写在前面

需熟悉常见的矩阵微积分表示方法及其具体含义。

1 变分法

F[y] 泛函。

$$F(y(x) + \epsilon \eta(x)) = F(y(x)) + \eta \int \frac{\partial F}{\partial y(x)} \eta(x) dx + O(\epsilon^2)$$

$$\int \frac{\partial F}{\partial y(x)} \eta(x) dx = 0$$

2 高斯分布的矩

一阶原点矩

$$E(x) = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \int \exp\left\{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right\} x dx$$

做换元 $z = x - \mu$ 后,有:

$$E(x) = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \int \exp\left\{-\frac{1}{2}z^T \Sigma^{-1} z\right\} (z + \mu) dz$$

而由对称性:

$$\int \exp\left\{-\frac{1}{2}z^T \Sigma^{-1}z\right\}(z)dz = 0$$

故有:

$$E(x) = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \int \exp\left\{-\frac{1}{2}z^T \Sigma^{-1} z\right\} (z + \mu) dz = \mu$$

二阶原点矩 类似地,做换元 $z = x - \mu$ 后,有:

$$E(x) = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \int \exp\left\{-\frac{1}{2}z^T \Sigma^{-1} z\right\} (z + \mu) (z + \mu)^T dz$$

将 $(z + \mu)(z + \mu)^T$ 展开,考虑对称性,有:

$$E(x) = \mu \mu^{T} + \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \int \exp\left\{-\frac{1}{2}z^{T}\Sigma^{-1}z\right\} zz^{T}dz$$

考虑 $I = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \int \exp\left\{-\frac{1}{2}z^T \Sigma^{-1}z\right\} z z^T dz$ 又有: $z = U^{-1}y = \Sigma y_j u_j$, 即 y = Uz

$$I = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \sum_{i,j} u_i u_j^T \int 1 \cdot \exp\left\{-\sum_{k=1}^D \frac{y_k^2}{2\lambda_k}\right\} y_i y_j d\vec{y}$$

再次利用对称性, 当且仅当 i = j 时, 有:

$$\sum_{i,j} u_i u_j^T \int 1 \cdot \exp\left\{-\sum_{k=1}^D \frac{y_k^2}{2\lambda_k}\right\} y_i y_j d\vec{y} \neq 0$$

所以:

$$I = \sum_{i=1}^{L} Du_{i}u_{i}^{T} \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \int 1 \cdot \exp\left\{-\sum_{k=1}^{D} \frac{y_{k}^{2}}{2\lambda_{k}}\right\} y_{i}y_{j}d\vec{y}$$
$$= \sum_{i=1}^{L} Du_{i}u_{i}^{T} \lambda_{i} = \Sigma$$

二阶中心矩

$$Var(x) = E((X - E(X))(X - E(X))^{T})$$
$$= E(xx^{T}) - E(x)(E(x))^{T} = \Sigma$$

3 条件高斯分布

划分向量

$$\begin{bmatrix} a_1 \\ \vdots \\ a_m \\ b_1 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}, \ \mu = \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \ \Sigma = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}$$

精度矩阵

$$\Lambda = \Sigma^{-1} = \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix}$$

值得注意的是: $\Lambda_{ij} \neq \Sigma_{ij}$ (分块的性质)