Calculating P-value Using Gaussians Models

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Abstract

One problem of modern Machine Learning classification methods is that they always hard predict a class, even if the given data is not from any of the classes. To solve this problem, our research focuses on finding the data point's P-value of each class. From previous work, we have a Nearest Neighbor Distance Model, which fits a distribution of nearest neighbor distances to calculate the given data point's P-value of each class. However, there are two issues: 1) it cannot detect an outlier. 2) it cannot predict if two clusters are differentiate not based on distance (overlap clusters).

I tried two ways to solve the problem. The first one is to use a Gaussian Naïve Bayes Model. The second one is to fit the data into Multivariate Gaussian Distribution. The main goal is to design a model that performs better on above two situations, and then we can use ensemble methods to combine all models. (Ensemble details are in another report).

Introduction

Gaussian Naïve Bayes Model will give us the posterior probability of each class given a data point. Using these posterior probabilities, we can empirically count how many more points are more extreme than the given one. This is an empirical way to calculate P-values.

Multivariate Gaussians Model calculates the mean and the covariance for each class, and then fit a Gaussian Distribution (a bell shape curve) for each of the class. When predicting, it gives P-value by calculating the given data point's CDF for each Gaussian Distribution, namely how many more extreme cases (in percent) are there. So close to 0 means unlikely, and close to 1 means likely. This is a theoretical way to calculate P-values.

Both methods will perform better on detecting outliers and overlap clusters compared to Nearest Neighbor Distance Model, because Gaussian models take not only distance but also covariance into account.

Detailed Approach

1) Gaussian Naïve Bayes Model

Gaussian Naïve Bayes Model train data by calculating the posterior probability using Naïve Bayes Rule:

$$\mathrm{p}(C_k|x) = \frac{p(C_k)p(x|C_k)}{p(x)}, for\ \ each\ \ class\ \ k$$

When predicting, it calculates P-values by empirically counting how many training data has lower posterior probability than itself for class k, then divide by the number of all training data in class k:

$$Pvalue\ of\ k = \frac{\#\ training\ data\ who\ has\ lower\ posterior\ prob\ in\ class\ k}{\#\ training\ data\ in\ class\ k}$$

2) Multivariate Gaussians Model

Multivariate Gaussians Model train data by fitting all the training data into multiple Gaussian Distributions as the following formula:

$$\mathrm{N}(x; \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{d}{2}}} |\Sigma|^{-\frac{1}{2}} \exp\{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\}$$

where *d* is a real k-dimensional column vector, and $|\Sigma|$ is the determinant of Σ. After that, we will get a "bell shape curve" *for each class.*

After fitting, Multivariate Gaussians Model gives P-values of class k by calculating the CDF of the given data in the kth Gaussian Distribution:

$$Pvalue\ of\ k = \ p(x < input\ data\ point \mid the\ kth\ Gaussian\ Distribution)$$

If we want to predict a class, we can simply pick the class who has the highest P-value:

$$\hat{y} = \ argmax_k(PValue_k)$$

Performance:

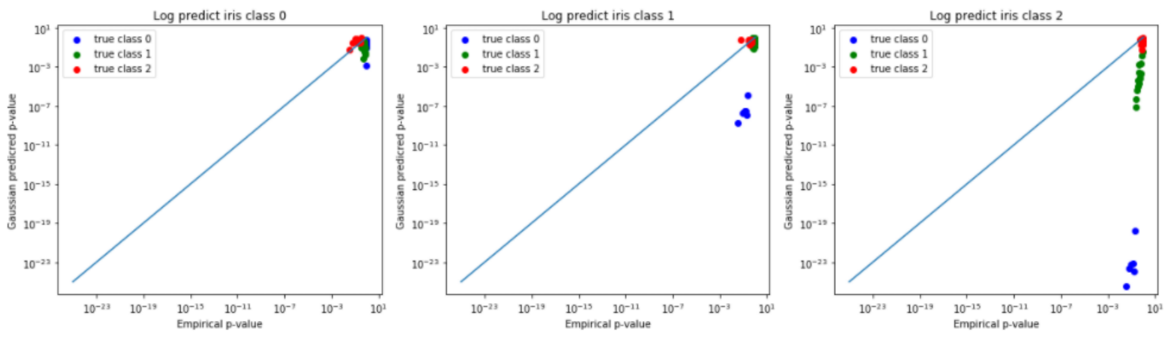
1) Accuracy (Train: 80%, Test: 20%)

Classifier/Dataset	Iris	Wine	Bio grid
Gaussian Naïve Bayes Model	0.9	0.91	0.39
Multivariate Gaussian Model	0.8	0.75	<0.1 & time-consuming

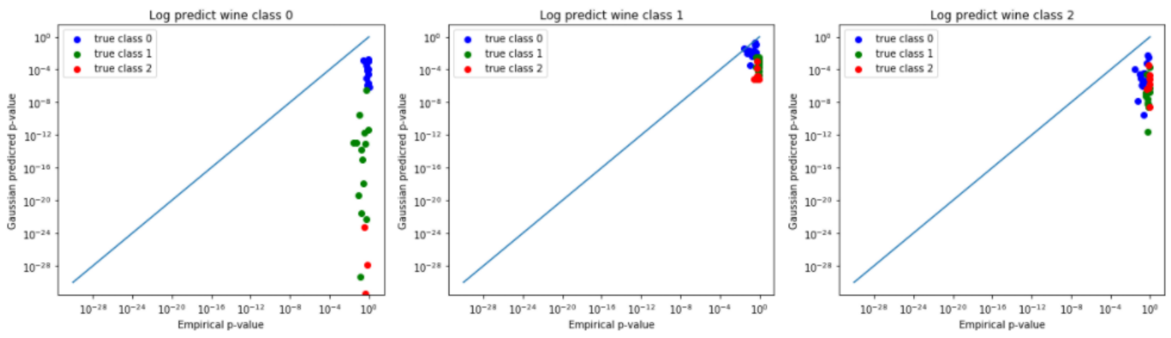
*Accuracy may flow because of random split of dataset

2) Plot

a) Iris dataset using Multivariate Gaussian Model:



b) Wine dataset using Multivariate Gaussian Model:



Conclusion:

We can see that Naïve Bayes Model has a better performance than Multivariate Gaussians Model. This may because the Multivariate Gaussians Model over-fits the dataset. Also, both models perform poor on Bio Grid dataset, because there are banana-shaped clusters, which is more suitable for Nearest Neighbor Distance Model. Having all these models, next step is to use an ensemble method to combine them and give a more reasonable result.