

Evolutionary Neural Architecture Search for Type 2 Diabetes Mellitus Diagnosis from Salivary ATR-FTIR Spectroscopy

Lucas Mendonça Andrade¹, Robinson Sabino-Silva², Murillo Guimarães Carneiro¹

¹Faculty of Computing, Federal University of Uberlandia, Uberlandia 38408-100, Minas Gerais, Brazil

²Innovation Center in Salivary Diagnostic and Nanotheranostics, Department of Physiology, Institute of Biomedical Sciences, Federal University of Uberlandia, Uberlandia 38408-100, Minas Gerais, Brazil

lucasmendonca@ufu.br, robinsonsabino@ufu.br, mgcarneiro@ufu.br

Abstract. *The blood diagnosis of diabetes mellitus (DM) is accurate, but invasive. Attenuated Total Reflectance by Fourier Transform Infrared Spectroscopy (ATR-FTIR) is a green technology adopted in the detection of several diseases resulting in a non-invasive and accurate diagnosis. The analysis of ATR-FTIR data using deep learning techniques like Convolutional Neural Network (CNN) is promising. However, the challenges to find optimized architectures are barely explored in the ATR-FTIR literature. In this paper, we propose an Evolutionary Neural Architecture Search technique able to find optimized CNN architectures for salivary ATR-FTIR spectra for type 2 DM diagnosis using Genetic Algorithm as optimization approach.*

1. Introduction

The diabetes mellitus (DM) is a condition in which the organism is not able to specifically use the insulin it produces or cannot produce it in sufficiently quantity. This illness can cause disfunctions in several organs such as kidneys, eyes, brain and others. This endocrine disorder is a worldwide epidemic and presents a significant rate of morbidity and mortality associated both with the condition of DM and the cost associated with its management and treatment [Azhar et al. 2020].

There are two types of DM: type 1 diabetes (DM1), in which the patients are unable to produce insulin, which leads to the need for hormone replacement and the type 2 (DM2), which is more common than type 1 DM where the causes are generally associated with obesity and overweight. It is characterized by insufficient insuline production or inappropriate use of the hormone [Cho et al. 2018].

Therefore, a quick and premature diagnoses of the disease is essential to avoid serious consequences and provide a better quality of life for the patient. The convencional methods for diagnoses are: glycated haemoglobin test (HbA1C), fasting plasma glucose test (FPG) and oral glucose tolerance test (OGTT). This thecniques use blood extraction to diagnosis, which causes discomfort to the patient and, in some cases, a high economic investment, that is due to the materials and procedures necessary to carry out the tests [Care and Suppl 2021].

The attenuated total reflection Fourier-transform infrared (ATR-FTIR) spectroscopy is an alternative for a rapid diagnosis, which can facilitate treatment and consequently improve the patient's quality of life. This technique is simple, sensitive and reproducible, being able to provide an objective diagnostic prediction for diabetes [Contreras-Rozo et al. 2023], [Nogueira et al. 2022].

Infrared spectroscopy analysis characterizes molecular bonds and functional groups in solid, liquid and gaseous samples, which allows its application for several purposes, such as: identification of animal species [Zhang et al. 2024] and bioscreening tool for breast cancer [Souza et al. 2023], for example. This technique is based on the principle that light changes the fundamental frequency of vibration of the molecules and that different materials have different absorption rates in the infrared wave band. According to these changes, the spectroscopy analysis can be used for both qualitative and quantitative analysis of a material [Yang et al. 2019].

Consequently, applying ATR-FTIR to a sample obtained with minimal patient invasion such as saliva can facilitate the diagnoses of diabetes, [Caixeta et al. 2020]. In this context, some approaches [Caixeta et al. 2023], [Sánchez-Brito et al. 2021] have proposed and analysed the usage of machine learning algorithms to perform diabetes mellitus diagnosis by classifying the spectra generated by ATR-FTIR spectroscopy.

Among the machine learning methods present in the literature, deep learning techniques, especially Convolutional Neural Networks (CNN), are considered promising in this matter [Zeng et al. 2024], [Santos et al. 2023]. However, the challenges to find optimized architectures are a barely explored topic in the ATR-FTIR literature. In view of it, the paper's main contribution is to propose the use of Evolutionary Neural Architecture Search as an approach to find a Convolutional Network that efficiently performs the diagnosis based on salivary ATR-FTIR samples. To this search, the Genetic Algorithm was applied as evolutionary optimization algorithm to find the best architecture from a macro space search point of view. The study was conducted with real salivary ATR-FTIR data collected at the Clinical Hospital of the Federal University of Uberlandia. It included 68 subjects: 23 non-diabetic individuals and 45 uncontrolled type 2 DM patients.

