according to the previous evaluation step, is deployed to cloud or on-premises infrastructures to enable its adoption by the final users.

ML model monitoring: The deployed model is continuously monitored for possible errors during real-world execution or even to detect potential accuracy degradation that might induce the implementation of additional iterations of the process shown in Figure 1.

3 COMPARISON METHODOLOGY

This section presents a specific instance of the workflow shown in the previous section, adapted to automatically evaluate the suitability of different existing ML models to address the problem of model classification. Although this problem has been investigated over the last few years by the MDE community, no systematic comparison of different ML techniques and encodings has been performed yet.

The proposed methodology aims at comparing existing ML/MDE tools as well as new implementations, and consists of a specific

instance of the workflow shown in Fig. 1. The methodology has been implemented in terms of a framework able to automatize the execution of the different tools under analysis. The existing approaches that have been analyzed in this paper are MAR [23, 24], a custom implementation of Lucene [34] specifically designed to classify metamodels, AURORA [28, 29] and MEMOCNN [30]. The rationale behind this selection is that these tools are based on solid ML techniques and demonstrated effectiveness in the metamodels classification. MAR is a search engine designed to work with models; nevertheless, the authors tested the capability of MAR to classify metamodels. The implementation of Lucene is based on the well-known Apache search engine and represents an attempt to employ a general-purpose tool to classify metamodels. AURORA is one of the first experiments to classify metamodels by exploiting feed-forward neural networks. Instead of relying on the original AURORA tools, we reimplemented the FFNN of AURORA because we could not integrate its tools that depend on external cloud-based technologies. Finally, MEMOCNN is the first attempt that represents metamodels using matrices and exploits a convolutional neural network to classify them. Additionally, we have implemented new classifiers based on Support Vector Machine, k -Nearest Neighbours, Naive Bayes Models, and Graph Neural Networks.

The framework automatizes and supports the activities shown in Fig. 2 and described below.

Data gathering. We have directly used an existing dataset, MODELSET, instead of creating a new one to address this step. MODELSET provides 5,000 Ecore models and 5,000 UML models, labelled with a category that reflects the application domain of the model (e.g., an Ecore model representing a state machine or a UML model describing the behaviour of an ATM). We use the provided Python library¹ to load and handle the labels of the dataset consistently.

Data preparation. To perform fair comparisons, we have pre-processed the original models as follows.

- **Detect duplicates.** We have observed that there are a large number of quasi-duplicate models for some categories of models. This seems to be due to the fact that MODELSET was built by gathering models from public repositories (GitHub and GenMyModel) in which users tend to copy-paste models. This may introduce a bias in the evaluation of the methods. Therefore, we have adapted to models the method to detect duplicates in program files devised by Allamanis in [1]. This pre-processing step is optional since we will perform experiments with duplicates and without them to compare the effect of duplication.
- **Filter.** Another issue is that some categories contain few models. Therefore, we filter out those categories with less than ten models as discussed and motivated later in the paper.
- **Prepared dataset.** After detecting duplicates and filtering categories, we obtain the list of models that we use for the evaluation. Finally, we apply this process to both UML and Ecore and save the list in a separate file to ensure that the evaluation of the different methods consistently uses the same models.

¹<http://github.com/modelset/modelset-py>

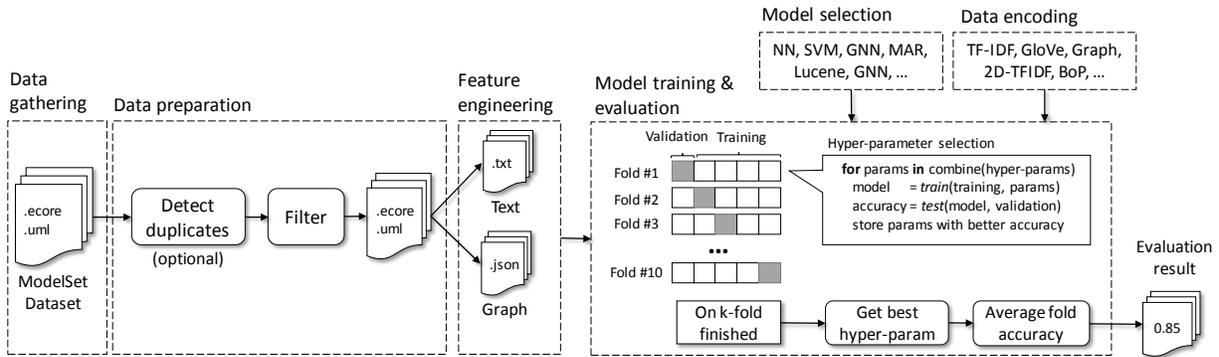


Figure 2: Overview of the methodology.

Feature engineering. Depending on the selected ML model, the features that need to be used to train the model are different. We are interested in experimenting with two different kinds of features. First, textual features are gathered by extracting the attribute values of the models, as suggested in [28]. This type of feature represents the models’ application domain (i.e., the names given by the user capture some meaning). Second, we convert the models into graphs that ML models can consume. The goal, in this case, is to study the effect of considering the model structure.

