

Contents

<i>Contents</i>	1
1 Data Mining and Analysis	3
1.7 Exercises	3
PART I DATA ANALYSIS FOUNDATIONS	5
2 Numeric Attributes	7
2.7 Exercises	7
3 Categorical Attributes	16
3.7 Exercises	16
4 Graph Data	20
4.6 Exercises	20
5 Kernel Methods	26
5.6 Exercises	26
6 High-dimensional Data	29
6.9 Exercises	29
7 Dimensionality Reduction	39
7.6 Exercises	39
PART II FREQUENT PATTERN MINING	45
8 Itemset Mining	47
8.5 Exercises	47
9 Summarizing Itemsets	56
9.6 Exercises	56
	1

10	Sequence Mining	63
	10.5 Exercises	63
11	Graph Pattern Mining	75
	11.5 Exercises	75
12	Pattern and Rule Assessment	84
	12.4 Exercises	84
PART III	CLUSTERING	89
13	Representative-based Clustering	91
	13.5 Exercises	91
14	Hierarchical Clustering	99
	14.4 Exercises	99
15	Density-based Clustering	106
	15.5 Exercises	106
16	Spectral and Graph Clustering	111
	16.5 Exercises	111
17	Clustering Validation	118
	17.5 Exercises	118
PART IV	CLASSIFICATION	123
18	Probabilistic Classification	125
	18.5 Exercises	125
19	Decision Tree Classifier	129
	19.4 Exercises	129
20	Linear Discriminant Analysis	137
	20.4 Exercises	137
21	Support Vector Machines	141
	21.7 Exercises	141
22	Classification Assessment	145
	22.5 Exercises	145

1.7 EXERCISES

Q1. Show that the mean of the centered data matrix \mathbf{Z} in Eq. (1.5) is $\mathbf{0}$.

Answer: Each centered point is given as: $\mathbf{z}_i = \mathbf{x}_i - \boldsymbol{\mu}$. Their mean is therefore:

$$\begin{aligned} \frac{1}{n} \sum_{i=0}^n \mathbf{z}_i &= \frac{1}{n} \sum_{i=0}^n (\mathbf{x}_i - \boldsymbol{\mu}) \\ &= \frac{1}{n} \sum_{i=0}^n \mathbf{x}_i - \frac{1}{n} \cdot n \cdot \boldsymbol{\mu} \\ &= \boldsymbol{\mu} - \boldsymbol{\mu} = \mathbf{0} \end{aligned}$$

Q2. Prove that for the L_p -distance in Eq. (1.2), we have

$$\delta_\infty(\mathbf{x}, \mathbf{y}) = \lim_{p \rightarrow \infty} \delta_p(\mathbf{x}, \mathbf{y}) = \max_{i=1}^d \{|x_i - y_i|\}$$

for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.

Answer: We have to show that

$$\lim_{p \rightarrow \infty} \left(\sum_{i=1}^d |x_i - y_i|^p \right)^{\frac{1}{p}} = \max_{i=1}^d \{|x_i - y_i|\}$$

Assume that dimension a is the max, and let $m = |x_a - y_a|$. For simplicity, we assume that $|x_i - y_i| < m$ for all $i \neq a$.

If we divide and multiply the left hand side with m^p we get:

$$\left(m^p \sum_{i=1}^d \left(\frac{|x_i - y_i|}{m} \right)^p \right)^{\frac{1}{p}} = m \left(1 + \sum_{i \neq a} \left(\frac{|x_i - y_i|}{m} \right)^p \right)^{\frac{1}{p}}$$

As $p \rightarrow \infty$, each term $\left(\frac{|x_i - y_i|}{m}\right)^p \rightarrow 0$, since $m > |x_i - y_i|$ for all $i \neq a$. The finite summation $\sum_{i \neq a} \left(\frac{|x_i - y_i|}{m}\right)^p$ converges to 0 as $p \rightarrow \infty$, as does $1/p$.

