PCA-based Category Encoder for Categorical to Numerical Variable Conversion

Hamed Farkhari†‡, Joseanne Viana ‡‡, Luis Miguel Campos ‡, Pedro Sebastiao∗ ‡‡, Rodolfo Oliveira §, Luis Bernardo §

†PDMFC, Rua Fradesso da Silveira, n. 4, Piso 1B, 1300-609, Lisboa, Portugal
‡ISCTE – Instituto Universitario de Lisboa, Av. das Forças Armadas, 1649-026 Lisbon, Portugal
§IT – Instituto de Telecomunicações, Av. Rovisco Pais, 1, Torre Norte, Piso 10, 1049-001 Lisboa, Portugal

∗FCT – Universidade Nova de Lisboa, Monte da Caparica, 2829-516 Caparica, Portugal;
Emails : Hamed Farkhari@iscte-iul.pt, joseanne cristina viana@iscte-iul.pt, luis.campos@pdmfc.com, pedro.sebastiao@iscte-iul.pt, rado@fct.unl.pt lflb@fct.unl.pt

Abstract—Increasing the cardinality of categorical variables might decrease the overall performance of ML algorithms. This paper presents a novel computational preprocessing method to convert categorical to numerical variables for machine learning (ML) algorithms. In this method, We select and convert three categorical features to numerical features. First, we choose the threshold parameter based on the distribution of categories in variables. Then, we use conditional probabilities to convert each categorical variable into two new numerical variables, resulting in six new numerical variables in total. After that, we feed these six numerical variables to the Principal Component Analysis (PCA) algorithm. Next, we select the whole or partial numbers of Principal Components (PCs). Finally, by applying binary classification with ten different classifiers, We measured the performance of the new encoder and compared it with the other 17 well-known category encoders. The proposed technique achieved the highest performance related to accuracy and Area under the curve (AUC) on high cardinality categorical variables using the well-known cybersecurity NSLKDD dataset. Also, we defined harmonic average metrics to find the best trade-off between train and test performance and prevent underfitting and overfitting. Ultimately, the number of newly created numerical variables is minimal. Consequently, this data reduction improves computational processing time which might reduce processing data in 5G future telecommunication networks.

Index Terms—Categorical Encoders, CyberSecurity, Dimensionality Reduction, Feature Selection, Machine Learning, NSLKDD, Principal Component Analyses

I. INTRODUCTION

Machine learning (ML) prediction problems require giving the model relevant features to represent the problem accurately. As a result, data preparation and feature engineering are critical activities in every machine learning algorithms [1]. As the amount of data accessible rises, the number of features diversity will increase. This expansion impacts categorical variables. First, the number of features grows, and then, the number of unique values detected in each feature (cardinality) increases [2]. The challenge of appropriately and effectively encoding categorical features influence the machine learning model’s performance in the second instance. Handling categorical characteristics is a well-known and widely used issue in data science and machine learning since many methods require numerical input [3]. This problem has several well-known solutions. Nevertheless, specific categorical data encoding schemes are more suited than others depending on the type of problems, such as classification or regression. This is critical when dealing with large volumes of data when errors and outliers are more common. Thus, making reliable statistical measures challenging to compute. We present a different approach to solve the categorical encoders modelling by using conditional probability in supervised learning and Principal Component Analysis (PCA). Further, We compare the performance of our method with several available categorical encoders and classifiers using the same dataset. We show that our method achieve the best performance by adjusting only two parameters. This paper starts by analyzing the results obtained from 17 different categorical to numerical encoders, using ten different classifiers, followed by a description of the metrics used to select the best combination. After that, we introduce our novel method to convert categorical to numerical variables based on the probability relationship between categories and target classes in supervised classification and the results are compared in accuracy and Area under the curve (AUC).

