

# Honours Multivariate Analysis

## Lecture 4 - Maximum Likelihood Estimation and Testing for Normality

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# Course Outline

- ① Introduction, Examples of Multivariate Data <sup>†</sup>
- ② TOOLS
  - ① Visualization and Summary Statistics <sup>†</sup>
  - ② Singular Value Decomposition, Eigenvalue Decomposition and Spectral Decomposition revisited <sup>†</sup>
  - ③ The Multivariate Normal Distribution <sup>†</sup>
  - ④ Multivariate Maximum Likelihood Estimation <sup>†</sup>
  - ⑤ Multivariate Inference <sup>†</sup>
- ③ EXPLORATORY ANALYSIS
  - ① Principal Component Analysis §
  - ② Factor Analysis §
  - ③ Correspondence Analysis §
- ④ CONFIRMATORY ANALYSIS
  - ① For grouped Multivariate Data:
    - ① Manova <sup>†</sup>
    - ② Discriminant Analysis §
  - ② Regression
    - ① Multivariate Regression §
    - ② Canonical Correlation Analysis §

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# The MVN Density and Likelihood

Consider a random sample,  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$  from the multivariate normal population  $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , with the  $\mathbf{X}_j$ 's mutually independent.

The joint density of  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$  is given by

$$\begin{aligned} f(\mathbf{x}_1, \dots, \mathbf{x}_n) &= \prod_{j=1}^n \frac{1}{(2\pi)^{\frac{p}{2}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp \left[ -\frac{1}{2} (\mathbf{x}_j - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x}_j - \boldsymbol{\mu}) \right] \\ &= \left( \frac{1}{(2\pi)^{\frac{p}{2}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \right)^n \exp \left[ -\frac{1}{2} \sum_{j=1}^n (\mathbf{x}_j - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x}_j - \boldsymbol{\mu}) \right] \end{aligned}$$

# The MVN Density and Likelihood

This joint density, written as a function of the variables, regards the parameters as fixed, albeit unknown, constants.

However, when observations are made, i.e. we are given values for  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ , then we can consider this expression to be a function of the parameters, referred to as the *likelihood*.

We are therefore trying to ascertain how likely specific values of the parameters  $\boldsymbol{\mu}$  and  $\boldsymbol{\Sigma}$  (viewed as variable) are, given our fixed observations.

$$\therefore L(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \left( \frac{1}{(2\pi)^{\frac{p}{2}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \right)^n \exp \left[ -\frac{1}{2} \sum_{j=1}^n (\mathbf{x}_j - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x}_j - \boldsymbol{\mu}) \right]$$

# The MVN Density and Likelihood

For ease of notation to follow, define

$$\mathbf{A} = (n - 1)\mathbf{S} = \mathbf{X}'\mathbf{X} - n\bar{\mathbf{x}}\bar{\mathbf{x}}' = \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})'$$

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The summation in the exponent of the likelihood function can then be written as

$$\sum_{j=1}^n (\mathbf{x}_j - \boldsymbol{\mu})'\boldsymbol{\Sigma}^{-1}(\mathbf{x}_j - \boldsymbol{\mu}) = \text{tr} [\boldsymbol{\Sigma}^{-1}\mathbf{A}] + n(\bar{\mathbf{x}} - \boldsymbol{\mu})'\boldsymbol{\Sigma}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu})$$

Make sure you go through the steps in the notes!

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Make sure you go through the steps in the notes!

We can now write the joint likelihood function as

$$L(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{np}{2}} |\boldsymbol{\Sigma}|^{-\frac{n}{2}} \exp \left[ -\frac{1}{2} \text{tr} [\boldsymbol{\Sigma}^{-1}\mathbf{A}] - \frac{n}{2} (\bar{\mathbf{x}} - \boldsymbol{\mu})'\boldsymbol{\Sigma}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu}) \right]$$

# MLE of $\mu$

We consider  $\Sigma$  as fixed and maximise

$$\begin{aligned}\log[L(\mu, \Sigma)] &= l(\mu, \Sigma) \\ &= -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{1}{2} \text{tr}[\Sigma^{-1} A] - \frac{n}{2} (\bar{x} - \mu)' \Sigma^{-1} (\bar{x} - \mu)\end{aligned}$$

with respect to  $\mu$ .

