Notes on Components Analysis
(Completing the square principle)

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Problem: Assume that we are given a multivariate Gaussian distribution $p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^F|\boldsymbol{\Sigma}|}} \exp\left\{-(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu})\right\}$. Let $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}$ we want to find $p(\mathbf{x}_1|\mathbf{x}_2)$.

Solution: Let us define

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{12}^T & \boldsymbol{\Sigma}_{22} \end{bmatrix} \Rightarrow$$

$$\boldsymbol{\Sigma}^{-1} = \begin{bmatrix} \mathbf{S}^{-1} & -\mathbf{S}^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1} \\ -\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T\mathbf{S}^{-1} & \boldsymbol{\Sigma}_{22}^{-1} + \boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T\mathbf{S}^{-1}\boldsymbol{\Sigma}_{22}^{-1} \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{D} \end{bmatrix}$$

and $\mathbf{S} = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T$.

Using the Schur complement we can compute the determinant as

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{12}^T & \boldsymbol{\Sigma}_{22} \end{bmatrix} \Rightarrow |\boldsymbol{\Sigma}| = |\boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}| \cdot |\boldsymbol{\Sigma}_{22}|$$

Using the Bayes rule $p(\mathbf{x}_1|\mathbf{x}_2) = \frac{p(\mathbf{x})}{p(\mathbf{x}_2)}$.

$$p(\mathbf{x}_2) = \int_{\mathbf{x}_1} p(\mathbf{x})d\mathbf{x}_1 = \int_{\mathbf{x}_1} \frac{1}{\sqrt{(2\pi)^F|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}\left(\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} - \boldsymbol{\mu}\right)^T \boldsymbol{\Sigma}^{-1} \left(\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} - \boldsymbol{\mu}\right)\right\} d\mathbf{x}_1$$

Let us now examine closely what is inside the $\exp$ function.

$$\left(\left[\begin{array}{c}\mathbf{x}_1\\ \mathbf{x}_2\end{array}\right]-\boldsymbol{\mu}\right)^T\left[\begin{array}{cc}\mathbf{A} & \mathbf{B}\\ \mathbf{B}^T & \mathbf{D}\end{array}\right]\left(\left[\begin{array}{c}\mathbf{x}_1\\ \mathbf{x}_2\end{array}\right]-\boldsymbol{\mu}\right)=\left(\left[\begin{array}{c}\overbrace{\mathbf{x}_1-\mu}^{\tilde{\mathbf{x}}_1}\\ \underbrace{\mathbf{x}_2-\mu}_{\tilde{\mathbf{x}}_2}\end{array}\right]\right)^T\left[\begin{array}{cc}\mathbf{A} & \mathbf{B}\\ \mathbf{B}^T & \mathbf{D}\end{array}\right]\left(\left[\begin{array}{c}\overbrace{\mathbf{x}_1-\boldsymbol{\mu}}^{\tilde{\mathbf{x}}_1}\\ \underbrace{\mathbf{x}_2-\boldsymbol{\mu}}_{\tilde{\mathbf{x}}_2}\end{array}\right]\right)$$

$$=[\tilde{\mathbf{x}}_1^T\mathbf{A}+\tilde{\mathbf{x}}_2^T\mathbf{B}^T \quad \tilde{\mathbf{x}}_1^T\mathbf{B}+\tilde{\mathbf{x}}_2^T\mathbf{D}]\left[\begin{array}{c}\tilde{\mathbf{x}}_1\\ \tilde{\mathbf{x}}_2\end{array}\right]=\tilde{\mathbf{x}}_1^T\mathbf{A}\tilde{\mathbf{x}}_1+\tilde{\mathbf{x}}_2^T\mathbf{B}^T\tilde{\mathbf{x}}_1+\tilde{\mathbf{x}}_1^T\mathbf{B}\tilde{\mathbf{x}}_2+\underbrace{\tilde{\mathbf{x}}_2^T\mathbf{D}\tilde{\mathbf{x}}_2}_{C_1}$$

$$=\tilde{\mathbf{x}}_1^T\mathbf{A}\tilde{\mathbf{x}}_1+2\tilde{\mathbf{x}}_2^T\mathbf{B}^T(\mathbf{x}_1-\boldsymbol{\mu}_1)+C_1$$

$$=\mathbf{x}_1^T\mathbf{A}\mathbf{x}_1-2\boldsymbol{\mu}_1^T\mathbf{A}\mathbf{x}_1+\underbrace{\boldsymbol{\mu}_1^T\mathbf{A}\boldsymbol{\mu}_1}+2\tilde{\mathbf{x}}_2^T\mathbf{B}^T\mathbf{x}_1-\underbrace{2\tilde{\mathbf{x}}_2^T\mathbf{B}^T\boldsymbol{\mu}_1}+\underbrace{C_1}$$

