

The Multivariate Normal Distribution

Edps/Soc 584 and Psych 594

Applied Multivariate Statistics

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Outline

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

Central Limit Theorem

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

Reading: Johnson & Wichern pages 149–176



Motivation

● Outline

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- To be able to make inferences about populations, we need a model for the distribution of random variables → 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.



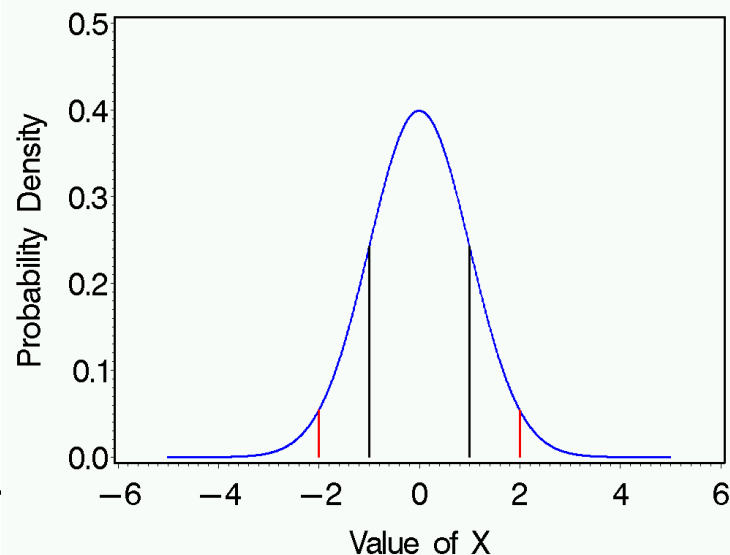
Introduction to the Multivariate Normal

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

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

- The parameters that completely characterize the distribution:
 - ◆ $\mu = E(X) = \text{mean}$
 - ◆ $\sigma^2 = \text{var}(X) = \text{variance}$
- Area corresponds to probability:
68% area between $\mu \pm \sigma$ and 95% between $\mu \pm 1.96\sigma$:

Standard Normal Distribution: $N(0,1)$



● Outline

Motivation

Intro. to Multivariate Normal

● Introduction to the Multivariate Normal

● Generalization to Multivariate Normal

● Proper Distribution

Bivariate Normal

More Properties

Estimation

Central Limit Theorem



Generalization to Multivariate Normal

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

This is a squared statistical distance of x from μ in standard deviation units.

Generalization to $p > 1$ variables:

- We have $x_{p \times 1}$ and parameters $\mu_{p \times 1}$ and $\Sigma_{p \times p}$.
- The exponent term for multivariate normal is

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

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

- ◆ 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

$$\int_{x_1} \dots \int_{x_p} \exp\left(-\frac{1}{2}(x - \mu)' \Sigma^{-1} (x - \mu)\right) = (2\pi)^{p/2} |\Sigma|^{1/2}$$

● Outline

Motivation

Intro. to Multivariate Normal

● Introduction to the

Multivariate Normal

● Generalization to Multivariate Normal

● Proper Distribution

Bivariate Normal

More Properties

Estimation

Central Limit Theorem



Proper Distribution

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

Multivariate Normal density function:

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

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

To denote this, we use

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

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

● Outline

Motivation

Intro. to Multivariate Normal

● Introduction to the

Multivariate Normal

● Generalization to Multivariate Normal

● Proper Distribution

Bivariate Normal

More Properties

Estimation

Central Limit Theorem



Bivariate Normal: $p = 2$

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad E(\mathbf{x}) = \begin{pmatrix} E(x_1) \\ E(x_2) \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \boldsymbol{\mu}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix}$$

and

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

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

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

● Bivariate Normal: $p = 2$

● Bivariate Normal & Statistical Distance

● Bivariate Normal & Independence

● Picture: $\mu_k = 0$, $\sigma_{kk} = 1$, $r = 0.0$

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

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● Summary: Comparing $r = 0.0$ vs $r = 0.75$

● Real Time Software Demo
● Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

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● Example: Axes of Ellipses & Prob. Contours

● Major Axis
Multivariate Normal Distribution
● Minor Axis

● Graph of 95% Probability



Bivariate Normal & Statistical Distance

The quantity in the exponent of the bivariate normal is

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

$$\begin{aligned}
&= ((x_1 - \mu_1), (x_2 - \mu_2)) \left(\frac{1}{\sigma_{11}\sigma_{22}(1 - \rho_{12}^2)} \right) \\
&\quad \times \begin{pmatrix} \sigma_{22} & -\rho_{12}\sqrt{\sigma_{11}\sigma_{22}} \\ -\rho_{12}\sqrt{\sigma_{11}\sigma_{22}} & \sigma_{11} \end{pmatrix} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix} \\
&= \frac{1}{1 - \rho_{12}^2} \left\{ \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right)^2 + \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right)^2 - 2\rho_{12} \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right) \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right) \right\} \\
&= \frac{1}{1 - \rho_{12}^2} \{ z_1^2 + z_2^2 - 2\rho_{12}z_1z_2 \}
\end{aligned}$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

● Bivariate Normal: $p = 2$

● Bivariate Normal & Statistical Distance

● Bivariate Normal &

Independence

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$\sigma_{kk} = 1, r = 0.0$

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● Summary: Comparing

$r = 0.0$ vs $r = 0.75$

● Real Time Software Demo

● Slices of Multivariate Normal

Density

● Example Probability Contours

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

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● Example: Axes of Ellipses &

Prob. Contours

● Major Axis
Multivariate Normal Distribution

● Minor Axis

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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**

$$\begin{aligned} f(\mathbf{x}) &= \frac{1}{2\pi\sqrt{\sigma_{11}\sigma_{22}}} \exp \left[\frac{-1}{2} \left\{ \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right)^2 + \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right)^2 \right\} \right] \\ &= \frac{1}{\sqrt{2\pi\sigma_{11}}} \exp \left[\frac{-1}{2} \left(\frac{x_1 - \mu_1}{\sqrt{\sigma_{11}}} \right)^2 \right] \frac{1}{\sqrt{2\pi\sigma_{22}}} \exp \left[\frac{-1}{2} \left(\frac{x_2 - \mu_2}{\sqrt{\sigma_{22}}} \right)^2 \right] \\ &= f_1(x_1) \times f_2(x_2) \end{aligned}$$

● Outline

Motivation

Intro. to Multivariate Normal

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- Real Time Software Demo
- Slices of Multivariate Normal Density

- Example Probability Contours
- Eigenvectors & Values

- Probability Contours: Axes of ellipsoid

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- Multivariate Normal Distribution
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Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$

● Outline

Motivation

Intro. to Multivariate Normal

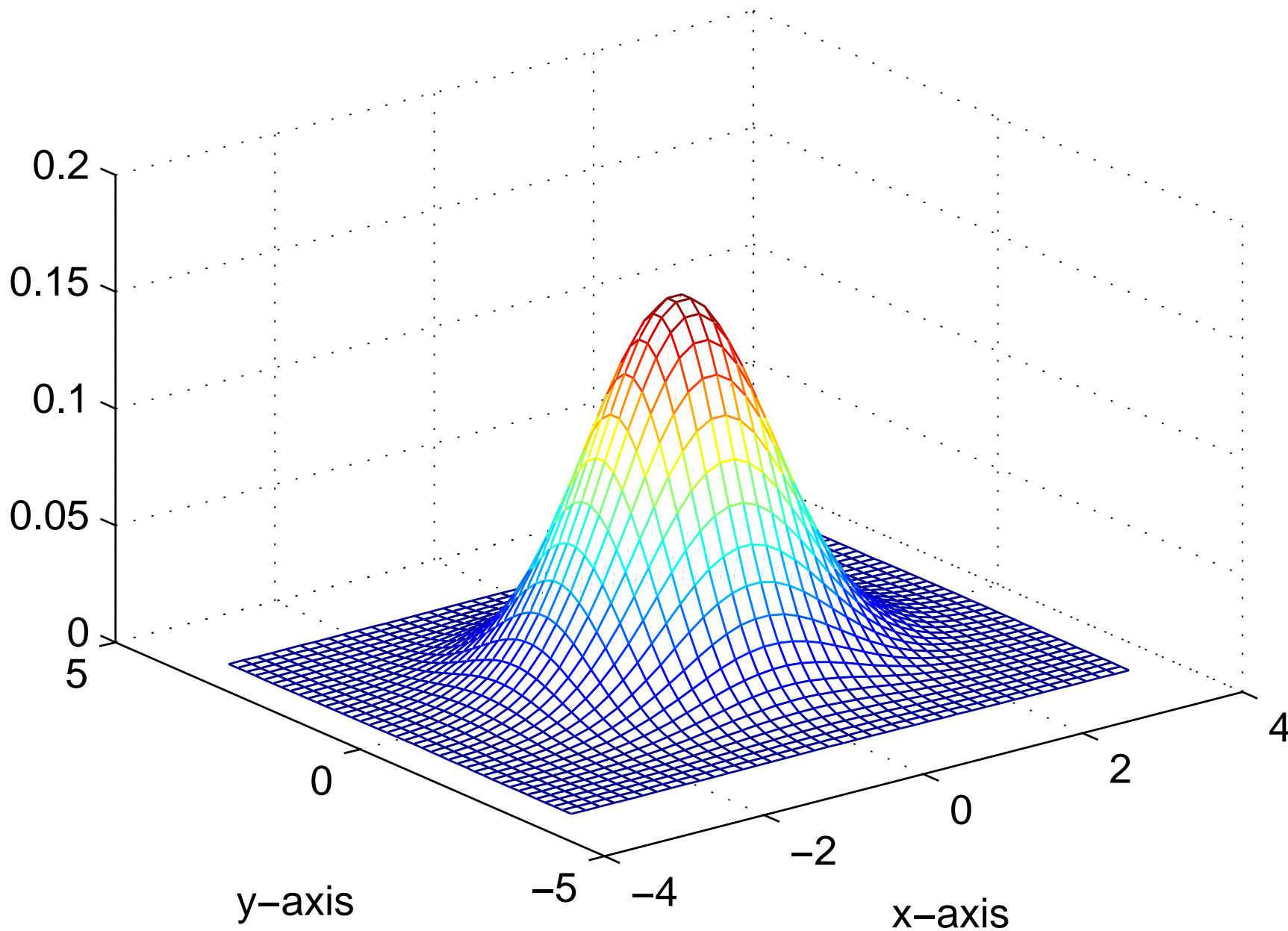
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- Summary: Comparing $r = 0.0$ vs $r = 0.75$
- Real Time Software Demo
- Slices of Multivariate Normal Density
- Example Probability Contours
- Eigenvectors & Values
- Probability Contours: Axes of ellipsoid
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μ_x

