Multivariate Normal Distribution Edps/Soc 584, Psych 594

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- Motivation
- The multivariate normal distribution
- The Bivariate Normal Distribution
- More properties of multivariate normal
- **E**stimation of μ and Σ
- Central Limit Theorem

Reading: Johnson & Wichern pages 149–176





Motivation

- ▶ To be able to make inferences about populations, we need a model for the distribution of random variables \longrightarrow We'll use the multivariate normal distribution, because...
- ▶ It's often a good population model. It's a reasonably good approximation of many phenomenon. A lot of variables are approximately normal (due to the central limit theorem for sums and averages).
- The sampling distribution of (test) statistics are often approximately multivariate or univariate normal due to the central limit theorem.
- ▶ Due to it's central importance, we need to thoroughly understand and know it's properties.



Estimation



Motivation

Introduction to the Multivariate Normal

▶ The probability density function of the Univariate normal distribution (p = 1 variables):

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2} \left(\frac{x-\mu}{\sigma}\right)^2\right\}$$
 for $-\infty < x < \infty$

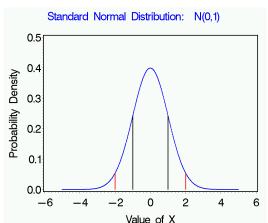
- ▶ The parameters that completely characterize the distribution:
 - $\mu = E(X) = \text{mean}$
 - $\sigma^2 = \text{var}(X) = \text{variance}$



Introduction to the Multivariate Normal (continued)

Area corresponds to probability:

68% area between $\mu \pm \sigma$ and 95% between $\mu \pm 1.96\sigma$:





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Generalization to Multivariate Normal

$$\left(\frac{x-\mu}{\sigma}\right)^2 = (x-\mu)(\sigma^2)^{-1}(x-\mu)$$

A squared statistical distance between x & μ in standard deviation units.

Generalization to p > 1 variables:

- ▶ We have $\mathbf{x}_{p \times 1}$ and parameters $\mu_{p \times 1}$ and $\mathbf{\Sigma}_{p \times p}$.
- ▶ The exponent term for multivariate normal is

$$(\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

where $-\infty < x_i < \infty$ for $i = 1, \ldots, p$.

- ▶ This is a scalar and reduces to what's at the top for p = 1.
- ▶ It is a squared statistical distance of x to μ (if Σ^{-1} exists). It takes into consideration both variability and covariability.
- Integrating

$$\int_{\mathbb{R}} \dots \int_{\mathbb{R}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right) = (2\pi)^{p/2} |\boldsymbol{\Sigma}|^{1/2}$$

Others



Proper Distribution

Since the sum of probabilities over all possible values must add up to 1, we need to divide by $(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}$ to get a "proper" density function.

Multivariate Normal density function:

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{p/2} |\mathbf{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$$

where
$$-\infty < x_i < \infty$$
 for $i = 1, \dots, p$.

To denote this, we use

$$\mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

For p = 1, this reduces to the univariate normal p.d.f.



Bivariate Normal: p = 2

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \qquad E(\mathbf{x}) = \begin{pmatrix} E(x_1) \\ E(x_2) \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \boldsymbol{\mu}$$
$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix}$$

and

$$\mathbf{\Sigma}^{-1} = \frac{1}{\sigma_{11}\sigma_{22} - \sigma_{12}^2} \begin{pmatrix} \sigma_{22} & -\sigma_{12} \\ -\sigma_{12} & \sigma_{11} \end{pmatrix}$$

If we replace σ_{12} by $\rho_{12}\sqrt{\sigma_{11}\sigma_{22}}$, then we get

$$\mathbf{\Sigma}^{-1} = \frac{1}{\sigma_{11}\sigma_{22}(1 - \rho_{12}^2)} \begin{pmatrix} \sigma_{22} & -\rho_{12}\sqrt{\sigma_{11}\sigma_{22}} \\ -\rho_{12}\sqrt{\sigma_{11}\sigma_{22}} & \sigma_{11} \end{pmatrix}$$

Using this, let's look at the statistical distance of \mathbf{x} from $\mu_{\mathbf{x}}$ from $\mu_{\mathbf{x}}$



Bivariate Normal & Statistical Distance

Bivariate Normal

The quantity in the exponent of the bivariate normal is

$$(\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

$$= ((x_{1} - \mu_{1}), (x_{2} - \mu_{2})) \left(\frac{1}{\sigma_{11}\sigma_{22}(1 - \rho_{12}^{2})}\right) \times \begin{pmatrix} \sigma_{22} & -\rho_{12}\sqrt{\sigma_{11}\sigma_{22}} - \rho_{12}\sqrt{\sigma_{11}\sigma_{22}} \\ \sigma_{11} \end{pmatrix} \begin{pmatrix} x_{1} - \mu_{1} \\ x_{2} - \mu_{2} \end{pmatrix}$$

$$= \frac{1}{1 - \rho_{12}^2} \left\{ \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right)^2 + \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right)^2 - 2\rho_{12} \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right) \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right) \right\}$$

$$= \frac{1}{1-\rho_{12}^2} \left\{ z_1^2 + z_2^2 - 2\rho_{12}z_1z_2 \right\}$$

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Bivariate Normal & Independence

$$f(\mathbf{x}) = \frac{1}{2\pi\sqrt{\sigma_{11}\sigma_{22}}} \exp\left[\frac{-1}{2(1-\rho_{12}^2)} \left\{ \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}}\right)^2 + \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}}\right)^2 - 2\rho_{12} \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}}\right) \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}}\right) \right\} \right]$$