ML model selection. In this work we are interested in comparing several ML models for the task of model classification. In particular, we have considered six models which are discussed in detail in Sect. 4.1.

Data encoding. A key element is how to map the model features of interest (attribute values and graph structure) into the kind of representation that can be manipulated by each underlying ML model (i.e., how to map strings into numeric vectors?). We have also considered several encodings and tested them systematically to address this issue. They are discussed in detail in Sect. 4.2.

Model training and evaluation: We aim to evaluate different ML models and encodings systematically. To do so, we rely on the k -fold cross-validation resampling method used in previous works [28–30]. First, the dataset is divided into k disjoint validation sets. Then, given a ML model and an encoding method, for each $j = 1, \dots, k$, the validation set j is used to assess the ML model trained with the other $k - 1$ sets. Finally, we report the average of the k performances. It is important to note that a ML model could admit several configurations of hyperparameters (e.g., number of neighbors in k -NN, and number of units in a hidden layer in FFNN). To select the best configuration we do the following: given a ML model and for each considered configuration, we run the k -fold and we compute the average accuracy. Finally, the best configuration is the one that achieve the highest accuracy. As it is done in [28–30], we consider 10 folds and run a 10-fold cross-validation procedure.

4 COMPARISON DIMENSIONS

The comparison of existing techniques and tools for model classification has been performed by considering two different aspects, i.e., the adopted ML algorithm (see Section 4.1) and the way software models are encoded (see Section 4.2). We developed a set of tools to

ML MODEL	ENCODING	IMPL.	INSPIRED BY/ ADAPTED FROM
FFNN	BoW TF-IDF	scikit	[22, 28]
	BoW word embeddings	scikit and gensim	[11]
SVM	BoW TF-IDF	scikit	[22]
	BoW word embeddings	scikit and gensim	[11]
k -NN	Graph kernel	scikit and GraKeL	[14, 15]
	BoW TF-IDF	scikit	[22]
	BoW word embeddings	scikit and gensim	[11]
	Raw BoW	Lucene	[34]
Naive Bayes models	BoP	MAR	[23]
	BoW TF-IDF	scikit	[16]
GNN	Raw graph	PyTorch	[25]
CNN	BoW 2D TF-IDF	Keras and TensorFlow	[30]

Table 1: Combination of ML models and input features considered in this paper.

automate the methodology presented in the previous section and thus simplify the investigation of all the possible encoding and ML algorithm combinations.

The considered combinations of model encodings and ML models are shown in Table 1 and graphically depicted in Fig 3. The choice of these combinations was driven by the compatibility of each encoding with the ML model (e.g., Naive Bayes models cannot handle word embeddings) and the techniques used in previous works about the application of ML to MDE (column INSPIRED BY/ADAPTED FROM). Specifically, there are two main families of representations i.e., **BoW** (Bag-of-Words) and **graph**. The former encodes the terms of the model (e.g., the names associated with the model elements), and the latter encodes the structure of the model plus some attributes of the model elements.

4.1 ML models

In this paper, we will focus on classification problems. Thus, in the rest of the section, we will present several ML algorithms used to solve this problem. From now on, we will assume that we have a dataset of pairs $\mathcal{D} = \{(x_i, y_i)\}_i$ where x_i is the input data and y_i is its associated label.

4.1.1 k -Nearest Neighbors (KNN). This one of the simplest classification algorithms. Given new data x , its k most similar/closest elements of the dataset \mathcal{D} are computed. Then, the label of the majority is assigned to x . The flexibility of this technique is given by the concept of *similarity* that has to be defined by the user.

An advantage of using k -NN is that one can use a well-known measure (e.g., euclidean distance) or create a user-defined one. In

