Part I: Linear Models

Chapter I.2

Multivariate Normal Distribution

Topics

To be discussed...

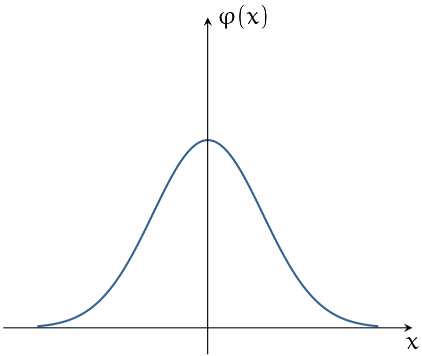
- definition of general multivariate normal distributions
- marginal & conditional distributions
- independence & correlation
- some illustrations (bivariate normal)
- linear transformations and applications

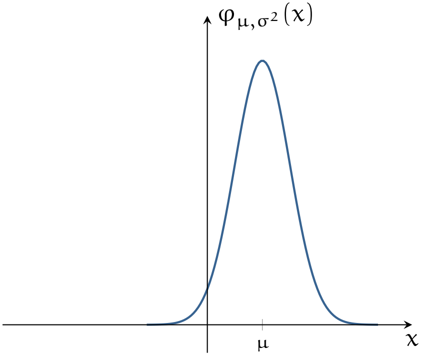
I.2.1 Univariate normal distribution $N(\mu, \sigma^2)$

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

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

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





I.2.2 Definition

Let $Z_1, \dots, Z_k \overset{\text{iid}}{\sim} N(0,1)$, $\mathbf{Z} = (Z_1, \dots, Z_k)'$, 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 $\mathbf{Z} \sim N_k(0, I_k)$).
- $\mathbf{X} = \boldsymbol{\mu} + A\mathbf{Z}$ has a **p dimensional normal distribution with parameters μ 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
  - $E\mathbf{X} = \boldsymbol{\mu}$, 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 $\Sigma \in \mathbb{R}^{p \times p}_{\geqslant 0}$**?

  ☞ 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 DF

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

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 $\mathbf{X} \sim N_p(\mu, \Sigma)$ with $\mu \in \mathbb{R}^p, \Sigma \in \mathbb{R}^{p \times p}_{\geqslant 0}$ and $\emptyset \neq K \subseteq \{1, \ldots, p\}$ and $\Sigma_{K,K} = \mathrm{Cov}\,(\mathbf{X}_K)$. Then:

1. $E\mathbf{X} = \mu$
2. $\mathrm{Cov}\,(\mathbf{X}) = \Sigma$
3. $\mathbf{X}_K \sim N(\mu_K, \Sigma_{K,K})$ ('**marginals of normals are normal**')

I.2.8 Theorem (conditionals of a multivariate normal distribution)

Let $\mathbf{X} \sim N_p(\mu, \Sigma)$ with $\mu \in \mathbb{R}^p, \Sigma \in \mathbb{R}^{p \times p}_{>0}$ and $\emptyset \neq K, L \subseteq \{1, \ldots, p\}$, $K \cap L = \emptyset$, $k = |K|$. Further, let $\Sigma_{K,L} = \mathrm{Cov}\,(\mathbf{X}_K, \mathbf{X}_L)$ and $\Sigma_{KK|L} = \Sigma_{K,K} - \Sigma_{K,L}\Sigma_{L,L}^{-1}\Sigma_{K,L}'$. Then:

1. $\mathbf{X}_K \mid \mathbf{X}_L = \mathbf{x}_L \sim N_k(\mu_K + \Sigma_{K,L}\Sigma_{L,L}^{-1}(\mathbf{x}_L - \mu_L), \Sigma_{KK|L})$

   ('**conditionals of normals are normal**')
2. $E(\mathbf{X}_K \mid \mathbf{X}_L = \mathbf{x}_L) = \mu_K + \Sigma_{K,L}\Sigma_{L,L}^{-1}(\mathbf{x}_L - \mu_L)$