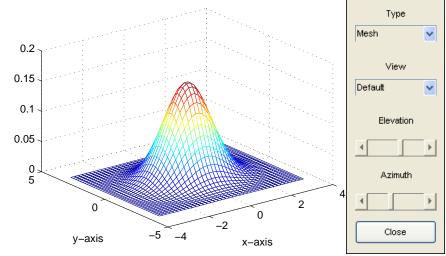
If $\sigma_{12} = 0$ or equivalently $\rho_{12} = 0$, then X_1 and X_2 are uncorrelated. For bivariate normal, $\sigma_{12} = 0$ implies that X_1 and X_2 are statistically independent, because the density factors

$$f(\mathbf{x}) = \frac{1}{2\pi\sqrt{\sigma_{11}\sigma_{22}}} \exp\left[\frac{-1}{2} \left\{ \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}}\right)^2 + \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}}\right)^2 \right\} \right]$$

$$= \frac{1}{\sqrt{2\pi\sigma_{11}}} \exp\left[\frac{-1}{2} \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}}\right)^2\right] \frac{1}{\sqrt{2\pi\sigma_{22}}} \exp\left[\frac{-1}{2} \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}}\right)^2\right]$$

$$= f_1(x_1) \times f_2(x_2)$$

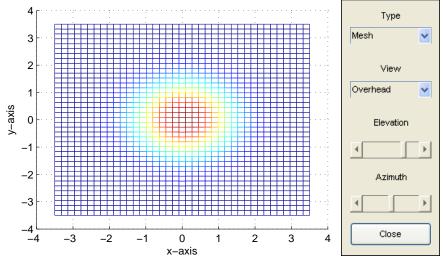
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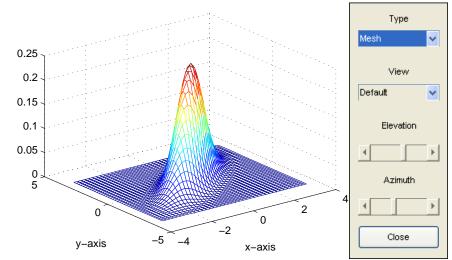
Others



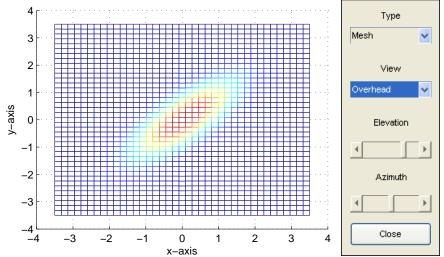
Overhead $\mu_k = 0$, $\sigma_{kk} = 1$, r = 0.0



Picture: $\mu_k = 0$, $\sigma_{kk} = 1$, r = 0.75



Overhead: $\mu_k = 0$, $\sigma_{kk} = 1$, r = 0.75





Summary: Comparing r = 0.0 vs r = 0.75

For the figures shown, $\mu_1 = \mu_2 = 0$ and $\sigma_{11} = \sigma_{22} = 1$:

• With r = 0.0.

Intro. to Multivariate Normal

- $\Sigma = \text{diag}(\sigma_{11}, \sigma_{22}), \text{ a diagonal matrix.}$
- Density is "random" in the x-y plane.
- ▶ When take a slice parallel to x-y, you get a circle.
- ▶ When r = .75.
 - Σ is not a diagonal.
 - Density is not random in x-y plane.
 - ▶ There is a linear tilt (ie., density is concentrated on a line).
 - When you take a slice you get an ellipse that's tilted.
 - ▶ Tilt depends on relative values of σ_{11} and σ_{22} (and scale used in plotting).
- ▶ When $\Sigma = \sigma^2 I$ (i.e., diagonal with equal variances), it's "spherical normal".

Others

Real Time Software Demo

- binormal.m (Peter Dunn)
- Graph_Bivariate_.R (http://www.stat.ucl.ac.be/ISpersonnel/lecoutre/stats/fichiers/~gall



Slices of Multivariate Normal Density

▶ For bi-variate normal, you get an ellipse whose equation is

$$(\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) = c^2$$

which gives all (x_1, x_2) pairs with constant probability.

- ▶ The ellipses are call contours and all are centered around μ .
- Definition:

A constant probability contour equals

$$= \ \, \{ \mathsf{all} \; \mathsf{x} \; \mathsf{such that} \; (\mathsf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathsf{x} - \boldsymbol{\mu}) = c^2 \}$$

= {surface of ellipsoid centered at μ }





Probability Contours: Axes of ellipsoid

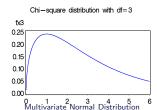
Important Points:

$$(\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \sim \chi_p^2 \qquad \text{(if } |\mathbf{\Sigma}| > 0)$$

► The solid ellipsoid of values x that satisfy

$$(\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \le c^2 = \chi^2_{p(\alpha)}$$

has probability $(1-\alpha)$ where $\chi^2_{p(\alpha)}$ is the $(1-\alpha)^{th}100\%$ point of the chi-square distribution with \vec{p} degrees of freedom.





Example: Axses of Ellipses & Prob. Contours

Back to the example where $\mathbf{x} \sim N_2$ with

$$m{\mu} = \left(egin{array}{c} 5 \\ 10 \end{array}
ight) \quad {\sf and} \quad {m{\Sigma}} = \left(egin{array}{cc} 9 & 16 \\ 16 & 64 \end{array}
ight)
ightarrow
ho = .667$$

and we want the "95% probability contour".

