COMP6245(20/21): Foundations of Machine Learning (MSc) Lab 1 Report

Yan Zhang (yz10u20@soton.ac.uk)

1 Introduction

The Gaussian distribution(also known as Normal distribution) is widely used in the area of machine learning. In this report, I use mathematical methods to give answer to the tasks listed in the Lab 1 pages.

2 Solution

2.1 Preliminaries

In the Preliminaries, the 3 by 3 symmetric matrix B is created. We found that the dot product of the first two column of the eigenvectors matrix is close to 0. We assume that the product of the eigenvectors of a symmetric matrix is orthogonal.

Let v_1, v_2 be eigenvectors of matrix B corresponding to the eigenvalues α,β, we have

$$Bv_1 = \alpha v_1, Bv_2 = \beta v_2 \tag{1}$$

To prove that u and v are orthogonal, we can conclude this by showing the inner product $v_1 v_2 = 0$. Then compute

$$\begin{aligned} \alpha(v_1 v_2) = (\alpha v_1)v_2 = Bv_1 v_2 = (Bv_1)^T v_2 \\ = v_1^T B^T v_2 = v_1^T Bv_2 = v_1^T \beta v_2 = \beta(v_1^T v_2) = \beta(v_1 v_2) \end{aligned} \tag{2}$$

we have

$$\begin{aligned} \alpha(v_1 v_2) = \beta(v_1 v_2) \\ (\alpha - \beta)v_1 v_2 = 0 \end{aligned} \tag{3}$$

Because $\alpha - \beta \neq 0$. Hence, we must have $v_1 v_2 = 0$ and the eigenvectors are orthogonal. We now come to the conclusion that eigenvectors of real symmetric matrices are orthogonal.

2.2 Random Numbers and Uni-variate Densities

Now we consider generate sample from continuous uniform distribution. we randomly generated two groups of 1000 sample from the U(0,1) distribution, one with the bins = 4 and another with the bins=40. The figure of the histogram is shown in figure 1.

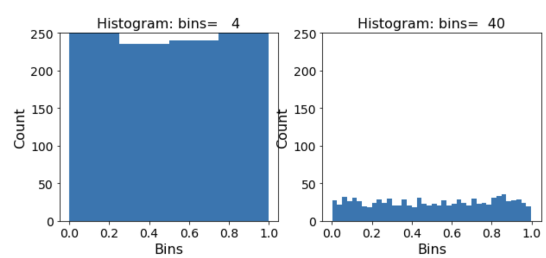


Figure 1: The two histograms showing the count of samples in each bin with bins=4 and bins=40.

The data is from a uniform distribution, where the probability of generating each data is equal. However, the figure does not appear flat, and there are some small ups and downs in the hist. This is because when sampling data from the uniform distribution, the sampling error exists. A sampling error is a statistical error that occurs when a sample is selected that does not represent the whole population. In this case, the sampling error is only an approximation of the population from which it is drawn, which means a certain range of bin could probably contain more data, and vice versa. After many repeated experiments, the plotted graph looks slightly different. Many reason could contribute to this result. Concretely, every time a sample is selected, there is a probability of being selected and a probability of not being selected. Hence, In every experiment, there might be some difference in the samples that were selected.

When starting with more data(10000 samples), the histogram appears flat. The smaller the sampling error is, the histogram appears flatter. In this case, when we start with a larger sample size, the sampling error is almost eliminated and most of the data points represent the whole population which overwhelm the disorder caused by a small part of the data points. Although it is good to have low sampling error, but large sampling size requires more resource and time.

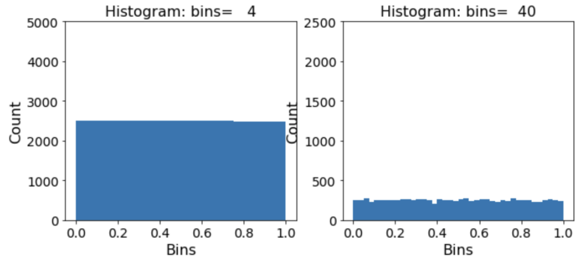


Figure 2: The two histograms showing the count of samples in each bin with bins=4 and bins=40.

Now, we add some uniform random numbers of size 1000, subtract the sum of each of them, and plot the histogram. The histogram looks like it is shaped like a curve approximate to normal distribution(shown in the first graph in Figure 3). The second graph in figure3 shows the histogram that when we started with more data. It appears that when the sample size goes up, the width of curve is getting gradually smaller. Hence larger sample gave us a more accurate estimate of the population mean. According to the central limit theorem, the mean of a sufficiently large number of independent random variables will itself be approximately normally distributed. In our case, the subtract of sum of samples is equal to the mean of the samples, because they both represent the center the whole samples.

