

Introduction to Multivariate Data Analysis

Final Project Report

José Antonio Álvarez Ocete - 917933752
jocete@ucdavis.edu

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1 Multiple Linear Regression

1.1 Introduction

In this first section, we will conduct a multiple linear regression following question 1 of the 5th homework assignment. We will estimate the regression coefficients (betas) following different several methods seen during the lectures and we will provide an estimation for a new response.

1.2 Summary

For this first analysis, I've selected the Battery Failure dataset. In this example, we want to predict the cycles of life of a certain battery before it fails. We are provided the following variables: Charge rate (amps), discharge rate (amps), depth of discharge (% of rated ampere-hours), temperature ($^{\circ}\text{C}$), and end of charge voltage (volts). These are the first three rows of data:

Charge rate (amps)	Discharge Rate (amps)	Depth of Discharge (% of rated ampere-hours)	Temperature ($^{\circ}\text{C}$)	End of Charge Voltage (volts)	Cicles to failure
0.375	3.13	60.0	40	2.00	101
1.000	3.13	76.8	30	1.99	141
1.000	3.13	60.0	20	2.00	96

1.3 Analysis

(1) Find the least square estimate beta hat

We obtain the least square estimate beta hat following out notes:

$$\hat{\vec{\beta}} = (Z^T \cdot Z)^{-1} \cdot Z^T \cdot \vec{Y}$$

Obtaining:

$$\hat{\vec{\beta}} = \begin{pmatrix} -2937.7571 \\ -33.7934 \\ -0.1798 \\ -1.7397 \\ 7.0627 \\ 1529.2897 \end{pmatrix}$$

(2) Find the R^2 statistic

We use:

$$R^2 = \frac{||\hat{\vec{Y}} - \bar{Y} \cdot \vec{1}_n||^2}{||\vec{Y} - \bar{Y} \cdot \vec{1}_n||^2}$$

Obtaining $R^2 = 0.4799$.

(3) Find sigma_hat_square and estimated Cov(beta square)

We use:

$$\hat{\sigma}^2 = \frac{1}{n - r - 1} ||\hat{\vec{\epsilon}}||^2$$

and

$$\hat{Cov}(\hat{\vec{\beta}}) = \hat{\sigma}^2 (Z^T Z)^{-1}$$

We obtain the following:

$$\hat{\sigma}^2 = 7138.186$$

$$\hat{Cov}(\hat{\vec{\beta}}) = \begin{pmatrix} 1.633e+07 & -2933.74 & 2980.4460 & -34.78143 & -991.73637 & -8.160e+06 \\ -2.934e+03 & 1880.55 & 18.5503 & 17.34897 & 10.28445 & -1.764e+02 \\ 2.980e+03 & 18.55 & 193.4117 & -3.23257 & 0.34449 & -1.696e+03 \\ -3.478e+01 & 17.35 & -3.2326 & 1.79944 & -0.08092 & -4.242e+01 \\ -9.917e+02 & 10.28 & 0.3445 & -0.08092 & 3.89193 & 4.549e+02 \\ -8.160e+06 & -176.39 & -1695.7845 & -42.42251 & 454.86652 & 4.081e+06 \end{pmatrix}$$

(4) 95% confidence interval for each β_j

We use one at a time confidence intervals for the betas:

$$\beta_j \in [\hat{\beta}_j \pm \hat{\sigma} \cdot \sqrt{\omega_{jj}} \cdot t_{n-r-1}(\frac{\alpha}{2})]$$

Obtaining:

$$\begin{aligned} \beta_0 &\in [-11604, 5729] \\ \beta_1 &\in [-126.8, 59.22] \\ \beta_2 &\in [-30.01, 29.65] \\ \beta_3 &\in [-4.617, 1.137] \\ \beta_4 &\in [2.831, 11.29] \\ \beta_5 &\in [-2804, 5862] \end{aligned}$$

(5) 95% simultaneous confidence intervals for all betas based on the confidence region