The upper 5% point of the chi-square distribution with 2 degrees of freedom is $\chi^2_{2(.05)} = 5.9915$, so $c = \sqrt{5.9915} = 2.4478$

Axes: $\mu \pm c\sqrt{\lambda_i}\mathbf{e}_i$ where $(\lambda_i, \mathbf{e}_i)$ is the i^{th} (i = 1, 2)eigenvalue/eigenvector pair of Σ .

$$\lambda_1 = 68.316$$
 $\mathbf{e}_1' = (.2604, .9655)$
 $\lambda_2 = 4.684$ $\mathbf{e}_2' = (.9655, -.2604)$



Major Axis

Using the largest eigenvalue and corresponding eigenvector:

Bivariate Normal

$$\underbrace{\begin{pmatrix} 5 \\ 10 \end{pmatrix}}_{\boldsymbol{\mu}} \pm \underbrace{2.45}_{\sqrt{\chi^{2}_{2(.05)}}} \underbrace{\sqrt{68.316}}_{\lambda_{1}} \underbrace{\begin{pmatrix} .2604 \\ .9655 \end{pmatrix}}_{\mathbf{e}_{1}}$$

$$\begin{pmatrix} 5 \\ 10 \end{pmatrix} \pm 20.250 \begin{pmatrix} .2604 \\ .9655 \end{pmatrix}$$

$$\begin{pmatrix} 5 \\ 10 \end{pmatrix} \pm \begin{pmatrix} 5.273 \\ 19.551 \end{pmatrix}$$

$$\longrightarrow \begin{pmatrix} -.273 \\ -9.551 \end{pmatrix}, \begin{pmatrix} 10.273 \\ 29.551 \end{pmatrix}$$

Estimation



Motivation

Minor Axis

Same process but now use λ_2 and \mathbf{e}_2 , the smallest eigenvalue and corresponding eigenvector:

Bivariate Normal

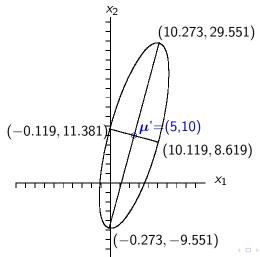
$$\begin{pmatrix} 5 \\ 10 \end{pmatrix} \pm 2.45\sqrt{4.684} \begin{pmatrix} .9655 \\ -.2604 \end{pmatrix}$$

$$\begin{pmatrix} 5 \\ 10 \end{pmatrix} \pm 5.30 \begin{pmatrix} .9655 \\ -.2604 \end{pmatrix}$$

$$\begin{pmatrix} 5 \\ 10 \end{pmatrix} \pm \begin{pmatrix} 5.119 \\ -1.381 \end{pmatrix}$$

$$\longrightarrow \begin{pmatrix} -.119 \\ 11.381 \end{pmatrix}, \begin{pmatrix} 10.119 \\ 8.619 \end{pmatrix}$$

Graph of 95% Probability Contour





Example: Equation for Contour

Equation for Contour:

$$(\mathbf{x} - \boldsymbol{\mu})'$$
 $\mathbf{\Sigma}^{-1}$ $(\mathbf{x} - \boldsymbol{\mu}) \leq 5.99$

Bivariate Normal

$$((x_1-5),(x_2-10))\begin{pmatrix} 9 & 16 \\ 16 & 64 \end{pmatrix}^{-1}\begin{pmatrix} (x_1-5) \\ (x_2-10) \end{pmatrix} \leq 5.99$$

$$((x_1-5),(x_2-10))\begin{pmatrix} .200 & -.050 \\ -.050 & .028 \end{pmatrix}\begin{pmatrix} (x_1-5) \\ (x_2-10) \end{pmatrix} \leq 5.99$$

$$.2(x_1-5)^2+.028(x_2-10)^2-.1(x_1-5)(x_2-10) \le 5.99$$

 $(\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$ is a quadratic form, which is equation for a polynomial

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Estimation



Motivation

Points inside or outside?

Are the following points inside or outside the 95% probability contour?

▶ Is the point (10,20) inside or outside the 95% probability contour?

$$(10,20) \longrightarrow .2(10-5)^2 + .028(20-10)^2 - .1(10-5)(20-10)$$

$$= .2(25) + .028(100) - .1(50)$$

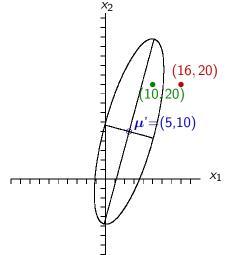
$$= 2.8$$

▶ Is the point (16,20) inside or outside the 95% probability contour?

$$(16,20) \longrightarrow .2(16-5)^2 + .028(20-10)^2 - .1(16-5)(20-10)$$
$$.2(121) + .028(100) - .1(11)(10)$$
$$= 16$$



Points Inside and Outside





More Properties that we'll Expand on

Bivariate Normal

If $\mathbf{X} \sim \mathcal{N}_{p}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then

- ▶ Linear combinations of components of **X** are (multivariate) normal.
- All sub-sets of the components of **X** are (multivariate) normal.
- Zero covariance implies that the corresponding components of X are statistical independent.
- The conditional distributions of the components of **X** are (multivariate) normal.





1: Linear Combinations

If $\mathbf{X} \sim \mathcal{N}_p(oldsymbol{\mu}, oldsymbol{\Sigma})$, then any linear combination

$$\mathbf{a}'\mathbf{X} = a_1X_1 + a_2X_2 + \cdots + a_pX_p$$

is distributed as

$$\mathbf{a}'\mathbf{X} \sim \mathcal{N}_1(\mathbf{a}'\boldsymbol{\mu},\mathbf{a}'\boldsymbol{\Sigma}\mathbf{a})$$

Also, If $\mathbf{a}'\mathbf{X}$ is normal $\mathcal{N}(\mathbf{a}'\mu,\mathbf{a}'\mathbf{\Sigma}\mathbf{a})$ for all possible \mathbf{a} , then \mathbf{X} must be $\mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

$$\mathbf{X} \sim \mathcal{N}\left(\left(\begin{array}{c} 5 \\ 10 \end{array}\right), \left(\begin{array}{cc} 16 & 12 \\ 12 & 36 \end{array}\right)\right) \qquad \begin{array}{c} \mathbf{a}' = (3,2) \\ Y = \mathbf{a}'\mathbf{X} = 3X_1 + 2X_2 \end{array}$$

$$\mu_Y = (3,2) \begin{pmatrix} 5 \\ 10 \end{pmatrix} = 35$$
 and $\sigma_Y^2 = (3,2) \begin{pmatrix} 16 & 12 \\ 12 & 36 \end{pmatrix} \begin{pmatrix} 3 \\ 2 \end{pmatrix} = 432$

 $Y \sim \mathcal{N}(35,432)$

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Others



Motivation

More Linear Combinations

If $X \sim \mathcal{N}_p(\mu, \Sigma)$, then the q linear combinations

$$\mathbf{Y}_{q \times 1} = \mathbf{A}_{q \times p} \mathbf{X} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{q1} & a_{q2} & \cdots & a_{qp} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_p \end{pmatrix}$$

Bivariate Normal

is distributed as $\mathcal{N}_{q}(\mathbf{A}\boldsymbol{\mu}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}')$.