**By inspection:**

$$\begin{aligned}l &= -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{1}{2} \text{tr}[\Sigma^{-1} A] - \frac{n}{2} (\bar{x} - \mu)' \Sigma^{-1} (\bar{x} - \mu) \\ &\leq -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{1}{2} \text{tr}[\Sigma^{-1} A]\end{aligned}$$

with equality when  $\frac{n}{2} (\bar{x} - \mu)' \Sigma^{-1} (\bar{x} - \mu) = 0$ , i.e., when

$$\hat{\mu} = \bar{x}.$$



# MLE of $\mu$

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$$\begin{aligned}\log[L(\mu, \Sigma)] &= l(\mu, \Sigma) \\ &= -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{1}{2} \text{tr}[\Sigma^{-1} \mathbf{A}] - \frac{n}{2} (\bar{x} - \mu)' \Sigma^{-1} (\bar{x} - \mu)\end{aligned}$$

with respect to  $\mu$ .

**By differentiation:**

$$\begin{aligned}\frac{\partial l}{\partial \mu} &= -\frac{n}{2} 2\Sigma^{-1}(\bar{x} - \mu)(-1) && \text{(See Theorem A.1)} \\ n\Sigma^{-1}(\bar{x} - \hat{\mu}) &= \mathbf{0} \\ \hat{\mu} &= \bar{x}\end{aligned}$$

# MLE of $\mu$

Showing that  $\hat{\mu} = \bar{x}$  is indeed a maximum and not a minimum or saddle point:

$$\frac{\partial^2 l}{\partial \mu \mu'} = \frac{\partial}{\partial \mu'} \{n \Sigma^{-1} \bar{x} - n \Sigma^{-1} \mu\} = -n \Sigma^{-1}$$

which is negative definite. Note that  $\Sigma^{-1}$  is positive definite since  $\Sigma$  is positive definite and symmetric.

# MLE of $\Sigma$

Let  $\hat{\mu} = \bar{x}$ . We first need to find the stationary point of  $l(\hat{\mu}, \Sigma)$  through differentiation with respect to  $\Sigma^{-1}$ , then show that the stationary point is a maximum. See Theorems A.2 & A.3.

$$\begin{aligned}l(\hat{\mu} = \bar{x}, \Sigma) &= -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{1}{2} \text{tr}[\Sigma^{-1} \mathbf{A}] \\&= -\frac{np}{2} \log(2\pi) + \frac{n}{2} \log |\Sigma^{-1}| - \frac{1}{2} \text{tr}[\Sigma^{-1} \mathbf{A}] \\ \frac{\partial l}{\partial \Sigma^{-1}} &= \frac{n}{2} [(\Sigma^{-1})^{-1}]' - \frac{1}{2} \mathbf{A}'\end{aligned}$$

$$\frac{n}{2} \hat{\Sigma} - \frac{1}{2} \mathbf{A} = \mathbf{0}$$

$$n \hat{\Sigma} = \mathbf{A}$$

$$\hat{\Sigma} = \frac{1}{n} \mathbf{A} = \frac{n-1}{n} \mathbf{S}$$

# MLE of $\Sigma$

To show that this stationary point is a maximum, taking the second order derivative with respect to  $\Sigma^{-1}$  is complicated. Therefore, the likelihood is reparameterised. See the course notes for the gory details.

When substituting  $\hat{\mu}$  and  $\hat{\Sigma}$  into the likelihood, we end up with the following expression for the maximised likelihood:

$$\begin{aligned} L(\hat{\mu}, \hat{\Sigma}) &= (2\pi)^{-\frac{np}{2}} |\hat{\Sigma}|^{-\frac{n}{2}} \exp \left[ -\frac{1}{2} \text{tr} \left[ \hat{\Sigma}^{-1} \mathbf{A} \right] - \frac{n}{2} (\bar{x} - \hat{\mu})' \hat{\Sigma}^{-1} (\bar{x} - \hat{\mu}) \right] \\ &= (2\pi)^{-\frac{np}{2}} \left| \frac{1}{n} \mathbf{A} \right|^{-\frac{n}{2}} \exp \left[ -\frac{1}{2} \text{tr} \left[ n \mathbf{A}^{-1} \mathbf{A} \right] \right] \\ &= (2\pi)^{-\frac{np}{2}} \left| \frac{1}{n} \mathbf{A} \right|^{-\frac{n}{2}} e^{-\frac{np}{2}} \end{aligned}$$

# Homework exercise 4.1

Johnson & Wichern exercise 4.18

Find the maximum likelihood estimates of  $\mu_{2 \times 1}$  and  $\Sigma_{2 \times 2}$  based on the random sample

$$\begin{bmatrix} 3 & 6 \\ 4 & 4 \\ 5 & 7 \\ 4 & 7 \end{bmatrix}$$

from a bivariate normal population.