Using the formula from the notes:

$$\beta_j \in [\hat{\beta}_j \pm \hat{\sigma} \cdot \sqrt{\omega_{jj}} \cdot \sqrt{(r+1) \cdot F_{r+1, n-r-1}(\alpha)}]$$

We obtain:

$$\begin{aligned} \beta_0 &\in [-19640, 13764] \\ \beta_1 &\in [-213, 145.5] \\ \beta_2 &\in [-57.67, 57.31] \\ \beta_3 &\in [-7.285, 3.805] \\ \beta_4 &\in [-1.092, 15.22] \\ \beta_5 &\in [-6822, 9880] \end{aligned}$$

(6) 95% simultaneous confidence intervals for all betas based on the Bonferroni correction

We compute a final set of intervals for the betas using the Bonferroni correction:

$$\beta_j \in [\hat{\beta}_j \pm \hat{\sigma} \cdot \sqrt{\omega_{jj}} \cdot t_{n-r-1}(\frac{\alpha}{2(r+1)})]$$

We obtain:

$$\begin{aligned}\beta_0 &\in [-15338, 9462] \\ \beta_1 &\in [-166.9, 99.29] \\ \beta_2 &\in [-42.86, 42.5] \\ \beta_3 &\in [-5.856, 2.377] \\ \beta_4 &\in [1.009, 13.12] \\ \beta_5 &\in [-4670, 7729]\end{aligned}$$

(7) Test $H_0 : \beta_1 = \beta_2 = 0$ at significance level $\alpha = 0.05$

Using this matrix for the linear transformation:

$$C = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

We can compute the F-test statistic:

$$\vec{\beta}_{(2)}^T \Omega_{22}^{-1} \vec{\beta}_{(2)} = 108296$$

And compare it to:

$$(r - q) \cdot \hat{\sigma}^2 \cdot F_{r-q, n-r-1}(\alpha) = 133445$$

Since $108296 < 133445$, we don't have sufficient evidence to assure that $\beta_1 = \beta_2 = 0$.

(8) 95% confidence interval for the mean response given $\mathbb{E}(Y_0) = \beta_0 + \sum_{i=1}^5 \beta_i \cdot \bar{z}_i$, where \bar{z}_i is the sample mean of $z_{i,j}$ for $i \in \{1, \dots, n\}$

First, compute \vec{z}_0 :

$$\vec{z}_0 = \begin{pmatrix} 1.000 \\ 1.031 \\ 3.034 \\ 62.840 \\ 19.500 \\ 1.999 \end{pmatrix}$$

And now compute the confidence intervals for it's associated value using the formula in the class notes:

$$\vec{z}_0^T \vec{\beta} \in [\vec{z}_0^T \hat{\vec{\beta}} \pm \hat{\sigma} \cdot t_{n-r-1}(\frac{\alpha}{2}) \sqrt{\vec{z}_0^T (Z^T Z)^{-1} \vec{z}_0}]$$

Obtaining the following interval: $\vec{z}_0^T \vec{\beta} \in [71.78, 152.8]$

(9) 95% confidence interval for a new response Y_0 given \vec{z}_0

Using a similiar formula:

$$\vec{z}_0^T \vec{\beta} \in [\vec{z}_0^T \hat{\vec{\beta}} \pm \hat{\sigma} \cdot t_{n-r-1}(\frac{\alpha}{2}) \sqrt{1 + \vec{z}_0^T (Z^T Z)^{-1} \vec{z}_0}]$$

And using that $Y_0 = \vec{z}_0^T \vec{\beta} + \epsilon_0$ we obtain:

$$Y_0 \in [-73.38, 298]$$

A substantially bigger interval than the over in (8), which makes sense since we are including the error now.

2 Principal Component Analysis

2.1 Introduction

Briefly summarize the goal of the analysis in your own words

2.2 Summary

Summarize your data by plots or sample estimates

2.3 Analysis

Implement the analysis based on what you have done in homework

3 Two-Sample test and Linear Discriminant Analysis

3.1 Introduction

For this final analysis we will conduct Linear Discriminant Analysis. That is, given enough data about tagged as two different classes, classify a new response into one of these classes. In order to do that we first need to conduct a two sample test to make sure that our populations are actually different.