Also, if

$$Y = AX + d$$

where $\mathbf{d}_{q\times 1}$ is a vector constants, then

$$\mathbf{Y} = \mathcal{N}(\mathbf{A}\boldsymbol{\mu} + \mathbf{d}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}').$$





Numerical Example with Multiple Combinations

$$\mathbf{X} \sim \mathcal{N}_2 \left(\left(egin{array}{c} 5 \\ 10 \end{array} \right) \left(egin{array}{c} 16 & 12 \\ 12 & 36 \end{array} \right)
ight)$$

$$egin{aligned} Y_1 &= X_1 + X_2 \ Y_2 &= X_1 - X_2 \end{aligned} \qquad ext{so} \qquad egin{aligned} oldsymbol{A}_{2 imes 2} &= \left(egin{array}{cc} 1 & 1 \ 1 & -1 \end{array}
ight) \end{aligned}$$

$$\mu_Y = \mathbf{A}\boldsymbol{\mu} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 5 \\ 10 \end{pmatrix} = \begin{pmatrix} 15 \\ -5 \end{pmatrix}$$

$$\mathbf{\Sigma}_{Y} = \mathbf{A}\mathbf{\Sigma}\mathbf{A}' = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 16 & 12 \\ 12 & 36 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 76 & -20 \\ -20 & 28 \end{pmatrix}$$

So

$$\mathbf{Y} \sim \mathcal{N}_2 \left(\left(\begin{array}{c} 15 \\ -5 \end{array} \right), \left(\begin{array}{cc} 76 & -20 \\ -20 & 28 \end{array} \right) \right)$$



Multiple Regression as an Example

This example will use what we know about linear combinations and now what we know about the distribution of linear combinations.

Linear Regression Model

- Y = response variable.
- \triangleright Z_1, Z_2, \dots, Z_r are predictor/explanatory variables, which are considered to be fixed.
- The model is

$$Y = \beta_o + \beta_1 Z_1 + \beta_2 Z_2 + \ldots + \beta_r Z_r + \epsilon$$

▶ The error of prediction ϵ is viewed as a random variable.

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Multiple Regression as an Example

Bivariate Normal

Suppose we have n observations on Y and have values of Z_i for all $i=1,\ldots,n$; that is,

$$Y_{1} = \beta_{o} + \beta_{1}Z_{11} + \beta_{2}Z_{12} + \dots + \beta_{r}Z_{1r} + \epsilon_{1}$$

$$Y_{2} = \beta_{o} + \beta_{1}Z_{21} + \beta_{2}Z_{22} + \dots + \beta_{r}Z_{2r} + \epsilon_{2}$$

$$\vdots \qquad \vdots$$

$$Y_{n} = \beta_{o} + \beta_{1}Z_{n1} + \beta_{2}Z_{n2} + \dots + \beta_{r}Z_{nr} + \epsilon_{n}$$

where $E(\epsilon_j)=0$, $var(\epsilon_j)=\sigma^2$ (a constant), and $cov(\epsilon_j,\epsilon_k)=0$ for $j\neq k$.

In terms of matrices,

$$\begin{pmatrix} Y_{1} \\ Y_{2} \\ \vdots \\ Y_{n} \end{pmatrix} = \begin{pmatrix} 1 & Z_{11} & Z_{12} & \dots & Z_{1r} \\ 1 & Z_{21} & Z_{22} & \dots & Z_{2r} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & Z_{n1} & Z_{n2} & \dots & Z_{nr} \end{pmatrix} \begin{pmatrix} \beta_{o} \\ \beta_{1} \\ \beta_{2} \\ \vdots \\ \beta_{r} \end{pmatrix} + \begin{pmatrix} \epsilon_{1} \\ \epsilon_{2} \\ \vdots \\ \epsilon_{n} \end{pmatrix}$$

$$\mathbf{Y} = \mathbf{Z}\boldsymbol{\beta} + \epsilon$$
 where $E(\epsilon) = \mathbf{0}$ and $\operatorname{cov}(\epsilon) = \sigma^2 \mathbf{I}$.

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Distribution of Y

$$\mathbf{Y} = \underbrace{\mathbf{Z}\boldsymbol{\beta}}_{\text{vector of constants}} + \underbrace{\epsilon}_{\text{random}} \quad \text{where } E(\epsilon) = \mathbf{0} \text{ and } \operatorname{cov}(\epsilon) = \sigma^2 \mathbf{I}.$$

So Y is a linear combination of a multivariate normally distributed variable, ϵ .

▶ Mean of Y:

$$\mu_{\mathbf{Y}} = E(\mathbf{Y}) = E(\mathbf{Z}\beta + \epsilon) = \mathbf{Z}\beta + E(\epsilon) = \mathbf{Z}\beta$$

Covariance of Y:

$$\mathbf{\Sigma_Y} = \sigma^2 \mathbf{I}$$

(the same as ϵ).

 \blacktriangleright Distribution of **Y** is multivariate normal because ϵ is multivariate normal:

$$\mathbf{Y} \sim \mathcal{N}(\mathbf{Z}\boldsymbol{\beta}, \sigma^2 \mathbf{I})$$

Estimation



Motivation

Least Square Estimation

$$\mathbf{Y} = \mathbf{Z}\boldsymbol{\beta} + \epsilon$$
 where $E(\epsilon) = \mathbf{0}$ and $cov(\epsilon) = \sigma^2 \mathbf{I}$

Bivariate Normal

 β and σ^2 are unknown parameters that need to be estimated from data.