# Sampling Distribution of $\bar{X}$

Reminder of the univariate case:

If  $X_1, X_2, \dots, X_n$  are i.i.d random observation from  $X \sim N(\mu, \sigma^2)$ , then

$$\bar{X} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$$

and

$$\frac{(n-1)s^2}{\sigma^2} \sim \chi_{n-1}^2$$

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**The multivariate case:**

Now suppose we observe  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$ , which are i.i.d random vectors drawn from  $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ .

For the sample mean we have

$$\bar{\mathbf{X}} \sim N_p\left(\boldsymbol{\mu}, \frac{1}{n}\boldsymbol{\Sigma}\right)$$

# Sampling Distribution of $S$

For the sample variance, note that the univariate case can be expressed as

$$\begin{aligned}(n-1)s^2 &\sim \sigma^2 \chi_{n-1}^2 \\ &= \sigma^2 (Z_1^2 + \dots + Z_{n-1}^2) \\ &= (\sigma Z_1)^2 + \dots + (\sigma Z_{n-1})^2\end{aligned}$$

with each  $\sigma Z_i = X_i - \mu \sim N(0, \sigma^2)$ .

This form is suitably generalized to the basic sampling distribution of the covariance matrix, namely the **Wishart distribution**.

This distribution is the multivariate analogue of the  $\chi^2$ -distribution.



# Sampling Distribution of $S$

If we define  $\mathbf{Y}_i = \mathbf{X}_i - \boldsymbol{\mu} \sim N_p(\mathbf{0}, \boldsymbol{\Sigma})$  and let  $\mathbf{Y}$  represent the  $p \times n$  matrix constructed from the  $n$  independent observations of  $\mathbf{X}_i$ , then

$$\mathbf{Y}\mathbf{Y}' = \sum_{i=1}^n (\mathbf{X}_i - \boldsymbol{\mu})(\mathbf{X}_i - \boldsymbol{\mu})' \sim W_p(n, \boldsymbol{\Sigma})$$

We say that  $\mathbf{Y}\mathbf{Y}'$  is  $p$ -dimensional Wishart distributed with  $n$  degrees of freedom.

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We say that  $\mathbf{Y}\mathbf{Y}'$  is  $p$ -dimensional Wishart distributed with  $n$  degrees of freedom.

Similar to the univariate case, when  $\bar{\mathbf{X}}$  is substituted for  $\boldsymbol{\mu}$ , the distribution remains Wishart, but with one less degree of freedom:

$$\sum_{i=1}^n (\mathbf{X}_i - \bar{\mathbf{X}})(\mathbf{X}_i - \bar{\mathbf{X}})' = \mathbf{A} = (n-1)\mathbf{S} \sim W_p(n-1, \boldsymbol{\Sigma})$$

$$\mathbf{S} \sim W_p\left(n-1, \frac{1}{n-1}\boldsymbol{\Sigma}\right)$$

# Properties of the Wishart distribution

Given  $\mathbf{A} \sim W_p(n, \mathbf{\Sigma})$ , we note the following properties:

- The Wishart distribution is a generalization of the  $\chi^2$ -distribution, where  $W_1(n, \sigma^2) = \sigma^2 \chi_n^2$ .

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- $\text{tr}(\mathbf{A}) \sim \chi_{np}^2$ .

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for  $\mathbf{A}$  positive definite.

- $\text{tr}(\mathbf{A}) \sim \chi_{np}^2$ .
- $E(\mathbf{A}) = n \mathbf{\Sigma}$ .