μ_y

σ_x

σ_y



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

● Outline

Motivation

Intro. to Multivariate Normal

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● Bivariate Normal & Statistical Distance

● Bivariate Normal & Independence

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● Real Time Software Demo

● Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

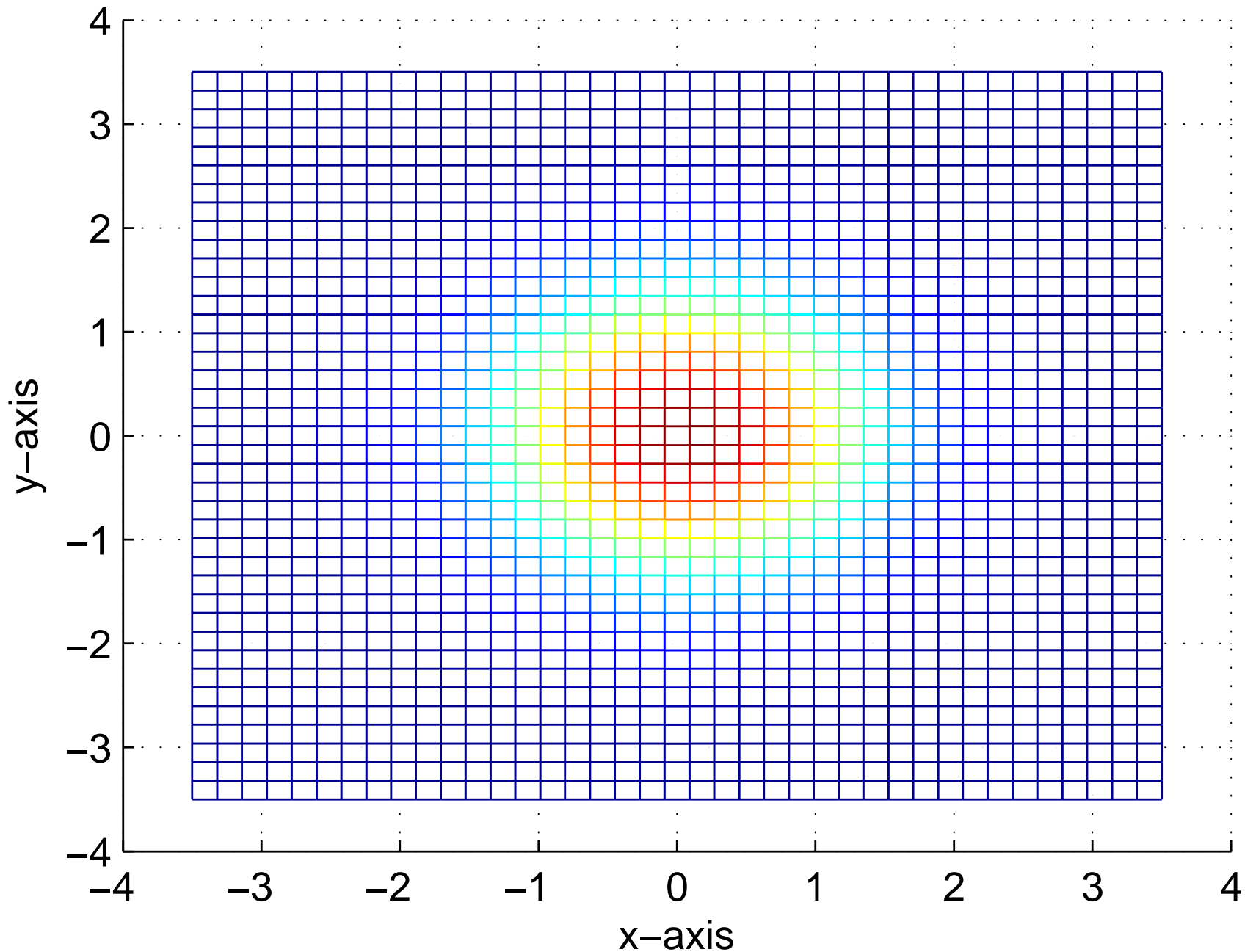
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mu x