Let define the constant $C_2=C_1+\boldsymbol{\mu}_1^T\mathbf{A}\boldsymbol{\mu}_1-2\tilde{\mathbf{x}}_2^T\mathbf{B}^T\boldsymbol{\mu}_1$

Let's we examine the part

$$\mathbf{x}_1^T\mathbf{A}\mathbf{x}_1-2\boldsymbol{\mu}_1^T\mathbf{A}\mathbf{x}_1+2\tilde{\mathbf{x}}_2^T\mathbf{B}^T\mathbf{x}_1=\mathbf{x}_1^T\mathbf{A}\mathbf{x}_1-2(\mathbf{A}\boldsymbol{\mu}_1-\mathbf{B}\tilde{\mathbf{x}}_2)^T\mathbf{x}_1. \qquad (1)$$

Our aim is to write the above (1) in a form as
$(\mathbf{x}_1-\boldsymbol{\rho})^T\mathbf{A}(\mathbf{x}_1-\boldsymbol{\rho})=\mathbf{x}_1^T\mathbf{A}\mathbf{x}_1-2\boldsymbol{\rho}^T\mathbf{A}\mathbf{x}_1+\boldsymbol{\rho}^T\boldsymbol{\rho}$.

Now we need to apply the "completing the square" principle as

$$\mathbf{x}_1^T\mathbf{A}\mathbf{x}_1-2\underbrace{(\boldsymbol{\mu}_1-\mathbf{A}^{-1}\mathbf{B}\tilde{\mathbf{x}}_2)^T}_{\boldsymbol{\rho}}\mathbf{A}\mathbf{x}_1+\boldsymbol{\rho}^T\mathbf{A}\boldsymbol{\rho}-\boldsymbol{\rho}^T\mathbf{A}\boldsymbol{\rho}$$

.

Hence, (1) can be written as

$$(\mathbf{x}_1-\boldsymbol{\rho})^T\mathbf{A}(\mathbf{x}_1-\boldsymbol{\rho})+C_3$$

where $C_3=-\boldsymbol{\rho}^T\mathbf{A}\boldsymbol{\rho}$.

Now let's have a closer look at the constant terms (constant terms with regards to $\mathbf{x}_1$)

$$\begin{aligned}\mathbf{C}_2-\boldsymbol{\rho}^T\mathbf{A}\boldsymbol{\rho}=&\mathbf{C}_2-(\boldsymbol{\mu}_1-\mathbf{A}^{-1}\mathbf{B}\tilde{\mathbf{x}}_2)^T\mathbf{A}(\boldsymbol{\mu}_1-\mathbf{A}^{-1}\mathbf{B}\tilde{\mathbf{x}}_2)\\ &=\mathbf{C}_2-[\boldsymbol{\mu}_1^T\mathbf{A}\boldsymbol{\mu}_1-2\boldsymbol{\mu}_1^T\mathbf{B}\tilde{\mathbf{x}}_2+\tilde{\mathbf{x}}_2^T\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B}\tilde{\mathbf{x}}_2]\\ &=\cancel{\boldsymbol{\mu}_1^T\mathbf{A}\boldsymbol{\mu}_1}-\cancel{2\boldsymbol{\mu}_1^T\mathbf{B}\tilde{\mathbf{x}}_2}+\tilde{\mathbf{x}}_2^T\mathbf{D}\mathbf{x}_2-[\cancel{\boldsymbol{\mu}_1^T\mathbf{A}\boldsymbol{\mu}_1}-\cancel{2\boldsymbol{\mu}_1^T\mathbf{B}\tilde{\mathbf{x}}_2}+\tilde{\mathbf{x}}_2^T\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B}\tilde{\mathbf{x}}_2]\\ &=\tilde{\mathbf{x}}_2^T(\mathbf{D}-\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B})\tilde{\mathbf{x}}_2\end{aligned}$$

