

# Multivariate Outlier Removing for the Risk Prediction of Gas Leakage based Methane Gas

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## 메탄 가스 기반 가스 누출 위험 예측을 위한 다변량 특이치 제거

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**Abstract** In this study, the relationship between natural gas (NG) data and gas-related environmental elements was performed using machine learning algorithms to predict the level of gas leakage risk without directly measuring gas leakage data. The study was based on open data provided by the server using the IoT-based remote control Picarro gas sensor specification. The natural gas leaks into the air, it is a big problem for air pollution, environment and the health. The proposed method is multivariate outlier removing method based Random Forest (RF) classification for predicting risk of NG leak. After, unsupervised k-means clustering, the experimental dataset has done imbalanced data. Therefore, we focusing our proposed models can predict medium and high risk so best. In this case, we compared the receiver operating characteristic (ROC) curve, accuracy, area under the ROC curve (AUC), and mean standard error (MSE) for each classification model. As a result of our experiments, the evaluation measurements include accuracy, area under the ROC curve (AUC), and MSE; 99.71%, 99.57%, and 0.0016 for MOL\_RF respectively.

**Key Words** : Natural, Gas, Leak prediction, Random Forest, Multivariate Outlier Detection, LN transform

**요약** 본 연구에서는, 천연가스(NG) 데이터와 가스 관련 환경 요소 간의 관계를 기계학습 알고리즘을 사용하여 가스 누출 데이터를 직접 측정하지 않고 가스 누출 위험 수준을 예측하였다. 이번 연구는 서버가 제공하는 오픈 데이터인 IoT 기반 원격 제어 피카로(Picarro) 가스 센서 사양을 기반으로 사용했다. 천연 가스는 공기 중으로 누출이 되며, 대기 오염, 환경, 그리고 건강에 큰 문제가 된다. 본 연구에서 제안하는 방법은 천연 가스의 누출 위험 예측을 위한 랜덤 포레스트(Random Forest) 분류 기반 다변량 특이치 제거 방법이다. 비지도 k-평균 클러스터링 후에 실험 데이터 집합은 불균형 데이터이다. 따라서 우리는 제안된 모델이 중간과 높은 위험 수준을 가장 잘 예측할 수 있다는 점에 초점을 맞춘다. 이 경우 각 분류 모델에 대한 수신자 조작 특성(ROC) 곡선, 정확도, 평균 표준 오차(MSE)를 비교했다. 실험 결과로 정확도, 수신자 조작 특성의 곡선 아래 영역(AUC, Area Under the ROC Curve), MSE가 각각 MOL\_RF의 경우 99.71%, 99.57%, 및 0.0016의 결과 값을 얻었다.

**주제어** : 천연 가스, 누출 예측, 랜덤 포레스트, 다변량 특이치 검출, LN 변환

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## 1. Introduction

A gas leak has had a serious impression on environmental pollution and health. Therefore, it is important to predict the level of risk related to gas leakage. Recent studies aim to predict leakage of natural gas and beware of such potential accidents in advance.

The researchers have studied a pilot project of this mapping to explore the first step in gaining a better understanding of the effects of NG leaks in [1,2]. NG mass was measured using a Picarro CH<sub>4</sub> sensor specification and a Google Street View machine in [3]. It is a gas sensor, fire-resistant, wired, and wireless transmitter that can be used in high-sensitivity facilities. In addition, this vehicle is an IoT-based remote monitoring system, a dual-antenna diagnostic solution used for real-time data aggregation analysis [4-7]. Further, we present a list of environmental and gas features raw data properties of NG found in mobile device-based methane gas studies from [15]. When NG is released into the air, it creates huge problems for the climate and the environment. The order of fluctuations in the sensitivity of the device used to measure the CH<sub>4</sub> level was higher. The related work of this study is [8], there, used OrdinalEncoder (OE) normalization for the target feature of CH<sub>4</sub> (g min). Then k-means clustering to the labeling of CH<sub>4</sub> for the data pre-processing part. The flow rate of the CH<sub>4</sub> leak is referred to in [1,2]. In recent years, a machine-based approach to environmental engineering has been widely used to predict natural gas leaks [4, 9]. They used factor analysis to reduce the size of the high-dimensional variables and to obtain the optical properties of the cluster analysis [10,11].