mu y

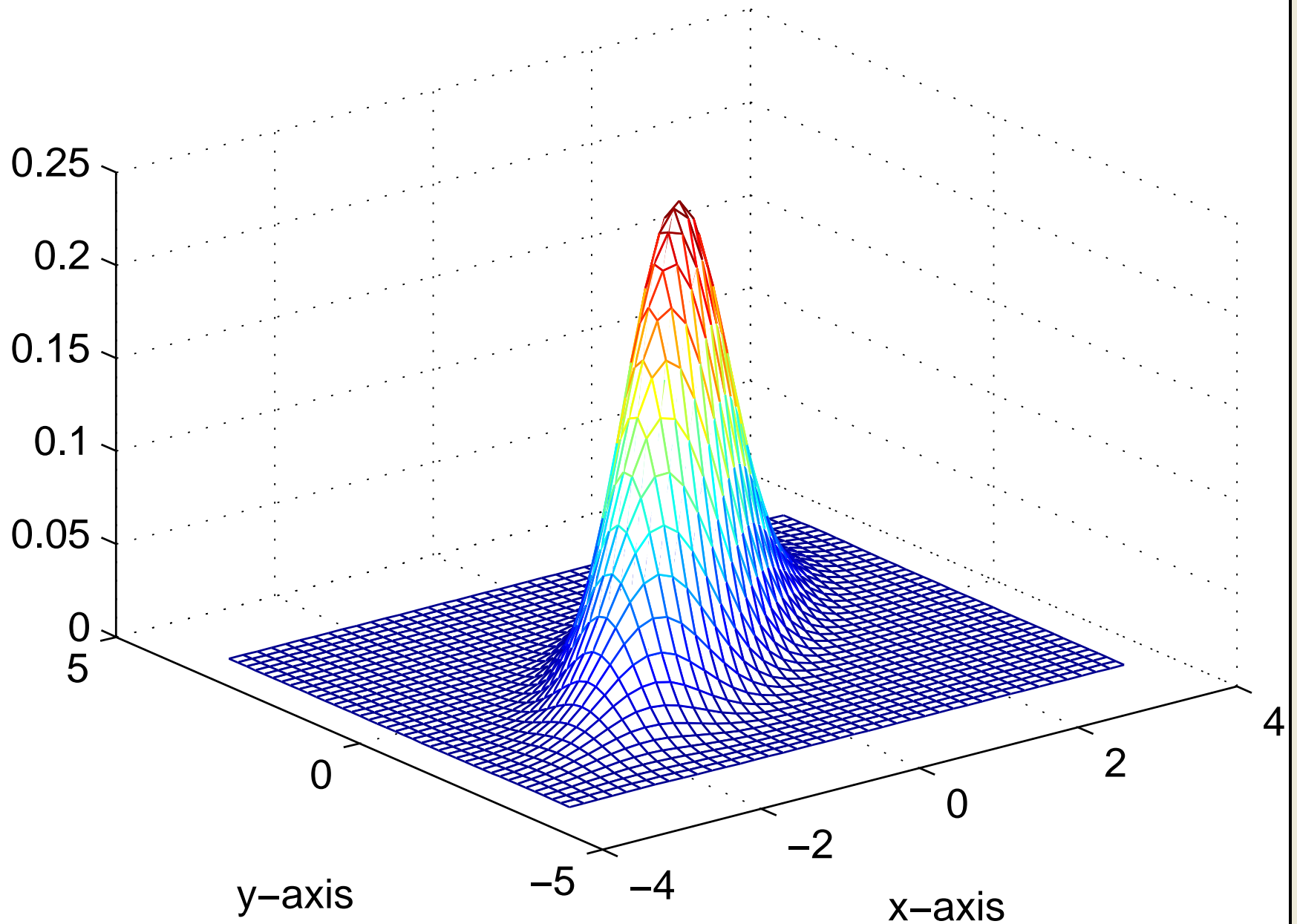
sigma x

sigma y



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

- Outline
- Motivation
- Intro. to Multivariate Normal
- Bivariate Normal
 - Bivariate Normal: $p = 2$
 - Bivariate Normal & Statistical Distance
 - Bivariate Normal & Independence
 - Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
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 - Summary: Comparing $r = 0.0$ vs $r = 0.75$
 - Real Time Software Demo
 - Slices of Multivariate Normal Density
 - Example Probability Contours
 - Eigenvectors & Values
 - Probability Contours: Axes of ellipsoid
 - Probability Contours: Axes of ellipsoid
 - Example: Axes of Ellipses & Prob. Contours

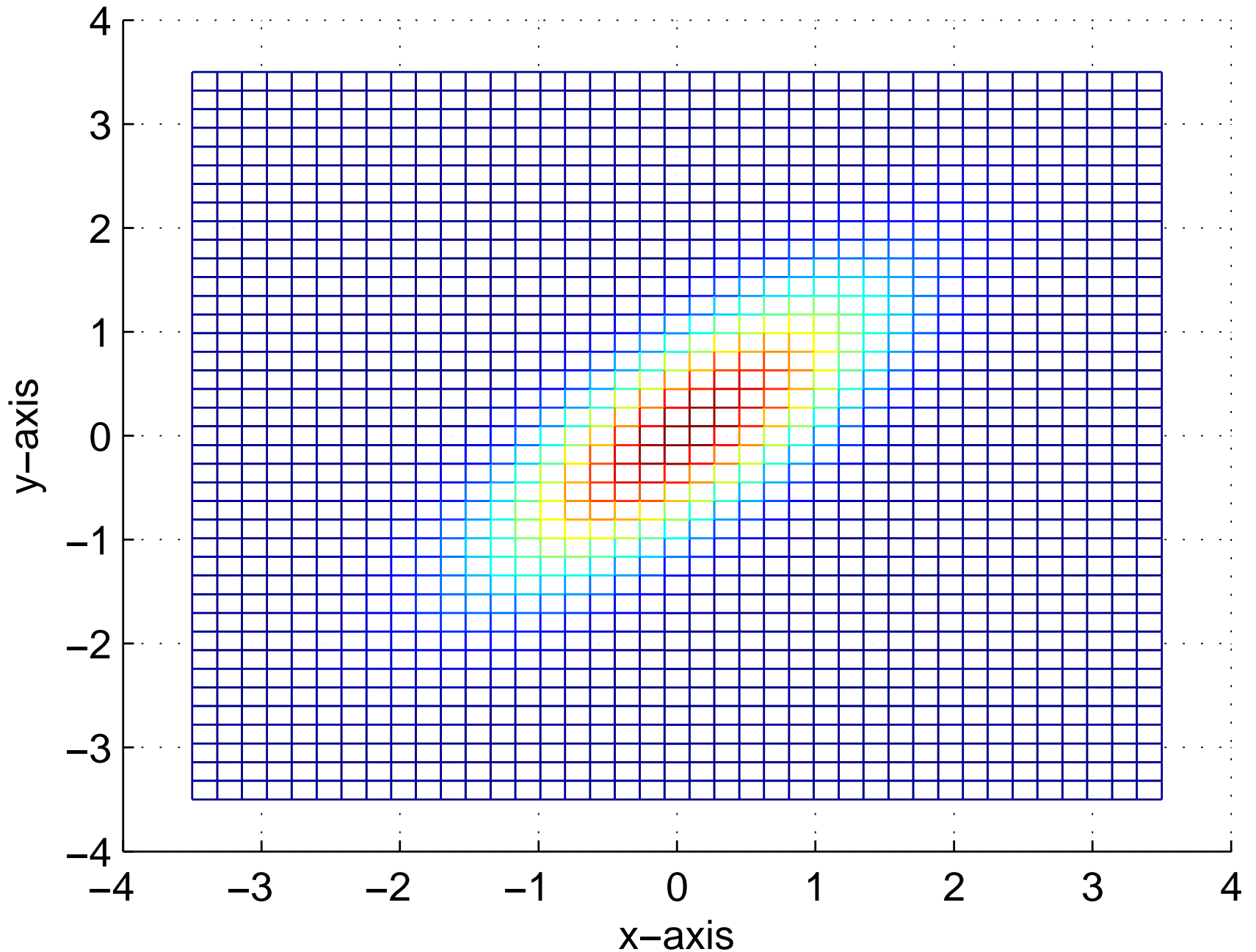


μ_x μ_y σ_x σ_y



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

- Outline
- Motivation
- Intro. to Multivariate Normal
- Bivariate Normal
 - Bivariate Normal: $p = 2$
 - Bivariate Normal & Statistical Distance
 - Bivariate Normal & Independence
 - Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
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 - Summary: Comparing $r = 0.0$ vs $r = 0.75$
 - Real Time Software Demo
 - Slices of Multivariate Normal Density
 - Example Probability Contours
 - Eigenvectors & Values
 - Probability Contours: Axes of ellipsoid
 - Probability Contours: Axes of ellipsoid
 - Example: Axes of Ellipses & Prob. Contours
 - Major Axis, Multivariate Normal Distribution
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μ_x

μ_y

σ_x

σ_y



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 $r = 0.0$,
 - ◆ $\Sigma = \text{diag}(\sigma_{11}, \sigma_{22})$, 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”.

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

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● Bivariate Normal & Statistical Distance

● Bivariate Normal & Independence

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● Real Time Software Demo

● Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

● Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

● Major Axis, Multivariate Normal Distribution

● Minor Axis

● Graph of 95% Probability



Real Time Software Demo

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

- Bivariate Normal: $p = 2$
- Bivariate Normal & Statistical Distance
- Bivariate Normal & Independence
- Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
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● **Real Time Software Demo**

- Slices of Multivariate Normal Density
- Example Probability Contours
- Eigenvectors & Values
- Probability Contours: Axes of ellipsoid
- Probability Contours: Axes of ellipsoid
- Example: Axes of Ellipses & Prob. Contours

- Major Axis
- Multivariate Normal Distribution
- Minor Axis

- Graph of 95% Probability

■ binormal.m (Peter Dunn)

■ Graph_Bivariate_.R

(<http://www.stat.ucl.ac.be/ISpersonnel/lecoutre/stats/fichiers/~gallery.pdf>)



Slices of Multivariate Normal Density

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

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

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

- The ellipses are call **contours** and all are centered around $\boldsymbol{\mu}$.

- Definition:

A constant probability contour equals

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

$$= \{ \text{surface of ellipsoid centered at } \boldsymbol{\mu} \}$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

- Bivariate Normal: $p = 2$
- Bivariate Normal & Statistical Distance
- Bivariate Normal & Independence
- Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
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- Summary: Comparing $r = 0.0$ vs $r = 0.75$

● Real Time Software Demo

● Slices of Multivariate Normal Density

- Example Probability Contours
- Eigenvectors & Values
- Probability Contours: Axes of ellipsoid
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● Example: Axes of Ellipses & Prob. Contours