# Summary of Sampling distribution results

Let  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$  be a random sample from  $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . Then

- ①  $\bar{\mathbf{X}} \sim N_p\left(\boldsymbol{\mu}, \frac{1}{n}\boldsymbol{\Sigma}\right)$
- ②  $(n-1)\mathbf{S} \sim W_p(n-1, \boldsymbol{\Sigma})$
- ③  $\bar{\mathbf{X}}$  and  $\mathbf{S}$  are independent.
- ④  $\bar{\mathbf{X}}$  and  $\mathbf{S}$  are *sufficient statistics* for  $\boldsymbol{\mu}$  and  $\boldsymbol{\Sigma}$ .

# Large Sample behaviour of $\bar{X}$ and $S$

If  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$  are independent observations from some population with mean  $\boldsymbol{\mu}$  and finite, nonsingular covariance  $\boldsymbol{\Sigma}$ , then

$$\bar{\mathbf{X}} \dot{\sim} N_p\left(\boldsymbol{\mu}, \frac{1}{n}\boldsymbol{\Sigma}\right) \text{ or, equivalently, } \sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu}) \dot{\sim} N_p(\mathbf{0}, \boldsymbol{\Sigma})$$

and

$$n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu}) \dot{\sim} \chi_p^2$$

for large  $n - p$ .

## Homework exercise 4.2

Johnson & Wichern exercises 4.19 & 4.21 (combined)

Let  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{60}$  be a random sample of size  $n = 60$  from an  $N_6(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  population. Specify each of the distributions completely (indicate if the distribution is approximate):

①  $\bar{\mathbf{X}}$  and  $\sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu})$

②  $(\mathbf{X}_1 - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{X}_1 - \boldsymbol{\mu})$

③  $(n - 1)\mathbf{S}$

④  $n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu})$

⑤  $n(\bar{\mathbf{X}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \boldsymbol{\mu})$

# Testing the Assumption of Normality

Up until now we have been **assuming** MVN observations.

To determine whether the observations  $\mathbf{X}_j$  appear to violate the assumption that they jointly came from a multivariate normal population, we address the following questions:

- 1 Do the marginal distributions of the elements of  $\mathbf{X}$  appear to be normal?
- 2 Do the scatter plots of the pairs of observations on different characteristics give the elliptical appearance expected from normal populations?
- 3 Are there any “wild” observations that should be checked?

# Univariate assessment – QQ-plots

QQ-plots, or quantile-quantile plots:

- Quick, visual way of assessing how closely the distribution of observed data matches some theoretical distribution
- Plot the sample quantile versus the quantile one would expect to observe if the observations were actually normally distributed

# Univariate assessment – QQ-plots

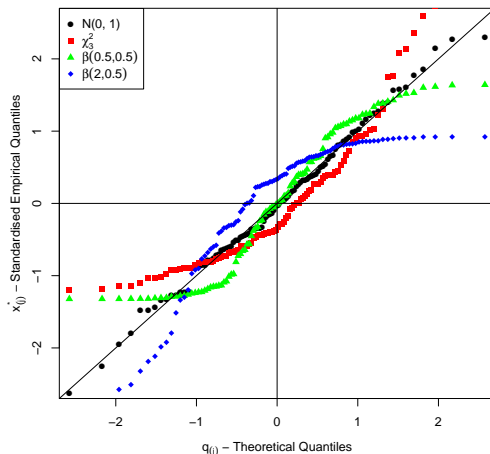
QQ-plots, or quantile-quantile plots:

- If we order the  $n$  observations such that  $x_{(1)} \leq x_{(2)} \leq \dots \leq x_{(n)}$ , then if the  $x_{(j)}$  are distinct, exactly  $j$  observations will be less than or equal to  $x_{(j)}$
- The proportion of the sample at or to the left of  $x_{(j)}$ , i.e.  $\frac{j}{n}$ , is often approximated by  $\frac{j - \frac{1}{2}}{n}$  for analytical convenience
- The quantiles for a standard normal distribution are defined as those values  $q_{(j)}$  such that

$$\Pr[Z \leq q_{(j)}] = \int_{-\infty}^{q_{(j)}} \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}} dz = p_{(j)} = \frac{j - \frac{1}{2}}{n}$$

# Univariate assessment – QQ-plots

Under the assumption of normality, a plot of  $(q_{(j)}, x_{(j)}^*)$  for all  $j$  should be a straight line through the origin, where  $x_{(j)}^*$  denotes the standardised values of  $x$



# Univariate assessment – correlation test

To formally test the linearity, we can calculate the correlation coefficient for the QQ plot, defined as

$$r_q = \frac{\sum_{j=1}^n (x_{(j)} - \bar{x})(q_{(j)} - \bar{q})}{\sqrt{\sum_{j=1}^n (x_{(j)} - \bar{x})^2} \sqrt{\sum_{j=1}^n (q_{(j)} - \bar{q})^2}}$$

and compare it to a table of critical values, given in Appendix B.



