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A Kernel k -Means-based Method for Diabetes Diagnosis

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Abstract: Diabetes diagnosis is important due to the death and complication consequences caused by the disease. It thus has attracted much research attention and effort in Artificial Intelligence to support human decisions. Our work proposes a kernel k -means-based predictive method and explores attribute selections for effective and robust diabetes diagnosis. This method uses homogeneous subclusters in the high dimensional kernelized feature space to compute the distance of a new instance to those subclusters and classify it accordingly. The PIMA and MIMIC data sets are respectively used for training and testing. Our experimental results could identify the best effective attribute groups and show that the proposed method outperforms existing ones for the task.

Keywords: *Disease diagnosis, feature selection, clustering, PIMA data set, MIMIC database*

1. INTRODUCTION

As reported in [20], diabetes is considered to be the seventh leading cause of death in 2030. It has risen from 108 million diabetic people in 1980 to 422 million ones in 2014. It is also a major cause of blindness, kidney failure, heart attacks, stroke, and lower limb amputation.

Diabetes diagnosis is thus important and has attracted much research effort in Artificial Intelligence to support doctors' decisions, as recently surveyed in [4]. In particular, machine learning methods were proposed, such as decision trees [6, 19], k -nearest neighbors [1], logistic regression [10, 14], neural networks [3, 5, 6, 7, 10, 11, 17], and support vector machines [12, 15]. In [2], electronic medical records were exploited for personalized diabetes management.

Besides prediction, [6, 8, 16] provided interpretable rules for decision making support in the disease diagnosis. Also, most of the above-mentioned works combined machine learning with other methods for data preprocessing such as genetic method [3], self-organizing maps [11], k -means [12], fuzzy c -means [16], random forests [14], and principal component analysis [11, 19].

Consequently, there were many different groups of attributes (i.e., feature) used for diabetes diagnosis as a machine learning task. However, to the best of our knowledge, there has been no extensive examination of attribute groups to identify the most effective ones for prediction. Meanwhile, doctors have relied on their medical knowledge to examine a patient's clinical and

paraclinical information to diagnose diabetes.

In this paper, we propose a novel method and explore various attribute groups for diabetes diagnosis. Our method is a kernel k -means-based one that classifies a new instance, i.e., as positive or negative, depending on its distances to the homogeneous subclusters obtained from a training dataset in a high dimensional kernelized feature space. We use the PIMA dataset [17] for training our model and diabetes cases from the MIMIC database [9] for testing it in comparison to some existing ones.

Next, Section 2 formulates the diabetes diagnosis problem and presents our proposed method. Section 3 presents our experiments evaluating the effectiveness of different attribute groups and the performance of the proposed method. Finally, Section 4 gives some concluding remarks.

2. THE PROPOSED METHOD

2.1 Problem definition

Given the information of a person, the problem is to predict if the person potentially has diabetes. The information includes his/her lab test results, current and past personal diseases, medication history, and family medical history. The prediction is binary, i.e., 1 if positive with diabetes, or 0 if negative.

2.2 Attribute groups

We summarize and name the attribute groups used in the corresponding works based on the attributes in the

PIMA data set, as presented in Table 1 below. The description of each attribute can be found in [17].

Group 8 was originally proposed for diabetes diagnosis in [17]. Group 2 in [6] was found in the extracted rules. Group 3_1 in [14] contained the top ranked attributes. Group 6_2 in [1] was the best case among several selected groups. Especially, Group 5 is what doctors rely on to diagnose diabetes, as provided in the decision support medical information visualization system [13].

Table 1: Different attribute groups in the existing works

Related Work	Named Group	Number of Attributes	Attributes
[6]	2	2	Glucose, BMI
[14]	3_1	3	Glucose, Insulin, BMI
[15]	3_2	3	Pregnancies, Glucose, Age
[3]	4	4	Glucose, Insulin, BMI, Age
[13]	5	5	Glucose, BloodPressure, Insulin, BMI, Age
[12]	6_1	6	Pregnancies, Glucose, Insulin, BMI, DiabetesPedigreeFunction, Age
[1]	6_2	6	Pregnancies, Glucose, BloodPressure, Insulin, BMI, DiabetesPedigreeFunction
[17]	8	8	Pregnancies, Glucose, BloodPressure, SkinThickness, Insulin, BMI, DiabetesPedigreeFunction, Age

3.2 The proposed kernel k -means-based method

Firstly, diabetes shares some symptoms and has common medical attribute values with some other diseases. This leads to data overlapping for diabetic people and non-diabetic people, as shown in [11] via visualization. Therefore, we propose to use a kernel to map the original diabetes data space to a higher dimensional one, so that instances can be more discriminated.

