Part I: Linear Models

Chapter I.2

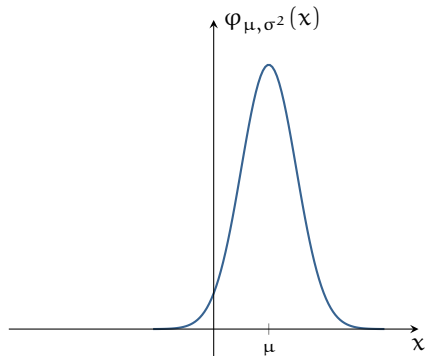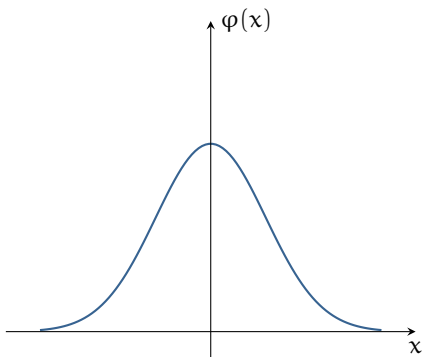## Multivariate Normal Distribution

Topics

To be discussed...
- definition of general multivariate normal distributions
- marginal & conditional distributions
- independence & correlation
- some illustrations (bivariate normal)
- linear transformations and applications

▶ I.2.1 Univariate normal distribution $N(\mu, \sigma^2)$

⯈ $X \sim N(\mu, \sigma^2)$ with parameters $\mu \in \mathbb{R}$ and $\sigma > 0$ has the PDF

$$\varphi_{\mu,\sigma^2}(x) = \frac{1}{\sqrt{2\pi}\,\sigma}\,\exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}, \quad x \in \mathbb{R}.$$

⯈ For $Z \sim N(0,1)$, we have $\boxed{X = \mu + \sigma Z}$; $\varphi = \varphi_{0,1}$.

▣ I.2.2 Definition

Let $Z_1, \ldots, Z_k \overset{\text{iid}}{\sim} N(0, 1)$, $\mathbf{Z} = (Z_1, \ldots, Z_k)'$, and $\boldsymbol{\mu} \in \mathbb{R}^p, A \in \mathbb{R}^{p \times k}$. Then:

- ❯ $\mathbf{Z}$ has a k-**dimensional standard normal distribution** (for short $\mathbf{Z} \sim N_k(\mathbf{0}, I_k)$).
- ❯ $\mathbf{X} = \boldsymbol{\mu} + A\mathbf{Z}$ has a p **dimensional normal distribution with parameters** $\boldsymbol{\mu}$ **and** $\Sigma = AA'$ (for short $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \Sigma)$).

▣ I.2.3 Remark

- ❯ In the situation of Definition I.2.2, we have
  - ❯ $E\mathbf{X} = \boldsymbol{\mu}$, $\text{Cov}(\mathbf{X}) = \Sigma$
  - ❯ Since $\text{rank}(\Sigma) = \text{rank}(A)$ may be less than p, Σ may be a singular matrix.
- ❯ How can a multivariate normal distribution be generated with a **given** $\boldsymbol{\mu} \in \mathbb{R}^p$ **and** $\Sigma \in \mathbb{R}_{\geqslant 0}^{p \times p}$?
  - ☞ How to choose A?

▶ I.2.4 Corollary

Let $Z_1, \ldots, Z_p \overset{\text{iid}}{\sim} N(0,1)$, $\mathbf{Z} = (Z_1, \ldots, Z_p)'$, and $\boldsymbol{\mu} \in \mathbb{R}^p, \Sigma \in \mathbb{R}^{p \times p}_{\geqslant 0}$. Then:

$$\mathbf{X} = \boldsymbol{\mu} + \Sigma^{1/2}\mathbf{Z} \sim N_p(\boldsymbol{\mu}, \Sigma).$$

▶ I.2.5 Theorem

Let $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \Sigma)$ with $\boldsymbol{\mu} \in \mathbb{R}^p, \Sigma \in \mathbb{R}^{p \times p}_{>0}$ and determinant $\det(\Sigma)$. Then, $\mathbf{X}$ has the PDF

$$f^{\mathbf{X}}(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^p \det(\Sigma)}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})'\Sigma^{-1}(\mathbf{x} - \boldsymbol{\mu})\right), \quad \mathbf{x} = (x_1, \ldots, x_p)' \in \mathbb{R}^p.$$

▶ I.2.6 Remark

A multivariate normal distribution $N_p(\boldsymbol{\mu}, \Sigma)$ with $\boldsymbol{\mu} \in \mathbb{R}^p$ and singular covariance-matrix $\Sigma \in \mathbb{R}^{p \times p}_{\geqslant 0}$ does not have a density function on $\mathbb{R}^p$!