Thus $\delta_\infty(\mathbf{x}, \mathbf{y}) = m \times 1^0 = m = |x_a - y_a| = \max_{i=1}^d \{|x_i - y_i|\}$

Note that the same result is obtained even if we assume that dimensions other than a achieve the maximum value m . In the worst case, we have $m = |x_i - y_i|$ for all d dimensions. In this case, the expression on LHS becomes

$$\lim_{p \rightarrow \infty} m \left(\sum_{i=1}^d 1^p \right)^{1/p} = \lim_{p \rightarrow \infty} m d^{1/p} = \lim_{p \rightarrow \infty} m d^0 = m$$

PART ONE

DATA ANALYSIS FOUNDATIONS

2.7 EXERCISES

Q1. True or False:

- (a) Mean is robust against outliers.

Answer: False

- (b) Median is robust against outliers.

Answer: True

- (c) Standard deviation is robust against outliers.

Answer: False

Q2. Let X and Y be two random variables, denoting age and weight, respectively. Consider a random sample of size $n = 20$ from these two variables

$$X = (69, 74, 68, 70, 72, 67, 66, 70, 76, 68, 72, 79, 74, 67, 66, 71, 74, 75, 75, 76)$$

$$Y = (153, 175, 155, 135, 172, 150, 115, 137, 200, 130, 140, 265, 185, 112, 140, \\ 150, 165, 185, 210, 220)$$

- (a) Find the mean, median, and mode for X .

Answer: The mean, median, and mode are:

$$\mu = \frac{1}{20} \sum_{i=1}^{20} x_i = 1429/20 = 71.45$$

$$\text{median} = (71 + 72)/2 = 71.5$$

$$\text{mode} = 74$$

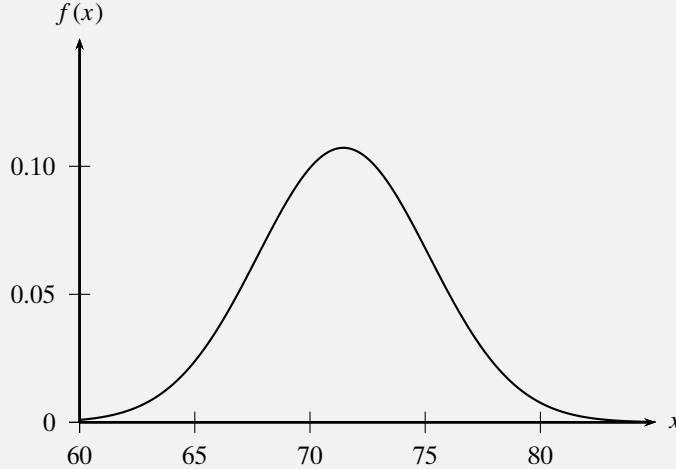
- (b) What is the variance for Y ?

Answer: The mean of Y is $\mu_Y = 3294/20 = 164.7$. The variance is:

$$\sigma_Y^2 = \frac{1}{20} \sum_{i=1}^2 0y_i - \mu_Y = 27384.2/20 = 1369.21$$

(c) Plot the normal distribution for X .

Answer: The mean for X is $\mu_X = 71.45$, and the variance is $\sigma_X^2 = 13.8475$, with a standard deviation of $\sigma_X = 3.72$.



(d) What is the probability of observing an age of 80 or higher?

Answer: If we leverage the empirical probability mass function, we get:

$$P(X \geq 80) = 0/20 = 0$$

since we do not have anyone with age 80 or more in our sample.

We can use the normal distribution modeling, with parameters $\mu_X = 71.45$ and $\sigma_X^2 = 13.8475$ to get:

$$P(X \geq 80) = \int_{80}^{\infty} N(x|\mu_X, \sigma_X) = 0.010769$$

(e) Find the 2-dimensional mean $\hat{\mu}$ and the covariance matrix $\hat{\Sigma}$ for these two variables.