● Major Axis
Multivariate Normal Distribution

● Minor Axis

● Graph of 95% Probability

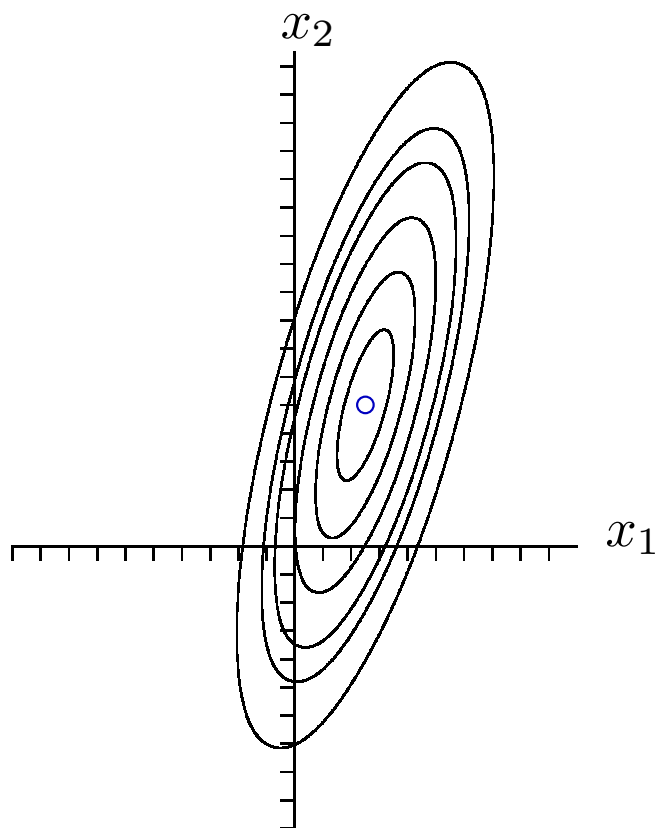


Example Probability Contours

Suppose that $x \sim N_2$ with

$$\mu = \begin{pmatrix} 5 \\ 10 \end{pmatrix} \quad \text{and} \quad \Sigma = \begin{pmatrix} 9 & 16 \\ 16 & 64 \end{pmatrix} \rightarrow \rho = .67$$

Probability contours for 99%, 95%, 90%, 75%, 50%, and 20%:



● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

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● Summary: Comparing $r = 0.0$ vs $r = 0.75$

● Real Time Software Demo

● Slices of Multivariate Normal Density

● **Example Probability Contours**

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

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● Example: Axes of Ellipses & Prob. Contours

● Major Axis, Multivariate Normal Distribution

● Minor Axis

● Graph of 95% Probability



Eigenvectors & Values

To get the axes of the ellipsoids of probability contours... a little more on eigenvectors and eigenvalues ...

- Recall that eigenvectors e_i and eigenvalues λ_i are solutions to

$$\Sigma e_i = \lambda_i e_i \quad i = 1, 2, \dots, p$$

where $\Sigma_{p \times p}$ symmetric and e_i is a $(p \times 1)$ vector.

- If Σ is positive definite (so that Σ^{-1} exists), then

$$\Sigma e = \lambda e \quad \text{implies} \quad \Sigma^{-1} e = \left(\frac{1}{\lambda} \right) e$$

● Outline

Motivation

Intro. to Multivariate Normal

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- Real Time Software Demo
- Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

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● Example: Axes of Ellipses & Prob. Contours

● Major Axis
Multivariate Normal Distribution

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Probability Contours: Axes of ellipsoid

- The axes of the ellipsoid are
 - ◆ In the direction of the eigenvectors of Σ^{-1} (or Σ)
 - ◆ Their lengths are proportional to the square roots of the eigenvalues of Σ (or reciprocals of square roots of eigenvalues of Σ^{-1}).

- Specifically:

$$\text{axes are } \mu \pm c\sqrt{\lambda_i}e_i$$

where e_i and λ_i are the i^{th} eigenvectors and eigenvalues of Σ .

- What's c ?

- The nature of Σ^{-1} determines the shape of the ellipses.

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● Real Time Software Demo

● Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

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● Example: Axes of Ellipses & Prob. Contours

● Major Axis
Multivariate Normal Distribution

● Minor Axis

● Graph of 0.5% Probability



Probability Contours: Axes of ellipsoid

Important Points:

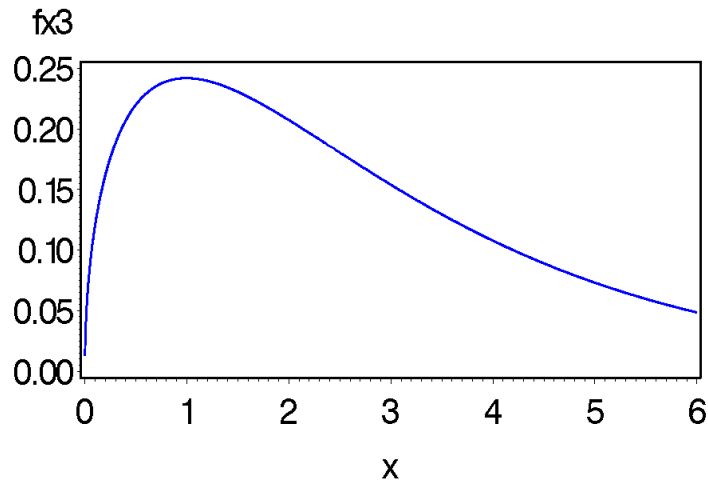
1. $(\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \sim \chi_p^2$ (if $|\boldsymbol{\Sigma}| > 0$)

2. The solid ellipsoid of values \mathbf{x} that satisfy

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

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

Chi-square distribution with df=3



- Outline
- Motivation
- Intro. to Multivariate Normal
- Bivariate Normal
 - Bivariate Normal: $p = 2$
 - Bivariate Normal & Statistical Distance
 - Bivariate Normal & Independence
 - Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
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 - 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 $r = 0.75$
 - Real Time Software Demo
 - Slices of Multivariate Normal Density
 - Example Probability Contours
 - Eigenvectors & Values
 - Probability Contours: Axes of ellipsoid
 - Probability Contours: Axes of ellipsoid

- Example: Axes of Ellipses & Prob. Contours

- Major Axis
- Multivariate Normal Distribution
- Minor Axis
- Graph of 95% Probability



Example: Axes of Ellipses & Prob. Contours

Back to the example where $x \sim N_2$ with

$$\mu = \begin{pmatrix} 5 \\ 10 \end{pmatrix} \quad \text{and} \quad \Sigma = \begin{pmatrix} 9 & 16 \\ 16 & 64 \end{pmatrix} \rightarrow \rho = .667$$

and we want the “95% probability contour”.

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

$$c = \sqrt{5.9915} = 2.4478$$

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

$$\lambda_1 = 68.316 \quad e'_1 = (.2604, .9655)$$

$$\lambda_2 = 4.684 \quad e'_2 = (.9655, -.2604)$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

- Bivariate Normal: $p = 2$
- Bivariate Normal & Statistical Distance
- Bivariate Normal & Independence
- Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
- 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 $r = 0.75$
- Real Time Software Demo
- Slices of Multivariate Normal Density
- Example Probability Contours
- Eigenvectors & Values
- Probability Contours: Axes of ellipsoid
- Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

- Major Axis
- Multivariate Normal Distribution
- Minor Axis
- Graph of 95% Probability



Major Axis

Using the largest eigenvalue and corresponding eigenvector:

$$\underbrace{\begin{pmatrix} 5 \\ 10 \end{pmatrix}}_{\mu} \pm \frac{2.45}{\sqrt{\chi^2_{2(.05)}}} \underbrace{\sqrt{68.316}}_{\lambda_1} \underbrace{\begin{pmatrix} .2604 \\ .9655 \end{pmatrix}}_{e_1}$$

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

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

● Bivariate Normal: $p = 2$

● Bivariate Normal & Statistical Distance

● Bivariate Normal & Independence

● Picture: $\mu_k = 0$, $\sigma_{kk} = 1, r = 0.0$

● 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 $r = 0.75$

● Real Time Software Demo

● Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

● Probability Contours: Axes of ellipsoid

● Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

● Major Axis

● Minor Axis

● Graph of 95% Probability



Minor Axis

Same process but now use λ_2 and e_2 , the smallest eigenvalue and corresponding eigenvector:

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

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

$$\begin{pmatrix} 5 \\ 10 \end{pmatrix} \pm \begin{pmatrix} 5.119 \\ -1.381 \end{pmatrix} \rightarrow \begin{pmatrix} -.119 \\ 11.381 \end{pmatrix}, \begin{pmatrix} 10.119 \\ 8.619 \end{pmatrix}$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

- Bivariate Normal: $p = 2$
- Bivariate Normal & Statistical Distance
- Bivariate Normal & Independence
- Picture: $\mu_k = 0$, $\sigma_{kk} = 1, r = 0.0$
- 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 $r = 0.75$
- Real Time Software Demo
- Slices of Multivariate Normal Density
- Example Probability Contours
- Eigenvectors & Values
- Probability Contours: Axes of ellipsoid
- Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