Secondly, in medical research, the k -nearest neighbor method has recently been used for personalized diabetes management in [2]. However, if k is small, this method is ineffective with noises and, if k is large, it causes class heterogeneity of the k returned nearest neighbors. To overcome it, in this work we propose to use the 1-nearest neighbor method at the prediction step but on the derived homogeneous subclusters, rather than on the main clusters obtained from the training step using kernel k -means [18].

Details of our proposed method for diabetes prediction are as follows:

Input:

- D_t is a training set of instances X_i with classes y_i ,
- D_u is a set of new instances X_j ,
- k is a predefined number of clusters,
- σ is a bandwidth of the Gaussian kernel function.

Output:

- Predicted class y_j of X_j for every $X_j \in D_u$.

Process:

Step 1: Construct a clustering model in the feature space of the training data

- 1.1. Compute a kernel matrix KM from the instances in D_t :

$$KM(X_r, X_q) = K_{rq} = e^{-\frac{\|X_r - X_q\|^2}{2\sigma^2}}$$

$$\text{where } \|X_r - X_q\| = \sqrt{\sum_{d=1..p} (x_{rd} - x_{qd})^2}$$

for $r=1..n_t$ and $q=1..n_t$

- 1.2. Establish a membership matrix γ between k clusters C_o and n_t instances X_i in D_t , for $o=1..k$, $i=1..n_t$. Each cell in γ is 1 if X_i belongs to C_o ; or 0, otherwise. This matrix is initialized with the traditional k -means method on D_t .

- 1.3. Repeat the following substeps until the membership matrix γ is unchanged:

- 1.3.1. Update the distance between each cluster C_o and each instance X_r in D_t in the feature space as follows:

$$\| \phi(X_r) - C_o \|^2 = K_{rr} - \frac{2 \sum_{q=1..n_t} \gamma_{oq} K_{rq}}{\sum_{q=1..n_t} \gamma_{oq}} + \frac{\sum_{v=1..n_t} \sum_{z=1..n_t} \gamma_{ov} \gamma_{oz} K_{vz}}{\sum_{v=1..n_t} \sum_{z=1..n_t} \gamma_{ov} \gamma_{oz}}$$

for $o=1..k$ and $r=1..n_t$

- 1.3.2. Update the membership γ_{or} between the instance X_r and the cluster C_o as follows:

$$\gamma_{or} = \begin{cases} 1, & \text{if } \| \phi(X_r) - C_o \|^2 = \argmin_{o'=1..k} (\| \phi(X_r) - C_{o'} \|^2) \\ 0, & \text{otherwise} \end{cases}$$

for $r=1..n_t$ and $o=1..k$

Step 2: Construct a predictive model

- 2.1. Derive homogeneous subclusters $HC_{o'}$ from the main clusters C_o in Step 1 for $o'=1..k*|Y|$, $o=1..k$

A homogeneous subcluster $HC_{o'}$ is defined as a smaller group of the instances in C_o that belong to the same class in Y . For each main cluster C_o , the maximum number of homogeneous subclusters $HC_{o'}$ is $|Y|$ when only one instance in C_o belongs to each class in Y . The minimum number is 1 when all of the instances in C_o belong to the same class.

- 2.2. Assign the common class $y_{o'}$ of all of the instances in a homogeneous subcluster $HC_{o'}$ to that homogeneous subcluster $HC_{o'}$ for $o' = 1..k*|Y|$

Step 3: Predict a class y_j of a new instance X_j for every $X_j \in D_u$

- 3.1. Calculate the kernel-induced Euclidean distance between X_j and each homogeneous subcluster $HC_{o'}$ via its mean vector:

$$distance(X_j, HC_o) = 2 - 2 * K(X_j, HC_o)$$

where $K()$ is the Gaussian kernel function, $j=1..n_u$,
 $o'=1..k*|Y|$.

- 3.2. Based on the smallest distance in the previous substep, assign the class $y_{o'}$ of the nearest homogeneous subcluster $HC_{o'}$ to the new instance X_j for prediction, i.e., $y_j = y_{o'}$.