Answer: The mean and covariance matrices are:

$$\begin{aligned} \mu &= (\mu_X, \mu_Y)^T = (71.45, 164.7)^T \\ \Sigma &= \begin{pmatrix} \sigma_X^2 & \sigma_{XY} \\ \sigma_{XY} & \sigma_Y^2 \end{pmatrix} = \begin{pmatrix} 13.8475 & 122.435 \\ 122.435 & 1369.21 \end{pmatrix} \end{aligned}$$

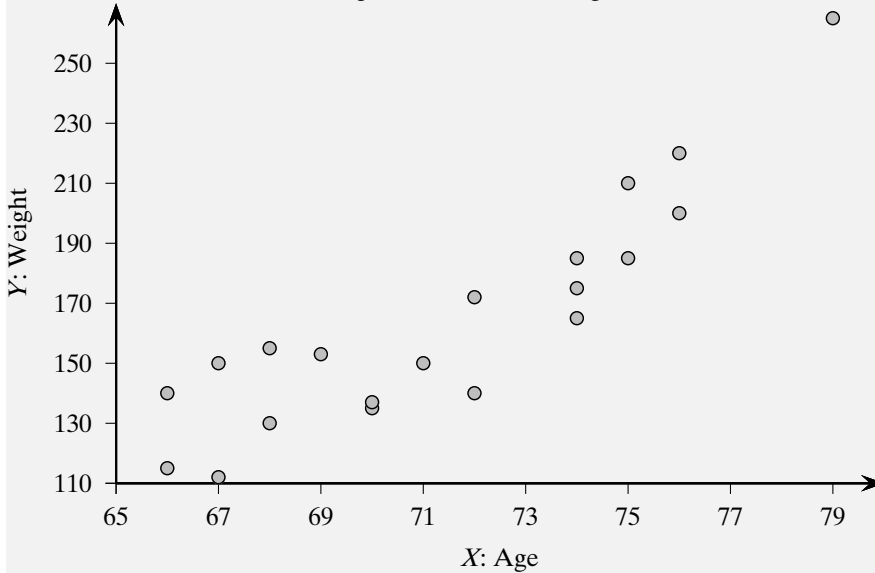
(f) What is the correlation between age and weight?

Answer:

$$\rho_{XY} = \sigma_{XY}/(\sigma_X\sigma_Y) = \frac{122.435}{\sqrt{13.845 \cdot 1369.21}} = 0.889$$

(g) Draw a scatterplot to show the relationship between age and weight.

Answer: The scatterplot is shown in the figure below.



Q3. Show that the identity in Eq. (2.15) holds, that is,

$$\sum_{i=1}^n (x_i - \mu)^2 = n(\hat{\mu} - \mu)^2 + \sum_{i=1}^n (x_i - \hat{\mu})^2$$

Answer: Consider the RHS

$$\begin{aligned} n(\hat{\mu} - \mu)^2 + \sum_{i=1}^n (x_i - \hat{\mu})^2 &= n(\hat{\mu}^2 - 2\hat{\mu}\mu + \mu^2) + \sum_{i=1}^n (x_i^2 - 2x_i\hat{\mu} + \hat{\mu}^2) \\ &= n\hat{\mu}^2 - 2n\hat{\mu}\mu + n\mu^2 + \left(\sum_{i=1}^n x_i^2 \right) - 2n\hat{\mu}^2 + n\hat{\mu}^2 \\ &= \left(\sum_{i=1}^n x_i^2 \right) - 2n\hat{\mu}\mu + n\mu^2 \\ &= \left(\sum_{i=1}^n x_i^2 \right) - 2n \left(\frac{\sum_{i=1}^n x_i}{n} \right) \mu + \sum_{i=1}^n \mu^2 \\ &= \sum_{i=1}^n (x_i - \mu)^2 \end{aligned}$$

Q4. Prove that if x_i are independent random variables, then

$$\text{var} \left(\sum_{i=1}^n x_i \right) = \sum_{i=1}^n \text{var}(x_i)$$

This fact was used in Eq. (2.12).

Answer: We assume for simplicity that all the variables are discrete. A similar approach can be used for continuous variables.