● Major Axis

● Minor Axis

● Graph of 95% Probability



Graph of 95% Probability Contour

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

● Bivariate Normal: $p = 2$

● Bivariate Normal & Statistical Distance

● Bivariate Normal & Independence

● Picture: $\mu_k = 0$,
 $\sigma_{kk} = 1, r = 0.0$

● 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 $r = 0.75$

● Real Time Software Demo

● Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

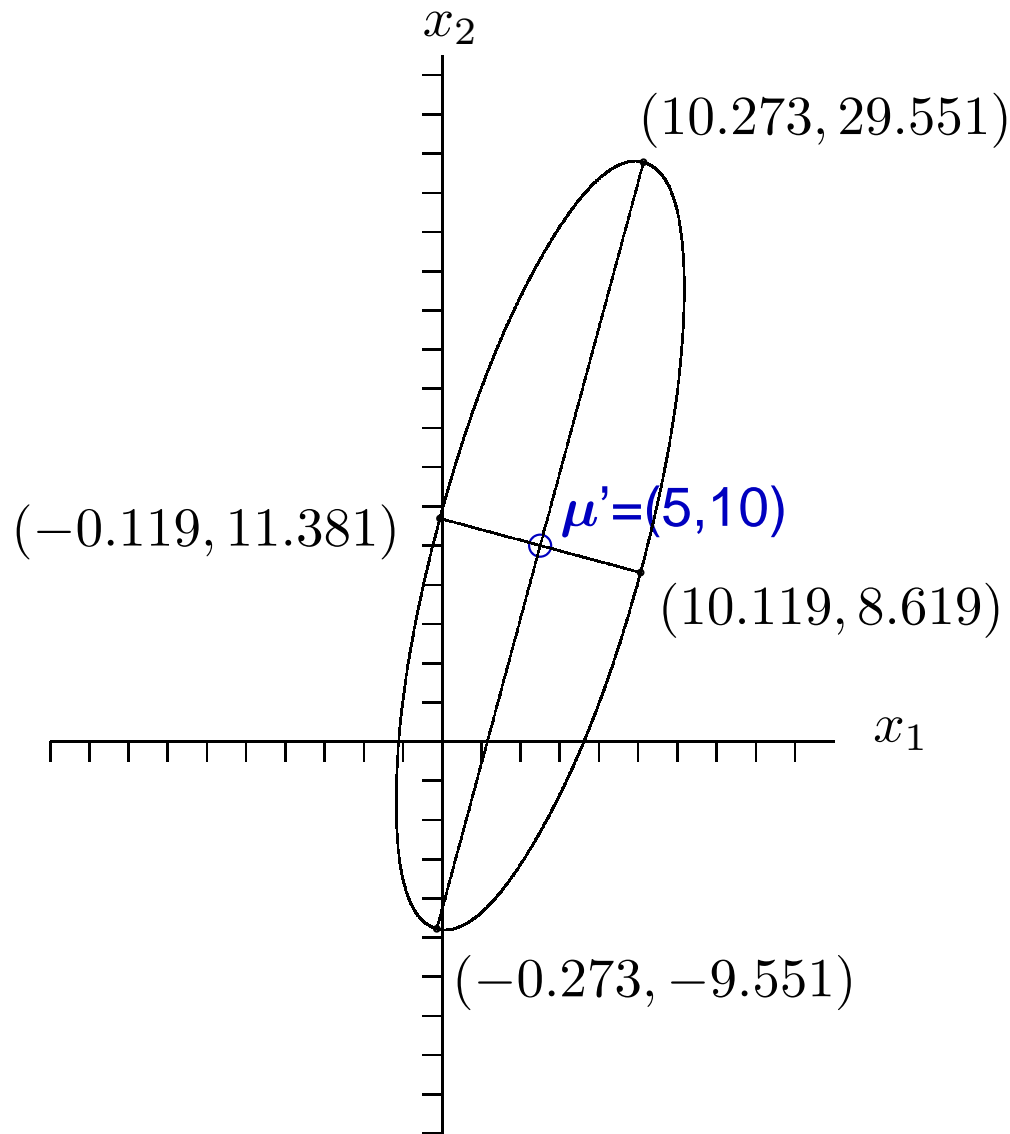
● Probability Contours: Axes of ellipsoid

● Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

● Major Axis
Multivariate Normal Distribution

● Minor Axis





Example: Equation for Contour

Equation for Contour:

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

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

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

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

- Bivariate Normal: $p = 2$
- Bivariate Normal & Statistical Distance
- Bivariate Normal & Independence
- Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
- 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 $r = 0.75$
- Real Time Software Demo
- Slices of Multivariate Normal Density
- Example Probability Contours
- Eigenvectors & Values
- Probability Contours: Axes of ellipsoid
- Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

- Major Axis
- Multivariate Normal Distribution
- Minor Axis
- Graph of 95% Probability



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?

$$\begin{aligned}(10, 20) &\longrightarrow .2(10 - 5)^2 + .028(20 - 10)^2 - .1(10 - 5)(20 - 10) \\ &= .2(25) + .028(100) - .1(50) \\ &= 2.8\end{aligned}$$

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

$$\begin{aligned}(16, 20) &\longrightarrow .2(16 - 5)^2 + .028(20 - 10)^2 - .1(16 - 5)(20 - 10) \\ &.2(121) + .028(100) - .1(11)(10) \\ &= 16\end{aligned}$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

- Bivariate Normal: $p = 2$
- Bivariate Normal & Statistical Distance
- Bivariate Normal & Independence
- Picture: $\mu_k = 0, \sigma_{kk} = 1, r = 0.0$
- 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 $r = 0.75$
- Real Time Software Demo
- Slices of Multivariate Normal Density
- Example Probability Contours
- Eigenvectors & Values
- Probability Contours: Axes of ellipsoid
- Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

- Major Axis
- Multivariate Normal Distribution
- Minor Axis
- Graph of 95% Probability



Points Inside and Outside

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

● Bivariate Normal: $p = 2$

● Bivariate Normal & Statistical Distance

● Bivariate Normal & Independence

● Picture: $\mu_k = 0$,
 $\sigma_{kk} = 1, r = 0.0$

● 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 $r = 0.75$

● Real Time Software Demo

● Slices of Multivariate Normal Density

● Example Probability Contours

● Eigenvectors & Values

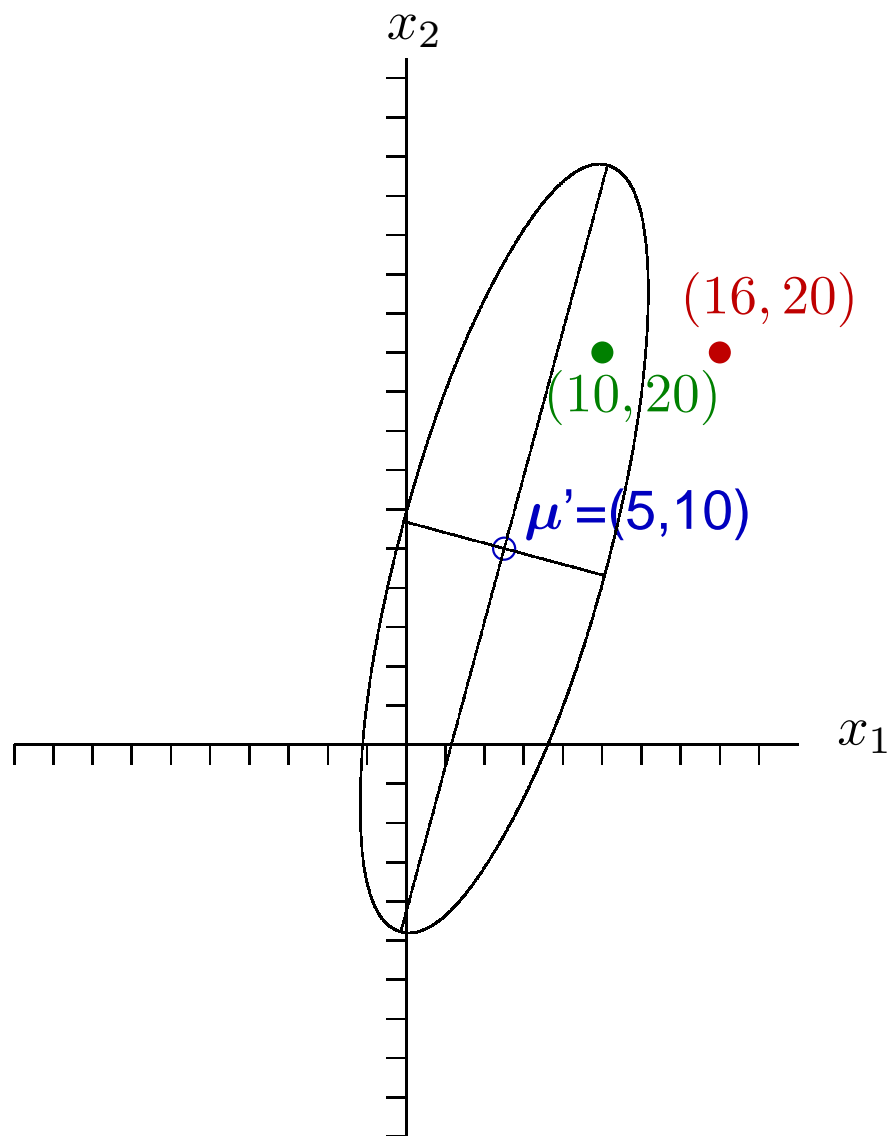
● Probability Contours: Axes of ellipsoid

● Probability Contours: Axes of ellipsoid

● Example: Axes of Ellipses & Prob. Contours

● Major Axis
Multivariate Normal Distribution

● Minor Axis
Graph of 95% Probability





More Properties that we'll Expand on

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

1. **Linear combinations** of components of \mathbf{X} are (multivariate) normal.
2. All **sub-sets** of the components of \mathbf{X} are (multivariate) normal.
3. **Zero covariance** implies that the corresponding components of \mathbf{X} are statistical independent.
4. The **conditional distributions** of the components of \mathbf{X} are (multivariate) normal.

