MS-E2112 Multivariate Statistical Analysis (5cr)
Lecture 1: Introduction, Multivariate Location and Scatter

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Practical Things

Practical Things

- Lecturer: Pauliina Ilmonen, pauliina.ilmonen(a)aalto.fi
- The first lecture is on Monday January 9th at 12.15-14.00
- Exercises: Jaakko Pere, jaakko.pere(a)aalto.fi
- There are four exercise groups, choose the one that fits best to your schedule

Self Study

Before the course starts, make sure that you know how to calculate the univariate means, medians, variances, and max and min values. Familiarize yourself with the correlation coefficients and common graphical presentations (boxplots, scatter plots, histograms, bar plots, pie charts) of data. Learn to calculate the multivariate mean vector and covariance matrix. Make sure that you know what is a cumulative distribution function, a probability density function, and a probability mass function. Make sure that you know what is the expected value of a random variable. Read about univariate and multivariate normal distributions and elliptical distributions. Make sure that you know what is meant by central symmetric distributions and skew distributions. Recall what are the determinant, eigenvectors and eigenvalues of a matrix and make sure that you know what is meant by a symmetric matrix and a positive definite matrix.

How to pass this course?

You are expected to

- Attend the lectures and be active - not compulsory, no points, but highly recommended.
- Submit your project work on time - THIS IS COMPULSORY - max 6 points.
- Take the exam - max 24 points. (The course examinations is on Friday 21.4.)
- Participate to weekly exercises (group 1, group 2, group 3 OR group 4) - not compulsory, but highly recommended - max 3 points.
- Be ready to present your homework solutions in the exercise group - not compulsory, but highly recommended - max 3 points.

Max total points $= 6 + 24 + 3 + 3 = 36$. You need at least 16 points in order to pass the course.

Exercises

Participate to weekly exercises (group 1, group 2, group 3 OR group 4) - not compulsory, but highly recommended - max 3 points. If you attend 2-3 times, you get 1 point. If you attend 4-5 times, you get 2 points. If you attend at least 6 times (out of 11 times), you get 3 points.

In order to earn the exercise points, you have to arrive on time to the exercise session. The names of the participants are collected at the beginning of each exercise class. You can not get any exercise points without attending the exercises.

Exercise session 11 is reserved for the project work and for summarizing the contents of the course.

Attending all the exercise sessions, including the last one, is highly recommended!

Homework

Solve the homework problems and be ready to present your solutions in the exercise group - not compulsory, but highly recommended - max 3 points. Note that your solution does not have to be perfect or even correct — trying your very best is enough! If you solve your homework assignments 2-3 times, you get 1 point. If you solve your homework assignments 4-5 times, you get 2 points. If you solve your homework assignments at least 6 times (out of 10 times), you get 3 points.

In order to earn the homework points, you have to arrive on time to the exercise session and write your name to the homework list. You can not get any homework points without attending the exercises.

Project Work

Find a multivariate (at least 3-variate) dataset (Statistics Finland (=Tilastokeskus), OECD, collect yourself, ...), set a research question, and perform multivariate analysis. Write a report (max 10 pages), and submit it in MyCourses before Friday 14.4. at 12.00 (midday).

Goals of the project work:

- Description of the research questions
- Description of the dataset
- Univariate and bivariate statistical analysis to present the variables
- Application of your chosen multivariate statistical methods to answer research questions (justification and output)
- Conclusions and answers to the question raised at the beginning
- Critical evaluation of the analysis

Remember that No findings is a finding! Note that you will automatically get 0 points from the exam if you will not submit your project work on time!

How to get a good grade?

- Attend the lectures and be active!
- Work hard on your project work.
- Be active in exercises!
- Study for the exam!

Grading is based on the total points as follows: 16p -> 1, 20p -> 2, 24p -> 3, 28p -> 4, 32p -> 5.