The remainder of this paper is organized as follows. In Section 2, related works with the analysis of ATR-FTIR with machine learning is discussed. In Section 3, the problem formulation and the materials and methods applied are discussed. In Section 4, the proposed evolutionary neural architecture search is presented. In Section 5, the experimental results obtained with the proposed work and the real data are detailed and discussed. And finally, in Section 6 the conclusions of this paper are presented.

2. Related Works

The usage and comparison of different Machine Learning techniques for classifying ATR-FTIR samples is well discussed in the literature. In [Dou et al. 2023], different implementations of SVM and LDA were compared when applied to gallbladder cancer diagnosis from dried serum samples. In [Nogueira et al. 2021], a model based on partial least squares (PLS) associated with cosine KNN was implemented for COVID-19 diagnosis from swab suspension fluids. Complementing this context, the usage of Artificial Neural Networks and Convolutional Networks has proven to be good machine

learning tools associated with ATR-FTIR samples. In [Guo et al. 2023], different machine learning techniques were analyzed as a tool for diagnosing lung cancer from blood samples, where the back propagation neural network obtained better results. In [Jiang et al. 2021], a CNN was used to classify 10 different types of plastic materials, obtaining an accuracy of 87 %. In [Zeng et al. 2024], again a CNN was implemented to detect and identify microplastics obtaining better results compared to other techniques.

Regarding the study of diabetes, the use of neural networks and other machine learning techniques for diagnosing and monitoring the disease is also common in the literature. In [Caixeta et al. 2023], the usage of SVM and LDA was tested to type 2 DM diagnosis. In this scenario, the SVM got the best results and the band areas values of 2962 cm⁻¹, 1641 cm⁻¹ and 1073 cm⁻¹ where higher in type 2 DM than in non-diabetic, which importance was clear in a SHAP graph obtained. In [Sanchez-Brito et al. 2021], a comparison is made between the usage of different techniques such as SVM and ANN for DM2 diagnosis with salivary ATR-FTIR spectroscopy, in which a suggested ANN architecture obtained the best results. In [Sánchez-Brito et al. 2021], again different machine learning techniques were evaluated for diagnosis with the addition of classifying patients between low, normal and high glucose values and a precise estimation of a specific glucose value from ATR-FTIR spectroscopy.

Among the usage of Genetic Algorithm (GA) with ATR-FTIR, the most frequent application is in the preprocessing step where it is used frequently to highlight the useful and most important ATR-FTIR wavelength to facilitate the prediction or classification by a Machine Learning Algorithm. In [Asghari 2020] and in [Mohammadi 2021], this preprocess was used in a comparison between PLS and Support Vector Regression for determination of oxygenate in gasoline and for a quantitative determination of resins in oil samples, respectively. In [Zandbaaf 2022], GA was used again for wavelength selection, but with an artificial neural network to predict the breakdown voltage for transformer oils samples.

Another implementation of evolutionary algorithms in conjunction with classifiers is the usage of these tools to find the ideal neural network architecture, which is known as Evolutionary Neural Architecture Search. Inspired by the possibility of using bio-inspired algorithms for this optimization purpose and by the fact that the application of this concept is not very common in ATR-FTIR samples, this paper is intended to be a proof of concept of this kind of implementation.

3. Materials and Methods

3.1. Data Collection

The data was collected at the Clinical Hospital of the Federal University of Uberlandia (HC-UFU, Uberlandia, Minas Gerais, Brazil) after approval of the Institutional Review Board of the Federal University of Uberlandia. The inclusion criterion were: adults between 18 and 85 years old, both genders, patients from the Endocrinology Outpatient Clinic of the Hospital mentioned, diagnosed with type 2 diabetes mellitus or patients without diabetes mellitus. The study group included 68 subjects: 23 non-diabetic individuals and 45 uncontrolled type 2 diabetic patients. Figure 1 shows the mean spectrum of non-diabetic and type 2 diabetic groups. Originally, this data was obtained for the study carried out in [Caixeta et al. 2023].