Standard, machine-learning techniques are divided into three categories as supervised, semi-supervised, and unsupervised. The data we use is unsupervised data without a label. The

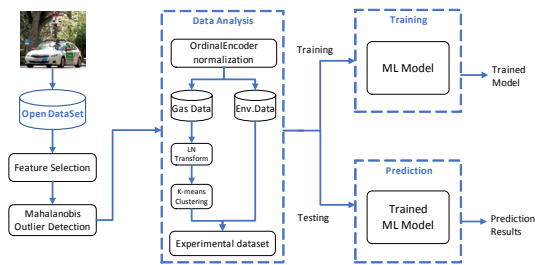
purpose of this study was to compare the KNN, DT, RF, NB, and MLP [10, 12,13] classification techniques for feature selection using factor analysis (FA) and OE normalization for risk prediction of NG' leaks. The model is evaluated on the accuracy, mean squared error (MSE), AUC, and receiver operating characteristic curve (ROC). The main contributions of this research are, we propose the multivariate outlier removing Mahalanobis distance [13, 14] and OE based ML method to predict NG leakage risk detection in the open data by the unsupervised mode. In addition, after we performed a natural logarithmic (Ln) transformation, the overall content distribution pattern of the original data did not change significantly until the k-mean cluster analysis was performed. Therefore, our method is suitable for the early prediction of NG leaks in the air.

Therefore, in this study, based on the relationship between the gas data and the environmental elements assume by the gas were identified in order to predict the level of gas leakage risk without directly measuring the gas leak data.

## 2. Methodology

In this paper, we used Picarro's vehicle-based methane gas open data. Initially, we cleaned data for null and constant values row and column data. In this case, we selected 17 features from 33 features [18]. Fig. 1 shown the general system architecture of the proposed method. In this method, initially, we cleaning data by null and constant variables row and column and selected features. Behind feature selection, we removed outliers using multivariate outlier detecting Mahalanobis distance method. After outlier eliminating, we normalized data by the OrdinalEncoder technique [8]. As well, we divided data into two parts with the Gas and

Environment dataset. In the gas dataset, we converted by Ln transform. Furthermore, we using unsupervised k-means clustering algorithms for labeling into CH<sub>4</sub> gas data. After labeling, we combined both data gas and environment by the labeled dataset. In this labeled dataset we make train machine learning models for predictive analysis. After the train, we had test predictive and evaluating models by accuracy measurement.



**Fig. 1. The general system architecture of the proposed method**

## 2.1 Mahalanobis Outlier Detection

Multivariate outliers can be identified with the use of Mahalanobis distance, which is the distance of a data point from the calculated centroid of the other cases where the centroid is calculated as the intersection of the mean of the variables being assessed. Each point is recognized as an X, Y combination and multivariate outliers lie a given distance from the other cases. The distances are interpreted using a  $p < 0.001$  and the corresponding  $\chi^2$  value with the degrees of freedom equal to the number of variables. Multivariate outliers can also be recognized using leverage, discrepancy, and influence. Leverage is related to Mahalanobis distance but is measured on a different scale so that the  $\chi^2$  distribution does not apply. Large scores indicate the case if further out however may still lie on the same line. Discrepancy assesses the extent that the case is in line with the other cases. Influence is determined by leverage and discrepancy and assesses changes in

coefficients when cases are removed. Cases  $> 1.00$  are likely to be considered the outliers.

It was introduced by Prof. P. C. Mahalanobis in 1936 and has been used in various statistical applications ever since. However, it's not so well known or used in the machine learning practice.

1. It transforms the columns into uncorrelated variables
2. Scale the columns to make their variance equal to 1
3. Finally, it calculates the Euclidean distance.

The formula to compute Mahalanobis distance is as follows:

$$D^2 = (x - m)^T C^{-1} (x - m) \quad (1)$$

where,  $D^2$  is the square of the Mahalanobis distance,  $x$  is the vector of the observation (row in a dataset),  $m$  is the vector of mean values of independent variables (mean of each column),  $C^{-1}$  is the inverse covariance matrix of independent variables and  $(x - m)$  is essentially the distance of the vector from the mean, then divide this by the covariance matrix (or multiply by the inverse of the covariance matrix).

