

The Accuracy of KNN, SVM, neural network, naive Bayes classifier and DBSCAN, kmeans for Determining the Cancer by Gene-expression signatures

Hsieh Cheng-Han, Hsu Ting-Hao, Sun Shih-Yu, Lu Che-Yuan, Huang Chia-Yen

May 2023

Abstract

Nowadays, using machine to give an early diagnosis of a cancer type is widely studied. In this paper, based on the gene-expression dataset on Synapse.org, we compare the performance of machine learning techniques, including data preprocessing, e.g., Principal components analysis (PCA), Autoencoder (AE), classification, e.g., k-nearest neighbors (KNN), support vector machine (SVM), neural network (NN), and clustering for dealing with unknown types, e.g., k-means, density-based spatial clustering of applications with noise (DBSCAN). The experiment results show that with PCA reducing the dimension of the dataset to 32, using KNN for classifying the known types, and finally use DBSCAN to cluster the unknown types, the accuracy of predicting can reach about 94%, which beats the other methods out.

breast invasive carcinoma (BRCA) colon adenocarcinoma (COAD) kidney renal clear cell carcinoma (KIRC) lung adenocarcinoma (LUAD) prostate adenocarcinoma (PRAD)

machine may determine the type of disease that this person may have by collecting the data from the person, and thereby achieve the goal of personalized medicine. As a result, machine learning methods have become a popular tool for medical researchers.

In real application, besides from the known cancers in the train data, there're numerous unknown types of cancers. When a new type of cancer appears, how shall the machine results? In ideal situation, this new type of cancer should be reported as an unknown type, which can be done by the combination of classification and clustering. However, how to choose the proper machine learning methods is a hot potato, since the different combinations of machine learning methods have different performance.

In this work, the dataset on Synapse.org is used, which contains 20531 RNA sequences and 3 types of cancer in the train data, and 2 new types in test data. To find out which techniques is more suitable to predict cancer by RNA sequence, this work examines the accuracy of the combinations of some major machine learning techniques, including PCA, AE, KNN, SVM, NN, k-means, DBSCAN.

1 Introduction

Over the years, machine learning methods for early predict various disease are widely used in medical field. [1] [2] From diabetes [3], heart disease [4], to lung adenocarcinoma [5] etc., machine learning methods is universally studied attributed to the promising perspective. With a well-built database of disease and a well-choose combination of machine learning methods, within seconds, a

2 Related works

Data preprocess

Autoencoder (AE): An AE is a type of neural network used for unsupervised learning and dimensionality reduction. It is designed to learn efficient representations or encodings of input data by training the network to recon-

struct its own inputs. The AE consists of an encoder and a decoder. The encoder compresses the input data into a lower-dimensional representation, often called the latent space or code. The decoder then aims to reconstruct the original input data from this compressed representation. By learning a compact representation of the input data, AEs can capture important features and discard noise or irrelevant information. This makes them effective in tasks such as image or text classification, where reducing the dimensionality of the data can improve performance.

Principal components analysis (PCA): PCA is a statistical technique used for dimensionality reduction and data exploration. It aims to transform a dataset with a large number of variables into a lower-dimensional space while preserving the most important information. PCA accomplishes this by identifying the principal components, which are linear combinations of the original variables. Applications of PCA span various fields, including image and signal processing, finance, genetics, and social sciences. It is particularly useful in scenarios where the dataset is high-dimensional and the interpretation and visualization of the data are challenging.

Classification algorithm

k-nearest neighbors (KNN) classification algorithm: The KNN classification algorithm is a supervised learning method which is first developed by Fix and Hodges [6]. The idea of KNN is based on the idiom, "birds of a feather flock together". By picking the k -nearest neighbors of a data point, the unknown class label can be determined. Lots of works [7] [8] [9] show the fact that KNN performs well for prediction of diabetes disease.

support vector machine (SVM): Given a set of training datas, where each data is labeled as a binary class, such as 0 and 1, SVM training algorithm creates a model that assigns new examples to the binary labels by making it a non-probabilistic binary linear classifier. In addition, according to [10] [11], SVM can also use a method called kernel trick to effectively perform non-linear classification by implicitly mapping its inputs into a high-dimensional feature space.

neural network (NN): Neural network have been used in many fields to deal with intricate datas. With input layer, hidden layer and output layer constructed by neurons, each data in dataset is processed while passing

through neurons, layer by layer. After the processing, the outcome can be used to predict. Using back propagation, the accuracy of predictions increase in each training. In order to construct the hidden layer more efficient, NAS (Neural Architecture Searching) is used to search suitable structure for hidden layer, increasing the accuracy. According to [12][13], many neural network have been constructed and trained already, with high efficiency and accuracy in prediction of diabetes.