   The matrix $\Sigma_{K,L}\Sigma_{L,L}^{-1}$ is called **regression matrix**.
3. $\mathrm{Cov}\,(\mathbf{X}_K \mid \mathbf{X}_L = \mathbf{x}_L) = \Sigma_{KK|L}$,

Independence & Correlation

I.2.9 Theorem (independence under multivariate normal distribution)

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

1. $\mathbf{X}_K$ and $\mathbf{X}_L$ are independent if and only if $\Sigma_{K,L} = \mathbf{0}$
2. $\mathbf{X} = (X_1, \ldots, X_p)' \sim N_p(\mathbf{0}, I_p) \iff X_1, \ldots, X_p \overset{\text{iid}}{\sim} N(0, 1)$
3. $\mathbf{X} = (X_1, \ldots, X_p)' \sim N_p(\boldsymbol{\mu}, \Sigma)$ 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** $\mathbf{X} = (X_1, X_2)'$ has the DF (for $x_1, x_2 \in \mathbb{R}$)

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

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:

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

with determinant $\det\Sigma = \sigma_1^2\sigma_2^2(1-\rho^2)$ and $\boldsymbol{\mu} = (\mu_1, \mu_2)' \in \mathbb{R}^2$

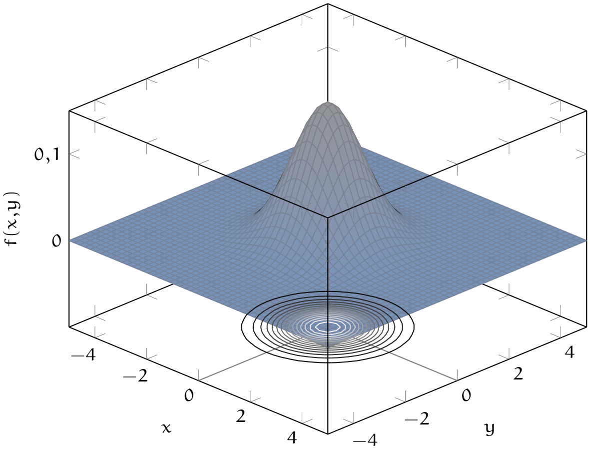


Figure: DF of bivariate standard normal distribution $N_2(0, 0, 1, 1, 0)$

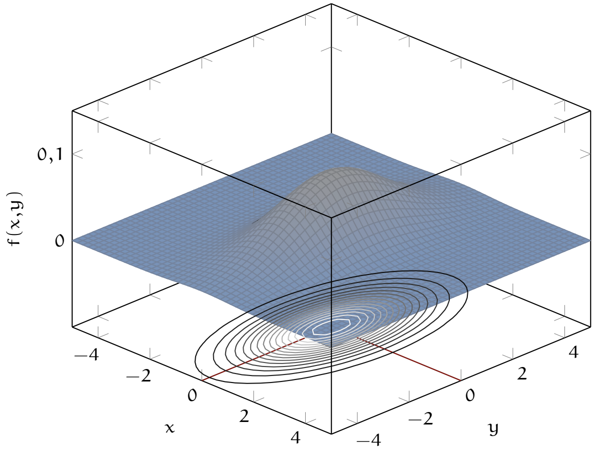


Figure: DF of bivariate normal distribution $N_2(0, 0, 1, 4, 0)$

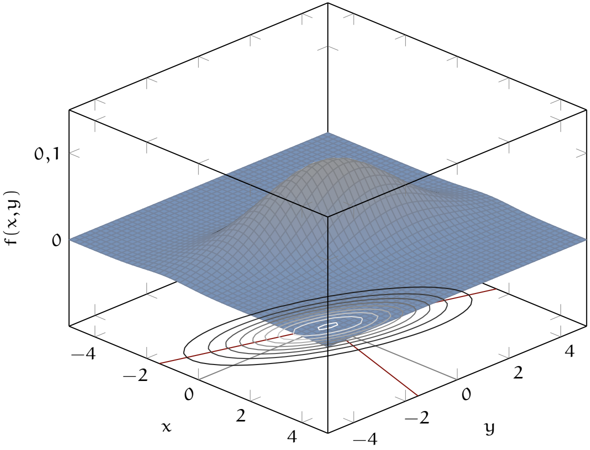


Figure: DF of bivariate normal distribution $N_2(0, 0, 1, 4, \frac{1}{2})$

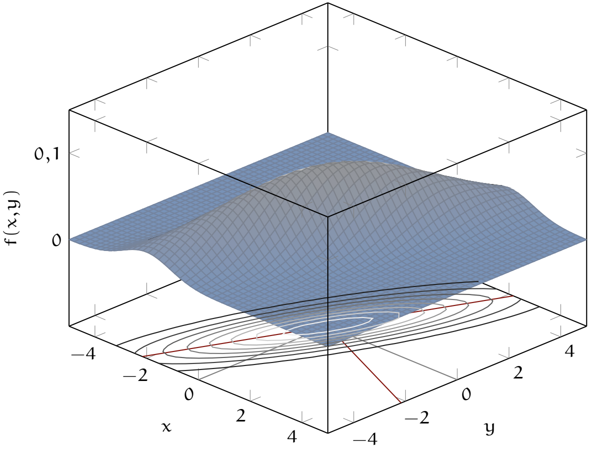


Figure: DF of bivariate normal distribution $N_2(0, 0, 1, 4, \frac{4}{5})$

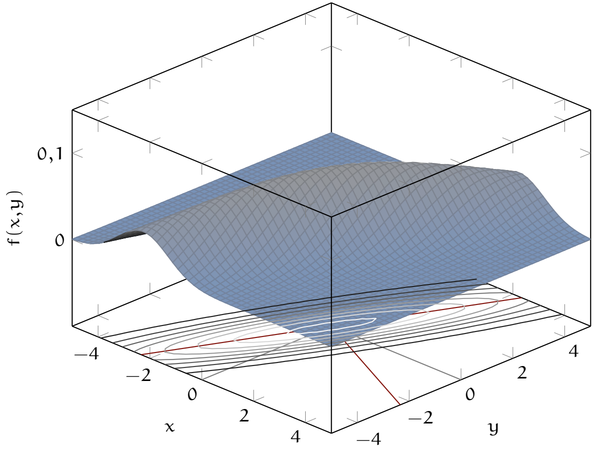
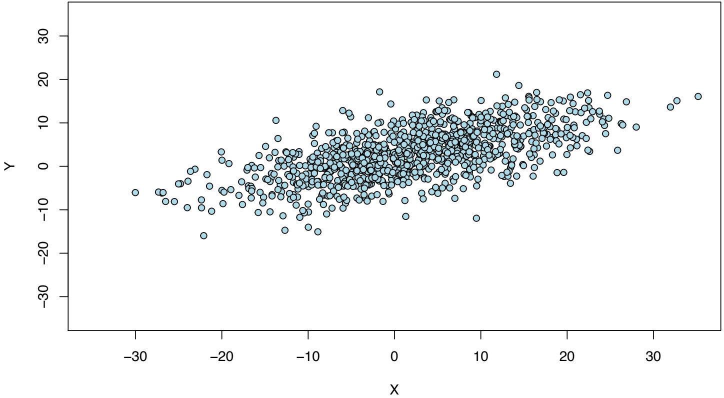
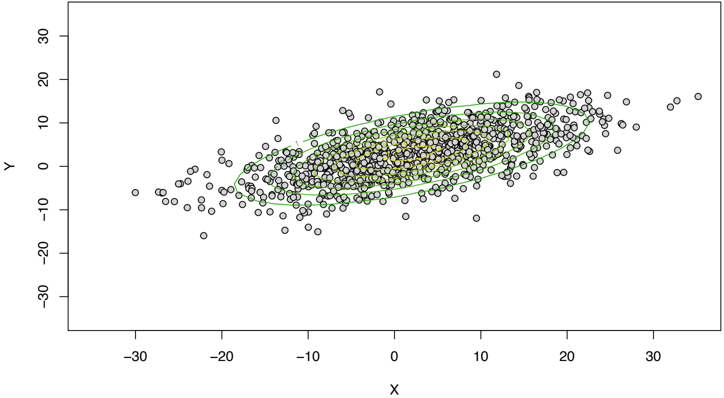