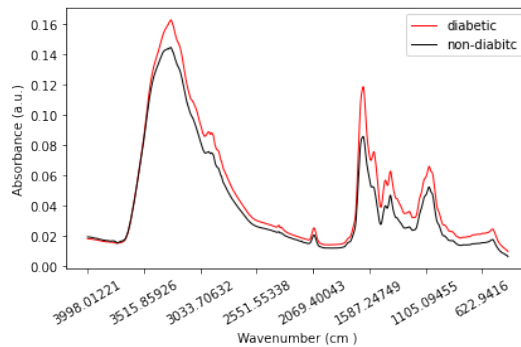


Figure 1. Representative average ATR-FTIR spectra in saliva of non-diabetic subjects and type 2 diabetes patients.

3.2. Genetic Algorithm

The Genetic Algorithm (GA) is an adaptative search method that is inspired by Charles Darwin's Theory of Evolution by natural selection, in which the individual best adapted to the environment has a greater chance of surviving compared to the less adapted. In this way, this method uses procedures and representations inspired by the process of evolution to find an approximate solution to search and optimization tasks.

In this context, the GA search space is scanned by a set of N individuals, called population. Each individual in this population is a potential solution to the problem and it is formed by a chain of genes, which are a numerical or binary representation of the parameters to be optimized in the problem.

The search and optimization process takes place through successive evolutions applied to the population, in which only individuals who present the best results, known as Fitness, are maintained. Generally, a convergence parameter is defined, which can be, for example, a number G of generations, to define the result, which in this case, is represented by the best individual of the last generation.

The process of evolution consists of 4 stages: selection, crossover, mutation and reinsertion. In the selection, pairs of individuals which will participate in the evolution process and generate new individuals for the search are selected.

In crossover, each pair of individuals goes through a gene exchange process, thus generating two new individuals. After the generation of new potential solutions, the mutation process occurs, which aims to further diversity the new individuals generated. Generally, in this process, some of the new individuals are selected to undergo random changes in their genes.

After the process of mutation, the reinsertion occurs, in which the new individuals become part of the population of the new generation or not. Initially, the fitness of these individuals is calculated, and a rule is applied to define which N individuals, based on their fitness, will be part of the new generation. For example, in ordered reinsertion, the new population is composed of the N individuals with the best fitness between the newly generated ones and the last generation's ones. Finally, the gene of the best individual in the last generation is decoded, thus generating a solution to the applied problem.

3.3. Neural Architecture Search (NAS)

Generally, the process of finding the ideal design for an artificial neural network is a laborious, often time-consuming task that depends on the expertise of the executor. In view of this, the goal of NAS is to automate the process of finding the ideal design formulating this task as an optimization problem.

According to [Elsken et al. 2019], a standard NAS pipeline involves three main components: the search space, which defines how the architecture is represented, the optimization algorithm that is responsible for generating architectures suitable for the problem with pre-established criteria and an evaluator to estimate performance between the different architectures tested.

The NAS application is divided into two types of search space: micro and macro space search. In micro space search, the objective is to obtain a computational module, known as cell, which is repeatedly stacked to form the network architecture following a prerequisite model. In turn, the macro space search consists of designing the skeleton of the network, maintaining the layers with pre-established designs, changing only the number of layers and the number of their channels and neurons, for example.

From an optimization point of view, NAS is intrinsically a multi-objective optimization problem, which makes the application of multi-objective evolutionary optimization reasonable [Cheng et al. 2022]. Therefore, the application of GA to this problem becomes trivial [Wen et al. 2022], [Garcia-Garcia et al. 2023].

4. GA Neural Architecture For ATR-FTIR Spectra Analysis

For the problem of diagnosing diabetes, a macro space search application was selected. In this context, the aim is to optimize the number of channels in the convolutional layers, the number of fully connected layers, in addition to the number of neurons that make up each layer, the dropout rate applied in the dropout layers and the learning rate.

Essentially, the base architecture to be optimized is represented in Figure 2, which is composed of two convolutional layers with kernel size equal to 5×5 and stride equals to 1, each of which is followed by a max pooling layer with kernel size equal to 2×2 and stride of 2. The fully-connected part can be composed of up to 3 layers, each layer being followed by a dropout layer. In the end of the architecture, the last layer is composed of a single neuron, which returns the classification result.