Consider the random variable $x_1 + x_2$. Its mean is given as

$$\mu_{x_1+x_2} = \sum_{x_1=a} \sum_{x_2=b} (a+b) f(a, b)$$

Since x_1 and x_2 are independent, their joint probability mass function is given as:

$$f(x_1, x_2) = f(x_1) \cdot f(x_2)$$

Thus, the mean is given as

$$\begin{aligned} \mu_{x_1+x_2} &= \sum_{x_1=a} \sum_{x_2=b} (a+b) f(a, b) \\ &= \sum_{x_1=a} \sum_{x_2=b} (a+b) f(a) f(b) \\ &= \sum_{x_1=a} f(a) \sum_{x_2=b} (a+b) f(b) \\ &= \sum_{x_1=a} f(a) \left(\sum_{x_2=b} a f(b) + \sum_{x_2=b} b f(b) \right) \\ &= \sum_{x_1=a} f(a) (a + \mu_{x_2}) \\ &= \mu_{x_1} + \mu_{x_2} \end{aligned}$$

In general, we can show that the expected value of the sum of the variables x_i is the sum of their expected values, i.e.,

$$E \left[\sum_{i=1}^n x_i \right] = \sum_{i=1}^n E[x_i]$$

Now, let us consider the variance of the sum of the random variables:

$$\begin{aligned} \text{var} \left(\sum_{i=1}^n x_i \right) &= E \left[\left(\sum_{i=1}^n x_i - E \left[\sum_{i=1}^n x_i \right] \right)^2 \right] \\ &= E \left[\left(\sum_{i=1}^n x_i - \sum_{i=1}^n E[x_i] \right)^2 \right] \\ &= E \left[\left(\sum_{i=1}^n (x_i - E[x_i]) \right)^2 \right] \end{aligned}$$

$$\begin{aligned}
&= E \left[\sum_{i=1}^n (x_i - E[x_i])^2 + 2 \sum_{i=1}^n \sum_{j>i} (x_i - E[x_i])(x_j - E[x_j]) \right] \\
&= \sum_{i=1}^n E \left[(x_i - E[x_i])^2 \right] + 2 \sum_{i=1}^n \sum_{j>i} \text{cov}(x_i, x_j) \\
&= \sum_{i=1}^n \text{var}(x_i)
\end{aligned}$$

The last step follows from the fact that $\text{cov}(x_i, x_j) = 0$ since they are independent.

- Q5.** Define a measure of deviation called *mean absolute deviation* for a random variable X as follows:

$$\frac{1}{n} \sum_{i=1}^n |x_i - \mu|$$

Is this measure robust? Why or why not?

Answer: No, it is not robust, since a single outlier can skew the mean absolute deviation.

- Q6.** Prove that the expected value of a vector random variable $\mathbf{X} = (X_1, X_2)^T$ is simply the vector of the expected value of the individual random variables X_1 and X_2 as given in Eq. (2.18).

Answer: This follows directly from the definition of expectation of a vector random variable. When both X_1 and X_2 are discrete we have

$$\boldsymbol{\mu} = E[\mathbf{X}] = \sum_{\mathbf{x}} \mathbf{x} f(\mathbf{x}) = \sum_{x_1} \sum_{x_2} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} f(x_1, x_2) = \begin{pmatrix} \mu_{X_1} \\ \mu_{X_2} \end{pmatrix}$$

Likewise, when both X_1 and X_2 are continuous we have

$$\boldsymbol{\mu} = E[\mathbf{X}] = \int_{\mathbf{x}} \mathbf{x} f(\mathbf{x}) d\mathbf{x} = \int_{x_1} \int_{x_2} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} f(x_1, x_2) dx_1 dx_2 = \begin{pmatrix} \mu_{X_1} \\ \mu_{X_2} \end{pmatrix}$$

In more detail, assume that both X_1 and X_2 are discrete, we have

$$\begin{aligned}
\boldsymbol{\mu} &= E \left[\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \right] = \sum_{x_1, x_2} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} f(x_1, x_2) = \begin{pmatrix} \sum_{x_1, x_2} x_1 f(x_1, x_2) \\ \sum_{x_1, x_2} x_2 f(x_1, x_2) \end{pmatrix} \\
&= \begin{pmatrix} \sum_{x_1} x_1 \sum_{x_2} f(x_1, x_2) \\ \sum_{x_2} x_2 \sum_{x_1} f(x_1, x_2) \end{pmatrix} = \begin{pmatrix} \sum_{x_1} x_1 f(x_1) \\ \sum_{x_2} x_2 f(x_2) \end{pmatrix} = \begin{pmatrix} E[X_1] \\ E[X_2] \end{pmatrix} = \begin{pmatrix} \mu_{X_1} \\ \mu_{X_2} \end{pmatrix}
\end{aligned}$$

where $f(x_1, x_2) = p(X_1 = x_1, X_2 = x_2)$ is the joint probability mass function of X_1 and X_2 , and $f(x_1) = \sum_{x_2} f(x_1, x_2)$ and $f(x_2) = \sum_{x_1} f(x_1, x_2)$ are the *marginal probability distributions* of X_1 and X_2 , respectively. Note that X_1 and X_2 do not have to be independent for the above to hold.