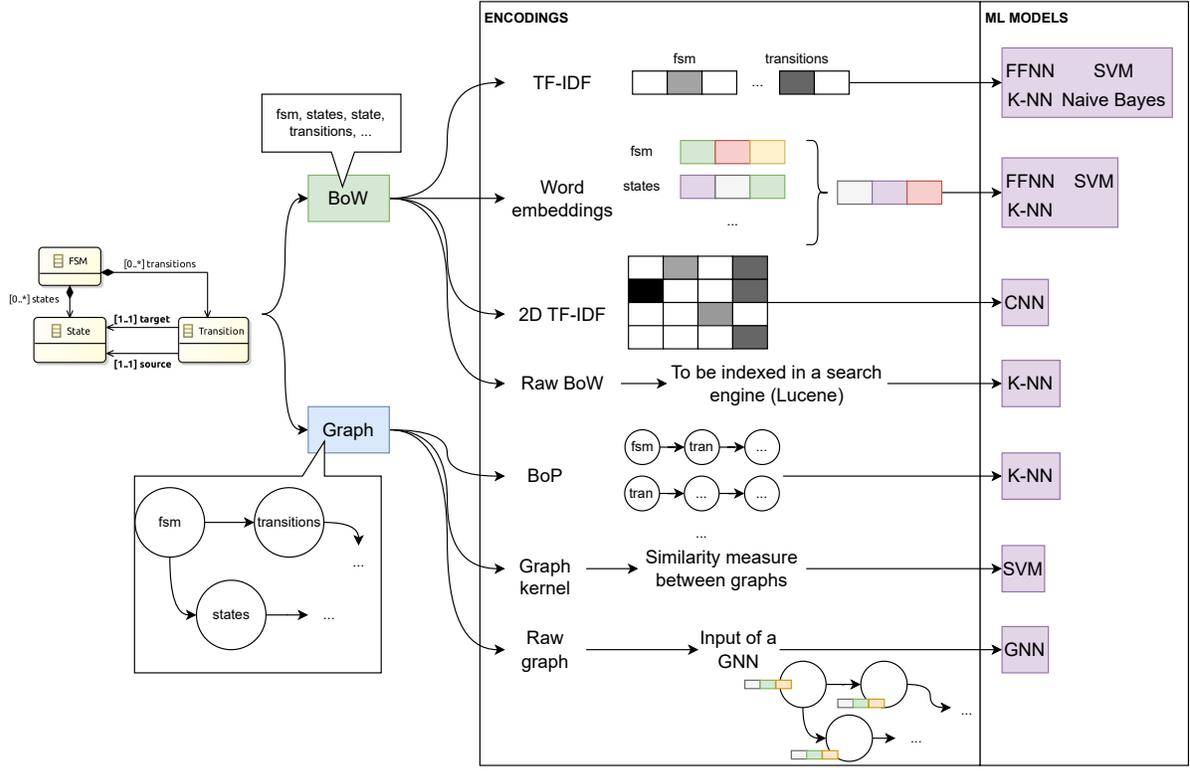


Figure 3: Input features and ML models.

particular, in this paper, we will use search engines to take advantage of their capabilities to compare and rank models according to their similarity to an input query. In our experiments, we consider k -NN using the following three different similarity measures (the first one is typically used in k -NN, whereas the other two are intended to evaluate the possibility of using off-the-shelf search engines to as a lightweight method to perform model classification):

- The euclidean distance over numeric vectors. In the next section we will show two strategies to encode models using a Bag-of-Words representation. This enables us to map software models to numeric vectors.
- The Lucene search engine. Lucene uses the scoring function Okapi BM25. It is a bag of words retrieval function that ranks a set of documents based on the query terms appearing in each document.

$$R(q, d) = \sum_{t \in q} \frac{f_t^d}{k_1 \left(1 - b + b \frac{l_d}{\text{avg}l_d}\right) + f_t^d} \quad (1)$$

where f_t^d is the frequency of term t in document d ; l_d is the length of the document d ; $\text{avg}l_d$ is the document average length along the collection; k is a free parameter usually set to 2 and $b \in [0, 1]$.

- The MAR search engine. MAR uses an adapted scoring function Okapi BM25 over BoPs. We use an approach similar to Lucene, that is, we use MAR as the similarity measure

of k -NN by performing a query using the given model and retrieving the top k more similar models.

4.1.2 Bayes Naive Classifiers (BNC). This is a simple ML technique that takes advantage of the independence assumption between the dimensions of the data. Given new data x , we want to assign it the label l such that

$$\text{argmax}_l P(y = y_l | x). \quad (2)$$

Using the Bayes theorem, we have the following:

$$P(y = y_l | x) = \frac{P(y_l)P(x|y = l)}{P(x)}$$

If we replace this formula into (2) and taking into account that $P(x)$ does not depend on l , we can transform (2) into

$$\text{argmax}_l P(y_l)P(x|y = l)$$

Now, using the independence assumption of the components, $P(x|y = l) = \prod_{j=1}^K P(x^j|y = l)$ and we have the following

$$\text{argmax}_l P(y_l) \prod_{j=1}^K P(x^j|y = l)$$

where each x^j is the j component or dimension of x . Normally, $P(y_l)$ is estimated by counting the proportion of the different classes of the dataset \mathcal{D} . Depending on how $P(x^j|y = l)$ is estimated using \mathcal{D} , BNC are divided in several types. We will to consider the following ones:

- Gaussian Naive Bayes (GNB). The $P(x^j|y = l)$ distribution is assumed to be Gaussian.
- Multinomial Naive Bayes (MNB). In this case, a multinomial distribution is considered.
- Complement Naive Bayes (CNB). This is an adaptation of the MNB for unbalanced datasets.

4.1.3 Support Vector Machine (SVM). Let us assume that we are facing a binary classification problem i.e., there are only two distinct labels. This ML algorithm tries to find a hyperplane in the data space that divides the group of data points x_i into two groups, one for each label. Given new data x , we just have to see in which side of the hyperplane it falls in. It is important to remark that this ML model has two important hyperparameters:

- The regularization term C it is used to control the overfitting, affecting the number of misclassified points in the training set.
- The kernel used: sometimes it is not possible to find a separation hyperplane, and it is necessary to map these points to a higher dimensional space (*kernel trick*). The kernel is the dot product in this new dimensional space.