Figure 3 presents the chromosome representation of the GA proposed for CNN architecture search. A population of 100 individuals was defined, in which each individual is composed of 10 genes with 3-digit binary values, that is, with a range from 000 to 111. The first two genes (CL1 and CL2) represent the number of channels of the two convolutional layers. From gene 3 to 8, the neuron numbers of each fully-connected layer are defined interspersed with the dropout rate value of the dropout layer. In gene 9, the learning rate is represented and in gene 10, the number of fully-connected layers implemented in the architecture is defined.

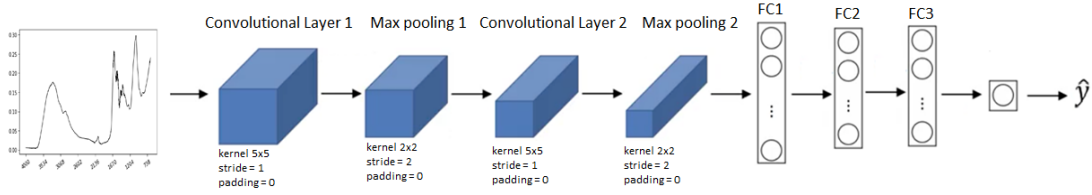


Figure 2. Base architecture defined for the Evolutionary NAS.

Gene representation	CL ₁	CL ₂	FC ₁	D ₁	FC ₂	D ₂	FC ₃	D ₃	LR	ARCH
Value	CL ₁ ∈ [000,111]	CL ₂ ∈ [000,111]	FC ₁ ∈ [000,111]	D ₁ ∈ [000,111]	FC ₂ ∈ [000,111]	D ₂ ∈ [000,111]	FC ₃ ∈ [000,111]	D ₃ ∈ [000,111]	LR ∈ [000,111]	ARCH ∈ [000,111]

Figure 3. Chromosome representation of the Genetic Algorithm applied.

To convert the gene value to the network parameters, initially they were transformed integers and then applied to the following relations. The numbers after the gene represent the position in the chromosome representation:

- Number of channels: $CL_1 = 2^{gene_1}$
- Number of channels: $CL_2 = 2^{gene_2}$
- Neurons number: $FC_{1,2,3} = 2^{(gene_{j+3})}$, with $j \in \{3, 5, 7\}$
- Dropout rate: $DL_{1,2,3} = 0,03(gene_j)$, with $j \in \{4, 6, 8\}$
- Learning rate: $LR = 10^{-gene_9}$
- Fully-connected configuration:
 - $gene_{10} = 1$ or 2 or 3 : 1 fully-connected layer
 - $gene_{10} = 3$ or 4 or 5 : 2 fully-connected layers
 - $gene_{10} = 6$ or 7 : 3 fully-connected layers

In all fully connected layers configurations, the layer is followed by a dropout layer with dropout rate set by the next gene on the chromosome. Figure 4 presents the main steps of the GA developed to optimize the CNN architecture. The overall technique can be understood in terms of the following steps:

Evaluate Population/new individuals. To evaluate the different models generated by the Genetic Algorithm, cross-validation with 4 folds was used. To train each model, balanced accuracy was used as the metric in a 5-epoch training. The fitness metric defined was the area under the ROC curve, which defines the quality of a classifier by how close this area is to 1. Furthermore, a penalty of 30% of the fitness value was applied if the individual presented an increasing number of neurons in two consecutive fully connected layers. The population size was defined as 100 individuals and the convergence parameter was defined as 50 generations.

Selection. Roulette with 30 pairs per generation was considered here. This method uses the individual fitness percentage value in relation to the sum of the fitness of the entire population. A number is drawn and the individual who occupies that range in the interval is selected. Therefore, the higher the fitness, the greater the probability of