A. Contributions and Motivation

The traditional categorical encoders did not provide the parameters to adjust them with classifiers. Considering this constraint, the main contributions of this paper are summarized as follows:

• New method to encode categorical features using only two hyperparameters embedding threshold and PCA to adjust with different classifiers for maximum performance achievement.
• Supervised category encoder, which is suitable to use for both linear and nonlinear classification algorithms.
• Comparison between the proposed solution with available categorical encoders using harmonic averages, accuracy, and AUC.
Our method achieves the highest performance using the lowest possible dimensionality in high cardinality categorical variables in the test set results, which did not include elements of the train set. Furthermore, it is possible to prevent or decrease underfitting and overfitting, defining new metrics using a different set of hyperparameters on our encoder to make adjustments in the classifiers in the preprocessing steps.

II. THE PROPOSED METHOD

The scheme offers a unique computational preprocessing approach for converting categorical to numerical variables for machine learning (ML) methods. Table I shows the dataset with categorical variables named from \( V \text{variable}_1 \) to \( V \text{variable}_N \). Each variable contains different numbers of categories. Target variable contains two classes for the purpose of binary classification.

| Variable\(_{1}\) | ... | Variable\(_{N}\) | Target |
|------------------|-----|----------------|--------|
| Category\(_{1,1}\) | ... | Category\(_{N,1}\) | Class \( C_1 \) or \( C_2 \) |
| Category\(_{1,2}\) | ... | Category\(_{N,2}\) | (Binary Classification) |
| ... | ... | ... | ... |
| Category\(_{1,J}\) | ... | Category\(_{N,J}\) | ... |

TABLE I: Categorical variables with different categories in binary classification.

Using the variables and the target in Table I, we define the conditional probabilities for each unique category in binary classification. The calculation for each category is based on the numbers of its occurrences for each class \( C_1 \) and \( C_2 \) per its total occurrences as illustrated in equations (1) and (2):

\[
P_{1,j} = P(Target = C_1 | V \text{variable}_j = \text{Category}_{j}) \tag{1}
\]

\[
P_{2,j} = P(Target = C_2 | V \text{variable}_j = \text{Category}_{j}) \tag{2}
\]

Before applying the threshold parameter, for each unique \( \text{Category}_{j} \) the following condition holds:

\[
P_{1,j} + P_{2,j} = 1, \ (3) \text{ where } i, j \text{ are defined}
\]

\{1,2, ..., \( M_j \), \( N \) is the number of total categorical variables, and \( M_i \) is the number of unique categories for variable \( i \). \( N \) and \( M_i \) are fixed for each variable. Thus, each variable \( V \text{variable}_i \) will produce two new numerical variables with three states.

\[
\begin{array}{c|ccc}
\hline
V \text{variable}_i & \text{New V ar1} & \text{New V ar2} & \text{Conditions} \\
\hline
\text{Category}_{i,j} & 1 & 0 & \text{If } P_{1,j} \geq P_{2,j}, \text{ AND } P_{1,j} > \text{threshold.} \\
\hline
\end{array}
\]

TABLE II: Converting each categorical variable to two numerical variables with conditions for each category.

In Table II, \( \text{Category}_{i,j} \), \( V \text{variable}_i \), \( \text{New V ar1} \), and \( \text{New V ar2} \) refers to \( \text{Category}_{i,j} \), categorical \( V \text{variable}_i \), first and second new created numerical variables for \( V \text{variable}_i \), respectively. New numerical variables will be created based on probability conditions on equations (1) and (2) and the value of threshold.

A. Threshold

The first hyperparameter denominated threshold is defined for categories with low occurrences in the probability calculation as demonstrated in \( P_{1,j} \) or \( P_{2,j} \) resulting in the last row in the Table II. These categories are rare, and the user configures the threshold for them. NSLKDD dataset contain three categorical variables. We used one unique threshold for all of them. Applying the threshold, using both equations (1) and (2), and estimating the conditions defined in Table II, the scheme creates two new numerical variables for each categorical variable. After applying the process for all categorical variables, six new numerical variables will be generated. After the procedure, if the new numerical variable contain only one unique value for all categories, i.e., only ones or zeroes, the new variable must be removed. All amounts of thresholds represented in our results are in percentage.