Marginals & Conditionals

For a vector $\mathbf{x} \in \mathbb{R}^p$ and $\emptyset \neq K \subseteq \{1, \ldots, p\}$, let $\mathbf{x}_K = (x_i)_{i \in K}$.

> **I.2.7 Theorem (parameters and marginals of a multivariate normal distribution)**
>
> Let $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \Sigma)$ with $\boldsymbol{\mu} \in \mathbb{R}^p, \Sigma \in \mathbb{R}_{\geq 0}^{p \times p}$ and $\emptyset \neq K \subseteq \{1, \ldots, p\}$ and $\Sigma_{K,K} = \text{Cov}(\mathbf{X}_K)$. Then:
>
> ❶ $E\mathbf{X} = \boldsymbol{\mu}$
>
> ❷ $\text{Cov}(\mathbf{X}) = \Sigma$
>
> ❸ $\mathbf{X}_K \sim N(\boldsymbol{\mu}_K, \Sigma_{K,K})$ ('**marginals of normals are normal**')

> **I.2.8 Theorem (conditionals of a multivariate normal distribution)**
>
> Let $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \Sigma)$ with $\boldsymbol{\mu} \in \mathbb{R}^p, \Sigma \in \mathbb{R}_{>0}^{p \times p}$ and $\emptyset \neq K, L \subseteq \{1, \ldots, p\}$, $K \cap L = \emptyset$, $k = |K|$. Further, let $\Sigma_{K,L} = \text{Cov}(\mathbf{X}_K, \mathbf{X}_L)$ and $\Sigma_{KK|L} = \Sigma_{K,K} - \Sigma_{K,L}\Sigma_{L,L}^{-1}\Sigma_{K,L}'$. Then:
>
> ❶ $\mathbf{X}_K \mid \mathbf{X}_L = \mathbf{x}_L \sim N_k(\boldsymbol{\mu}_K + \Sigma_{K,L}\Sigma_{L,L}^{-1}(\mathbf{x}_L - \boldsymbol{\mu}_L), \Sigma_{KK|L})$
>
>   ('**conditionals of normals are normal**')
>
> ❷ $E(\mathbf{X}_K \mid \mathbf{X}_L = \mathbf{x}_L) = \boldsymbol{\mu}_K + \Sigma_{K,L}\Sigma_{L,L}^{-1}(\mathbf{x}_L - \boldsymbol{\mu}_L)$
>
>   The matrix $\Sigma_{K,L}\Sigma_{L,L}^{-1}$ is called **regression matrix**.
>
> ❸ $\text{Cov}(\mathbf{X}_K \mid \mathbf{X}_L = \mathbf{x}_L) = \Sigma_{KK|L}$,

Independence & Correlation

Let $X \sim N_p(\mu, \Sigma)$ with $\mu \in \mathbb{R}^p$, $\Sigma \in \mathbb{R}^{p \times p}_{\geqslant 0}$ and $\emptyset \neq K, L \subseteq \{1, \ldots, p\}$, $K \cap L = \emptyset$, $k = |K|$. Further, let $\Sigma_{K,L} = \text{Cov}(X_K, X_L)$. Then:

1. X_K and X_L are independent if and only if $\Sigma_{K,L} = 0$

2. $X = (X_1, \ldots, X_p)' \sim N_p(0, I_p) \iff X_1, \ldots, X_p \overset{iid}{\sim} N(0, 1)$

3. $X = (X_1, \ldots, X_p)' \sim N_p(\mu, \Sigma)$ with a diagonal matrix $\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_p^2)$

   $\iff X_1, \ldots, X_p$ are independent random variables with $X_j \sim N(\mu_j, \sigma_j^2)$, $1 \leqslant j \leqslant p$

Bivariate normal distribution

▶ I.2.10 Example (Bivariate normal distribution)

A **bivariate normal distributed random vector** $X = (X_1, X_2)'$ has the PDF (for $x_1, x_2 \in \mathbb{R}$)

$$f^{X_1,X_2}(x_1,x_2) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \exp\left(-\frac{1}{2(1-\rho^2)}\left[\frac{(x_1-\mu_1)^2}{\sigma_1^2}\right.\right.$$
$$\left.\left. - 2\rho\frac{(x_1-\mu_1)(x_2-\mu_2)}{\sigma_1\sigma_2} + \frac{(x_2-\mu_2)^2}{\sigma_2^2}\right]\right) \quad \text{(C.1)}$$

with parameters $\mu_1, \mu_2 \in \mathbb{R}$, $\sigma_1^2, \sigma_2^2 > 0$ and $\rho \in (-1, 1)$;