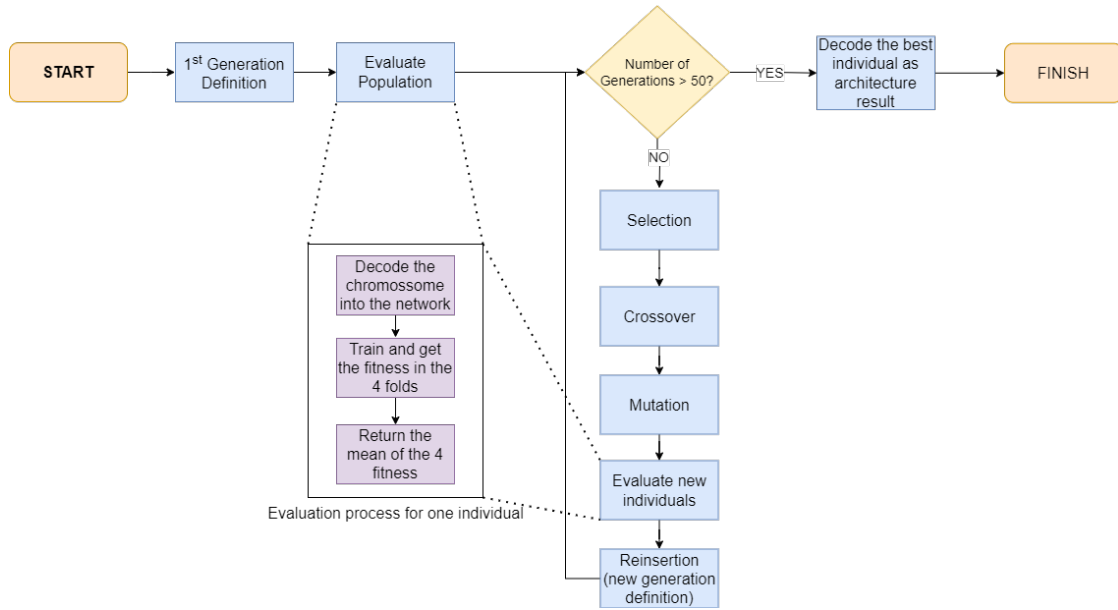


Figure 4. Search process fluxogram.

selection. As there are 30 pairs, 60 individuals are drawn, with the possibility of repetition, to generate the groups.

Crossover. The method used was the simple crossover, in which a random cutoff point is defined for each pair of selected individuals. Each individual in the pair generates a new one that is composed of its genes up to the cut point and the genes of the other individual in the pair in the rest of the chromosome.

Mutation. The mutation was carried out in 10 individuals chosen at random from the 60 generated ones in the crossover. For implementation, one bit was selected from the 30 that make up the chromosome to be replaced by its complement.

Reinsertion. Ordered reinsertion was used to define the individuals from subsequent generations.

5. Experimental Results

To evaluate the implementation of the proposed GA for CNN architecture search, the original 68 ATR-FTIR spectra dataset was divided into a training set with 51 instances and a test set to validate the architecture with 17 instances defined randomly.

The best solution obtained by GA was implemented according to the CNN architecture search step, however 200 epochs were used to fit the final CNN model instead of 5 in the training set. The GA was also executed 3 times to better evaluate the proposed encoding. The metrics used in the evaluation on the test set were balanced accuracy, macro F1 score, recall, precision, specificity and the area under the curve.

5.1. Architectures, Hyperparameters and Predictive Performance

Table 1 shows the architectures and hyperparameters found by our technique over each one of the three executions, and Table 2 presents the predictive results obtained by each one of those configurations on the test set. For example, in first execution, GA obtained

a CNN with 2 and 64 neurons respectively at first and second convolutional layers, and two fully connected layers with 128 and 16 neurons, with 0 and 0.21 of dropout rate, respectively. Such a configuration achieved a balanced accuracy of 0.83 and macro F1 of 0.86.

As one can see, all the configurations obtained by GA presented good values for most measures. The recall (a.k.a sensitivity) values for the three models are very high, which indicates that the positive class classification is generally good. In other words, the correct diagnosis of a patient with diabetes is well performed by the models. The value of 1 indicates that the first and the second design made the correct diagnosis for all the patients with diabetes.

In general, although the three configurations obtained by our technique presented competitive performance in terms of GA fitness (close to 0.7), the first configuration presented the best results compared to the others. The second and third configurations presented difficulty in the classification of the non-diabetic patients. In relation to the architectural parameters, the difference of the first model is the convolutional layers. It has more filters, which proved to be fundamental for the classification of the minority class of the dataset, resulting in a better specificity.