P value probability is shown as following equation

$$P = 1 - \chi^2(MAH, df) \quad (2)$$

In this paper, outliers are removed based on the Mahalanobis Distance for detection of multivariate outliers. We have 16 features for environments data and 1 feature for gas data, totally 17 features. There dependent variable is CH<sub>4</sub>, predictor variables are "CavityPressure", "CavityTemp", "DasTemp", "EtalonTemp", "WarmBoxTemp", "OutletValve", "GPS\_ABS\_LAT", "GPS\_ABS\_LONG", "WS\_WIND\_LON", "WS\_WIND\_LAT", "WS\_COS\_HEADING", "WS\_SIN\_HEADING", "WIND\_N", "WIND\_E", "WIND\_DIR\_SDEV", "CAR\_SPEED".

In Fig. 2(a), outliers detected by Mahalanobis distance using a  $p < 0.001$  and the corresponding  $\chi^2$  value with the degrees of freedom. Fig. 2(b)

shows removed outliers from dataset by rank  $p$  value. Where, degree of freedom has  $df=13$ .

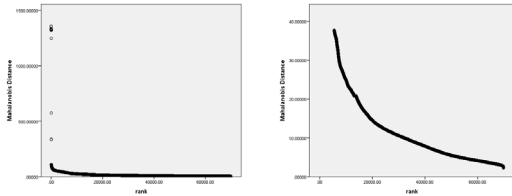


Fig. 2. Comparison between before and after Mahalanobis outlier.

### 2.2 Ordinal Encoder

Encode categorical variables as an integer array. The input of this transformer is the same as an integer or string array and represents a value obtained by a category (discrete) characteristic. There converts feature to the ordinal integers. As a result, one integer column (0 to  $n-1$ ) appears in one feature, and  $n$  is the number of categories. We implemented the OE normalization for all components. Fig. 3 shows plots of component 6 with and without OE. Additionally, after OE, we transformed the log10 scale transform with all seven components. The results are shown in Fig. 4. It can be seen that the distribution of the initial values of the data mentioned in [1] is similar

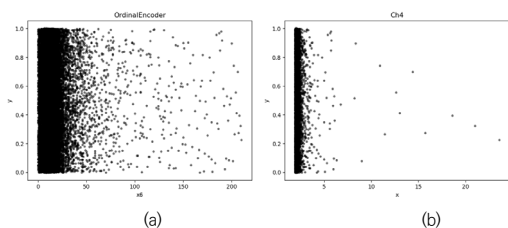


Fig. 3. Plots of with and without OE normalization for CH4 data. (a) with OE, (b) without OE.

After outlier detecting we have removed zero valued column as “GPS\_ABS\_LON\_OE”, and after OE normalization we removed “CavityPressure”. Now we have 14 features for environmental data.

Additionally, after OE, we transformed the Ln

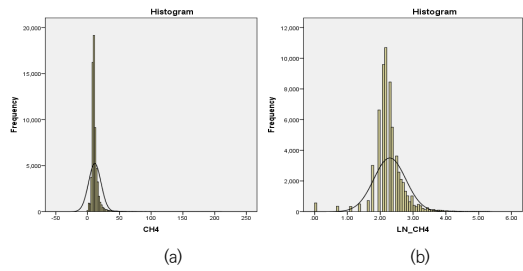


Fig. 4. Histogram of with and without Ln transform for CH4. a) without Ln, b) with Ln.

scale transform with all features. Fig. 5 is the results before and after Ln transform of CH4 were compared. It can be seen that the distribution of the initial values of the data mentioned in [1] is similar.

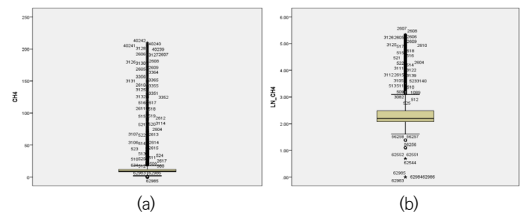


Fig. 5. Comparison between before and after Ln transform. (a) without Ln, (b) with Ln.