Finally, we will use the one-vs-one schema to extend this approach to multiclass classification. First, we train one SVM that distinguishes between these two labels for each pair of different labels. Then, given a new data point, we run all these SVMs over this data point, and we assign it the label of the majority.

We will run SVMs over a Bag-of-Words representation (using two different encodings). Furthermore, we will consider the kernel presented in MORGAN [15] in order to run SVMs over graphs.

4.1.4 Neural networks (NNs). A neural network is an almost everywhere differentiable function $f_\theta(x)$ that tries to approximate the probability distribution $P(y|x)$ i.e., given new data, it returns the probabilities of belonging to each class. The training process is basically solving an optimization problem:

$$\operatorname{argmax}_\theta \sum_{(x,y) \in \mathcal{D}} \mathcal{L}(f_\theta(x), P(y|x)),$$

where θ represents the trainable weights of the NN, \mathcal{L} is the loss function (i.e., a measure that compares the expected output with the actual one). That is, the idea is to find a θ such that $f_\theta(x)$ performs very well in the dataset \mathcal{D} .

There exists several types of NN depending on the architecture of the function f_θ and the shape of the input. In this paper, we consider the following ones:

- FeedForward Neural Network (FFNN). This neural network is the first and the simplest among the neural networks. Essentially is composed of three types of layers, i.e., one input, one output, and one or several hidden layers. The simplest type of feedforward neural network is the perceptron, a feedforward neural network with no hidden layers. Given the input, a non-linearity function (normally ReLU) is used to compute the output. A FeedForward network is made of several connected layers of neurons, and the output of one layer becomes the input of the next one.
- Convolutional Neural Network (CNN) [20]. This network has been specifically conceived to process images. A CNN

consists of three layers, i.e., convolutional, pooling, and fully-connected layers. The convolutional layer extracts the features from the input image. The pooling reduces the spatial size of the convolved features. The last layer works like a multilayer perceptron in which every layer is fully connected to the previous one.

- Graph Neural Network (GNN) [35]. This neural network receives as input the nodes of a graph and generates node embeddings based on local network neighborhoods. More specifically, each node of the graph is initialized with an initial vector. Then, in each step (i.e., after the application of each layer), it is updated with the vectors of its neighborhood.

We have applied FFNN using BoW representations. Also, we have experimented with a GNN (which can directly used a graph representation) with two convolutional layers with the GraphSAGE operator [19] and a mean global pooling. Finally, we have also applied a CNN by encoding a model as a special BoW representation mapped to a 2D matrix to emulate an input image. The input image transits three convolutional layers. In each transition, a convolutional filter is applied together with a pooling procedure to decrease the size of the feature. Finally, the output of this pipeline is passed through two fully-connected layers to perform the classification.

4.2 Encoding of software models

A ML model cannot receive a raw software model as input, but it has to be transformed to a set of features which can be processed by the target ML model (e.g., a numeric vector). Therefore, an important task to use ML models with software models is to choose the proper encoding and implement it effectively. In the following, we present different encoding techniques with which we have experimented in this work.

Models as a Bags of Words (BoW). For each model, we extract the string attribute values² and we split them taking into account the *whitespace*, *snake case* and *camel case* conventions. As a result, a multiset (bag) of words is obtained from an input model. For instance, the BoW associated to the Ecore model in Fig. 3 is {fsm, states, state, target, source, transition, transitions}. In this way, the vocabulary associated to the dataset is the set of words extracted from it. Finally, each bag is transformed into a real valued vector. For this, we have considered the following alternatives:

- **TF-IDF.** Each bag of words is represented by a high dimensional vector whose number of dimensions is the size of the global vocabulary (i.e., one dimension per different word). More concretely, each bag b is transformed into a vector v and the component associated to the word i of the vocabulary is the following:

$$v_i = \operatorname{tf}(b, i) \times \log \frac{1 + n}{1 + \operatorname{df}(i)} + 1.$$

Where $\operatorname{tf}(b, i)$ is the number of times i appears in b , n is the number of bags and $\operatorname{df}(i)$ is the number of bags that contain the term i . Finally, we normalize the vector v by its norm. The final vector is a high-dimensional vector in which a zero means the absence of a term and the higher

²e.g., in the case of Ecore, the most notable attribute is `ENamedElement.name`.

the component associated to a concept is the stronger it is in the model. For instance, in the graphical representation of the TD-IDF encoding of the simple FSM metamodel in Fig. 3, the `fsm` term is represented with a lighter grey than the transitions.