- ▸ for short: $(X_1, X_2)' \sim N_2(\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \rho)$
- ▸ covariance matrix Σ as in Theorem I.2.7:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} \in \mathbb{R}^{2\times 2}$$

with determinant $\det\Sigma = \sigma_1^2\sigma_2^2(1-\rho^2)$ and $\mu = (\mu_1, \mu_2)' \in \mathbb{R}^2$
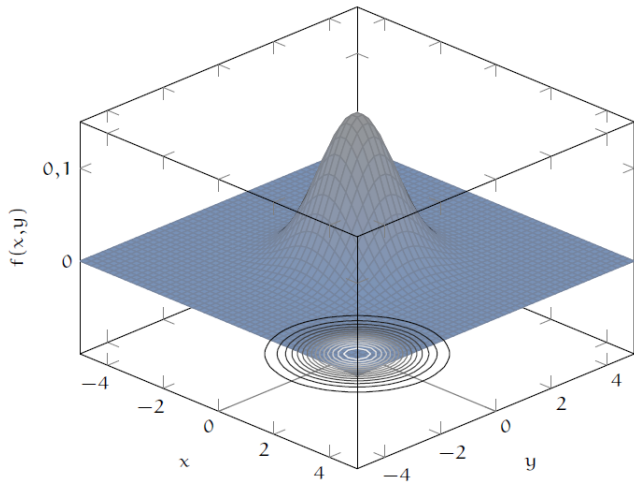
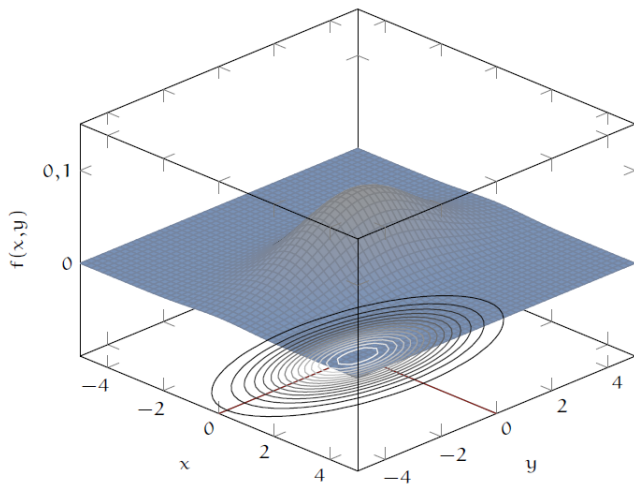Figure: PDF of bivariate standard normal distribution $N_2(0, 0, 1, 1, 0)$

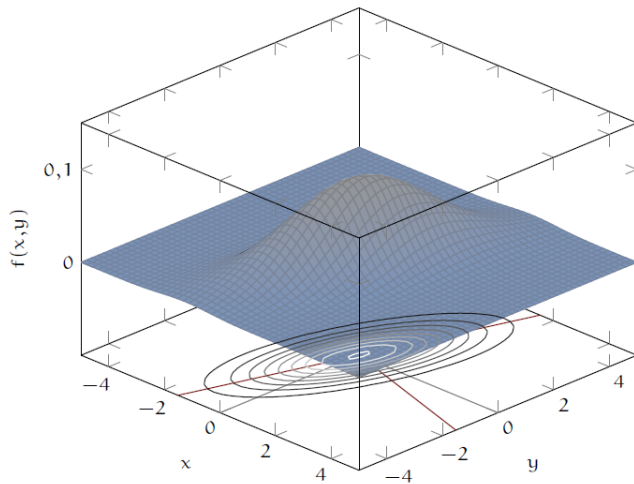Figure: PDF of bivariate normal distribution $N_2(0, 0, 1, 4, 0)$