### 2.3 K-means Clustering

In this session we will explain one of the most popular ML unsupervised algorithm K-means clustering classification used to CH4 gas data. The K-means is a multi-variable classification method developed by MacQueen in 1967 [11]. The main concept is to distribute the variables to the nearest class  $n$  values into  $k$  subgroups. The basic concept is to divide the variables into  $k$  subgroups of  $n$  values in the nearest class. We divided into three levels for gas leakage by low, medium, and high.

In Fig. 6, we illustrated k-means clustering results by the boxplot for CH4. Here final cluster center includes low, medium, and high reached 2.59, 3.65, and 4.48, respectively as almost the same with the [1] median threshold value (ppm) for defining elevated CH4. The cluster values

have as low-51582, medium-12104, and high-460. From the value of the clusters, it can be seen that the imbalanced data with CH<sub>4</sub>.

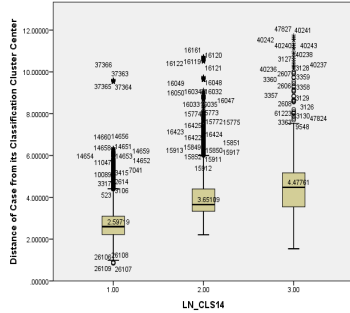


Fig. 6. Box plot of clusters for the gas data.

We also analyzed factors for depend variable is CH<sub>4</sub> with other environment data. Table 2 shows descriptive statistics of features for CH<sub>4</sub>. Which is the cluster 1, 2, and 3 are low, medium and high. There have means and standard deviations of the features used in the factor analysis. The number of cases has N=69831.

Table 1. Descriptive Statistics of CH<sub>4</sub> for Cluster Number of 1, 2, and 3 are used in the analysis phase (N=64146)

	Cluster1 (N=51582)		Cluster2 (N= 12104)		Cluster3 (N=460)	
	Mean	Std. Deviation	Mean	Std. Deviation	Mean	Std. Deviation
CavityTemp	1.92	.272	2.63	2.216	1.96	.307
DasTemp	88.11	33.882	145.2	42.511	82.88	39.29
EtalonTemp	2.00	.164	2.49	.552	2.08	.272
WarmBox Temp	1.99	.107	2.35	.504	2.06	.243
OutletValve	7.06	2.735	13.94	2.711	6.50	3.63
WS_WIND_LAT	1718.9	868.4	1946.1	926.2	1802.7	890.4
WS_COS_HEADING	1232.2	987.1	1402.9	984.4	1458.0	1040.8
WS_SIN_HEADING	1822.8	1099.9	1337.2	1007.3	1823.9	1185.8
WIND_N	1366.2	1014.1	1225.3	977.9	1510.5	1120.0
WIND_E	1729.4	626.2	1433.3	675.8	1639.4	535.9
WIND_DIR_SDEV	2329.5	1284.4	1845.2	1269.5	2891.1	832.4
CAR_SPEED	11.04	5.413	9.23	5.258	97.62	41.5

Table 2 we can show communalities value for each clusters and extracted by PCA. From these results, it can be shown as the percentage of features of the value explained by the coefficient for the given variable. In other words, we obtain

indicating that about 87.0% of the variation in DasTemp\_OE is explained by the cluster 1 factor model. Likewise, 81.6% in cluster 2, and 82.1% in cluster 3.

Table 2. Communalities of Factor model for each clusters (Initial = 1, Extraction Method: Principal Component Analysis. Only cases for which Cluster Number of 1, 2 and 3 are used in the analysis phase.)

	Extraction		
	Cluster 1	Cluster 2	Cluster 3
CavityTemp_OE	.400	<b>.748</b>	.549
DasTemp_OE	<b>.870</b>	<b>.816</b>	<b>.821</b>
EtalonTemp_OE	<b>.781</b>	<b>.825</b>	<b>.851</b>
OutletValve_OE	<b>.821</b>	<b>.766</b>	<b>.873</b>
WS_WIND_LON_OE	<b>.896</b>	<b>.827</b>	<b>.904</b>
WS_WIND_LAT_OE	.572	.565	.624
WS_COS_HEADING_OE	.630	<b>.780</b>	<b>.769</b>
WS_SIN_HEADING_OE	.693	.683	<b>.787</b>
WIND_N_OE	.069	.587	.277
WIND_E_OE	.525	.601	.673
WIND_DIR_SDEV_OE	<b>.705</b>	<b>.759</b>	<b>.831</b>
CAR_SPEED_OE	.134	.241	.192