B. Principal Component Analysis

The second hyperparameter is the number of Principal Components (PCs) available after the PCA processing. The main objective of PCA in our methodology is to remove the correlation between the six new numerical features described in Table II. PCs can varied from 1 to \( K \), where \( K \leq 6 \). Generally, \( K \) is defined as the minimum PCs needed to capture most of the data variances. By choosing \( K \) PCs, the cumulative data variance is one, while for \( K - 1 \), it is less than one. We describe the combination of the first and second hyperparameters in the grid search section.

C. Scaling

Usually, scaling is applied before PCA to prevent the dominance effect of some features over others caused by different scales. In our method, the six new numerical features are normalized between zero and one; consequently, there is no need for scaling. However, after the PCA process, the standardization scale using mean and standard deviation is applied for faster convergence in some classifiers such as Support Vector Machines (SVMs).
D. Dataset

We chose NSLKDD [4] dataset for testing different encoding methods and classifiers which is frequently used in cybersecurity research (for instance, for network intrusion detection). NSLKDD is divided into four different partitions namely, KDDTrain+, KDDTrain+ _20Percent, KDDTest+ and KDDTest-21. All partitions are freely available for download from [4]. We used exclusively and entirely KDDTrain+ for training, and KDDTest+ as a complete test dataset for test purposes which is including all the test instances. A quick analysis of NSLKDD shows that the KDDTrain+, KDDTest+, KDDTrain+20Percent, and KDDTest-21 contain 125973, 22544, 25192, and 11850 records, respectively. Among all variables in the dataset, only three are categorical, namely protocol type, service, and flag. We convert the categorical variables to numerical using different encoders to compare the performance of each method in binary classification.

E. Categorical Encoders Dimensionality

One of the main challenges related to the Categorical variables with high cardinality is high dimensionality after converting them to numerical features. Methods such as One Hot Encoding presents such constraints. In the proposed method, the number of dimensions of new numerical features varies in the range of one to six. The protocol_type and flag variables in both KDDTrain+ and KDDTest+ sets contain the same cardinality. However, for service variable, the cardinality is greater and different between the train and test sets which makes the available encoder may present low performance. Table III shows the difference of dimensionality for newly created numerical features for each of the encoding schemes used. These categorical encoders are used from category encoders library version 2.2.2. According to the Table III, other encoder schemes create at least three dimensions for the new numerical features, in our system it is possible to reduce it to one.

| Encoding Scheme (abbreviation) | Dim. |
|-------------------------------|------|
| (Proposed)                    | 1-5  |
| Backward Difference Encoder (Backward Difference) [5] | 81  |
| BaseN Encoder (BaseN) [6]     | 13   |
| Binary Encoder (Binary) [7]   | 13   |
| Cat Boost Encoder (Cat Boost) [8] | 3    |
| Count Encoder (Count) [9]     | 3    |
| Generalized Linear Mixed Model Encoder (GLMM) [10] | 3    |
| Hashing Encoder (Hash) [11]   | 8    |
| Helmet Encoder (Helmet) [5]   | 81   |
| James-Stein Encoder (James-Stein) [12] | 3    |
| Leave One Out Encoder (LOOE) [13] | 3    |
| M-estimate Encoder (MEestimate) [14] | 3    |
| One Hot Encoder (One Hot) [5] | 84   |
| Ordinal Encoder (Ordinal) [5] | 3    |
| Polynomial Encoder (Polynomial) [5] | 81   |
| Sum Encoder (Sum) [5]         | 81   |
| Target Encoder (Target) [14]  | 3    |

F. Classifiers

Ten classifiers with different configurations in Python v3.6.9 and Sci-kit learn library v0.23.2 were used to make results comparable. These classifiers with hyperparameters are shown in Table IV. For replication purposes, the seed value of randomness (random state) in all classifiers was considered as zero.