Let y_1, y_2, \dots, y_n be a random sample with values $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_r$ on the explanatory variables. The least squares estimate of β is the vector b that minimizes

$$\sum_{j=1}^{n} (y_j - \mathbf{z}_j' \mathbf{b})^2 = \sum_{j=1}^{n} (y_j - b_o - b_1 z_{j1} - b_2 z_{j2} - \dots - b_r z_{jr})^2$$

$$= (\mathbf{y} - \mathbf{Z}\mathbf{b})'(\mathbf{y} - \mathbf{Z}\mathbf{b})$$

$$= \epsilon' \epsilon$$

where \mathbf{z}_i' is the j^{th} row of \mathbf{Z} , and $\mathbf{b} = (b_o, b_1, b_2, \dots, b_r)'$. If **Z** has full rank (i.e., the rank of **Z** is $r + 1 \le n$), then the least squares estimate of β is

$$\hat{\boldsymbol{\beta}} = (\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{y}$$





What's the distribution of $\hat{\beta}$?

Bivariate Normal

$$\hat{\boldsymbol{\beta}} = (\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{y} = \mathbf{A}\mathbf{y}$$

We showed that $\mathbf{Y} \sim \mathcal{N}_n(\mathbf{Z}\boldsymbol{\beta}, \sigma^2 \mathbf{I})$.

Mean of Â:

$$\mu_{\hat{\boldsymbol{\beta}}} = E(\hat{\boldsymbol{\beta}}) = E(\mathbf{AY})$$

$$= \mathbf{A}E(\mathbf{Y})$$

$$= \mathbf{AZ}\boldsymbol{\beta}$$

$$= (\mathbf{Z'Z})^{-1}\mathbf{Z'Z}\boldsymbol{\beta} = \boldsymbol{\beta}$$

▶ Covariance matrix for $\hat{\beta}$

$$\begin{split} \mathbf{\Sigma}_{\hat{\boldsymbol{\beta}}} &= \mathbf{A}\mathbf{\Sigma}_{\mathbf{Y}}\mathbf{A}' \\ &= ((\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}')(\sigma^2\mathbf{I})(\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1}) \\ &= \sigma^2(\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1} \\ &= \sigma^2(\mathbf{Z}'\mathbf{Z})^{-1} \end{split}$$

▶ The distribution of $\hat{\beta}$: $\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2(\mathbf{Z}'\mathbf{Z})^{-1})$.





The distribution of \hat{Y}

The "fitted values" or predicted values are

$$\hat{\mathbf{y}} = \mathbf{Z}\hat{\boldsymbol{\beta}} = \mathbf{H}\mathbf{y}$$

where $\mathbf{H} = \mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'$. The matrix \mathbf{H} is the "hat" matrix.

- ▶ We just showed that $\hat{\boldsymbol{\beta}} \sim \mathcal{N}(\boldsymbol{\beta}, \sigma^2(\mathbf{Z}'\mathbf{Z})^{-1})$, and so $\hat{\mathbf{y}}$ is a linear combination of a vector that's multivariate normal.
- Mean of Ŷ:

$$\mu_{\hat{\mathbf{Y}}} = E(\mathbf{Z}\hat{oldsymbol{eta}}) = \mathbf{Z}E(\hat{oldsymbol{eta}}) = \mathbf{Z}oldsymbol{eta}$$

Covariance matrix for Ŷ

$$\mathbf{Z}\mathbf{\Sigma}_{\hat{\boldsymbol{\beta}}}\mathbf{Z}' = \mathbf{Z}(\sigma^2\underbrace{(\mathbf{Z}'\mathbf{Z})^{-1}})\underbrace{\mathbf{Z}'} = \sigma^2\mathbf{Z}'\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1} = \sigma^2\mathbf{I}$$

Distribution of Ŷ:

$$\hat{\mathbf{Y}} \sim \mathcal{N}(\mathbf{Z}\boldsymbol{\beta}, \sigma^2 \mathbf{I})$$

Estimation



Motivation

The distribution of $\hat{\epsilon}$

The estimated residuals are

$$\hat{\epsilon} = \mathbf{y} - \hat{\mathbf{y}} = (\mathbf{I} - \mathbf{H})\mathbf{y}$$

and they contain the information necessary to estimate σ^2 .

The least squares estimate of σ^2 is

$$s^2 = \frac{\hat{\epsilon}' \hat{\epsilon}}{n - (r+1)}$$

The estimates $\hat{\beta}$ and $\hat{\epsilon}$ are uncorrelated.

Multivariate Normality Assumption $\epsilon \sim N_n(\mathbf{0}, \sigma^2 \mathbf{I})$ and what we know about linear combinations of random variables allowed us to derive the distribution of various random variables.

The distribution of $\hat{\epsilon}$

Last few comments on this example:

▶ The least squares estimates of β and ϵ are also the maximum likelihood estimates.

Bivariate Normal

- ▶ The maximum likelihood estimate of σ^2 is $\hat{\sigma}^2 = \hat{\epsilon}' \hat{\epsilon}/n$
- $ightharpoonup \hat{\beta}$ and $\hat{\epsilon}$ are statistically independent.



2: Sub-sets of Variables

If $\mathbf{X} \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then all sub-sets of \mathbf{X} are (multivariate) normally distributed.