- **Word embeddings.** A word embedding is a representation of text where each word has an associated vector, and words with similar meanings have similar vectors (i.e., geometrically close vectors). A valuable property of word embeddings is that once learned (from a certain collection of documents), it is possible to reuse them for several projects. Thus, there are several already trained word embeddings ready to be used. In this work, we consider the 300-d GloVe [31] embeddings trained with Wikipedia and Gigaword 5. Since each word already has a vector associated that encodes its meaning, we transform each bag into a vector by computing the average of the vectors associated with the words of the bag.
- **2D TF-IDF.** We follow the encoding technique used in [30] to encode the features. The TF-IDF vectors are split into sequences of consecutive cells and then they are stacked vertically to generate 2D matrices.

Models as graphs. Software models typically have a graph-like structure. Hence, this representation is particularly suitable to enable ML models to learn the structure of the models. In particular, we transform each model of the dataset into a graph following this procedure:

- Each object of the model is mapped to a node in the graph.
- Each reference of the model is mapped to an edge in the graph.
- Each node is given two attributes: an identifier for the object if available (e.g., a name attribute) and the name of its meta-class. In general, an object may have more than one attribute, but ML graph algorithms typically require a fixed number of attributes. Thus, we have chosen these two pieces of information as the most representative ones for classification. Nevertheless, other tasks may require the selection of different types of attributes.

If the target ML model is SVM (see Sect. 4.1.3), we consider graph kernels [14] and we can run SVM directly over the raw graphs. A graph kernel can be seen as a dot product between graphs in a high-dimensional vector space.

If the target ML model is GNN (see Sect. 4.1.4), the raw graph is introduced into the ML model. However, to adequately handle attribute values (which are strings), we need to map the vocabulary to numeric vectors. This is done in three steps. First of all, each word in the vocabulary is assigned a unique integer value. Then, the node attributes are converted into a numeric vector (with size 2 because we are considering only two attributes). Finally, the GNN requires an embedding layer to map the node attributes into a larger numeric vector which is learned during training and represents the meaning of the node.

Finally, we use MAR as an alternative means to encode the model structure. MAR is a search engine designed to perform query-by-example [23]. In MAR each model is encoded as *bag-of-paths* (BoPs), where paths are computed between attribute values. For instance, for the metamodel shown in Fig. 3, the path (*FSM*, *name*, *EClass*) has length 1 and simply encodes the name of class. However, (*FSM*,

name, *EClass*, *transitions*, *name*, *EStructuralFeature*) has length 2 and encodes the existence of a reference named *transition* associated to the *FSM*. A configuration parameter of MAR is the maximum length of the paths. The longer the path is, the more model structure is encoded. In this work, we set the path length to 3, which is the standard value used by MAR (as reported in [24]).

5 EXPERIMENTS

In this section, we explain our experimental setup and report the results of our experiments. Through the performed experiments, we aim to answer the following research questions:

- **RQ1:** Which model achieves a greater performance in the task of model classification?
- **RQ2:** How the chosen encoding of software models affects the task of model classification?
- **RQ3:** Which is the effect of data duplication on the performance of the ML models?

The first research question aims at providing insights into which ML model to choose when faced with a classification task. Then, RQ2 complements RQ1 by studying the importance of the selected encoding in the performance of the models. Finally, RQ3 addresses the question of whether the results can be biased due to the presence of duplicates, which is a typical scenario when data is downloaded from public sources. It is important to remark that the experiments have been facilitated by the methodology explained in Sect. 3, instantiated and automated for the task of model classification.

5.1 Replication package

The results of the experiments and detailed instructions to run them from scratch are described in a replication package available at <https://figshare.com/s/5904baec3dbd0a48036c>.

The replication package is built using standard Python ML libraries like scikit-learn, PyTorch, Pandas, etc. Moreover, we provide a Python execution environment to make sure that the same dependencies are used. Finally, the results of the paper are automatically generated from the outputs of the experiments.

5.2 Data

We use MODELSET [22] as the source dataset to perform our experiments. It contains about 5,000 Ecore models and 5,000 UML models labelled with their categories and gathered from GitHub and GenMyModel respectively. The main reason for choosing it is that, currently, it is the largest dataset of labelled models available. In this work, we are interested in classification which is a supervised task and requires a labelled dataset. Although other datasets have been used in previous works, they are very small [3] which contains only 555 Ecore metamodels, and this hinders the possibility of obtaining reliable conclusions from its use. The Lindholmen dataset, instead, contains more than 90,000 UML models [33], but they are not labelled. Moreover, the dataset is not curated, and actually, many of the models are broken.

An important aspect to consider when using MODELSET is that it contains duplicate and quasi-duplicate models, which is a typical issue in datasets extracted from public sources like GitHub. Therefore, we have built an implementation of the algorithm proposed

	Ecore			UML	
	All	No-dups		All	No-dups
Num. models	4167	2068	Num. models	3720	1317
Num. categories	67	48	Num. categories	44	28
Avg. elements	219	145	Avg. elements	126	129
Classes	28	19	Class diagrams	9	9
Attributes	16	12	Use case diag.	3	3
References	29	22	Others	1.25	1.5

Table 2: Statistics of the used dataset, after filtering. We report the statistics with and without duplicates.

by Allamanis [1] but adapted it to detect and remove duplication in modeling datasets.