The results suggested the best job of explaining variation in DasTemp\_OE, EtalonTemp\_OE, OutletValve\_OE, and WS\_WIND\_LON\_OE reached 87.0%, 78.1%, 82.1%, and 89.6% for the first cluster of CH<sub>4</sub>; DasTemp\_OE, EtalonTemp\_OE, and WS\_WIND\_LON\_OE reached 81.6%, 82.5%, and 82.7% for the second cluster of CH<sub>4</sub>; DasTemp\_OE, EtalonTemp\_OE, OutletValve\_OE, WS\_WIND\_LON\_OE, and WIND\_DIR\_SDEV\_OE reached 82.1%, 85.1%, 87.3%, 90.4%, and 83.1% for the third cluster of CH<sub>4</sub>. We can to see values that are close to the initial value one. This model shows that most of the features of these variables are explained. In this case, the model is better for some variables than for others. The model explains DasTemp\_OE, EtalonTemp\_OE, OutletValve\_OE, WS\_WIND\_LON\_OE, and WIND\_DIR\_SDEV\_OE are the best for CH<sub>4</sub> features. In additionally, not bad for other variables such as CavityTemp\_OE, WS\_WIND\_LAT\_OE, WS\_COS\_HEADING\_OE, WS\_SIN\_HEADING\_OE, WIND\_N\_OE, WIND\_E\_OE, WIND\_DIR\_SDEV\_OE, and CAR\_SPEED. However, for other variables such as CAR\_SPEED\_OE, the

model does not work very well and only explains about 24% of the changes. This model extracted by PCA.

### 3. Evaluation Metrics

The performance evaluation of this paper was completed using accuracy, AUC, F1-score, and MSE. We can find precisions and recall as follows [4]:

$$Precision = \frac{TP}{TP+FP} \quad \text{and} \quad Recall = \frac{TP}{TP+FN} \quad (3)$$

The F1 score is the harmonic mean of precision and recall as follows:

$$F1 = \frac{2 \cdot Precision \cdot Recall}{Precision + Recall} \quad (4)$$

We have studied on the multi-class case, there the average of the F1-score of each class label with weighting depending on the average parameter as Eq. (4).

The accuracy is a measure of the degree for the nearness of calculated value to its actual value. Accuracy is the sum of true positive fraction and true negative fraction among all the test data as Eq. (5).

$$Accuracy = \frac{TP + TN}{TP + FP + FN + TN} \quad (5)$$

In addition, one of our evaluated metrics is the mean squared error (MSE) for the predicted leaks to relative to actual values was used:

$$MSE = \frac{1}{mn} \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} (X(i,j) - Y(i,j))^2 \quad (6)$$

with  $m$  and  $n$  being the number of observations, which  $m$  is the number of data and  $n$  is predicting NG. The  $X$  and  $Y$  being the actual and predicted values for the  $i, j$  - th data point, respectively.

### 4. Experimental Results

The dataset is selected on [1, 8, 15] experimental data which named as "03/15/2017-0.3/25/2017"

for Sample\_Raw open data [6]. In the default setting of training (70%) and testing (30%) set. The descriptive statistics for experimental data have described in the Table 3.

Table 3. Descriptive statistics of classes for experimental dataset

Class	Total	Train 70%	Test 30%
Low	51582	36136	15446
Medium	12104	8462	3642
High	460	304	156
<b>Total</b>	<b>64146</b>	<b>44902</b>	<b>19244</b>

Table 4. Evaluation comparison of the proposed algorithms for experimental dataset(%).

	Accuracy	AUC	MSE
<b>MOL-RF</b>	<b>99.71</b>	<b>99.57</b>	<b>0.0016</b>
MOL-KNN	92.23	79.05	0.051
<b>MOL-DT</b>	<b>99.62</b>	<b>99.60</b>	<b>0.002</b>
MOL-NB	92.60	94.61	0.04
MOL-MLP	93.32	86.47	0.034
RF	90.98	82.64	0.11
KNN	88.54	81.34	0.14
DT	85.93	80.36	0.16
NB	59.51	68.70	0.42
MLP	80.26	50.00	0.22