Bivariate Normal

For example, let's partition X into two sub-sets

$$\mathbf{X}_{p\times 1} = \begin{pmatrix} X_1 \\ \vdots \\ X_q \\ \hline X_{q+1} \\ \vdots \\ X_p \end{pmatrix} = \begin{pmatrix} \mathbf{X}_{1(q\times 1)} \\ \hline \mathbf{X}_{2((p-q)\times 1)} \end{pmatrix} \text{ and } \boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_q \\ \hline \mu_{q+1} \\ \vdots \\ \mu_p \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu}_{1(q\times 1)} \\ \hline \boldsymbol{\mu}_{2((p-q)\times 1)} \end{pmatrix}$$

$$\mathbf{\Sigma}_{p\times p} = \begin{pmatrix} \mathbf{\Sigma}_{11(q\times q)} & \mathbf{\Sigma}_{12(q\times (p-q))} \\ \mathbf{\Sigma}_{21((p-q)\times p)} & \mathbf{\Sigma}_{22((p-q)\times (p-q))} \end{pmatrix} = \begin{pmatrix} \mathbf{\Sigma}_{11} & \mathbf{\Sigma}_{12} \\ \mathbf{\Sigma}_{21} & \mathbf{\Sigma}_{22} \end{pmatrix}$$



Sub-sets of Variables continued

Then for

$$\mathbf{X} = \left(rac{\mathbf{X}_{1(q imes 1)}}{\mathbf{X}_{2((p-q) imes 1)}}
ight)$$

The distributions of the sub-sets are

$$\mathbf{X}_1 \sim \mathcal{N}(oldsymbol{\mu}_1, oldsymbol{\Sigma}_{11}) \qquad ext{and} \qquad \mathbf{X}_2 \sim \mathcal{N}(oldsymbol{\mu}_2, oldsymbol{\Sigma}_{22})$$

The result means that

- Each of the X_i's are univariate normals (next page)
- All possible sub-sets are multivariate normal.
- All marginal distributions are (multivariate) normal.





Little Example on Sub-sets

Suppose that

$$\mathbf{X} = \left(egin{array}{c} X_1 \ X_2 \ X_3 \end{array}
ight) \sim \mathcal{N}_3(oldsymbol{\mu}, oldsymbol{\Sigma})$$

Bivariate Normal

Due to the result on sub-sets of multivariate normals,

$$X_1 \sim \mathcal{N}(\mu_1, \sigma_{11})$$

 $X_2 \sim \mathcal{N}(\mu_2, \sigma_{22})$
 $X_3 \sim \mathcal{N}(\mu_3, \sigma_{33})$

Also

$$\left(\begin{array}{c}X_2\\X_3\end{array}\right) \sim \mathcal{N}\left(\left(\begin{array}{c}\mu_2\\\mu_3\end{array}\right)\left(\begin{array}{cc}\sigma_{22}&\sigma_{23}\\\sigma_{32}&\sigma_{33}\end{array}\right)\right)$$

3: Zero Covariance & Statistical Independence

Bivariate Normal

There are three parts to this one:

- ▶ If \mathbf{X}_1 is $(q_1 \times 1)$ and \mathbf{X}_2 is $(q_2 \times 1)$ are statistically independent, then $cov(\mathbf{X}_1, \mathbf{X}_2) = \mathbf{\Sigma}_{12} = \mathbf{0}$.
- If

$$\left(\begin{array}{c|c} \mathbf{X}_1 \\ \hline \mathbf{X}_2 \end{array}\right) \sim \mathcal{N}_{q_1+q_2}\left(\left(\begin{array}{c|c} \boldsymbol{\mu}_1 \\ \hline \boldsymbol{\mu}_2 \end{array}\right), \left(\begin{array}{c|c} \mathbf{\Sigma}_{11} & \mathbf{\Sigma}_{12} \\ \hline \mathbf{\Sigma}_{21} & \mathbf{\Sigma}_{22} \end{array}\right)\right),$$

Then \mathbf{X}_1 and \mathbf{X}_2 are statistically independent if and only if $\mathbf{\Sigma}_{12} = \mathbf{\Sigma}'_{21} = \mathbf{0}$.

If X_1 and X_2 are statistically independent and distributed as $\mathcal{N}_{q_1}(\mu_1, \Sigma_{11})$ and $\overline{\mathcal{N}_{q_2}(\mu_2, \Sigma_2)}$, respectively, then

$$\left(egin{array}{c|c} oldsymbol{\mathsf{X}}_1 \ \hline oldsymbol{\mathsf{X}}_2 \end{array}
ight) \sim \mathcal{N}_{q_1+q_2}\left(\left(egin{array}{c|c} oldsymbol{\mu}_1 \ \hline oldsymbol{\mu}_2 \end{array}
ight), \left(egin{array}{c|c} oldsymbol{\Sigma}_{11} & oldsymbol{0} \ \hline oldsymbol{0} & oldsymbol{\Sigma}_{22} \end{array}
ight)
ight).$$





Example

$$\mathbf{Y}_{4 \times 1} = \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{pmatrix}$$
 and $\mathbf{\Sigma}_{\mathbf{Y}} = \begin{pmatrix} 2 & 1 & 0 & .5 \\ 1 & 3 & 0 & .5 \\ 0 & 0 & 4 & 0 \\ .5 & .5 & 0 & 1 \end{pmatrix}$

and $\mathbf{Y} \sim \mathcal{N}_4(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

Let's take $\mathbf{X}'_1 = (Y_1, Y_2, Y_4)$ and $\mathbf{X}'_2 = (Y_3)$.

Then

$$\left(\begin{array}{c} \mathbf{X}_{1} \\ \hline \mathbf{X}_{2} \end{array}\right) \sim \mathcal{N}_{4} \left(\left(\begin{array}{ccc|c} \mu_{1} \\ \mu_{2} \\ \hline \mu_{4} \\ \hline \mu_{3} \end{array}\right), \left(\begin{array}{ccc|c} 2 & 1 & .5 & 0 \\ 1 & 3 & .5 & 0 \\ \hline .5 & .5 & 1 & 0 \\ \hline 0 & 0 & 0 & 4 \end{array}\right) \right)$$

So set X_1 is statistically independent of X_2 .