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll Expand on

- 1: Linear Combinations
- More Linear Combinations
- Numerical Example with Multiple Combinations
- Multiple Regression as an Example
- Multiple Regression as an Example
- Distribution of \mathbf{Y}
- Least Square Estimation
- What's the distribution of $\hat{\beta}$?
- The distribution of $\hat{\mathbf{Y}}$
- The distribution of $\hat{\epsilon}$
- 2: Sub-sets of Variables
- Sub-sets of Variables continued
- Little Example on Sub-sets
- 3: Zero Covariance & Statistical Independence
- Example
- 4: Conditional Distributions
- Conditional Distribution for $q_1 = q_2 = 1$
- Multivariate Normal Distribution as a Multiple Regression as a Conditional Dist.



1: Linear Combinations

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

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

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● **1: Linear Combinations**

● More Linear Combinations

● Numerical Example with Multiple Combinations

● Multiple Regression as an Example

● Multiple Regression as an Example

● Distribution of \hat{Y}

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance & Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



More Linear Combinations

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

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

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

Also, if

$$\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{d},$$

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll Expand on

● 1: Linear Combinations

● **More Linear Combinations**

● Numerical Example with Multiple Combinations

● Multiple Regression as an Example

● Multiple Regression as an Example

● Distribution of \mathbf{Y}

● Least Square Estimation

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

● The distribution of $\hat{\mathbf{Y}}$

● The distribution of $\hat{\boldsymbol{\epsilon}}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



Numerical Example with Multiple Combinations

- Outline
- Motivation
- Intro. to Multivariate Normal
- Bivariate Normal
- More Properties
 - More Properties that we'll Expand on
 - 1: Linear Combinations
 - More Linear Combinations
 - Numerical Example with Multiple Combinations
 - Multiple Regression as an Example
 - Multiple Regression as an Example
 - Distribution of \hat{Y}
 - Least Square Estimation
 - What's the distribution of $\hat{\beta}$?
 - The distribution of \hat{Y}
 - The distribution of $\hat{\epsilon}$
 - 2: Sub-sets of Variables
 - Sub-sets of Variables continued
 - Little Example on Sub-sets
 - 3: Zero Covariance & Statistical Independence
 - Example
 - 4: Conditional Distributions
 - Conditional Distribution for $q_1 = q_2 = 1$
 - Multivariate Normal Distribution
 - Multiple Regression as a Conditional Dist.

$$\mathbf{X} \sim \mathcal{N}_2 \left(\begin{pmatrix} 5 \\ 10 \end{pmatrix}, \begin{pmatrix} 16 & 12 \\ 12 & 36 \end{pmatrix} \right)$$

$$\begin{aligned} Y_1 &= X_1 + X_2 \\ Y_2 &= X_1 - X_2 \end{aligned} \quad \text{so} \quad \mathbf{A}_{2 \times 2} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

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

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

So

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



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.
- Z_1, Z_2, \dots, Z_r are predictor/explanatory variables, which are considered to be fixed.

- The model is

$$Y = \beta_0 + \beta_1 Z_1 + \beta_2 Z_2 + \dots + \beta_r Z_r + \epsilon$$

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with
Multiple Combinations

● Multiple Regression as an
Example

● Multiple Regression as an
Example

● Distribution of \hat{Y}

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



Multiple Regression as an Example

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

$$Y_1 = \beta_o + \beta_1 Z_{11} + \beta_2 Z_{12} + \dots + \beta_r Z_{1r} + \epsilon_1$$

$$Y_2 = \beta_o + \beta_1 Z_{21} + \beta_2 Z_{22} + \dots + \beta_r Z_{2r} + \epsilon_2$$

$$\vdots \quad \vdots$$

$$Y_n = \beta_o + \beta_1 Z_{n1} + \beta_2 Z_{n2} + \dots + \beta_r Z_{nr} + \epsilon_n$$

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

In terms of matrices,

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = \begin{pmatrix} 1 & Z_{11} & Z_{12} & \dots & Z_{1r} \\ 1 & Z_{21} & Z_{22} & \dots & Z_{2r} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & Z_{n1} & Z_{n2} & \dots & Z_{nr} \end{pmatrix} \begin{pmatrix} \beta_o \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_r \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with Multiple Combinations

● Multiple Regression as an Example

● Multiple Regression as an Example

● Distribution of Y

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



Distribution of Y

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

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

■ Mean of Y :

$$\mu_Y = E(Y) = E(Z\beta + \epsilon) = Z\beta + E(\epsilon) = Z\beta$$

■ Covariance of Y :

$$\Sigma_Y = \sigma^2 I$$

(the same as ϵ).

■ Distribution of Y is multivariate normal because ϵ is multivariate normal:

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with

Multiple Combinations

● Multiple Regression as an Example

● Multiple Regression as an Example

● Distribution of Y

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



Least Square Estimation

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

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 z_1, z_2, \dots, z_r on the explanatory variables. The least squares estimate of β is the vector b that minimizes

$$\begin{aligned} \sum_{j=1}^n (y_j - z'_j b)^2 &= \sum_{j=1}^n (y_j - b_0 - b_1 z_{j1} - b_2 z_{j2} - \dots - b_r z_{jr})^2 \\ &= (\mathbf{y} - \mathbf{Zb})'(\mathbf{y} - \mathbf{Zb}) \\ &= \epsilon' \epsilon \end{aligned}$$

where z'_j is the j^{th} row of Z , and $b = (b_0, b_1, b_2, \dots, b_r)'$.

If Z has full rank (i.e., the rank of Z is $r + 1 \leq n$), then the least squares estimate of β is

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with

Multiple Combinations

● Multiple Regression as an

Example

● Multiple Regression as an

Example

● Distribution of Y

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



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

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

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

■ Mean of $\hat{\beta}$:

$$\begin{aligned} \mu_{\hat{\beta}} = E(\hat{\beta}) &= E(\mathbf{A}\mathbf{Y}) \\ &= \mathbf{A}E(\mathbf{Y}) \\ &= \mathbf{A}\mathbf{Z}\boldsymbol{\beta} \\ &= \underbrace{(\mathbf{Z}'\mathbf{Z})^{-1}} \underbrace{\mathbf{Z}'\mathbf{Z}}\boldsymbol{\beta} = \boldsymbol{\beta} \end{aligned}$$

■ Covariance matrix for $\hat{\beta}$

$$\begin{aligned} \Sigma_{\hat{\beta}} &= \mathbf{A}\Sigma_{\mathbf{Y}}\mathbf{A}' \\ &= ((\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}')(\sigma^2\mathbf{I})(\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1}) \\ &= \sigma^2(\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{Z}(\mathbf{Z}'\mathbf{Z})^{-1} \\ &= \sigma^2(\mathbf{Z}'\mathbf{Z})^{-1} \end{aligned}$$

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with Multiple Combinations

● Multiple Regression as an Example

● Multiple Regression as an Example

● Distribution of \mathbf{Y}

● Least Square Estimation

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

● The distribution of $\hat{\mathbf{Y}}$

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance & Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

● Multiple Regression as a Conditional Dist.



The distribution of \hat{Y}

The “fitted values” or predicted values are

$$\hat{y} = Z\hat{\beta} = Hy$$

where $H = Z(Z'Z)^{-1}Z'$. The matrix H is the “hat” matrix.

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

■ Mean of \hat{Y} :

$$\mu_{\hat{Y}} = E(Z\hat{\beta}) = ZE(\hat{\beta}) = Z\beta$$

■ Covariance matrix for \hat{Y}

$$Z\Sigma_{\hat{\beta}}Z' = Z(\sigma^2 \underbrace{(Z'Z)^{-1}}) \underbrace{Z'} = \sigma^2 Z'Z(Z'Z)^{-1} = \sigma^2 I$$

■ Distribution of \hat{Y} :

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with

Multiple Combinations

● Multiple Regression as an

Example

● Multiple Regression as an

Example

● Distribution of Y

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

● Multiple Regression as a
Conditional Dist.



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.