The accuracy, ROC, AUC, and MSE measurements of the performance results are shown in Table 4, which can support us to know how the models perform when the normalization is not selected properly. The OE, machine learning algorithms implemented in Python, and cluster analysis and Mahalanobis outlier detection removing implemented in SPSS 20.0. The accuracy, AUC, MSE, and ROC curve measurements of the performance results are shown in Table 4, which can support us to know how the models perform when the normalization is not selected properly. The RF algorithm had the highest accuracy of 90.98%, AUC 82.64, MSE 0.11, and ROC 72.38% than other algorithms such as KNN, DT, NB, and MLP. We increased these performances by the Mahalanobis with OE and LN transform (MOL) model, and then the DNN model was improved by prediction

measurements. Our proposed MOL\_RF has made accuracy, AUC, and MSE; 99.71%, 99.57%, and 0.0016 respectively. In addition, MOL\_DT has made accuracy, AUC, and MSE; 99.62%, 99.60%, and 0.002 respectively.

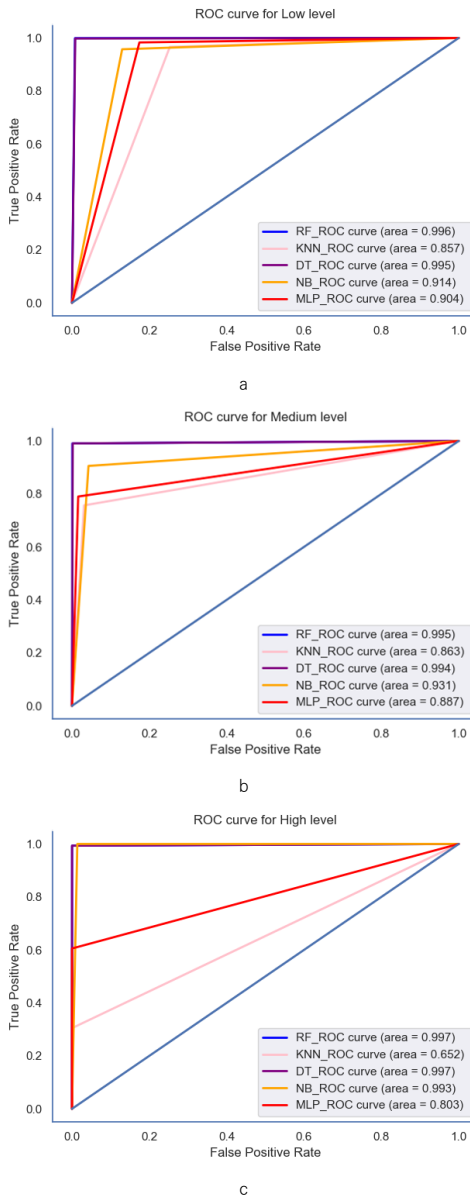


Fig. 7. Multi-class ROC curves by the compared F-OE algorithms for low, medium and high levels. a) Low level class. b) Medium level class. c) High level class.

We provided multi-class ROC curves of compared some prediction model in Fig. 7. As mentioned before, we proposed to find a better model performance to predict medium and high-level classes for the experimental dataset. The factor analysis with OE based RF shows higher ROC scores low-level 99.9%, medium-level 99.7%, and high-level 99.7% than others for all class level.

## 5. Conclusion

In this paper, we present relationship between NG data and environmental elements was performed using machine learning algorithms to predict the level of gas leakage risk without directly measuring gas leakage data on vehicle-based open data factor analysis. We eliminated outlier values using multivariate outlier detecting Mahalanobis distance method; normalized them using the OrdinalEncoder, and then classified them using the k-mean cluster on the new CH<sub>4</sub> value. We performed a Ln transformation, the overall content distribution pattern of the original data did not change significantly until the k-mean cluster analysis was performed. It is suggested to find a better model performance to predict the medium and high-levels for the unbalanced experimental data set. Our proposed MOL\_RF methods predict the risk of leakage in the suggested algorithms, with accuracy, AUC, and MSE, reaching 99.71%, 99.57%, and 0.0016 respectively. In addition, MOL\_DT has made accuracy, AUC, and MSE; 99.62%, 99.60%, and 0.002 respectively. The system has implemented the SPSS and Python, including its performance, is tested on open real data.

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