4: Conditional Distributions

Let $\mathbf{X}'=(\mathbf{X}'_{1(q1 imes1)},\mathbf{X}'_{2(q_2 imes1)})$ be distributed at $\mathcal{N}_{q1+q2}(\mu,\mathbf{\Sigma})$

Bivariate Normal

$$oldsymbol{\mu} = \left(egin{array}{c|c} oldsymbol{\mu}_1 \\ \hline oldsymbol{\mu}_2 \end{array}
ight) \quad ext{and} \quad oldsymbol{\Sigma} = \left(egin{array}{c|c} oldsymbol{\Sigma}_{11} & oldsymbol{\Sigma}_{12} \\ \hline oldsymbol{\Sigma}_{21} & oldsymbol{\Sigma}_{22} \end{array}
ight)$$

 $|\Sigma| > 0$ (i.e., positive definite). Then conditional distribution of X_1 given $X_2 = x_2$ is (multivariate) normal with mean and covariance matrix

$$\mu_1 + \mathbf{\Sigma}_{12} \mathbf{\Sigma}_{22}^{-1} (\mathbf{x}_2 - \mu_2)$$
 and $\mathbf{\Sigma}_{11} - \mathbf{\Sigma}_{12} \mathbf{\Sigma}_{22}^{-1} \mathbf{\Sigma}_{21}$

Let's look more closely at this for a simple case of $q_1 = q_2 = 1$.



Conditional Distribution for $q_1 = q_2 = 1$

Bivariate normal distribution

Intro. to Multivariate Normal

$$\left(\begin{array}{c} X_1 \\ X_2 \end{array}\right) \sim \mathcal{N}_2 \left(\left(\begin{array}{c} \mu_1 \\ \mu_2 \end{array}\right), \left(\begin{array}{cc} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{array}\right)\right)$$

$$f(x_1|x_2)$$
 is $\mathcal{N}_1\left(\mu_1 + \frac{\sigma_{12}}{\sigma_{22}}(x_2 - \mu_2), \sigma_{11} - \sigma_{12}\left(\frac{\sigma_{12}}{\sigma_{22}}\right)\right)$

Notes:

•
$$\sigma_{12} = \rho_{12} \sqrt{\sigma_{11}} \sqrt{\sigma_{22}}$$

$$\Sigma_{12}\Sigma_{22}^{-1} = \sigma_{12}/\sigma_{22} = \rho_{12}(\sqrt{\sigma_{11}}/\sqrt{\sigma_{22}})$$

$$\boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12} \boldsymbol{\Sigma}_{22}^{-1} \boldsymbol{\Sigma}_{21} = \sigma_{11} - \sigma_{12}^2 / \sigma_{22} = \sigma_{11} (1 - \rho_{12}^2)$$

Alternative way to write $f(x_1|x_2)$:

$$f(x_1|x_2)$$
 is $\mathcal{N}_1\left(\mu_1+\rho_{12}\frac{\sqrt{\sigma_{11}}}{\sqrt{\sigma_{22}}}(x_2-\mu_2),\sigma_{11}(1-\rho_{12}^2)\right)$ Spring 2015 A4.1/56

Multiple Regression as a Conditional Dist.

Bivariate Normal

Consider the case where $q_1 = 1$ and $q_2 > 1$.

- All conditional distributions are normal.
- ▶ The conditional covariance matrix $\Sigma_{11} \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$ does not depend on the values of the conditioning variables.
- The conditional means have the following form:

Let
$$\mathbf{\Sigma}_{12}\mathbf{\Sigma}_{22}^{-1} = \boldsymbol{\beta}_{q_1 \times q_2} = \begin{pmatrix} \beta_{1,q_1+1} & \beta_{1,q_1+2} & \cdots & \beta_{1,q_1+q_2} \\ \beta_{2,q_1+1} & \beta_{2,q_1+2} & \cdots & \beta_{2,q_1+q_2} \\ \cdots & \cdots & \ddots & \cdots \\ \beta_{q_1,q_1+1} & \beta_{q_1,q_1+2} & \cdots & \beta_{q_1,q_1+q_2} \end{pmatrix}$$

Condtional means
$$\begin{pmatrix} \mu_1 + \sum_{i=q_1+1}^{q_1+q_2} \beta_{1i}(x_i - \mu_i) \\ \mu_2 + \sum_{i=q_1+1}^{q_1+q_2} \beta_{2i}(x_i - \mu_i) \\ \vdots \\ \mu_{q_1} + \sum_{i=q_1+1}^{q_1+q_2} \beta_{q_1i}(x_i - \mu_i) \end{pmatrix}$$



Estimation of μ and Σ

& sampling distribution of estimators.

Suppose we have a p dimensional normal distribution with mean μ and covariance matrix **\(\Sigma**

Take *n* observations $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ (these are each $(p \times 1)$ vectors).

$$\mathbf{X}_{j} \sim \mathcal{N}_{p}(oldsymbol{\mu}, oldsymbol{\Sigma})$$
 $j=1,2,\ldots,n$ and independent

For p = 1, we know that the MLEs are

$$\hat{\mu} = \bar{x} = \frac{1}{n} \sum_{j=1}^{n} x_j \sim \mathcal{N}\left(\mu, \frac{1}{n}\sigma^2\right)$$

And
$$n\hat{\sigma}^2 = \sum_{j=1}^n (x_j - \bar{x})^2$$
 and $\frac{1}{\sigma^2} \sum_{j=1}^n (x_j - \bar{x})^2 \sim \chi^2_{(n-1)}$

Or
$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (x_j - \bar{x})^2 \sim \sigma^2 \chi_{(n-1)}^2$$





Estimation of μ and Σ : Multivariate Case

The maximum likelihood estimator of μ is

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{X}} = \frac{1}{n} \sum_{i=1}^{n} X_{i}$$

and the ML estimator of Σ is

$$\hat{\mathbf{\Sigma}} = \frac{n-1}{n} \mathbf{S}^2 = \mathbf{S}_n = \frac{1}{n} \sum_{i=1}^n (\mathbf{X}_j - \hat{\boldsymbol{\mu}}) (\mathbf{X}_j - \hat{\boldsymbol{\mu}})'$$

Sampling Distribution of $\hat{\mu}$:

The estimator is a linear combination of normal random vectors each from $\mathcal{N}_{p}(\mu, \Sigma)$ i.i.d.:

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{X}} = \frac{1}{n} \mathbf{X}_1 + \frac{1}{n} \mathbf{X}_2 + \dots + \frac{1}{n} \mathbf{X}_n$$

So $\hat{\mu}$ also has a normal distribution, Multivariate Normal Distribution

Estimation



Sampling Distribution of $\hat{\Sigma}$

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

The matrix

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

is distributed as a Wishart random matrix with (n-1) degrees of freedom.