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and compare it to a table of critical values, given in Appendix B.

Many other formal tests for univariate normality exist, for example:

- Shapiro-Wilk
- Anderson-Darling
- Jarque-Bera
- Lilliefors test
- etc.

# Multivariate assessment

We can now compare the contours of constant density from observed data with the ellipsoid as defined in chapter 3.3, where a set of bivariate outcomes  $\mathbf{x}$  such that

$$(\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \leq \chi_p^2(\alpha)$$

has probability  $1 - \alpha$ .

- Typically we calculate the above for  $\alpha = 0.5$  and calculate the proportion of points for which the squared distance is less than  $\chi_p^2(0.5)$ .
- If this deviates from 50%, it is evidence against the assumption of normality.

# Multivariate assessment

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Again, many other formal test can be applied:

- Mardia
- Henze-Zirkler
- Royston
- etc.

# Multivariate assessment

We can also construct a chi-square plot based on the assumption that, given underlying normality, the squared distances,  $d_j^2 = (\mathbf{x}_j - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}_j - \bar{\mathbf{x}})$  should behave like chi-square random variables.

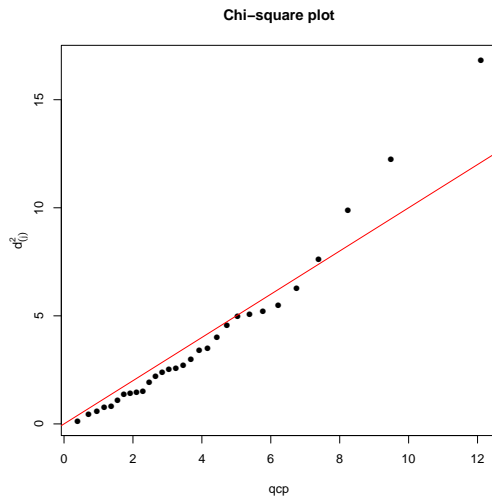
To construct these plots,

- 1 Calculate  $d_j^2 = (\mathbf{x}_j - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}_j - \bar{\mathbf{x}})$ .
- 2 Order the squared distances from smallest to largest as  $d_{(1)}^2 \leq d_{(2)}^2 \leq \dots \leq d_{(n)}^2$ .
- 3 Graph the pairs  $\left( q_{c,p} \left( \frac{j - \frac{1}{2}}{n} \right), d_{(j)}^2 \right)$  where  $q_{c,p} \left( \frac{j - \frac{1}{2}}{n} \right) = \chi_p^2 \left( \frac{n - j + \frac{1}{2}}{n} \right)$ .

If the variables are multivariate normal distributed, the plot should be a straight line through the origin.

# Example

Example 4.14 on page 186 of Johnson & Wichern. Solution in `Lecture4.R`.



# Caution!

It is important to note the following crucial drawbacks of all measures of fit:

With small samples, only severe deviations will indicate lack of fit, whilst very large samples will invariably produce statistically significant lack of fit.

# Homework exercise 4.3

Johnson & Wichern exercises 4.28 & 4.29 (combined)

Consider the air pollution data

- 1 Construct a QQ-plot for the solar radiation measurements and carry out a test for normality based on the correlation coefficient  $r_q$ . You are not prescribed to use a specific  $\alpha$ -value; what can you report based on Table B.1?

Now examine the pairs  $X_5 = \text{NO}_2$  and  $X_6 = \text{O}_3$  for bivariate normality.

- 2 Calculate the distances  $(\mathbf{x}_j - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}_j - \bar{\mathbf{x}})$ ,  $j = 1, 2, \dots, 42$ , where  $\mathbf{x}'_j = [x_{j5}, x_{j6}]$ .
- 3 Determine the proportion of observations  $\mathbf{x}'_j = [x_{j5}, x_{j6}]$ ,  $j = 1, 2, \dots, 42$  falling within the approximate 50% probability contour of a bivariate normal distribution.
- 4 Construct a chi-square plot for the ordered distances in Part 3.