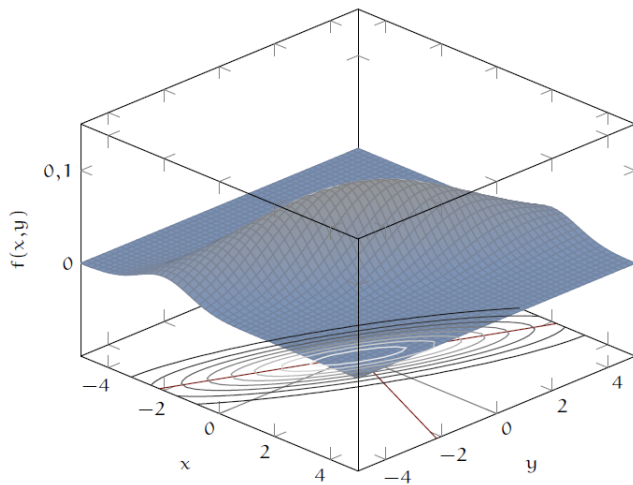Figure: PDF of bivariate normal distribution $N_2(0, 0, 1, 4, \frac{1}{2})$

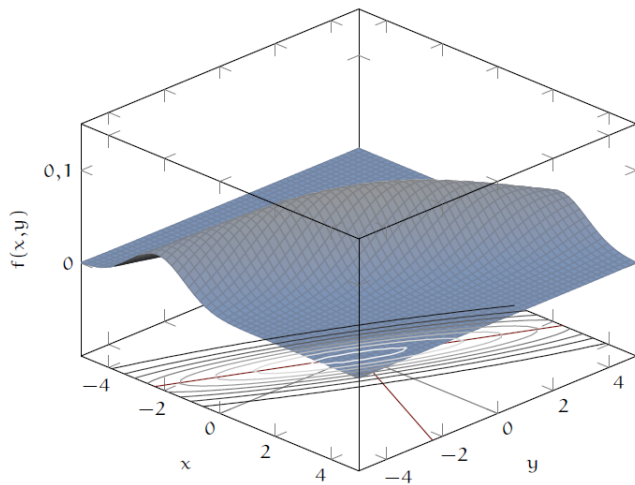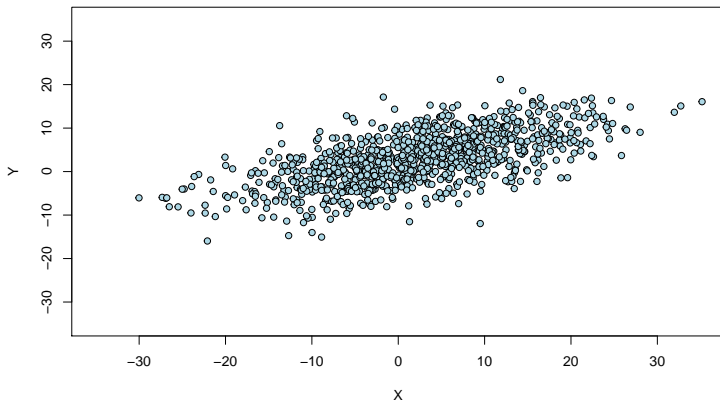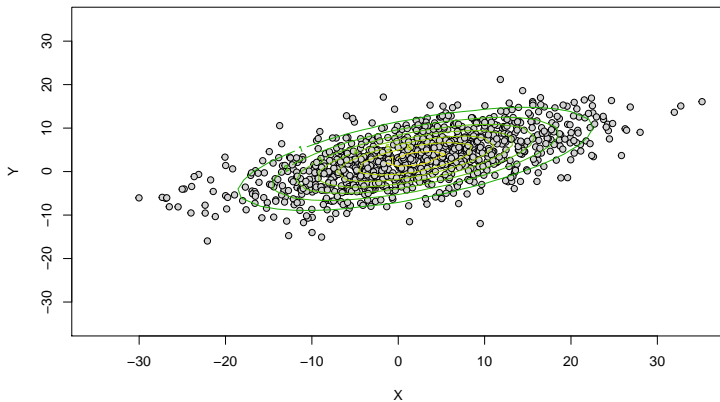Figure: PDF of bivariate normal distribution $N_2(0, 0, 1, 4, \frac{4}{5})$

Figure: PDF of bivariate normal distribution $N_2(0, 0, 1, 4, \frac{9}{10})$

Simulated bivariate normal data

Simulated bivariate normal data with ellipses

⊠ I.2.11 Theorem

Let $X \sim N_p(\mu, \Sigma)$ with $\mu \in \mathbb{R}^p, \Sigma \in \mathbb{R}_{\geqslant 0}^{p \times p}$ and $a \in \mathbb{R}^k, B \in \mathbb{R}^{k \times p}, 1 \leqslant k \leqslant p$. Then:

$$Y = a + BX \sim N_k(a + B\mu, B\Sigma B').$$

In particular, we get for $\Sigma \in \mathbb{R}_{>0}^{p \times p}$ and $\Sigma^{-1/2} = (\Sigma^{1/2})^{-1}$

$$Y = \Sigma^{-1/2}(X - \mu) \sim N_p(0, I_p).$$

⊠ I.2.12 Remark

❯ The transformation

$$Y = \Sigma^{-1/2}(X - \mu)$$

considered in Theorem I.2.11 is called **Mahalanobis transformation**.