Last few comments on this example:

1. The least squares estimates of β and ϵ are also the maximum likelihood estimates.
2. The maximum likelihood estimate of σ^2 is $\hat{\sigma}^2 = \hat{\epsilon}'\hat{\epsilon}/n$
3. $\hat{\beta}$ and $\hat{\epsilon}$ are statistically independent.

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with Multiple Combinations

● Multiple Regression as an Example

● Multiple Regression as an Example

● Distribution of \mathbf{Y}

● Least Square Estimation

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

● The distribution of $\hat{\mathbf{Y}}$

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables continued

● Little Example on Sub-sets

● 3: Zero Covariance & Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



2: Sub-sets of Variables

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

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

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with

Multiple Combinations

● Multiple Regression as an

Example

● Multiple Regression as an

Example

● Distribution of Y

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

● Multiple Regression as a

Conditional Dist.



Sub-sets of Variables continued

Then for

$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_{1(q \times 1)} \\ \mathbf{X}_{2((p-q) \times 1)} \end{pmatrix}$$

The distributions of the sub-sets are

$$\mathbf{X}_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11}) \quad \text{and} \quad \mathbf{X}_2 \sim \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{22})$$

The result means that

- Each of the \mathbf{X}_i 's are univariate normals (next page)
- All possible sub-sets are multivariate normal.
- All marginal distributions are (multivariate) normal.

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with

Multiple Combinations

● Multiple Regression as an

Example

● Multiple Regression as an

Example

● Distribution of \mathbf{Y}

● Least Square Estimation

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

● The distribution of $\hat{\mathbf{Y}}$

● The distribution of $\hat{\boldsymbol{\epsilon}}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

● Multiple Regression as a

Conditional Dist.



Little Example on Sub-sets

Suppose that

$$\mathbf{X} = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}_3(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with

Multiple Combinations

● Multiple Regression as an

Example

● Multiple Regression as an

Example

● Distribution of \hat{Y}

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

● Multiple Regression as a

Conditional Dist.



3: Zero Covariance & Statistical Independence

There are three parts to this one:

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

2. If

$$\begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix} \sim \mathcal{N}_{q_1+q_2} \left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \right),$$

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

3. If \mathbf{X}_1 and \mathbf{X}_2 are statistically independent and distributed as $\mathcal{N}_{q_1}(\mu_1, \Sigma_{11})$ and $\mathcal{N}_{q_2}(\mu_2, \Sigma_2)$, respectively, then

$$\begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix} \sim \mathcal{N}_{q_1+q_2} \left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \mathbf{0} \\ \mathbf{0} & \Sigma_{22} \end{pmatrix} \right).$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with Multiple Combinations

● Multiple Regression as an Example

● Multiple Regression as an Example

● Distribution of \mathbf{Y}

● Least Square Estimation

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

● The distribution of $\hat{\mathbf{Y}}$

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance & Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



Example

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

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

$$\begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix} \sim \mathcal{N}_4 \left(\begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_4 \\ \mu_3 \end{pmatrix}, \begin{pmatrix} 2 & 1 & .5 & 0 \\ 1 & 3 & .5 & 0 \\ .5 & .5 & 1 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix} \right)$$

So set \mathbf{X}_1 is statistically independent of \mathbf{X}_2 .

- Outline

- Motivation

- Intro. to Multivariate Normal

- Bivariate Normal

- More Properties

- More Properties that we'll

- Expand on

- 1: Linear Combinations

- More Linear Combinations

- Numerical Example with

- Multiple Combinations

- Multiple Regression as an Example

- Multiple Regression as an Example

- Distribution of $\hat{\mathbf{Y}}$

- Least Square Estimation

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

- The distribution of $\hat{\mathbf{Y}}$

- The distribution of $\hat{\epsilon}$

- 2: Sub-sets of Variables

- Sub-sets of Variables

- continued

- Little Example on Sub-sets

- 3: Zero Covariance &

- Statistical Independence

- Example

- 4: Conditional Distributions

- Conditional Distribution for

- $q_1 = q_2 = 1$

- Multivariate Normal Distribution

- Conditional Dist.



4: Conditional Distributions

Let $\mathbf{X}' = (\mathbf{X}_{1(q_1 \times 1)}, \mathbf{X}_{2(q_2 \times 1)})$ be distributed at $\mathcal{N}_{q_1+q_2}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\Sigma} = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

and $|\boldsymbol{\Sigma}| > 0$ (i.e., positive definite). Then the conditional distribution of \mathbf{X}_1 given $\mathbf{X}_2 = \mathbf{x}_2$ is (multivariate) normal with mean and covariance matrix

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

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

- Outline
- Motivation
- Intro. to Multivariate Normal
- Bivariate Normal
- More Properties
 - More Properties that we'll Expand on
 - 1: Linear Combinations
 - More Linear Combinations
 - Numerical Example with Multiple Combinations
 - Multiple Regression as an Example
 - Multiple Regression as an Example
 - Distribution of \hat{Y}
 - Least Square Estimation
 - What's the distribution of $\hat{\beta}$?
 - The distribution of \hat{Y}
 - The distribution of $\hat{\epsilon}$
 - 2: Sub-sets of Variables
 - Sub-sets of Variables continued
 - Little Example on Sub-sets
 - 3: Zero Covariance & Statistical Independence
 - Example
 - 4: Conditional Distributions
 - Conditional Distribution for $q_1 = q_2 = 1$
 - Multivariate Normal Distribution
 - Multiple Regression as a Conditional Dist.



Conditional Distribution for $q_1 = q_2 = 1$

Bivariate normal distribution

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

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

Notes:

- $\sigma_{12} = \rho_{12} \sqrt{\sigma_{11}} \sqrt{\sigma_{22}}$
- $\Sigma_{12} \Sigma_{22}^{-1} = \sigma_{12} / \sigma_{22} = \rho_{12} (\sqrt{\sigma_{11}} / \sqrt{\sigma_{22}})$
- $\Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} = \sigma_{11} - \sigma_{12}^2 / \sigma_{22} = \sigma_{11} (1 - \rho_{12}^2)$

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

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

What is this?

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

● More Properties that we'll

Expand on

● 1: Linear Combinations

● More Linear Combinations

● Numerical Example with

Multiple Combinations

● Multiple Regression as an

Example

● Multiple Regression as an

Example

● Distribution of \hat{Y}

● Least Square Estimation

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

● The distribution of \hat{Y}

● The distribution of $\hat{\epsilon}$

● 2: Sub-sets of Variables

● Sub-sets of Variables

continued

● Little Example on Sub-sets

● 3: Zero Covariance &

Statistical Independence

● Example

● 4: Conditional Distributions

● Conditional Distribution for

$q_1 = q_2 = 1$

● Multivariate Normal Distribution

Conditional Dist.



Multiple Regression as a Conditional Dist.

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:

$$\text{Let } \Sigma_{12}\Sigma_{22}^{-1} = \beta_{q_1 \times q_2} \begin{pmatrix} \beta_{1,q_1+1} & \beta_{1,q_1+2} & \cdots & \beta_{1,q_1+q_2} \\ \beta_{2,q_1+1} & \beta_{2,q_1+2} & \cdots & \beta_{2,q_1+q_2} \\ \cdots & \cdots & \ddots & \cdots \\ \beta_{q_1,q_1+1} & \beta_{q_1,q_1+2} & \cdots & \beta_{q_1,q_1+q_2} \end{pmatrix}$$

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

- Outline
- Motivation
- Intro. to Multivariate Normal
- Bivariate Normal
- More Properties
 - More Properties that we'll Expand on
 - 1: Linear Combinations
 - More Linear Combinations
 - Numerical Example with Multiple Combinations
 - Multiple Regression as an Example
 - Multiple Regression as an Example
 - Distribution of Y
 - Least Square Estimation
 - What's the distribution of $\hat{\beta}$?
 - The distribution of \hat{Y}
 - The distribution of $\hat{\epsilon}$
 - 2: Sub-sets of Variables
 - Sub-sets of Variables continued
 - Little Example on Sub-sets
 - 3: Zero Covariance & Statistical Independence
 - Example
 - 4: Conditional Distributions
 - Conditional Distribution for $q_1 = q_2 = 1$



Estimation of μ and Σ

& sampling distribution of estimators.

Suppose we have a p dimensional normal distribution with mean μ and covariance matrix Σ .