Table 2 shows some statistics about the models of the datasets, after filtering for removing models whose associated category has less than 10 models. For both Ecore and UML datasets and the variants with duplicates removed, we report the number of models, the number of categories, and the average number of elements per model. In addition, we also report the average number of objects per meta-type for some types of elements to give hints about the structure of the models (e.g., number of classes, attributes, and references for Ecore and the number of class diagrams, use case diagrams, and an aggregation of the other UML diagrams).

In MODELSET, each model has a main label called *category* which we use as the target variable for the classification task. The category of a model refers to its main application domain. For instance, models intended to describe conference systems (e.g., like EasyChair or HotCRP) are labelled with *conference*. As can be observed, after removing duplicates, the dataset size is halved, and the number of categories is reduced. Nevertheless, the number of models is large enough to perform the classification task adequately.

5.3 Considered hyper-parameters

Table 3 shows the hyper-parameters considered for each ML model. In the case of FFNN, we consider one layer and several hidden units. For SVM, we consider several values of C (the regularization parameter). If the input of the SVM is a vector, we study the performance of the *rbf* kernel and the *linear* one. If the input is a graph, then we use the *graph kernel* used in MORGAN [15]. For k -NN models, we test several values of k . In the case of CNB and MNB, we vary the smoothing parameter (α). GNB does not admit any hyper-parameters. Our experiments consider a GNN with a fixed initial embedding dimension, hidden dimension, and two layers. We do not systematically vary these hyper-parameters because the training procedure of these networks is expensive. Through ad-hoc experiments, we observed that these values are adequate. Finally, we consider the architecture used in [30] for the CNN.

5.4 Evaluation metric

We evaluate how well the presented models are able to classify metamodels. Initially, we considered *Accuracy*, that is, the correctly classified models over the total models analysed:

$$Accuracy = \frac{\text{Correctly classified models}}{\text{Total models}} \quad (3)$$

ML MODEL	HYPER-PARAMETERS	VALUES
FFNN	Hidden size	[50, 100, 150, 200]
SVM	C	[0.01, 0.1, 1, 10, 100]
	Kernel	rbf, linear, graph kernel
k -NN	k	[1, 2, 3, 4, 5]
CNB, MNB	α	[0.1, 0.6, 1.1, 1.6]
GNB	-	-
GNN	Initial embedding dimension	256
	Layers	2
	Hidden dimension	128
CNN	-	-

Table 3: Hyper-parameters considered for each model

However, to make sure that we take into account the potential bias due to the unbalanced of the dataset (i.e., there may be categories with much less instances than other category), we have considered the *Balanced Accuracy*. This is a modified version of the accuracy that takes into account unbalanced categories. It is defined as the average of the recalls for each category. More concretely, for each category k , its associated recall is defined as:

$$Recall_k = \frac{TP_k}{\text{Number of samples}_k},$$

where TP_k is the number of corrected identified models of the category k . Finally, the balanced accuracy is defined as:

$$\text{Balanced accuracy} = \frac{\sum_{k=1}^K Recall_k}{K}$$

In practice, it means that all categories will have the same importance even if they contain a small number of samples.

5.5 Addressing RQs

To support our experiments we have developed a framework to easily plug-in new classification methods and evaluate them consistently. To this end, we have relied on the Python library *sci-kit learn*. To integrate a ML method in our framework, there are three main scenarios:

- Using an ML algorithm already supported by sci-kit. This is straightforward.
- Using an ML algorithm which can be implemented in Python. In this case, a scikit classifier needs to be created. This requires essentially implementing a training procedure (a fit method) and a prediction procedure (predict method). In this case, integration is straightforward as well, although additional work maybe need in the implementation. This is the case of our implementation of GNN for models which rely on Pytorch and PyG.
- Integrate a third-party tool, typically not implemented as a Python library. This is the case with the MAR and Lucene search engines and the MEMOCNN classifier. In this case, the strategy is similar to before. A scikit classifier is created, but it is much more complex since it needs to wrap the third-party tool by calling external programs and processing their results.

The column IMPL. in Table 1 shows which tool we have used to implement each ML method and encoding. We have implemented a TF-IDF encoding using the scikit facilities, word embeddings using

	Model	Encoding	B. accuracy	Best hyper.
1	FFNN	TF-IDF	0.898511	hidden size = 200
2	SVM	TF-IDF	0.895735	kernel = linear, $C = 100$
3	GNN	Raw graph	0.888875	–
4	CNN	2D TF-IDF	0.885606	–
5	k -NN	Lucene (BoW)	0.882907	$k = 1$
6	SVM	WordE	0.880327	kernel = linear, $C = 10$
7	k -NN	TF-IDF	0.879817	$k = 1$
8	FFNN	WordE	0.877892	hidden size = 50
9	k -NN	MAR (BoP)	0.873174	$k = 1$
10	k -NN	WordE	0.852933	$k = 1$
11	GNB	TF-IDF	0.809371	–
12	SVM	Graph kernel	0.792745	$C = 0.1$
13	CNB	TF-IDF	0.775844	$\alpha = 0.1$
14	MNB	TF-IDF	0.754884	$\alpha = 0.1$