Introduction

Introduction

The first step of all statistical analysis is the univariate and bivariate analysis. First calculate the univariate means, medians, variances, max and min values. Then calculate the correlation coefficients. And take a look at your data — literally! Make histograms of continuous variables and pie charts of categorical variables. Make boxplots to detect univariate outliers, and make scatter plots to detect bivariate structures.

Note that visualization is not always easy when the data contains a large number of individuals, but do not skip plotting your data! It is very important that you get familiar with your data before you conduct any large multivariate analysis.

Multivariate Location and Scatter

Multivariate Data

Let x denote a p-variate random vector with a cumulative distribution function F_x. Let X denote a $n \times p$ data matrix of independent and identically distributed (i.i.d.) observations $x_1, x_2, ..., x_n$ from the distribution F_x.

Location Functionals

Definition

A $p \times 1$ vector-valued functional $T(F_x)$, which is affine equivariant in the sense that

$$T(F_{Ax+b}) = AT(F_x) + b$$

for all nonsingular $p \times p$ matrices A and for all p-vectors b, is called a location functional.

Scatter Functionals

Definition

A $p \times p$ matrix-valued functional $S(F_x)$ which is positive definite and affine equivariant in the sense that

$$S(F_{Ax+b}) = AS(F_x)A^T$$

for all nonsingular $p \times p$ matrices A and for all p-vectors b, is called a scatter functional.

Location and Scatter Estimates

The corresponding sample statistics are obtained if the functionals are applied to the empirical cumulative distribution F_n based on a sample $x_1, x_2, \ldots, x_n$. Notation $T(F_n)$ and $S(F_n)$ or $T(X)$ and $S(X)$ is used for the sample statistics. The location and scatter sample statistics then also satisfy

$$T(XA^T + 1_n b^T) = AT(X) + b$$

and

$$S(XA^T + 1_n b^T) = AS(X)A^T$$

for all nonsingular $p \times p$ matrices A and for all p-vectors b.

Scatter Functionals

Scatter matrix functionals are usually standardized such that in the case of standard multivariate normal distribution $S(F_x) = I$.

Shape Functionals

Definition

If a positive definite $p \times p$ matrix-valued functional $S(F_x)$ satisfies that $S(F_{Ax+b})$ is proportional to $AS(F_x)A^T$ for all nonsingular $p \times p$ matrices A and for all p-vectors b, then $S(F_x)$ is called a shape functional.

Traditional Functionals

The first examples of location and scatter functionals are the mean vector and the regular covariance matrix:

$$T_1(F_x) = E(x) \text{ and } S_1(F_x) = Cov(F_x) = E\left((x - E(x))(x - E(x))^T\right).$$

The Sample Mean Vector and the Sample Covariance Matrix

Traditional estimates of the mean vector and the covariance matrix are calculated as follows:

$$T_1(X) = \frac{1}{n}\sum_{i=1}^{n} x_i$$

and

$$S_1(X) = Cov(X) = \frac{1}{n-1}\sum_{i=1}^{n}\left((x_i - T_1(X))(x_i - T_1(X))^T\right).$$

Why do we need other location and scatter measures???

Scatter Functionals

There are several other location and scatter functionals, even families of them, having different desirable properties (robustness, efficiency, limiting multivariate normality, fast computations, etc).

Moment Based Functionals

Location and scatter functionals can be based on the third and fourth moments as well. A location functional based on third moments is

$$T_2(F_x) = \frac{1}{p} E\left((x - E(x))^T Cov(F_x)^{-1}(x - E(x))x\right)$$

and a scatter matrix functional based on fourth moments is

$$S_2(F_x) = \frac{1}{p+2} E\left((x - E(x))(x - E(x))^T Cov(F_x)^{-1}(x - E(x))(x - E(x))^T\right).$$