4. EVALUATION

The evaluation of our proposed method is to answer the following questions:

Question 1: Given a data set and a method, which attribute group is more effective for diabetes diagnosis?

Question 2: Given a data set and an attribute group, which method is more effective for diabetes diagnosis?

Question 3: Given a data set, which method is more robust to missing values of attributes of instances?

The effectiveness is measured by the Accuracy, Recall, Precision, and F measures. In this context, Accuracy is the percentage of correctly predicted people to be either positive or negative with diabetes. Recall is the percentage of all true diabetic patients that are predicted. Meanwhile, Precision is the percentage of positively predicted people who are truly diabetic patients.

The robustness is addressed because, without preprocessing, there are many instances in the training and testing data sets that miss some attribute values. Table 2 presents the details of the two data sets PIMA and MIMIC that we use for training and testing, respectively.

We compare the proposed method with the following typical baseline methods: k -nearest neighbors (k -NN) [1], logistic regression (LR) [10, 14], neural networks (NN) [3, 5, 6, 7, 10, 11, 17], and support vector machines (SVM) [12, 15].

Table 2: Data descriptions for training and testing

Data set	Role	Number of Instances	Percentage of Positives	Percentage of Negatives	Percentage of Missing Values
PIMA	Training	768	34.9%	65.1%	12.1%
MIMIC	Testing	180	38.9%	61.1%	15.4%

For parameter settings, we use k in $\{1, 3, 5\}$ for k -NN; feedforward multiplayer perceptrons with the default network configuration, learning rate = 0.01, and training time = 1,000 epochs for NN; the radial basis function as a kernel with $gamma = 0.01$ and $C = 50$ for SVM. As for the

proposed kernel k -means-based method (KK), we use the Gaussian kernel function with the $sigma$ computed from the attribute variances in $\{0.1, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02, 0.01, 0.009, 0.008, 0.007, 0.006, 0.005, 0.004, 0.003, 0.002, 0.001, 0.0009, 0.0008, 0.0007, 0.0006, 0.0005, 0.0004, 0.0003, 0.0002, 0.0001\}$ and k in $\{2, 4, 6, 8, 10, 12, 14\}$. The grid search scheme was used.

For the results, Accuracy is presented in percent (%) in the range $[0, 100]$, while Recall, Precision, and F-measure are shown in the range $[0, 1]$. For Question 1, Table 3 and Table 4 respectively show the attribute group that gives a certain method the highest Accuracy or the highest F-measure. For each method and each attribute group, the highest measures are obtained with the best tuned parameters. In both cases, our proposed method has the best performance, with attribute group 3_1.

Table 3: The highest Accuracy for each method

Method	Attribute Group	Accuracy	Recall	Precision	F-measure
KK	3_1	92.78	0.81	1.00	0.90
k -NN	2	67.78	0.40	0.64	0.49
LR	2	69.44	0.46	0.65	0.54
NN	6_1	71.11	0.41	0.73	0.53
SVM	6_1	69.44	0.44	0.66	0.53
SVM	8	69.44	0.46	0.65	0.54

Table 4: The highest F-measure for each method

Method	Attribute Group	Accuracy	Recall	Precision	F-measure
KK	3_1	92.78	0.81	1.00	0.90
k -NN	3_2	60.00	0.56	0.49	0.52
LR	5	63.89	0.56	0.53	0.55
NN	3_1	67.78	0.49	0.61	0.54
SVM	5	62.22	0.59	0.51	0.55

For Question 2, Tables 5-7 respectively present the highest Accuracy, Recall, and F-measure of each method for each attribute group. For each measure, the highest values are obtained with the best tuned parameters. It shows that our proposed method outperforms all of the compared ones on every measure and every attribute group.

Note that group 3_1 consists of only three attributes, namely, Glucose, Insulin, and BMI. However, for our proposed method, it gives the same Recall as, but better Accuracy and F-measure than any other group, including group 8 (with 8 attributes) that doctors have used for diabetes diagnosis. For the other methods, it also give better results than, or comparable to, the other attribute groups. That is, machines can support doctors to have simpler but more accurate diagnosis.