Table 4: Results for Ecore, with duplicate models

	Model	Encoding	B. Accuracy	Best hyper.
1	FFNN	TF-IDF	0.824972	hidden size = 150
2	SVM	TF-IDF	0.815609	kernel = linear, $C = 10$
3	GNN	Raw graph	0.807656	–
4	SVM	WordE	0.786988	kernel = linear, $C = 100$
5	k -NN	Lucene (BoW)	0.786793	$k = 1$
6	CNN	2D TF-IDF	0.778440	–
7	FFNN	WordE	0.777899	hidden size = 150
8	k -NN	MAR (BoP)	0.775339	$k = 3$
9	k -NN	TFIDF	0.764505	$k = 1$
10	CNB	TFIDF	0.733788	$\alpha = 0.1$
11	k -NN	WordE	0.723883	$k = 1$
12	MNB	TF-IDF	0.716409	$\alpha = 0.1$
13	GNB	TF-IDF	0.607369	–
14	SVM	Graph kernel	0.593098	$C = 0.1$

Table 5: Results for Ecore, removing duplicate models

GloVe (through the gensim library) and a graph kernel using GraKeL. Then, we have used scikit to implement FFNN, SVM, k -NN and Naive Bayes models over these encodings. Additionally, we have created a GNN specifically designed for model classification using PyTorch. We have reused the MAR search engine to experiment with its BoP encoding. We have also used Lucene as an alternative search engine, following [34]. Finally, we have reused the CNN implementation presented in [30] based on Keras and TensorFlow. A limitation of the experiments is that, since CNN and Lucene are third-party implementation, we could not experiment with UML models because they are not currently supported.

6 RESULTS

Using the experimental setup presented in the previous section, we have obtained the following results. Table 4 shows the results for Ecore without discarding duplicates. Table 5 shows the results for Ecore, but applying the pre-processing phase to discard duplicates. Table 6 shows the results for UML without discarding duplicates. Table 7 shows the results for UML, but discarding duplicates. In the rest of the section we analyse these results.

	Model	Encoding	B. Accuracy	Best hyper.
1	SVM	WordE	0.873906	kernel = linear, $C = 10$
2	FFNN	WordE	0.872578	hidden size = 150
3	SVM	TF-IDF	0.870490	kernel = linear, $C = 100$
4	FFNN	TF-IDF	0.864192	hidden size = 100
5	k -NN	MAR (BoP)	0.859487	$k = 1$
6	k -NN	WordE	0.849309	$k = 1$
7	k -NN	TF-IDF	0.848727	$k = 1$
8	GNN	Raw graph	0.843559	–
9	GNB	TF-IDF	0.798754	–
10	SVM	Graph kernel	0.769627	$C = 0.1$
11	CNB	TF-IDF	0.760579	$\alpha = 0.1$
12	MNB	TF-IDF	0.745817	$\alpha = 0.1$

Table 6: Results for UML, with duplicate models

	Model	Encoding	B. Accuracy	Best hyper.
1	FFNN	WordE	0.775893	hidden size = 150
2	FFNN	TF-IDF	0.758389	hidden size = 50
3	SVM	WordE	0.756125	kernel = rbf, $C = 100$
4	SVM	TF-IDF	0.744753	kernel = linear, $C = 10$
5	k -NN	MAR (BoP)	0.716452	$k = 3$
6	GNN	Raw graph	0.713418	–
7	CNB	TF-IDF	0.703389	$\alpha = 0.1$
8	k -NN	WordE	0.694383	$k = 1$
9	k -NN	TF-IDF	0.686937	$k = 1$
10	GNB	TF-IDF	0.630084	–
11	MNB	TF-IDF	0.628251	$\alpha = 0.1$
12	SVM	Graph kernel	0.530019	$C = 0.1$

Table 7: Results for UML, removing duplicate models

6.1 RQ1: Best model

The best models are *feed-forward neural network* (FFNN) and SVM in the four scenarios (Ecore and UML with and without duplicates). Moreover, FFNN outperforms the SVM for 3 out of the 4 scenarios.

Using a “lightweight method” like k -NN plus MAR (or Lucene) obtains consistently worse results than more advanced ML methods, particularly neural networks and SVMs. However, the loss of accuracy when using MAR or Lucene is not very high, which means that these models are still competitive. This suggests that the classification tasks could be effectively addressed with simple, off-the-shelf machinery. We foresee two scenarios in which lightweight methods can be a good fit: *a)* for teams with little experience with ML and the additional complexity that it brings for testing and deploying the ML models and *b)* when there already exist search engines with a large number of indexed models, and thus, it is possible to profit from them with little effort.

Finally, it is worth mentioning that FFNN and SVM, which can be considered simple ML models, outperforms more complex models like CNN and GNN which can be considered *deep learning models* since they have much more learnable parameters. One reason could be that the dataset size is not large enough for the usage of complex models.

