

Machine learning

September 2021

1. Multivariate Gaussian distribution
Proof Multivariate Gaussian distribution normalization

$$p(x | \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

Gaussian Distribution normalize :

$$\Leftrightarrow \int_{-\infty}^{\infty} p(x | \mu, \sigma^2) = 1$$

Have mean:

$$E[x] = \int_{-\infty}^{\infty} p(x | \mu, \sigma^2) = \mu$$

Variance:

$$Var[x] = \int_{-\infty}^{\infty} (x - \mu)^2 p(x | \mu, \sigma^2) = \sigma^2$$

Where the μ is a D -dimensional mean Σ is $D \times D$ covariance, and $|\Sigma|$ denotes the of σ

Set :

$$\Delta^2 = \frac{-1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu) = \frac{-1}{2}(x^T - \mu^T) \Sigma^{-1}(x - \mu)$$

$$= \frac{-1}{2}x^T \Sigma^{-1}x + \frac{1}{2}x^T \Sigma^{-1}\mu + \frac{1}{2}\mu^T \Sigma^{-1}x + \frac{-1}{2}\mu^T \Sigma^{-1}\mu$$

Proof : Σ : symmetric, then Σ^{-1} is symmetric

We have : $\Sigma \Sigma^{-1} = I$

$$I = I^T$$

$$\Sigma \Sigma^{-1} = (\Sigma \Sigma^{-1})^T$$

$$\Sigma \Sigma^{-1} = (\Sigma^{-1})^T \Sigma^T$$

$$\Sigma^{-1} \Sigma \Sigma^{-1} = \Sigma^{-1} (\Sigma^{-1})^T \Sigma$$

$$\Sigma^{-1} = (\Sigma^{-1})^T$$

Then Σ^{-1} is symmetric
So that:

$$\Delta^2 = \frac{-1}{2}x^T\Sigma^{-1}x + x^T\Sigma^{-1}\mu + const$$

Consider eigenvalues and eigenvectors of Σ

$$\Sigma u_i = \lambda_i u_i, i = 1, \dots, D$$

Because Σ is a real, symmetric matrix, its eigenvalues will be real and its eigenvector form an orthonormal set.

$$\text{Proof: } \Sigma = \sum_{i=1}^D \lambda_i u_i u_i^T \Rightarrow \Sigma^{-1} = \sum_{i=1}^D \frac{1}{\lambda_i} u_i u_i^T$$

$$\text{Let : } \Sigma = \sum_{i=1}^D \lambda_i u_i u_i^T = U D U^T$$

U has dimension $D \times D$

D is diagonal matrix with the eigenvalue λ its diagonal

U is orthogonal matrix so $U^{-1} = U^T$

$$\Sigma^{-1} = (U D U^T)^{-1} = (U^T)^{-1} D^{-1} U^{-1} = U D^{-1} U^T = \Sigma^{-1} = \sum_{i=1}^D \frac{1}{\lambda_i} u_i u_i^T$$

$$\Delta^2 = (x - \mu)^T \Sigma^{-1} (x - \mu) = \sum_{i=1}^D \lambda_i u_i u_i^T = \sum_{i=1}^D \frac{1}{\lambda_i} (x - \mu)^T u_i u_i^T (x - \mu)$$

With : $y_i = u_i^T (x - \mu)$

$$\Delta^2 = \sum_{i=1}^D \frac{y_i^2}{\lambda_i}$$

$$|\Sigma|^{-\frac{1}{2}} = \prod_{j=1}^D \lambda_j^{-\frac{1}{2}}$$

$$p(y) = \prod_{j=1}^D \left(\frac{1}{2\pi\lambda_j} \right)^{\frac{1}{2}} \exp\left\{ -\frac{y_j^2}{2\lambda_j} \right\}$$

$$\Rightarrow \int_{-\infty}^{\infty} p(y) dy = \prod_{j=1}^D \int_{-\infty}^{\infty} \left(\frac{1}{2\pi\lambda_j} \right)^{\frac{1}{2}} \exp\left\{ -\frac{y_j^2}{2\lambda_j} \right\} dy_j = 1$$