Clustering algorithm

k-means: k-means is a popular and easily implemented clustering method in machine learning and data analysis. With n data points in a dataset, k-means algorithm partition them into k distinct clusters. The algorithm works iteratively and converges to a solution by minimizing the sum of squared distance between the data points and the center of their cluster. K-means is a useful algorithm for clustering data, which is widely applied on many researches, e.g. [?], [?], [?].

Density-based spatial clustering of applications with noise (DBSCAN): DBSCAN is a data clustering algorithm proposed by Ester et al. [14] DBSCAN is particularly effective in discovering clusters of arbitrary shapes and handling noise in the data. Unlike k-means need user specify how many clusters, DBSCAN determine the clusters and noise automatically by the density of data points. This characteristic makes it particularly useful when addressing the datasets where the number of cluster is unknown. DBSCAN is the major clustering algorithm in machine learning field, since the ability to discover the number of clusters automatically. And the variants of DBSCAN [15] is also developed widely.

Table 1: COMPARISON OF CLASSIFICATION TECHNIQUES. (ARRHYTHMIA DATA SET)

Method	Search (s)	acc	acc (normalized)	acc (PCA-32)	acc (PCA-32-normalized)	acc (PCA-32-normalized)
KNN-Brute-Force + DBSCAN	0.014	44.3038 \pm 0	46.2025 \pm 0	38.6076 \pm 0	42.4051 \pm 0	34.81
SVM (linear) + DBSCAN	1.048	25.9494 \pm 0	35.4430 \pm 0	32.2785 \pm 0	29.7468 \pm 0	31.64
SVM (polynomial) + DBSCAN	0.765	25.9494 \pm 0	25.3165 \pm 0	1.2658 \pm 0	33.5443 \pm 0	30.37
SVM (RBF) + DBSCAN	5.298	25.9494 \pm 0	22.7848 \pm 0	0.6329 \pm 0	30.3797 \pm 0	22.15
SVM (sigmoid) + DBSCAN	2.298	28.4810 \pm 0	20.2532 \pm 0	30.3797 \pm 0	36.0759 \pm 0	22.15
KNN-Brute-Force + kmeans	0.014	44.3038 \pm 0	41.7722 \pm 0	43.0380 \pm 0	43.0380 \pm 0	36.07
SVM (linear) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0
SVM (polynomial) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0
SVM (linear) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0
SVM (sigmoid) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0

Table 2: COMPARISON OF CLASSIFICATION TECHNIQUES. (GENE EXPRESSION CANCER RNA-SEQ DATA SET)

Method	Search (s)	acc	acc (normalized)	acc (PCA-30)	acc (PCA-30-normalized)	acc (PCA-30-normalized)
KNN-Brute-Force + DBSCAN	4.317	59.0361 \pm 0	66.5663 \pm 0	94.5783 \pm 0	78.3133 \pm 0	64.45
SVM (linear) + DBSCAN	131.809	61.7470 \pm 0	9.9398 \pm 0	9.9398 \pm 0	10.5422 \pm 0	63.25
SVM (polynomial) + DBSCAN	31.221	61.7470 \pm 0	1.2048 \pm 0	64.4578 \pm 0	61.1446 \pm 0	63.25
SVM (RBF) + DBSCAN	3.988	X	X	9.9398 \pm 0	63.2530 \pm 0	40.36
SVM (sigmoid) + DBSCAN	0.446	X	X	71.6867 \pm 0	65.9639 \pm 0	44.27
KNN-Brute-Force + kmeans	4.859	74.0964 \pm 0	53.6145 \pm 0	94.8795 \pm 0	84.9398 \pm 0	42.16
SVM (linear) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0
SVM (polynomial) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0
SVM (linear) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0
SVM (sigmoid) + kmeans	X	X \pm 0	X \pm 0	X \pm 0	X \pm 0	0

3 main section

4 Experiment result

5 Conclusion

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