Q7. Show that the correlation [Eq. (2.23)] between any two random variables X_1 and X_2 lies in the range $[-1, 1]$.

Answer: The Cauchy-Schwartz inequality states that for any two vectors \mathbf{x} and \mathbf{y} in an inner product space, they satisfy:

$$|\langle \mathbf{x}, \mathbf{y} \rangle|^2 \leq \langle \mathbf{x}, \mathbf{x} \rangle \cdot \langle \mathbf{y}, \mathbf{y} \rangle$$

Define the inner product between two random variables X_1 and X_2 as follows:

$$\langle X_1, X_2 \rangle = E[X_1 X_2]$$

Expectation is a valid inner product since it satisfies the three conditions: i) symmetric: $E[X_1 X_2] = E[X_2 X_1]$, ii) positive-semidefinite: $E[X_1 X_1] = E[X_1^2] \geq 0$, and iii) linear: $E[aX_1 X_2] = aE[X_1 X_2]$ and $E[(X_1 + Z)X_2] = E[X_1 X_2] + E[Z X_2]$.

Then, we have

$$\begin{aligned} |\sigma_{12}| &= \left| cov(X_1, X_2) \right|^2 \\ &= \left| E[(X_1 - \mu_1)(X_2 - \mu_2)] \right|^2 \\ &= \left| \langle (X_1 - \mu_1), (X_2 - \mu_2) \rangle \right|^2 \\ &\leq \langle X_1 - \mu_1, X_1 - \mu_1 \rangle \cdot \langle X_2 - \mu_2, X_2 - \mu_2 \rangle \\ &= E[X_1 - \mu_1] \cdot E[X_2 - \mu_2] \\ &= \sigma_1 \cdot \sigma_2 \end{aligned}$$

Since $|\sigma_{12}| \leq \sigma_1 \cdot \sigma_2$, it follows that the correlation $\rho_{12} = \sigma_{12}/\sigma_1\sigma_2$ lies in the range $[-1, 1]$.

Q8. Given the dataset in Table 2.1, compute the covariance matrix and the generalized variance.

Table 2.1. Dataset for Q8

	X_1	X_2	X_3
\mathbf{x}_1	17	17	12
\mathbf{x}_2	11	9	13
\mathbf{x}_3	11	8	19

Answer: The covariance matrix is:

$$\Sigma = \begin{pmatrix} 8.0 & 11.33 & -5.33 \\ 11.33 & 16.22 & -8.56 \\ -5.33 & -8.56 & 9.56 \end{pmatrix}$$

The generalized variance is:

$$\det(\Sigma) = -1.38 \times 10^{-13}$$

- Q9.** Show that the outer-product in Eq.(2.31) for the sample covariance matrix is equivalent to Eq. (2.29).

Answer: Let $\mathbf{z}_i = \mathbf{x}_i - \hat{\boldsymbol{\mu}}$ denote a centered data point. The outer product form of covariance matrix is given as:

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_{i=1}^n \mathbf{z}_i \mathbf{z}_i^T$$

Let us consider the entry in cell (j, k) ; we have:

$$\hat{\boldsymbol{\Sigma}}(j, k) = \frac{1}{n} \sum_{i=1}^n z_{ij} z_{ik} = \frac{1}{n} \sum_{i=1}^n (x_{ij} - \hat{\mu}_j)(x_{ik} - \hat{\mu}_k) = \hat{\sigma}_{jk}$$

which is exactly the covariance between the j -th and k -th attribute.