3.2 Summary

The dataset selection for this example was a little trickier since I wanted to display nice graphs about the data. In order to achieve this the more convenient way was to pick up a two-variate dataset with a nice visual separation between its classes. We will see why in the analysis.

The dataset selected was the Anaconda one. It has two variates: Snout vent length and weight. The class we want to predict is the snake gender: either male (M) or female (F). These are the first 5 rows of our dataset from each class:

Snout Vent Length	Weight	Gender	Snout Vent Length	Weight	Gender
271.0	18.50	F	176.7	3.00	M
477.0	82.50	F	259.5	9.75	M
306.3	23.40	F	258.0	10.07	M
365.3	33.50	F	229.8	7.50	M
466.0	69.00	F	233.0	6.25	M
440.7	54.00	F	237.5	9.85	M

Our dataset is completely balanced, having the same number of males than females.

3.3 Analysis

As stated in the introduction we start by conducting a two sample test with the null hypothesis $H_0 : \mu_1 = \mu_2$. We start by extracting the basic stats from the data and computing the Hotelling's T^2 statistic:

$$\begin{aligned}\bar{\vec{x}}_1 &= \begin{pmatrix} 348.28 \\ 37.26 \end{pmatrix}, \bar{\vec{x}}_2 = \begin{pmatrix} 228.75 \\ 7.29 \end{pmatrix} \\ S_{pooled} &= \begin{pmatrix} 2606.4 & 667.9 \\ 667.9 & 204.2 \end{pmatrix} \\ T^2 &= (\bar{\vec{x}}_1 - \bar{\vec{x}}_2)^T \left(\frac{1}{n_1} + \frac{1}{n_2} \right) S_{pooled}^{-1} (\bar{\vec{x}}_1 - \bar{\vec{x}}_2) = 76.92\end{aligned}$$

We compare this value to:

$$F = \frac{(n_1 + n_2 - 2)p}{n_1 + n_2 - 1 - p} \cdot F_{p, n_1 + n_2 - 1 - p}(\alpha) = 6.463$$

Since $76.92 > 6.463$, we reject H_0 , concluding that both populations are, indeed, different. We can now proceed with linear discrimination analysis. For a given new response \vec{x}_0 we will classify it in the first population if and only if:

$$(\bar{\vec{x}}_1 - \bar{\vec{x}}_2)^T \cdot S_{pooled}^{-1} \cdot (\vec{x}_0 - \frac{1}{2}(\bar{\vec{x}}_1 - \bar{\vec{x}}_2)) \geq 0$$

That is, if and only if:

$$0.05095 - 0.01986 \cdot (\vec{x}_0 - \begin{pmatrix} 288.5 \\ 22.28 \end{pmatrix}) \geq 0$$

In order to measure how good this classifier is we use two methods:

- The Apparent Error Rate (AER): Try to predict every single sample by training the model with every point in the dataset (including the one we will predict), and then use it for the prediction.
- The Expected Actual Error Rate (EAER): Using the same technique but exclude the point that we will predict from the train set.

In this case we obtain the same value for both measures: a $0.08929 = \frac{5}{56}$ error rate, missing 5 samples. Finally, let's plot our populations and their respective mean-centered mahalanobis-distance ellipses to gain a geometry perspective of what is going on here:

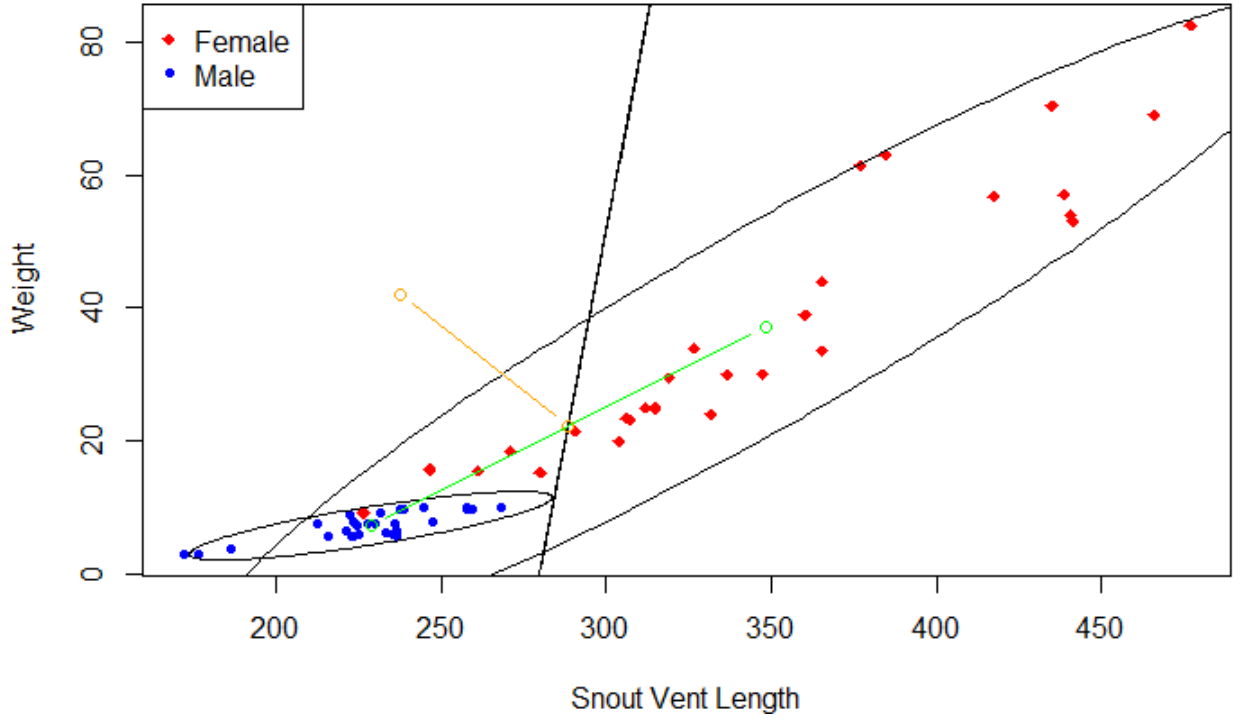


Figure 1: Anaconda dataset partition

In this figure we can see the two different classes in red (female) and blue (male). We have also plotted each population mean-centered ellipse and a green line joining their centers. We can rewrite our test using the following: \vec{x}_0 will be classified as Female (class 1) if and only if:

$$\vec{\omega}^T \cdot \vec{\omega}_0 \geq 0$$

Where:

$$\vec{\omega} = (\vec{x}_1 - \vec{x}_2)^T \cdot S_{pooled}^{-1}$$

$$\vec{\omega}_0 = (\vec{x}_0 - \frac{1}{2}(\vec{x}_1 - \vec{x}_2))$$

What we are computing here is the cosine of the angle between $\vec{\omega}$ and $\vec{\omega}_0$. If the absolute value of the angle is less than 90° , the cosine will be positive, so we are just studying this angle. In 1, we plot $\vec{\omega}$ in orange, while $\vec{\omega}_0$ will be a vector from the middle point of the green segment to the given new response \vec{x}_0 .

The easiest way to see this geometrically is to plot a perpendicular line to $\vec{\omega}$. This is the black line (although it doesn't seem perpendicular, this is because of the different scale in the axis). If the point is on the right side of the line, $\vec{\omega}_0$ and $\vec{\omega}$ will create an angle smaller than 90° , classifying \vec{x}_0 as Female, while if the point is on the left side of the line, $\vec{\omega}_0$ and $\vec{\omega}$ will create an angle greater than 90° , classifying \vec{x}_0 as Male.