Example 1: Bivariate Normal Distribution

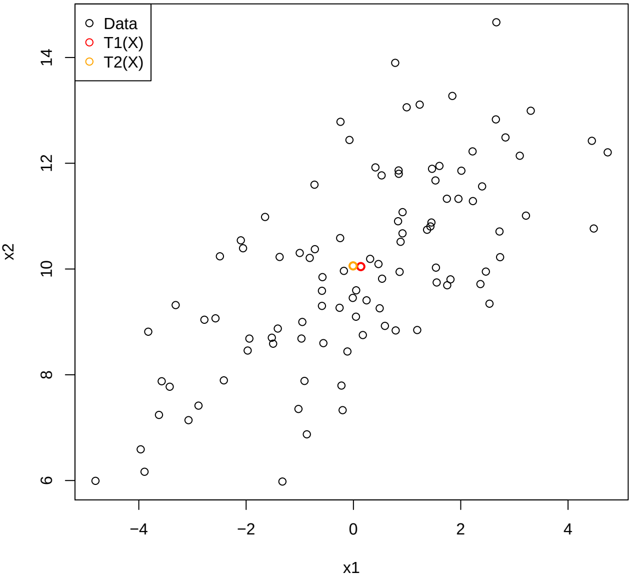
In this example we consider bivariate normal distribution $N(\mu, \mathrm{A})$, where

$$\mathrm{A} = \begin{bmatrix} 4 & 2 \\ 2 & 3 \end{bmatrix}$$

and

$$\mu = \begin{bmatrix} 0 & 10 \end{bmatrix}.$$

Example 1: Bivariate Normal Distribution



Example 1: Bivariate Normal Distribution

We simulated 100 samples from $N(\mu, \mathrm{A})$ and we then calculated the sample mean vector $T_1(X)$, the location vector based on third moments $T_2(X)$, the sample covariance matrix $S_1(X)$ and the scatter matrix based on fourth moments $S_2(X)$ of each sample. In order to compare $T_1(X)$, $T_2(X)$, $S_1(X)$, and $S_2(X)$, we calculated the means of the estimates.

$$T_1(X): \begin{bmatrix} 0.006703295 \\ 10.001765054 \end{bmatrix} \qquad T_2(X): \begin{bmatrix} 0.01626947 \\ 9.99082058 \end{bmatrix}$$

$$S_1(X): \begin{bmatrix} 4.029396 & 2.034711 \\ 2.034711 & 2.968536 \end{bmatrix} \qquad S_2(X): \begin{bmatrix} 3.9197916 & 2.003406 \\ 2.003406 & 2.924344 \end{bmatrix}$$

Both location estimates seem to estimate the parameter μ and both scatter estimates seem to estimate the parameter A.

Example 2: Independent Components, Skewed Distributions

In this example we consider $\mathrm{Gamma}(\alpha, \beta)$ and $\chi^2(k)$ distributions, where

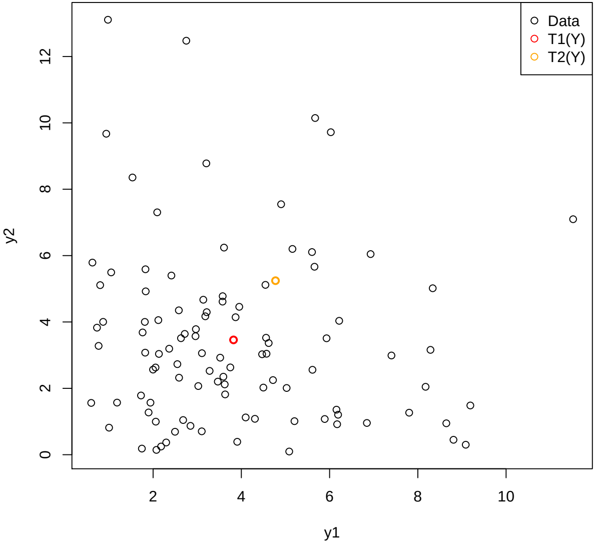
$$\alpha = 2,$$

$$\beta = 0.5$$

and

$$k = 3.$$

Example 2: Independent Components, Skewed Distributions



Example 2: Independent Components, Skewed Distribution

As in Example 1, we ran the simulation 100 times and calculated the means.