2. Conditional Gaussian Distribution

Suppose x is a D-dimensional vector with Gaussian distribution $N(x | \mu, \Sigma)$ and that we partition x into two disjoint subsets x_a and x_b

$$x_a = \begin{pmatrix} x_a \\ x_b \end{pmatrix}$$

We also define corresponding partitions of the mean vector μ given by

$$\mu = \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix}$$

and of the covariance matrix Σ given by

$$\Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix} \Rightarrow A = \Sigma^{-1} = \begin{pmatrix} A_{aa} & A_{ab} \\ A_{ba} & A_{bb} \end{pmatrix}$$

Σ is symmetric so Σ_{aa} and Σ_{bb} are symmetric while $\Sigma_{ab} = \Sigma_{ba}^T$

We have:

$$\begin{aligned} & -\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu) = -\frac{1}{2}(x - \mu)^T A(x - \mu) \\ & = -\frac{1}{2}(x_a - \mu_a)^T A_{aa}(x_a - \mu_a) - \frac{1}{2}(x_a - \mu_a)^T A_{ab}(x_b - \mu_b) - \frac{1}{2}(x_b - \mu_b)^T A_{ba}(x_a - \mu_a) - \frac{1}{2}(x_b - \mu_b)^T A_{bb}(x_b - \mu_b) \\ & = -\frac{1}{2}x^T A_{aa}^{-1}x_a + x_a^T(A_{aa}\mu_a - A_{ab}(x_b - \mu_b)) + const \end{aligned}$$

Compare with Gaussian distribution:

$$\Sigma_{a|b} = A_{aa}^{-1}$$

$$\mu_{a|b} = \Sigma_{a|b}(A_{aa}\mu_a - A_{ab}(x_b - \mu_b)) = \mu_a - A_{aa}^{-1}A_{ab}(x_b - \mu_b)$$

By using Schur complement,

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} M & -MBD^{-1} \\ -D^{-1}CMD^{-1} & D^{-1}CMBD^{-1} \end{pmatrix}, M = (A - BD^{-1}C)^{-1}$$

$$\Rightarrow A_{aa} = (\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba})^{-1}\Sigma_{ab}\Sigma_{bb}^{-1}$$

As a result :

$$\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b)$$

$$\Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$$

$$\Rightarrow p(x_a | x_b) = N(x_{a|b} | \mu_{a|b}, \Sigma_{a|b})$$

3. Marginal Gaussian distribution

The marginal distribution given by

$$p(x_a) = \int p(x_a, x_b) dx_b$$

We need to integrate out x_b by looking the quadratic form related to x_b

$$-\frac{1}{2}x_b^T A_{bb}x_b + x_b^T m = -\frac{1}{2}(x_b - A_{bb}^{-1}m)^T A_{bb}(x_b - A_{bb}^{-1}m) + \frac{1}{2}m^T A_{bb}^{-1}m$$

with $m = A_{bb}\mu_b - A_{ba}(x_a - \mu_a)$

We can integrate over unnormalized Gaussian :

$$\int \exp\{-\frac{1}{2}(x_b - A_{bb}^{-1}m)^T A_{bb}(x_b - A_{bb}^{-1}m)\} dx_b$$

The remaining term:

$$-\frac{1}{2}x_a^T(A_{aa} - A_{ab}A_{bb}^{-1}A_{ba})x_a + x_a^T(A_{aa} - A_{ab}A_{bb}^{-1}A_{ba})\mu_a + const$$

Similarly, we have:

$$E[x_a] = \mu_a \text{cov}[x_a] = \Sigma_{aa} \Rightarrow p(x_a) = N(x_a | \mu_a, \Sigma_{aa})$$