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

$$\mathbf{X}_j \sim \mathcal{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \quad j = 1, 2, \dots, n \text{ and independent}$$

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

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

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

● Estimation of μ and Σ

● Estimation of μ and Σ :

Multivariate Case

● Sampling Distribution of $\hat{\Sigma}$

Central Limit Theorem



Estimation of μ and Σ : Multivariate Case

The maximum likelihood estimator of μ is

$$\hat{\mu} = \bar{\mathbf{X}} = \frac{1}{n} \sum_{j=1}^n \mathbf{X}_j$$

and the ML estimator of Σ is

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

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.*:

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

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

$$\bar{\mathbf{X}} \sim \mathcal{N}_p\left(\mu, \frac{1}{n} \Sigma\right)$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

● Estimation of μ and Σ

● Estimation of μ and Σ :
Multivariate Case

● Sampling Distribution of $\hat{\Sigma}$

Central Limit Theorem



Sampling Distribution of $\hat{\Sigma}$

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

The matrix

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

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

Wishart distribution:

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

$W_m(\cdot | \Sigma)$ = Wishart distribution with m degrees of freedom

= The distribution of $\sum_{j=1}^m \mathbf{Z}_j \mathbf{Z}_j'$

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

Note : $\bar{\mathbf{X}}$ and S are independent.

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

● Estimation of μ and Σ

● Estimation of μ and Σ :

Multivariate Case

● Sampling Distribution of $\hat{\Sigma}$

Central Limit Theorem



Law of Large Numbers

Data are not always (multivariate) normal

The Law of Large Numbers (for multivariate data):

Let $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$ be independent observations from a population with mean $E(\mathbf{X}) = \boldsymbol{\mu}$.

Then $\bar{\mathbf{X}} = (1/n) \sum_{j=1}^n \mathbf{X}_j$ converges in probability to $\boldsymbol{\mu}$ as n gets large; that is,

$$\bar{\mathbf{X}} \rightarrow \boldsymbol{\mu} \text{ for large samples}$$

And

S (or S_n) approach Σ for large samples

These are true regardless of the true distribution of the \mathbf{X}_j 's.

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

Central Limit Theorem

● Law of Large Numbers

● Central Limit Theorem

● Few more comments

● Comparison of Probability

Contours

● Why So Much a Difference with Only 20?



Central Limit Theorem

Let Y_1, Y_2, \dots, Y_n be independent observations from a population with mean $E(Y) = \mu$ and finite (non-singular, full rank), covariance matrix Σ .

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

So, for “large” n

$$\bar{X} = \text{Sample mean vector} \approx \mathcal{N}\left(\mu, \frac{1}{n}\Sigma\right),$$

regardless of the underlying distribution of the Y_j 's.

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

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

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

$$n(\bar{X} - \mu)' S^{-1} (\bar{X} - \mu) \approx \chi_p^2$$

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

Central Limit Theorem

● Law of Large Numbers

● Central Limit Theorem

● Few more comments

● Comparison of Probability

Contours

● Why So Much a Difference with Only 20?



Few more comments

- 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{X} are tighter than those for X since we have $(1/n)\Sigma$ for \bar{X} rather than Σ for X .

See next slide for an example of the latter.

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

Central Limit Theorem

● Law of Large Numbers

● Central Limit Theorem

● Few more comments

● Comparison of Probability

Contours

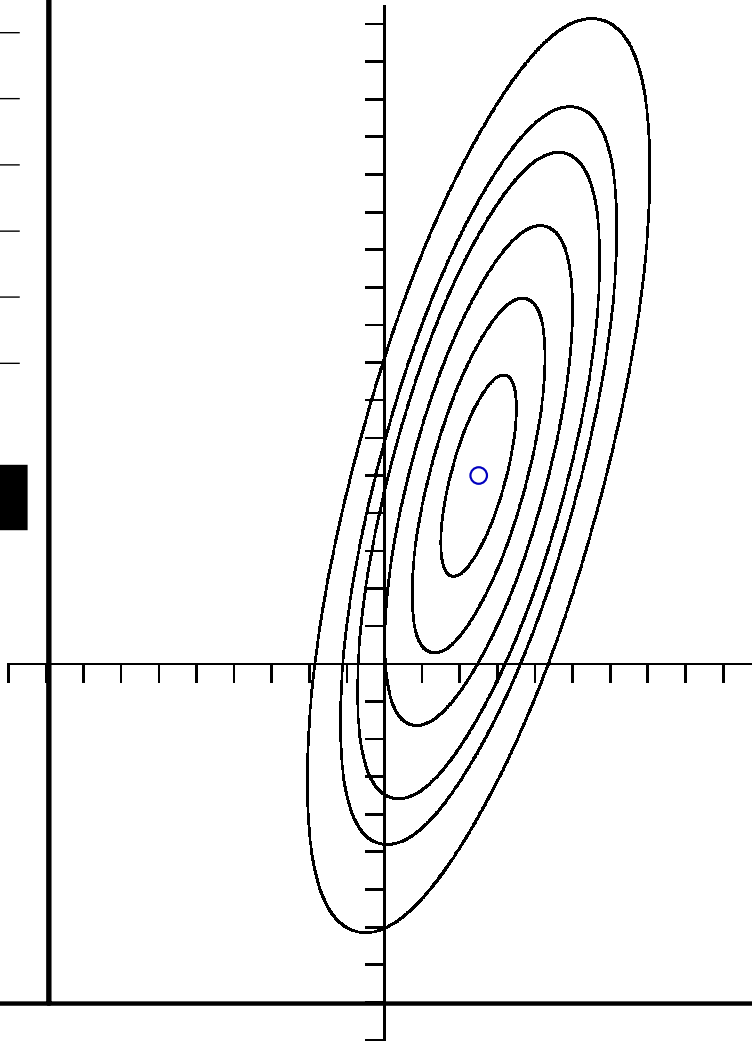
● Why So Much a Difference
with Only 20?



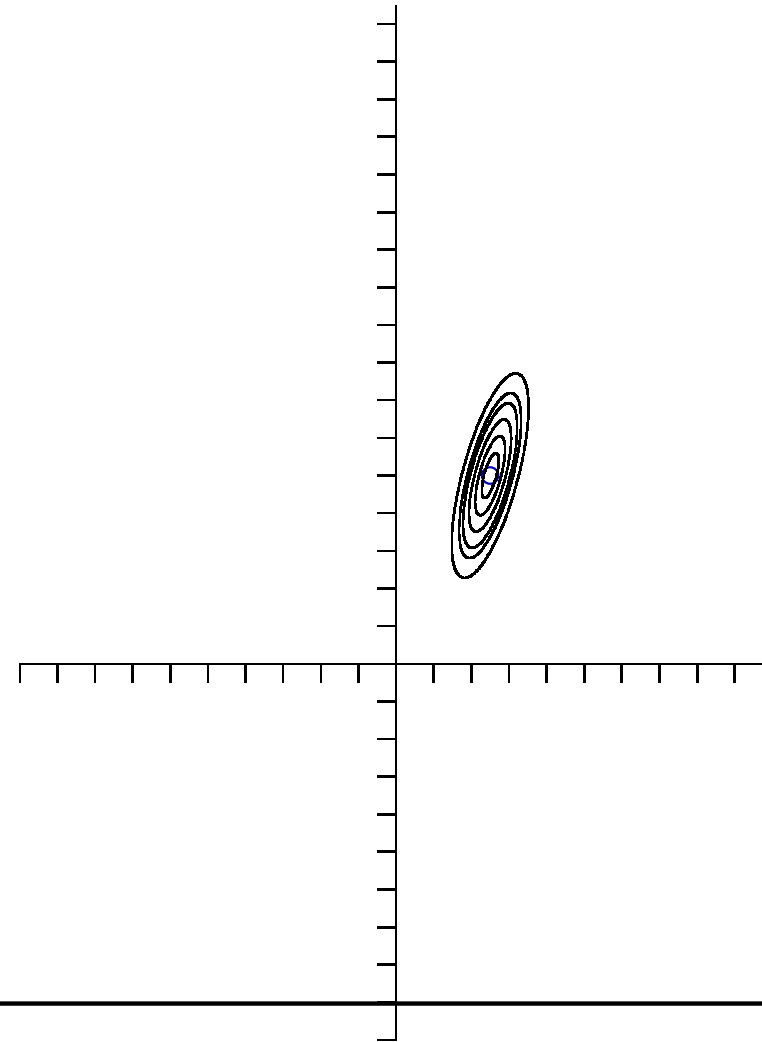
Comparison of Probability Contours

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

Contours for X_j



Contours for \bar{X}



● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

Central Limit Theorem

● Law of Large Numbers

● Central Limit Theorem

● Few more comments

● Comparison of Probability

Contours

● Why So Much a Difference with Only 20?



Why So Much a Difference with Only 20?

● Outline

Motivation

Intro. to Multivariate Normal

Bivariate Normal

More Properties

Estimation

Central Limit Theorem

● Law of Large Numbers

● Central Limit Theorem

● Few more comments

● Comparison of Probability

Contours

● Why So Much a Difference
with Only 20?

For X_j

$$\Sigma = \begin{pmatrix} 9 & 16 \\ 16 & 64 \end{pmatrix} \longrightarrow \lambda_1 = 68.316 \text{ and } \lambda_2 = 4.684$$

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

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

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