G. Metrics

Metrics such as accuracy can be simply measured in multiclass problems. However, other metrics such as precision, recall, FPR, F1-Score, and the sum of the Area Under the Curve (AUC) of Receiver Operating Characteristic (ROC), cannot be calculated easily [16]. Thus, in practice, only accuracy is enough to check performance in multi-class problems. It is essential to choose the proper metrics to compare the results between the available encoders and the proposed system. We used binary classification and divided the target labels to attack and regular internet traffic (normal labels). The proportion of

| Classifiers       | hyperparameters                           |
|-------------------|--------------------------------------------|
| Logistic Regression (LR) | solver = 'saga', penalty = 'l2', c = 1.0 |
| Multilayer Perceptron (MLP) | solver = 'adam', alpha = 0.0001, hidden_layer sizes = 100, activation = relu, learning rate init = 0.001('constant'), batch size=200 |
| SVM 1             | kernel = rbf, gamma = 'auto', c=1.0        |
| SVM 2             | kernel = poly, gamma='auto', c=1.0, degree=5 |
| SVM 3             | kernel = linear, c=1.0                     |
| Decision Tree(DT) | max depth=5, split quality measure = 'gini', max features considered for each best split = min(8, number of new numerical features) |
| Ada Boost Classifier (ADA 1) | base estimator=DecisionTreeClassifier (max depth=1), n_estimators=50 |
| Ada Boost Classifier (ADA 2) | base estimator=DecisionTreeClassifier (max depth=5), n_estimators=10 |
| Random Forest (Forest) | max depth=5, no. of estimators = 10, split quality measure = 'gini', max features considered for each best split = min (5, number of new numerical features) |
| Gaussian Naive Bays (GBN) | default sci-kit learn parameters |

TABLE IV: Classifiers with hyperparameters used for classification.
attack and normal labels in the train set is 46.54% and 53.46%. In the test set, the ratios are 56.92% and 43.08%, respectively. The percentage of labels in two classes shows that the number of instances is balanced in train and test sets. The accuracy and AUC are usually used for balanced classification. The precision, F1-score, and other metrics are used for unbalanced classification.

H. New Metrics

Usually, the attacks and normal data in train and test are not equal, making sense for the algorithms learning proposes. For example, the NSLKDD test set contains only 15% of the total data. The excellent performance exhibited on the test set cannot guarantee equally good performance for the train set and vice versa. We should therefore consider a trading-off between the performances of train and test sets. If we change the amount of data available for the test in 1% if the accuracy of the algorithm change 1% in the test, it affects only 15% in the total data, for our data set is 22544 samples. On the other hand, 1% changes in the training data affect the other 85% of data containing 125973 samples. For the first time, we want to define new metrics to consider both train and test performance because by ignoring minimal changes in test performance, extensive changes may occur in the train performance. In cybersecurity, these changes mean our systems can detect more attacks, and protection increases. We defined new metrics and compared our system’s performance using both previous and new metrics considering the above explanation. These new metrics are the distance to the ideal point as the error to calculate mean squares errors (MSE) and a harmonic average of the same metrics in train and test sets. Using only one of these three metrics is adequate for sorting the performance of encoders and fine-tuning hyperparameters in our proposed encoder. In addition, using these metrics avoid overfitting or underfitting problems, which will be discussed in the following sections based on our results. Equations 4, 5, and 6 express the new metrics used to estimate performance:

- Mean Square Errors (MSE) to the ideal point for **accuracy**:
  \[ MSE = 0.5[(100 - a)^2 + (100 - b)^2] \]  \( (4) \)

- Mean Square Errors (MSE) to the ideal point for **AUC**:
  \[ MSE = 0.5[(1 - a)^2 + (1 - b)^2] \]  \( (5) \)

- Harmonic average of the same metrics (**accuracy or AUC**) in train and test:
  \[ Harmonic\_avg = \frac{2.a.b}{(a + b)} \]  \( (6) \)

Where \( a \) and \( b \) in equation (4), are accuracies in percentage in train and test while in equation (5), \( a \) and \( b \) are **AUCs**, in train and test, and the harmonic averages in equation (6) defines \( a \) and \( b \) using **accuracy** or **AUCs** in train and test, respectively. The harmonic average is defined to calculate the average between train and test sets for the same metric.