5.2. Interpretability Analysis

To complement the performance of the first model the Shapley Additive Explanations (SHAP) was obtained. The SHAP is an approach that calculates the contribution of each

Table 1. Genetic Algorithm's Design results

EXECUTION NUMBER	CL ₁	CL ₂	FC ₁	D ₁	FC ₂	D ₂	FC ₃	D ₃	LR
1	2	64	128	0	16	0.21	0	0	0.0001
2	4	32	16	0	16	0.03	32	0.12	0.001
3	2	32	128	0.18	0	0	0	0	0.001

Table 2. Network's performance

EXECUTION NUMBER	BALANCED ACCURACY	MACRO F1 SCORE	RECALL	PRECISION	AREA UNDER THE CURVE	SPECIFICITY	GA'S FITNESS
1	0.83	0.86	1	0.85	0.91	0.67	0.73
2	0.75	0.77	1	0.80	0.83	0.5	0.7
3	0.70	0.72	0.91	0.77	0.76	0.5	0.71

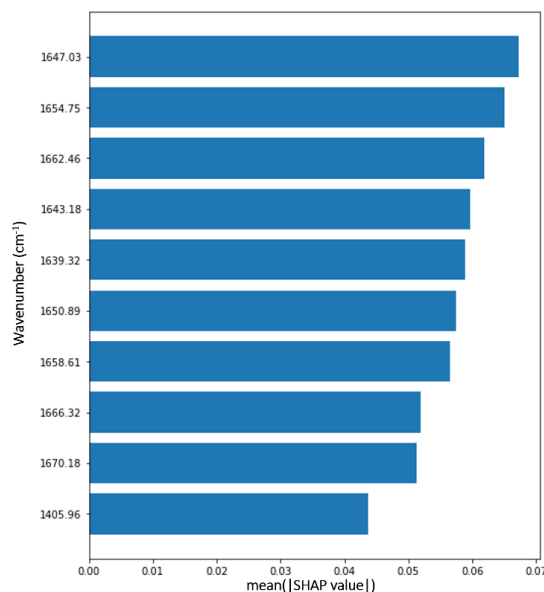


Figure 5. Feature importance (SHAP value) graph for the first design.

feature to the target value [Akulich et al. 2022]. This SHAP value obtained for each feature helps to understand which bands in ATR-FTIR are the most important to discriminate non-diabetic individuals and type 2 diabetic patients. The SHAP feature importance is presented in Figure 5, which indicates the main vibrational modes responsible for the detection of type 2 diabetic patients. Most of these modes indicates that proteins have contributed in the detection of diabetic and non-diabetic individuals.

6. Conclusion

Early diabetes diagnosis can reduce complications of the disease through treatment. With progress in the application of portable ATR-FTIR devices [Butler et al. 2019], the development of non-invasive methods for diagnosis as well as monitoring has great potential to be applied at any place, which can be help for disease prevention and control.

The present study seeks to contribute to the application of ATR-FTIR devices in medical environments, providing a more accurate, non-invasive and low-cost DM diagnostic. In this context, different works have applied the concepts of machine learning with these spectroscopic signals to be able to recognize diabetes. In the case of using CNNs, the results are directly influenced by their architecture and the chosen hyperparameters, which definition is not a trivial task. In this paper the concept of Evolutionary Neural Architecture Search was applied using a GA to automate the definition of the architecture and hyperparameters without the need for deeper knowledge of the data and neural network architecture design to obtain good results.

With the GA encode defined in this paper, a convolutional network architecture was obtained that presented a balanced accuracy of 0.83, macro F1 score of 0.86 and specificity of 0.67. Therefore, it was possible to obtain a good convolutional network model applied to the diagnosis of diabetes through salivary ATR-FTIR spectroscopy without the need for pre-processing, specific modifications to the original samples and

in-depth knowledge on the subject. As future works, the improvement of the NAS strategy in order to achieve even better predictive performance can be done.

Acknowledgment

Authors thank the financial support given the Brazilian National Council for Scientific and Technological Development - CNPq (grants n. 420212/2023-0), the Minas Gerais Research Foundation – FAPEMIG (grant n. APQ-00410-21), the INCT in Theranostics and Nanobiotechnology (grant n. CNPq-465669/2014-0), and the INCT in Oral Health and Odontology (grant n. CNPq-406840/2022-9). We also thank NVIDIA Corporation by the donation of a Titan V GPU used in this research.

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