Figure: DF of bivariate normal distribution $N_2(0, 0, 1, 4, \frac{9}{10})$

Simulated bivariate normal data



Simulated bivariate normal data with ellipses



I.2.11 Theorem

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

$$\mathbf{Y} = \mathbf{a} + B\mathbf{X} \sim N_k(\mathbf{a} + B\boldsymbol{\mu}, B\Sigma B').$$

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

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

I.2.12 Remark

- The transformation

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

  considered in Theorem I.2.11 is called **Mahalanobis transformation**.
- Considering the Euclidean norm $\|\mathbf{Y}\|$ of $\mathbf{Y}$, we get

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

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

I.2.13 Corollary

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

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

2. If $X_1, \ldots, X_n \overset{\text{iid}}{\sim} N(\mu, \sigma^2)$, $\sigma^2 > 0$, then
   - $\overline{X} \sim N(\mu, \frac{\sigma^2}{n})$
   - $\boxed{\sqrt{n}\,\frac{\overline{X} - \mu}{\sigma} \sim N(0, 1)}$

I.2.14 Theorem

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

- $A\mathbf{X}$ and $B\mathbf{X}$ are independent if and only if $A\Sigma B' = 0$.

I.2.15 Theorem

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

- $\overline{Z}$ and $\mathbf{Z} - \overline{Z}\mathbb{1}_p = E_p\mathbf{Z}$ 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:

1. $X_1^2 \sim \chi^2(1)$
2. $\sum_{i=1}^{n} X_i^2 \sim \chi^2(n)$

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:

1. $\frac{n}{\sigma^2} \widehat{\sigma}_\mu^2 \sim \chi^2(n)$.
2. $\overline{X}$ and $\widehat{\sigma}^2$ are independent.
3. $\frac{n-1}{\sigma^2} \widehat{\sigma}^2 \sim \chi^2(n-1)$ (if $n \geqslant 2$)

Proof. $Z_j := \frac{X_j - \mu}{\sigma}$; $X_j = \mu + \sigma Z_j$, $1 \le j \le n$. , $Z_1, \dots, Z_n \overset{iid}{\sim} N(0,1)$

$$\hat{\sigma}_\mu^2 = \frac{1}{n} \sum_{j=1}^{n} (X_j - \mu)^2 = \frac{1}{n} \sum_{j=1}^{n} (\sigma Z_j)^2 = \frac{\sigma^2}{n} \cdot \sum_{j=1}^{n} Z_j^2$$

$$\hookrightarrow \frac{n}{\sigma^2} \cdot \hat{\sigma}_\mu^2 = \sum_{j=1}^{n} Z_j^2 \underset{I.2.16}{\sim} \chi^2(n)$$

$$\bar{X} = \mu + \sigma \bar{Z} \ ; \quad \hat{\sigma}^2 = \frac{1}{n-1} \sum_{j=1}^{n} \left(\cancel{\mu} + \sigma Z_j - (\cancel{\mu} + \sigma \bar{Z}) \right)^2$$

$$= \frac{\sigma^2}{n-1} \sum_{j=1}^{n} (Z_j - \bar{Z})^2 = \sigma^2 \cdot S_Z$$

By Th. I.2.15, we get the result.