Hence, the quadratic term inside the exponential $\exp$ can be written as

$$\left(\left[\begin{array}{c}\mathbf{x}_1\\ \mathbf{x}_2\end{array}\right]-\boldsymbol{\mu}\right)^T\left[\begin{array}{cc}\mathbf{A} & \mathbf{B}\\ \mathbf{B}^T & \mathbf{D}\end{array}\right]\left(\left[\begin{array}{c}\mathbf{x}_1\\ \mathbf{x}_2\end{array}\right]-\boldsymbol{\mu}\right)=$$

$$=(\mathbf{x}_1-\underbrace{(\boldsymbol{\mu}_1-\mathbf{A}^{-1}\mathbf{B}(\mathbf{x}_2-\boldsymbol{\mu}_2))^T\mathbf{A}(\mathbf{x}_1-(\boldsymbol{\mu}_1-\mathbf{A}^{-1}\mathbf{B}(\mathbf{x}_2-\boldsymbol{\mu}_2))}_{\text{used to define } p(\mathbf{x}_1|\mathbf{x}_2)})+\underbrace{(\mathbf{x}_2-\boldsymbol{\mu}_2)^T(\mathbf{D}-\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B})(\mathbf{x}_2-\boldsymbol{\mu}_2)}_{\text{used to define } p(\mathbf{x}_2)}$$

Using Schur complement we can simplify the above as

$$\mathbf{D} - \mathbf{B}^T\mathbf{A}^{-1}\mathbf{B} = \boldsymbol{\Sigma}_{22}^{-1} + \cancel{\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T\mathbf{S}^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}} - \cancel{\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T\mathbf{S}^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}} = \boldsymbol{\Sigma}_{22}^{-1}$$

Hence, the second part is

$$(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T(\mathbf{D} - \mathbf{B}^T\mathbf{A}^{-1}\mathbf{B})(\mathbf{x}_2 - \boldsymbol{\mu}_2) = (\mathbf{x}_2 - \boldsymbol{\mu}_2)^T\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$$

Furthermore, since

$$\mathbf{A} = (\boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T)^{-1} \text{ Schur complement}$$

$$\mathbf{A}^{-1}\mathbf{B} = -\mathbf{A}^{-1}\mathbf{A}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}$$

Then, the first part can be written as

$$(\mathbf{x}_1 - \underbrace{(\boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2))}_{\overline{\mu}})^T(\underbrace{\boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T}_{\overline{\boldsymbol{\Sigma}}})^{-1}(\mathbf{x}_1 - \underbrace{(\boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)}_{\overline{\mu}}))$$

Hence, the quadratic part can be written as

$$(\mathbf{x}_1 - \tilde{\boldsymbol{\mu}})^T\overline{\boldsymbol{\Sigma}}^{-1}(\mathbf{x}_1 - \tilde{\boldsymbol{\mu}}) + (\mathbf{x}_2 - \boldsymbol{\mu}_2)^T\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$$

Using the above the initially probability can written as

$$p(\mathbf{x}_2) = \int_{\mathbf{x}_1} \frac{1}{\sqrt{(2\pi)^F|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}})^T\overline{\boldsymbol{\Sigma}}^{-1}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}}) - \frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)\right\} d\mathbf{x}_1$$

$$= \int_{\mathbf{x}_1} \frac{1}{\sqrt{(2\pi)^{F_1+F_2}|\overline{\boldsymbol{\Sigma}}||\boldsymbol{\Sigma}_{22}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}})^T\overline{\boldsymbol{\Sigma}}^{-1}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}})\right\} \exp\left\{-\frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)\right\} d\mathbf{x}_1$$

$$= \frac{1}{\sqrt{(2\pi)^{F_2}|\boldsymbol{\Sigma}_{22}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)\right\}$$

$$\cancelto{1}{\int_{\mathbf{x}_1} \frac{1}{\sqrt{(2\pi)^{F_1}|\overline{\boldsymbol{\Sigma}}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}})^T\overline{\boldsymbol{\Sigma}}^{-1}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}})\right\} d\mathbf{x}_1} \quad .$$

From the above it is evident that

$$p(\mathbf{x}_2) = \frac{1}{\sqrt{(2\pi)^{F_2}|\boldsymbol{\Sigma}_{22}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)\right\} \tag{2}$$

and

$$p(\mathbf{x}_1|\mathbf{x}_2) = \frac{1}{\sqrt{(2\pi)^{F_1}|\overline{\boldsymbol{\Sigma}}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}})^T\overline{\boldsymbol{\Sigma}}^{-1}(\mathbf{x}_1 - \overline{\boldsymbol{\mu}})\right\}. \tag{3}$$