6.2 RQ2: Encoding schemes

In the case of Ecore, the best encoding scheme is TF-IDF. In Tables 4 and 5 the first two models use as encoding technique TF-IDF. Interestingly, TF-IDF outperforms word embedding, which is a more sophisticated encoding. We believe that this can be caused by the

fact that we use a word embedding model trained on general texts, which may not be a good fit for software models. Thus, a potential future direction is to train word embeddings based on modelling texts.

On the other hand, for UML, the best encoding is word embedding. This confirms our previous argument. The rationale, in this case, is that UML models are often used to describe non-technical domains: e.g., a shopping center, a bank, etc. Therefore, the pre-trained embeddings capture the meaning of the model elements much better.

In the same line, the performance of the GNN drops for UML (in relative terms with respect to FFNN and SVM). This can be caused by the fact that the embedding layer is simply initialized with the vocabulary. A potential solution to improve the GNN performance for UML could be to initialize the embedding layer directly with word embeddings.

An interesting observation is related to the choice between simple or more complex encodings. One could expect that structured encoding schemes based on graphs (as used by MAR and models like GNN and SVM with kernel) should be superior. The rationale is that they are a good match for the graph-based nature of software models. However, our experiments reject this idea for the classification task. The main reason that we have observed is that the domain of application of a software model is mainly associated with the *names* given to its model elements. For example, most meta-models about *Petri nets* have words like *petri*, *net*, *place*, *transition*, *arc*, etc and the main difference with e.g., a *state machine* model is not the structure but the naming.

Thus, for ML tasks similar to the one in our experiments, possibly a simple encoding scheme based on extracting the strings is enough.

6.3 RQ3: The effect of (near) duplication

There is an important reduction in the accuracy of all the methods when duplicates are discarded. As expected, the type of model whose performance decays the most is the k -NN. This model is considered a *naive* memorization method [1]. If a model of the training set is duplicated in the test set, likely, this model appears first in the list of nearest neighbors.

Previous works [29] have obtained similar results using a feed-forward neural network, with a similar TF-IDF encoding (i.e., precision above 90%). However, our results show that these experiments could be biased due to the existence of duplicates. These results suggest that future works applying ML for MDE tasks should carefully consider the presence of duplicates.

Arguably, having duplicates in the dataset may reflect well scenarios in which the data has been obtained from public repositories (i.e., MODELSET was built from GitHub and GenMyModel). Nevertheless, our results show that there is still room to improve classification methods applied to software models.

6.4 Assessment

Our experiments have shown that the performance of the tested ML models (which are standard models) for the task of model classification is good (around 80% when duplicates are removed) but not excellent. This contrasts with previous works [16, 22, 28, 30].

The reason can be due to a variety of factors that makes the classification harder for the ML models, namely: the fact that we have used a larger dataset (with more categories), the removal of duplicates, and the use of UML models, which may be more complex than Ecore models. In practice, this means that model classification is not yet a solved problem. Instead, more research is needed to propose specific ML models to obtain better performance.

The internal threats to our approach are essentially related to the dataset we adopted. We identified some specific threats: MODELSET is composed of ~5000 Ecore and UML models, which could not be enough to train some ML models properly, but its size is enough to draw initial results. Moreover, to the best of our knowledge, it is the largest curated and labeled dataset publicly available. Another possible threat is related to the quality of MODELSET, the existence of duplicates is a relevant problem which affects different datasets. We alleviate this problem by considering two versions of the original dataset, with and without duplicates. Some of the employed tools are not able to classify UML models. We plan to extend these tools to analyze their performance in this task. An external threat that affects the generalization of the results is that we have only considered one kind of ML task. To partially mitigate this, we have performed the task with two with both Ecore and UML. Nevertheless, the proposed framework can boost the experimentation with other relevant ML tasks in the context of MDE.

7 CONCLUSION AND FUTURE WORK

In the last years, the application of ML techniques to enhance MDE-related scenarios has been increasingly researched. However, the current body of knowledge lacks a good understanding of which ML models and encodings are best suited. This paper aims to fill this gap, focussing on the task of model classification. To this end, we have considered six ML models and six possible encodings, and we have systematically combined and evaluated them. Finally, we applied these two datasets of about 5,000 Ecore models and 5,000 UML models. The results show that a feed-forward neural network using a TF-IDF encoding is generally the best approach. However, simpler models like k -NN combined with a search engine provide almost comparable results. In general, for model classification, the model structure is irrelevant (i.e., it is not needed to use more complex models like GNNs). Moreover, we have shown that the performance of all ML models is reduced when (quasi-)duplicate models are discarded.

In future works, we plan to apply this framework to other ML tasks in the MDE domain to generalise our results. Regarding extensions for the task of model classification, we plan to consider multi-classification as done in [22] (e.g., multiple labels per model) as well as using other performance metrics. We also plan to investigate other ML models which can generalize better and improve the accuracy of the tested models.

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