❯ Considering the Euclidean norm $\|Y\|$ of Y, we get

$$\|Y\|^2 = Y'Y = (\Sigma^{-1/2}(X - \mu))'\Sigma^{-1/2}(X - \mu) = (X - \mu)'\Sigma^{-1}(X - \mu) = \|X - \mu\|_\Sigma^2, \text{ say.}$$

$\|X\|_\Sigma^2$ is called **Mahalanobis norm** of X. For random vectors X and Y of the same dimension p, $\|X - Y\|_\Sigma^2$ is called **Mahalanobis distance** of X and Y.

▶ I.2.13 Corollary

1 Let $X = (X_1, \ldots, X_p)' \sim N_p(\mu, \Sigma)$ with $\Sigma = (\sigma_{ij})_{i,j}$ and $\overline{X} = \frac{1}{p} \sum\limits_{j=1}^p X_j$. Then:

$$\overline{X} = \frac{1}{p} \mathbb{1}_p' X \sim N\Big(\frac{1}{p} \sum_{j=1}^p \mu_j, \frac{1}{p^2} \mathbb{1}_p' \Sigma \mathbb{1}_p \Big) = N\Big(\frac{1}{p} \sum_{j=1}^p \mu_j, \frac{1}{p^2} \sum_{i,j} \sigma_{ij} \Big).$$

2 If $X_1, \ldots, X_n \overset{iid}{\sim} N(\mu, \sigma^2)$, $\sigma^2 > 0$, then

> ● $\overline{X} \sim N(\mu, \frac{\sigma^2}{n})$

> ● $\boxed{\sqrt{n} \dfrac{\overline{X} - \mu}{\sigma} \sim N(0, 1)}$

▶ I.2.14 Theorem

Let $X \sim N_p(\mu, \Sigma)$ with $\mu \in \mathbb{R}^p, \Sigma \in \mathbb{R}_{\geqslant 0}^{p \times p}$. Then, for $A \in \mathbb{R}^{k \times p}, B \in \mathbb{R}^{r \times p}$ with $k, r \in \mathbb{N}$, we get:

- ❯ AX and BX are independent if and only if $A\Sigma B' = 0$.

▶ I.2.15 Theorem

Let $p \geqslant 2$, $Z = (Z_1, \ldots, Z_p)' \sim N_p(0, \sigma^2 I_p)$, $\overline{Z} = \frac{1}{p} \sum_{j=1}^p Z_j$, and $E_p = I_p - \frac{1}{p} \mathbb{1}_{p \times p}$. Then:

- ❯ $\overline{Z}$ and $Z - \overline{Z} \mathbb{1}_p = E_p Z$ are independent.
- ❯ $\overline{Z}$ and $S_Z = \frac{1}{p-1} \sum_{j=1}^p (Z_j - \overline{Z})^2$ are independent.

▶ I.2.16 Lemma

Let $X_1, \ldots, X_n \overset{\text{iid}}{\sim} N(0, 1)$. Then:

❶ $X_1^2 \sim \chi^2(1)$

❷ $\sum\limits_{i=1}^{n} X_i^2 \sim \chi^2(n)$

▶ I.2.17 Corollary

Let $X_1, \ldots, X_n \overset{\text{iid}}{\sim} N(\mu, \sigma^2)$ with $\mu \in \mathbb{R}$, $\sigma > 0$ and

$$\widehat{\sigma}_\mu^2 = \frac{1}{n} \sum_{j=1}^{n} (X_j - \mu)^2, \quad \widehat{\sigma}^2 = \frac{1}{n-1} \sum_{j=1}^{n} (X_j - \overline{X})^2.$$

Then:

❶ $\dfrac{n}{\sigma^2} \widehat{\sigma}_\mu^2 \sim \chi^2(n)$.

❷ $\overline{X}$ and $\widehat{\sigma}^2$ are independent.

❸ $\dfrac{n-1}{\sigma^2} \widehat{\sigma}^2 \sim \chi^2(n-1)$ (if $n \geqslant 2$)