$$T_1(Y): \begin{bmatrix} 4.031022 \\ 2.964918 \end{bmatrix} \qquad T_2(Y): \begin{bmatrix} 5.944029 \\ 4.740199 \end{bmatrix}$$

$$S_1(Y): \begin{bmatrix} 8.16111692 & 0.04234064 \\ 0.04234064 & 5.76640662 \end{bmatrix} \qquad S_2(Y): \begin{bmatrix} 13.4080726 & 0.1142734 \\ 0.1142734 & 9.8194396 \end{bmatrix}$$

Here the location estimates differ significantly from each other. Also the scatter estimates differ significantly from each other. Note also that the off-diagonal elements of both scatter estimates are small.

Location and Scatter Functionals Under Symmetry Assumptions

We now consider the behavior of scatter and location functionals under some symmetry assumptions.

Theorem

Under the assumption of central symmetry, all location functionals are equal to the center of symmetry.

Proof

Let x denote a p-variate random vector with a cumulative distribution function F_x. Let $\theta \in \mathbb{R}^p$ and assume that $x - \theta \sim -(x - \theta)$. Let T be an affine equivariant location functional and assume that $T(F_x)$ exists as finite quantity.

Since T is affine equivariance and since x is symmetric about θ, we have that

$$T(F_x) - \theta = T(F_{x-\theta}) = T(F_{-(x-\theta)}) = T(F_{-x+\theta}) = -T(F_x) + \theta.$$

Thus

$$2T(F_x) = 2\theta$$

and it follows that

$$T(F_x) = \theta.$$

Since T was an arbitrarily chosen location functional, this completes the proof.

Theorem

Under the assumption of multivariate elliptical distribution, all scatter functionals are proportional.

Proof (1/3)

Let x denote a p-variate random vector with a cumulative distribution function F_x. Assume that

$$x = \Omega z + \mu,$$

where $\mu \in \mathbb{R}^p$, $\Omega \in \mathbb{R}^{p \times p}$, Ω is full rank, and $z \sim Oz$ for all orthogonal $O \in \mathbb{R}^{p \times p}$. Let S be an affine equivariant scatter functional and assume that $S(F_x)$ exists as finite quantity.

Proof (2/3)

Since $z \sim Oz$ for all orthogonal $O \in \mathbb{R}^{p \times p}$, it holds that $z \sim PJz$ for all permutation matrices $P \in \mathbb{R}^{p \times p}$ and for all sign change matrices $J \in \mathbb{R}^{p \times p}$. Now it follows from affine equivariance of S that

$$S(F_{PJz}) = PJS(F_z)(PJ)^T$$

and from the property $PJz \sim z$ that

$$S(F_{PJz}) = S(F_z).$$

Thus

$$S(F_z) = PJS(F_z)(PJ)^T.$$

As $S(F_z) = PJS(F_z)(PJ)^T$ holds for all permutation matrices $P \in \mathbb{R}^{p \times p}$ and for all sign change matrices $J \in \mathbb{R}^{p \times p}$, we have that

$$(S(F_z))_{ij} = -(S(F_z))_{ji}, \; i \neq j$$

and

$$(S(F_z))_{ii} = (S(F_z))_{jj}.$$

Thus

$$S(F_z) \propto I.$$

Proof (3/3)

It now follows from above and from affine equivariance of S that

$$S(F_x) = S(F_{\Omega z+\mu}) = \Omega S(F_z)\Omega^T = \Omega c \cdot I\Omega^T = c\Omega\Omega^T,$$

where c is a constant that may depend on S.

Since S was an arbitrarily chosen scatter functional, this completes the proof.

Note that in general different location functionals do not measure the same population quantities. That is true also for scatter functionals — different scatter functional do not necessarily measure the same population quantities!

Next Week

Next week we will talk about principal component analysis (PCA).

References

References I

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