Whishart distribution:

- A multivariate analogue to the chi-square distribution.
- It's defined as

$$W_m(\cdot|\mathbf{\Sigma})$$
 = Wishart distribution with m degrees of freedom = The distribution of $\sum_{i=1}^{m} \mathbf{Z}_i \mathbf{Z}_j'$

where $\mathbf{Z}_i \sim \mathcal{N}_p(\mathbf{0}, \mathbf{\Sigma})$ and independent.

Note: \bar{X} and S are independent. 4□ → 4周 → 4 重 → 4 重 → 9 Q @

More Properties



Motivation

Law of Large Numbers

Data are not always (multivariate) normal

The Law of Large Numbers (for multivariate data):

Let X_1, X_2, \dots, X_n be independent observations from a population with mean $E(\mathbf{X}) = \mu$.

Then $\bar{\mathbf{X}} = (1/n) \sum_{i=1}^{n} \mathbf{X}_{i}$ converges in probability to μ as n gets large; that is,

 $\bar{\mathbf{X}}
ightarrow \mu$ for large samples

And

 $S(\text{or } S_n)$ approach Σ for large samples

These are true regardless of the true distribution of the X_i 's.





Central Limit Theorem

Let $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$ be independent observations from a population with mean $E(\mathbf{X}) = \mu$ and finite (non-singular, full rank), covariance matrix $\mathbf{\Sigma}$.

Then $\sqrt{n}(\mathbf{X}-\boldsymbol{\mu})$ has an approximate $\mathcal{N}(\mathbf{0},\boldsymbol{\Sigma})$ distribution if n>>p (i.e., "much larger than").

So, for "large" n

$$ar{\mathbf{X}} = \text{Sample mean vector } pprox \mathcal{N}(\boldsymbol{\mu}, \frac{1}{n} \mathbf{\Sigma}),$$

regardless of the underlying distribution of the X_j 's.

What if Σ is unknown? If n is large "enough", S will be close to Σ , so

$$\sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu}) \approx \mathcal{N}_p(\mathbf{0}, \mathbf{S}) \text{ or } \bar{\mathbf{X}} \approx \mathcal{N}_p(\boldsymbol{\mu}, \frac{1}{n}\mathbf{S}).$$

Since
$$n(\bar{\mathbf{X}} - \mu)' \mathbf{\Sigma}^{-1} (\bar{\mathbf{X}} - \mu) \sim \chi_p^2$$
,
 $n(\bar{\mathbf{X}} - \mu)' \mathbf{S}^{-1} (\bar{\mathbf{X}} - \mu) \approx \chi_p^2$



Few more comments

Intro. to Multivariate Normal

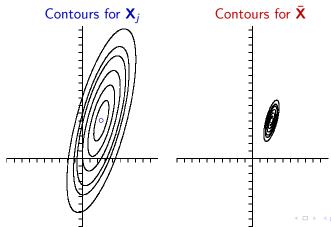
- ▶ Using **S** instead of Σ does not seriously effect approximation.
- ▶ *n* must be large relative to *p*; that is, (n p) is large.
- ▶ The probability contours for $\bar{\mathbf{X}}$ are tighter than those for \mathbf{X} since we have $(1/n)\mathbf{\Sigma}$ for $\bar{\mathbf{X}}$ rather than $\mathbf{\Sigma}$ for \mathbf{X} .

See next slide for an example of the latter.



Comparison of Probability Contours

Returning to our example and pretending we have n = 20. Below are contours for 99%, 95%, 90%, 75%, 50% and 20%:



CLT

Others



Why So Much a Difference with Only 20?

For X_i

$$\mathbf{\Sigma}=\left(egin{array}{cc}9&16\\16&64\end{array}
ight)\longrightarrow\lambda_1=68.316$$
 and $\lambda_2=4.684$

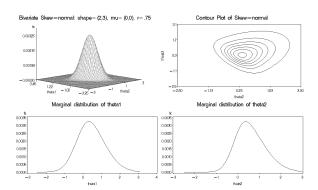
For $\bar{\mathbf{X}}$ with n=20

$$\mathbf{\Sigma} = \frac{1}{20} \begin{pmatrix} 9 & 16 \\ 16 & 64 \end{pmatrix} = \begin{pmatrix} 0.45 & 0.80 \\ 0.80 & 3.20 \end{pmatrix} \longrightarrow \lambda_1 = 3.42 \text{ and } \lambda_2 = 0.23$$

Note that 68.316/20 = 3.42 and 4.684/20 = 0.23.



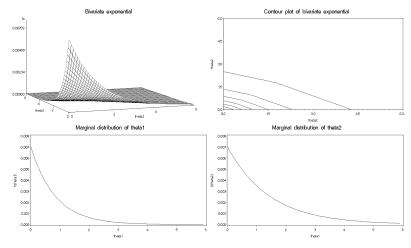
Other Multivariate Distributions: Skew-Normal

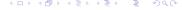




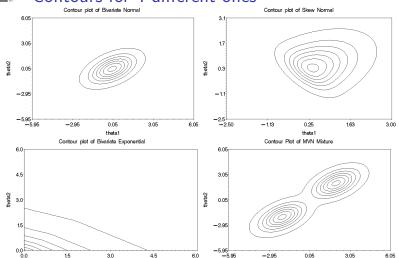


Marshall-Olkin bivariate exponential





Contours for 4 different ones





theta1

theta1