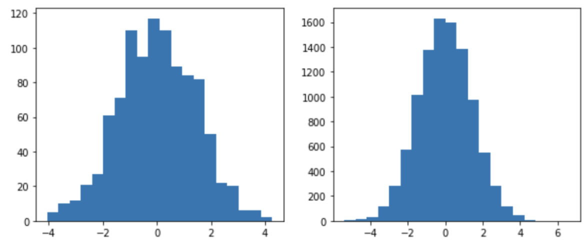


Figure 3: Distribution of the subtract of sum of uniform random distribution of size 1000 and 10000

2.3 Uncertainty in Estimation

There are many uncertainties in estimating the parameters in machine learning model. we want to estimate the variance of a uni-variate Gaussian, and the Figure 4 shows that as the sample size go up, the variation will be small. The sample size dictates the amount of information we have, and determine the precision that our estimation has. The uncertainty in our estimation is also determined by in confidence interval we made.

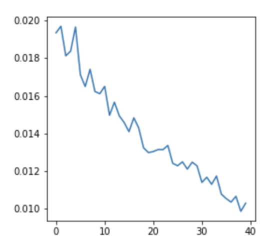


Figure 4: The variance of a uni-variate Gaussian density

For a known standard deviation, the confidence interval is the form:

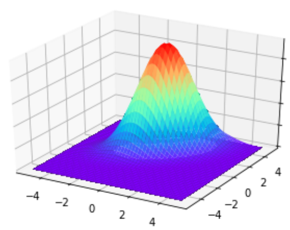
$$\left(\overline{x} - z^* \frac{\sigma}{\sqrt{n}}, \overline{x} + z^* \frac{\sigma}{\sqrt{n}}\right) \tag{4}$$

where $z^* = \Phi^{-1}\left(1 - \frac{\alpha}{2}\right) = -\Phi^{-1}\left(\frac{\alpha}{2}\right)$

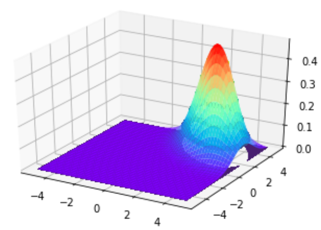
As the sample size n increases, confidence interval gets larger so the uncertainty in the estimation decreases.

2.4 Bi-variate Gaussian Distribution

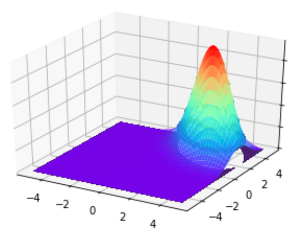
The Bi-variate Gaussian distribution is clearly visualized by the 3 dimension contour plot, which is shown in Figure 5.



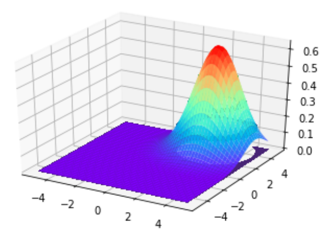
(a) $\mu = \begin{bmatrix}0, & 2\end{bmatrix}$ $\sigma = \begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}$



(b) $\mu = \begin{bmatrix}2.4, & 3.2\end{bmatrix}$ $\sigma = \begin{bmatrix}2 & -1\\-1 & 2\end{bmatrix}$



(c) $\mu = \begin{bmatrix}1.2, & 0.2\end{bmatrix}$ $\sigma = \begin{bmatrix}2 & 0\\0 & 4\end{bmatrix}$



(d) $\mu = \begin{bmatrix}2.4, & 3.2\end{bmatrix}$ $\sigma = \begin{bmatrix}2 & 0\\0 & 2\end{bmatrix}$

Figure 5: 3-dimension contours of Bi-variate Gaussian distribution

2.5 Distribution of Projections

Matrix decomposition is the factorization of a matrix into a product of matrices. The LU decomposition and Cholesky decomposition are the most frequently used one. In cholesky decomposition, the matrix A is decomposed into a product of a unique lower triangular matrix L and its transpose: $A = LL^T$. In our case, the original data is generated by the product of a uniform random data matrix(matrix X) and the transpose of the cholesky matrix(matrix A) of the covariance matrix C: $Y = XA^T$. Then matrix X and A are plot in Figure 6 to show the change of the dimension.

Projection is a technique used to reduce the dimension of a set of points. In this section, the data is projected onto a vector $u = \begin{bmatrix}\sin\theta & \cos\theta\end{bmatrix}$, where θ is a parameter that varies from 0 to 2π. With the change of θ, the data can be projected onto any vector in the area. And, therefore, the variance of the projected data varies with θ. By calculating all the variances of possible projections, we plot a graph(Figure 7) to show how the variance changes as theta varies.

The calculated maxima and minama of the variance are approximately 3.08 and 0.98. And the corresponding angle of projection when variance reaches maxima and minima are 44.08 degress and 315.91 degrees respectively.