- Q10.** Assume that we are given two univariate normal distributions, N_A and N_B , and let their mean and standard deviation be as follows: $\mu_A = 4, \sigma_A = 1$ and $\mu_B = 8, \sigma_B = 2$.
- (a) For each of the following values $x_i \in \{5, 6, 7\}$ find out which is the more likely normal distribution to have produced it.

Answer: If we plug-in x_i in the equation for the normal distribution, we obtain the following:

$$\begin{array}{ll} N_A(5) = 0.242 & N_B(5) = 0.065 \\ N_A(6) = 0.054 & N_B(6) = 0.121 \\ N_A(7) = 0.004 & N_B(7) = 0.176 \end{array}$$

Based on these values, we can claim that N_A is more likely to have produced 5, but N_B is more likely to have produced 6 and 7.

We can also solve this problem by finding the z -score for each value. We can then assign a point to the distribution for which it has a lower z -score (in terms of absolute value). For example, for 5, we have $z_A(5) = (5 - 4)/1 = 1$, and $z_B(5) = (5 - 8)/2 = -1.5$. Since $|z_B| > |z_A|$ we can claim that 5 comes from N_A .

For 6 and 7 we have:

$$\begin{array}{ll} z_A(6) = (6 - 4)/1 = 2 & z_B(6) = (6 - 8)/2 = -1 \\ z_A(7) = (7 - 4)/1 = 3 & z_B(7) = (7 - 8)/2 = -0.5 \end{array}$$

Thus, these values are more likely to have been generated from N_B .

- (b) Derive an expression for the point for which the probability of having been produced by both the normals is the same.

Answer: Plugging in the parameters of N_A and N_B into the equation for the normal distribution, and after setting up the equality, we obtain:

$$\frac{1}{\sqrt{2\pi}} e^{-\frac{(x-4)^2}{2}} = \frac{1}{2\sqrt{2\pi}} e^{-\frac{(x-8)^2}{8}}$$

$$2e^{\frac{(x-8)^2}{8}} = e^{\frac{(x-4)^2}{2}}$$

taking ln on both sides yields

$$\begin{aligned} \ln(2) + \frac{(x-8)^2}{8} &= \frac{(x-4)^2}{2} \\ \frac{8\ln(2) + x^2 + 64 - 16x}{8} &= \frac{x^2 + 16 - 8x}{2} \\ 2\ln(2) + x^2/4 - 4x &= x^2 - 8x \\ \frac{3}{4}x^2 - 4x - 2\ln(2) &= 0 \\ 0.75x^2 - 4x - 1.4 &= 0 \end{aligned}$$

We can solve this equation using the general solution for a quadratic equation: $\frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$. Plugging in the values from above we get $x = 5.67$.

Q11. Consider Table 2.2. Assume that both the attributes X and Y are numeric, and the table represents the entire population. If we know that the correlation between X and Y is zero, what can you infer about the values of Y ?

Table 2.2. Dataset for Q11

X	Y
1	a
0	b
1	c
0	a
0	c

Answer: Since the correlation is zero, we have $cov(X, Y) = 0$, which implies that $E[XY] = E[X]E[Y]$. From the data we have

$$E[XY] = (a + c)/5 \quad E[X] = 2/5 \quad E[Y] = (2a + 2c + b)/5$$

Equating these we get

$$\begin{aligned} (a + c)/5 &= 2(2a + 2c + b)/25 \\ 5a + 5c &= 4a + 4c + 2b \\ a + c &= 2b \end{aligned}$$

Q12. Under what conditions will the covariance matrix Σ be identical to the correlation matrix, whose (i, j) entry gives the correlation between attributes X_i and X_j ? What can you conclude about the two variables?

Answer: If the covariance matrix equals the correlation matrix, this means that for all i and j , we have

$$\begin{aligned}\rho_{ij} &= \sigma_{ij} \\ \frac{\sigma_{ij}}{\sigma_i \sigma_j} &= \sigma_{ij} \\ \sigma_i \sigma_j &= 1\end{aligned}$$

Thus, for the covariance matrix to equal the correlation matrix, X_i and X_j must be perfectly correlated; either $\sigma_i = \sigma_j = 1$ or $\sigma_i = \sigma_j = -1$.