III. EXPERIMENTAL RESULTS

A. Categorical Encoders Comparison

The performance of the combination of 17 different encoders, plus ours from Table III, with the ten classifiers from Table IV, was measured to compare our new proposed encoder algorithm with the other existing encoders. Table V summarizes the performance results for these 18 Encoders identified by their abbreviation names. Each column associate the encoding scheme with the best suitable classifier according to train or test for **accuracy** or **AUC**. In the fourth column, we use the maximum Harmonic average of train and test **accuracies** to compare the results and sort encoders from best to worst performance. For example, the Polynomial encoder achieved 89.9549% test **accuracy**, which was the highest that this encoder could be achieved by using GNB classifier. All the encoders were tested with all classifiers and the classifier with the highest performance is presented in the Table V. In our method, the hyperparameters Thre(1.87) and PCs(3) means 1.87 as a threshold in percentage and top three principal components, respectively. Our proposed method could achieve the highest test **accuracy** of 89.638041 percent among the others by feeding only the first principal component to the SVM2 classifier from Table IV, and with two different thresholds of 3.64 and 5.45 in percentage. This **accuracy** is the highest among all combinations of categorical encoders and classifiers tested and places our encoder on the first rank. By choosing the Harmonic average of **accuracies** as sorting metric, our method with the same hyperparameters after the Polynomial Contrast coding was placed in the second rank, as shown in Table V.

Figures 1 and 2 compare the 18 encoders, with ten different classifiers based on train versus test for **accuracies** and
Fig. 1: Scatter of train vs test sets accuracies achieved by combination of 18 category encoders.

**TABLE V:** 18 different encoders with the best classifier for each one, compared and sorted based on max harmonic average of accuracies. The amount of thresholds for our proposed method are in percentage.

| Encoding Scheme | Classifiers with Max. Train accuracy (%) | Classifiers with Max. Test accuracy (%) | Classifiers with Max. harmonic avg. of accuracies (%) | Classifiers with Max. Train AUC | Classifiers with Max. Test AUC |
|-----------------|----------------------------------------|----------------------------------------|------------------------------------------------------|-------------------------------|-------------------------------|
| Polynomial      | ADA2, 96.3167                          | GNB, 88.9549                           | ADA2, 90.0538                                        | ADA2, 0.9629                  | GNB, 0.888                    |
| Proposed        | All except GNB, Thres(1.19), PCs(1-5), 95.380756 | SVM3, Thres(1.87), PCs(3), 90.6161 | SVM3, Thres(1.87), PCs(3), 90.6161 | SVM2, Thres(3.64, 5.45), PCs(1), 0.953976 | SVM2, Thres(3.64, 5.45), PCs(1), 0.893252 |
| Ordinal         | ADA2, 96.3151                          | LR, 83.388                             | ADA2, 90.0538                                        | ADA2, 0.9629                  | LR, 0.8514                    |
| One Hot         | SVM1, 96.3127                          | DT, 83.7252                            | ADA2, 90.0538                                        | ADA2, 0.9629                  | DT, 0.8274                    |
| Sum             | MLP, 96.3143                           | ADA2, 79.5245                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | MLP, 0.9628                   |
| Target          | ADA2, 96.3167                          | ADA2, 79.5067                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| Backward Diff.  | ADA2, 96.315                           | Forest, 80.6112                        | ADA2, 90.0538                                        | ADA2, 0.9629                  | Forest, 0.8165                |
| Helment         | ADA2, 96.3127                          | Forest, 81.2145                        | ADA2, 90.0538                                        | ADA2, 0.9629                  | Forest, 0.822                 |
| Base-N          | SVM2, 96.3127                          | GNB, 83.6542                           | ADA2, 90.0538                                        | ADA2, 0.9629                  | GNB, 0.8534                   |
| Binary          | SVM2, 96.3127                          | GNB, 83.6542                           | ADA2, 90.0538                                        | ADA2, 0.9629                  | GNB, 0.8534                   |
| James-Stein     | ADA2, 96.3167                          | ADA2, 79.4979                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| Cat Boost       | ADA2, 96.3159                          | ADA2, 79.4979                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| GLMM            | ADA2, 96.3167                          | ADA2, 79.4934                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| LOOE            | ADA2, 96.3167                          | ADA2, 79.4934                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| WOE             | ADA2, 96.3151                          | ADA2, 79.4934                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| Count           | ADA2, 96.3143                          | ADA2, 79.4535                          | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| MEstimate       | ADA2, 96.3159                          | ADA2, 79.112                           | ADA2, 90.0538                                        | ADA2, 0.9629                  | ADA2, 0.808                   |
| Hash            | MLP, 91.9959                           | GNB, 77.8921                           | MLP, 0.917                                           | GNB, 0.8534                   |

