Marginal and conditional distributions of multivariate normal distribution

Assume an n-dimensional random vector

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}$$

has a normal distribution $N(\mathbf{x}, \mu, \Sigma)$ with

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

where $\mathbf{x}_1$ and $\mathbf{x}_2$ are two subvectors of respective dimensions p and q with $p+q=n$. Note that $\Sigma = \Sigma^T$, and $\Sigma_{21} = \Sigma_{21}^T$.

Theorem 4:

Part a The marginal distributions of $\mathbf{x}_1$ and $\mathbf{x}_2$ are also normal with mean vector μ_i and covariance matrix Σ_{ii} ($i = 1, 2$), respectively.

Part b The conditional distribution of $\mathbf{x}_i$ given $\mathbf{x}_j$ is also normal with mean vector

$$\mu_{i|j} = \mu_i + \Sigma_{ij}\Sigma_{jj}^{-1}(\mathbf{x}_j - \mu_j)$$

and covariance matrix

$$\Sigma_{i|j} = \Sigma_{jj} - \Sigma_{ij}^T\Sigma_{ii}^{-1}\Sigma_{ij}$$

Proof: The joint density of $\mathbf{x}$ is:

$$f(\mathbf{x}) = f(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp[-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)] = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp[-\frac{1}{2}Q(\mathbf{x}_1, \mathbf{x}_2)]$$

where Q is defined as

$$\begin{aligned} Q(\mathbf{x}_1, \mathbf{x}_2) &= (\mathbf{x} - \mu)^T\Sigma^{-1}(\mathbf{x} - \mu) \\ &= [(\mathbf{x}_1 - \mu_1)^T, (\mathbf{x} - \mu_2)^T] \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 - \mu_1 \\ \mathbf{x}_2 - \mu_2 \end{bmatrix} \\ &= (\mathbf{x}_1 - \mu_1)^T\Sigma^{11}(\mathbf{x}_1 - \mu_1) + 2(\mathbf{x}_1 - \mu_1)^T\Sigma^{12}(\mathbf{x}_2 - \mu_2) + (\mathbf{x}_2 - \mu_2)^T\Sigma^{22}(\mathbf{x}_2 - \mu_2) \end{aligned}$$

Here we have assumed

$$\Sigma^{-1} = \left[\begin{array}{cc} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{array} \right]^{-1} = \left[\begin{array}{cc} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{array} \right]$$

According to theorem 2, we have

$$\Sigma^{11} = (\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^T)^{-1} = \Sigma_{11}^{-1}+\Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22}-A_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}\Sigma_{12}^T\Sigma_{11}^{-1}$$

$$\Sigma^{22} = (\Sigma_{22}-\Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1} = \Sigma_{22}^{-1}+\Sigma_{22}^{-1}\Sigma_{12}^T(\Sigma_{11}-\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^T)^{-1}\Sigma_{12}\Sigma_{22}^{-1}$$

$$\Sigma^{12} = -\Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22} - \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1} = (\Sigma^{21})^T$$

Substituting the second expression for Σ^{11}, first expression for Σ^{22}, and Σ^{12} into $Q(\mathbf{x}_1,\mathbf{x}_2)$ to get:

$$\begin{aligned}
Q(\mathbf{x}_1,\mathbf{x}_2) &= (\mathbf{x}_1-\mu_1)^T[\Sigma_{11}^{-1} + \Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22} - A_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}\Sigma_{12}^T\Sigma_{11}^{-1}](\mathbf{x}_1-\mu_1) \\
&\quad -2(\mathbf{x}_1-\mu_1)^T[\Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22} - \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}](\mathbf{x}_2-\mu_2) \\
&\quad +(\mathbf{x}_2-\mu_2)^T[(\Sigma_{22} - \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}](\mathbf{x}_2-\mu_2) \\
&= (\mathbf{x}_1-\mu_1)^T\Sigma_{11}^{-1}(\mathbf{x}_1-\mu_1) \\
&\quad +(\mathbf{x}_1-\mu_1)^T\Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22} - A_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}\Sigma_{12}^T\Sigma_{11}^{-1}](\mathbf{x}_1-\mu_1) \\
&\quad -2(\mathbf{x}_1-\mu_1)^T[\Sigma_{11}^{-1}\Sigma_{12}(\Sigma_{22} - \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}](\mathbf{x}_2-\mu_2) \\
&\quad +(\mathbf{x}_2-\mu_2)^T[(\Sigma_{22} - \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}](\mathbf{x}_2-\mu_2) \\
&= (\mathbf{x}_1-\mu_1)^T\Sigma_{11}^{-1}(\mathbf{x}_1-\mu_1) \\
&\quad +[(\mathbf{x}_2-\mu_2) - \Sigma_{12}^T\Sigma_{11}^{-1}(\mathbf{x}_1-\mu_1)]^T(\Sigma_{22} - \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12})^{-1}[(\mathbf{x}_2-\mu_2) - \Sigma_{12}^T\Sigma_{11}^{-1}(\mathbf{x}_1-\mu_1)]
\end{aligned}$$

The last equal sign is due to the following equations for any vectors u and v and a symmetric matrix $A = A^T$:

$$u^TAu - 2u^TAv + v^TAv = u^TAu - u^TAv - u^TAv + v^TAv$$

$$= u^TA(u-v) - (u-v)^TAv = u^TA(u-v) - v^TA(u-v)$$

$$= (u-v)^T A(u-v) = (v-u)^T A(v-u)$$

We define

$$b \triangleq \mu_2 + \Sigma_{12}^T \Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1)$$

$$A \triangleq \Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}$$

and

$$\begin{cases} Q_1(\mathbf{x}_1) & \triangleq (\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1) \\ Q_2(\mathbf{x}_1, \mathbf{x}_2) & \triangleq [(\mathbf{x}_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1)]^T (\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12})^{-1} [(\mathbf{x}_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1)] \\ & = (\mathbf{x}_2 - b)^T A^{-1}(\mathbf{x}_2 - b) \end{cases}$$

and get

$$Q(\mathbf{x}_1, \mathbf{x}_2) = Q_1(\mathbf{x}_1) + Q_2(\mathbf{x}_1, \mathbf{x}_2)$$

Now the joint distribution can be written as:

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp[-\frac{1}{2}Q(\mathbf{x}_1, \mathbf{x}_2)] \\ &= \frac{1}{(2\pi)^{n/2}|\Sigma_{11}|^{1/2}|\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}|^{1/2}} exp[-\frac{1}{2}Q(\mathbf{x}_1, \mathbf{x}_2)] \\ &= \frac{1}{(2\pi)^{p/2}|\Sigma_{11}|^{1/2}} exp[-\frac{1}{2}(\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1)] \frac{1}{(2\pi)^{q/2}|A|^{1/2}} exp[-\frac{1}{2}(\mathbf{x}_2 - b)^T A^{-1}(\mathbf{x}_2 - b)] \\ &= N(\mathbf{x}_1, \mu_1, \Sigma_{11}) \; N(\mathbf{x}_2, b, A) \end{aligned}$$

The third equal sign is due to theorem 3:

$$|\Sigma| = |\Sigma_{11}||\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}|$$

The marginal distribution of $\mathbf{x}_1$ is

$$f_1(\mathbf{x}_1) = \int f(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x_2} = \frac{1}{(2\pi)^{p/2}|\Sigma_{11}|^{1/2}} exp[-\frac{1}{2}(\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1)]$$

and the conditional distribution of $\mathbf{x}_2$ given $\mathbf{x}_1$ is

$$f_{2|1}(\mathbf{x}_2|\mathbf{x}_1) = \frac{f(\mathbf{x}_1, \mathbf{x}_2)}{f(\mathbf{x}_1)} = \frac{1}{(2\pi)^{q/2}|A|^{1/2}} exp[-\frac{1}{2}(\mathbf{x}_2 - b)^T A^{-1}(\mathbf{x}_2 - b)]$$

with

$$b = \mu_2 + \Sigma_{12}^T \Sigma_{11}^{-1}(\mathbf{x}_1 - \mu_1)$$

$$A = \Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}$$