Table 5: The highest Accuracy of each method for each attribute group

Attribute Group	KK	k-NN	LR	NN	SVM
2	77.78	67.78	69.44	68.33	68.33
3_1	92.78	67.22	68.33	67.78	67.78
3_2	63.89	60	63.33	60	62.22
4	91.67	65.56	66.67	67.78	64.44
5	88.33	66.67	63.89	66.67	62.22
6_1	79.44	62.78	68.89	71.11	69.44
6_2	75.56	60.56	67.22	68.89	68.89
8	74.44	63.89	67.78	70.56	69.44

Table 6: The highest Recall of each method for each attribute group

Attribute Group	KK	k-NN	LR	NN	SVM
2	1.00	0.40	0.46	0.47	0.49
3_1	1.00	0.39	0.46	0.49	0.49
3_2	1.00	0.59	0.54	0.57	0.51
4	1.00	0.34	0.51	0.44	0.54
5	1.00	0.34	0.56	0.47	0.59
6_1	1.00	0.14	0.41	0.41	0.44
6_2	1.00	0.13	0.39	0.43	0.43
8	1.00	0.30	0.44	0.41	0.46

Table 7: The highest F-measure of each method for each attribute group

Attribute Group	KK	k-NN	LR	NN	SVM
2	0.78	0.49	0.54	0.54	0.54
3_1	0.90	0.48	0.53	0.54	0.54
3_2	0.60	0.52	0.54	0.53	0.51
4	0.88	0.44	0.55	0.52	0.54
5	0.84	0.44	0.55	0.52	0.55
6_1	0.76	0.22	0.51	0.53	0.53
6_2	0.73	0.19	0.48	0.52	0.52
8	0.68	0.39	0.52	0.52	0.54

Table 8 and Table 9 focus on the proposed method. For each attribute group, Table 8 presents the corresponding Recall, Precision, and F-measure of the proposed method when it achieves the highest Accuracy. Meanwhile, Table 9 presents the corresponding Accuracy, Recall, and Precision of the proposed method when it achieves the highest F-measure. The results show that the proposed method has the highest values for the Accuracy at the same time as for the F-measure. Also, they are with groups 3_1, 4, and 5, which consist of only 3 to 5 attributes.

For Question 3, although there are respectively 12.1% and 15.4% of missing attribute values in the PIMA and MIMIC data sets, our proposed method still achieves high Accuracy and F-measure as compared to the baseline ones. This proves its robustness to such noises in the data.

Table 8: The Recall, Precision, and F-measure corresponding to the highest Accuracy of the proposed method for each attribute group

Attribute Group	Accuracy	Recall	Precision	F-measure
2	77.78	1.00	0.64	0.78
3_1	92.78	0.81	1.00	0.90
3_2	63.89	0.60	0.54	0.56
4	91.67	0.79	1.00	0.88
5	88.33	0.81	0.88	0.84
6_1	79.44	0.80	0.71	0.75
6_2	75.56	0.86	0.64	0.73
8	74.44	0.60	0.70	0.65

Table 9: The Accuracy, Recall, Precision corresponding to the highest F-measure of the proposed method for each attribute group

Attribute Group	Accuracy	Recall	Precision	F-measure
2	77.78	1.00	0.64	0.78
3_1	92.78	0.81	1.00	0.90
3_2	58.89	0.79	0.48	0.60
4	91.67	0.79	1.00	0.88
5	88.33	0.81	0.88	0.84
6_1	76.67	0.94	0.63	0.76
6_2	75.56	0.86	0.64	0.73
8	71.67	0.76	0.61	0.68

5. CONCLUSIONS

In this paper, diabetes diagnosis has been studied as a binary classification task with our new proposed method. The method generates the clusters of similar instances in a high dimensional feature space using the Gaussian kernel function. Homogeneous subclusters are derived from the main clusters. A new instance is then predicted to belong to the class of the instances in its nearest subcluster.

Besides, our work has also conducted the experiments with several attribute groups used the related works and one used by medical doctors in practice. A new diabetes data set from the MIMIC database has been built as a testing data set for evaluating these attribute groups and the compared methods. The results have showed that the proposed method outperforms the others on every attribute group, and that the group of 3 attributes Glucose, Insulin, and BMI are sufficient for diabetes diagnosis.

For future work, a parameter-free version of the proposed method is considered for its stability and friendliness in practical use. Enhancing a medical information visualization system with the findings of this work is also of our interest. Such an enhancement is helpful for bridging a gap between human experts and computer systems in disease diagnosis.

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