Fig. 2: Scatter of train vs test sets AUC achieved by combination of 18 category encoders.

AUCs. In the figure 1, the point at [100, 100] represents the maximum train and test accuracy which is the ideal point of all encoders. Analyzing the existent encoders, the polynomial achieved the greatest train and test accuracies with the ADA2 and GNB classifiers, respectively. Our method performance achieved the highest test accuracy(89.64) with the SVM2 classifier compared with polynomial(88.95). Using the harmonic averages of accuracies as a metric, our method achieved 89.11 % during the test phase, which is still the highest test accuracy but lower than the usual metric(89.64). However, the amount of train accuracy increased from (89.5 to 92.18) and the difference between the usual metric and the harmonic averages is only 0.53% in the test set, which
we may consider irrelevant. We can conclude that the new metrics provide a better trade-off between train and test performances with these results. Figure 2 describes the results based on the \textit{AUC} metric for the same encoders and classifiers previously summarized. The ideal point is \([1.0, 1.0]\) for \textit{AUC}s train and test sets. We showed that the polynomial and our encoder performances presented nearly the same results using the new and usual metrics considering two floating points approximation for the test set. The performance for both of them was 0.89 on the test. The difference is in the train in which the polynomial reached 0.93 while our method achieved 0.92.

\textbf{B. Grid Search}

As described in the previous sections, our new proposed category encoder contains two hyperparameters: threshold and the number of principal components of PCA. We did a grid search for all of the possible combinations of these two parameters to find the best values for each one. For threshold, we checked different values from 0.01 to 50 in percentage. Categories appear in less than 1 or 5 percent of instances, usually known as rare by researchers. However, our results show a little more than five percent. The best test accuracy achieved 89.64 by choosing 5.45 or 3.64 percent as a threshold. We checked all numbers in the threshold range combined with different PC numbers varied from 1 to 6 as the second hyperparameter.

Figures. 3 and 4 depict the scatter results of \textit{accuracies} and \textit{AUC}s for train versus test sets. Table V shows more information about thresholds, PCs, and classifiers for gaining maximum values for different metrics.

\textbf{IV. CONCLUSION}

This paper proposed a new method for converting categorical features to numerical, which can be adapted with different classifiers by choosing the correct threshold and PCs. Furthermore, it produces the low dimensional outputs from high cardinality categorical variables. We used \textit{accuracy} and \textit{AUC} metric to compare performance between our method and 17 existent encoders. Additionally, we defined new metrics to estimate the trade-off between train and test set performances. Our results overcome the best encoder available for

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