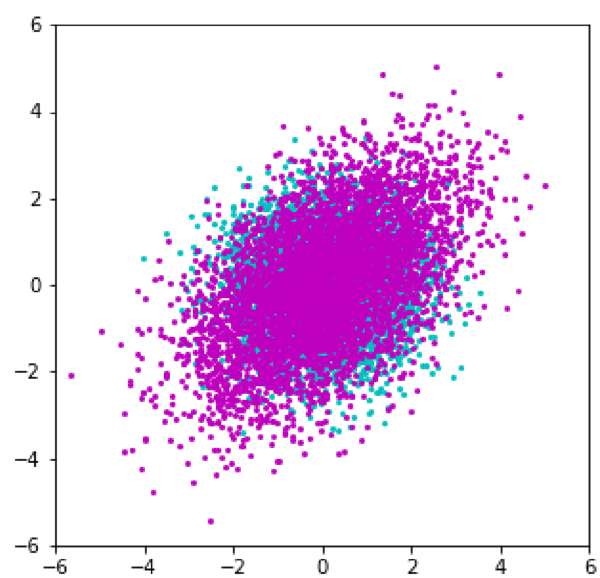


Figure 6: The scatter plot of X and Y

Eigen decomposition is the decomposition of a matrix into matrices composed of its eigenvectors and eigenvalues. We can compute the eigenvalues of the covariance matrix C:

$$\lambda_1 = 3, \lambda_2 = 1 \tag{5}$$

And the corresponding eigenvectors are:

$$u_1 = \begin{bmatrix} 0.70710678, & 0.70710678 \end{bmatrix}, u_2 = \begin{bmatrix} -0.70710678, & 0.70710678 \end{bmatrix} \tag{6}$$

The angle of the eigenvector corresponding to the larger eigenvalue is 45 degrees, which is very close to 44.08, and the angle of projection when variance reaches maxima. And, inversely, the angle of the eigenvector corresponding to the smaller eigenvalue is -45 degrees, which is close to approximately equal to 315.91 degrees. In addition, the larger eigenvalue 3 is close to the maxima of variance, and the smaller eigenvalue 1 is close to the minima of variance.

Say μ is the mean of projected data, e_j is the j^{th} element of the eigenvector e. The variance of projected data($x^T e$):

$$\begin{aligned} \frac{1}{n}\sum_{n=1}^{n}\big(\sum_{j=1}^{d} x_{ij}e_j - \mu\big)^2 &= \frac{1}{n}\sum_{n=1}^{n}\big(\sum_{j=1}^{d} x_{ij}e_j\big)^2 \\ &= \frac{1}{n}\sum_{n=1}^{n}\big(\sum_{j=1}^{d} x_{ij}e_j\big)\big(\sum_{a=1}^{d} x_{ia}e_a\big) \\ &= \sum_{j=1}^{d}\sum_{a=1}^{d}\big(\frac{1}{n}\sum_{i=1}^{n} x_{ia}x_{ij}\big)e_j e_a \\ &= \sum_{a=1}^{d}\big(\sum_{j=1}^{d} cov(a,j)e_j\big)e_a \\ &= \sum_{a=1}^{d}(\lambda e_a)e_a = \lambda \parallel e \parallel^2 = \lambda \end{aligned} \tag{7}$$

where $\mu = \frac{1}{n}\sum_{i=1}^{n}\big(\sum_{ij}^{d} x_{ij}e_j\big) = \sum_{j=1}^{d}\big(\frac{1}{n}\sum_{i=1}^{d} x_{ij}\big)e_j = 0$. Then we come to the conclusion, when the eigenvectors are unit vectors, the corresponding eigenvalues are the maximal variance of the projected data. Also, the maxima and minima of the variance always exist in the direction of projection where the eigenvectors are.

We use the Cholesky matrix to create correlations among random variables. For example, suppose that the two columns in matrix X are independent standard normal variables. The matrix A can be used to create new variables Y such that the covariance of the two columns in Y equals C. Then Y has a distribution:$Y \sim N\big(m, C\big) = N\big(0, C\big)$. Then, provided with a unit vector $u = \begin{bmatrix} \sin\theta & \cos\theta \end{bmatrix}$, we make product of them: $Yp = Yu$.

The variance of Yp can be computed as:

$$\begin{aligned} u^T C u &= \begin{bmatrix} \sin\theta, & \cos\theta \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} \sin\theta \\ \cos\theta \end{bmatrix} \\ &= 2 + \sin 2\theta \end{aligned} \tag{8}$$

The shape of the graph have looked sinusoidal, with a period equal to π.

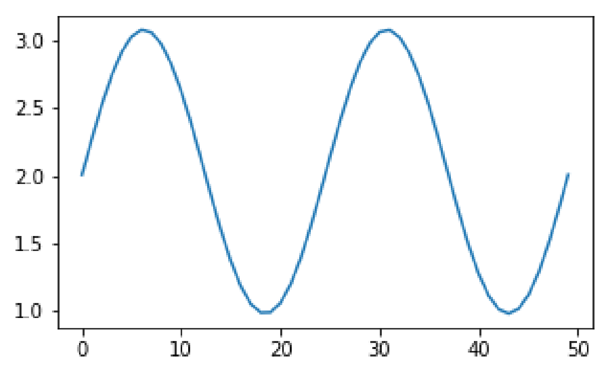


Figure 7: Variance of the projected data