多元高斯分布的kl距离

0.1 问题描述

假设p和q分别表示两个正态分布的概率密度, 其中μ_1和$\mu 2$分别表示p和q的均值向量, Σ_1和Σ_2分别表示p和q的协方差矩阵, 求p和q这两个分布之间的$Kullback$-$Leibler$距离 是多少?写出推导过程。

0.2 结果

$$D_{KL}\left(p\|q\right)=\frac{1}{2}\left(\ln\frac{|\Sigma_1|}{|\Sigma_2|}-n+tr\left(\Sigma_2^{-1}\Sigma_1\right)+\left(\mu_1-\mu_2\right)^T\Sigma_2^{-1}\left(\mu_1-\mu_2\right)\right)$$

0.3 推导过程

$$\begin{aligned}
D_{KL}\left(p\|q\right) &= \int_x p(x)\ln\frac{p(x)}{q(x)}dx && (1)\\
&= \int_x p(x)\ln\left((2\pi)^{\frac{n-n}{2}}\right)\left(\frac{|\Sigma_1|}{|\Sigma_2|}\right)^{\frac{1}{2}} && (2)\\
& \quad exp\left(\frac{1}{2}\left(\left(x-\mu_2\right)^T\Sigma_2^{-1}\left(x-\mu_2\right)-\left(x-\mu_1\right)^T\Sigma_1^{-1}\left(x-\mu_1\right)\right)\right)dx && (3)\\
&= \frac{1}{2}\int_x p(x)\left(\ln\frac{|\Sigma_1|}{|\Sigma_2|}+\left(\left(x-\mu_2\right)^T\Sigma_2^{-1}\left(x-\mu_2\right)-\left(x-\mu_1\right)^T\Sigma_1^{-1}\left(x-\mu_1\right)\right)\right)dx && (4)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}+\frac{1}{2}\int_x p(x)\left(\left(x-\mu_2\right)^T\Sigma_2^{-1}\left(x-\mu_2\right)-\left(x-\mu_1\right)^T\Sigma_1^{-1}\left(x-\mu_1\right)\right)dx && (5)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}+\frac{1}{2}E_p\left[\left(x-\mu_2\right)^T\Sigma_2^{-1}\left(x-\mu_2\right)-\left(x-\mu_1\right)^T\Sigma_1^{-1}\left(x-\mu_1\right)\right] && (6)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{1}{2}E_p\left[tr\left(\Sigma_1^{-1}\left(x-\mu_1\right)\left(x-\mu_1\right)^T\right)\right]+\frac{1}{2}E_p\left[tr\left(\Sigma_2^{-1}\left(x-\mu_2\right)\left(x-\mu_2\right)^T\right)\right] && (7)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{1}{2}tr\left(E_p\left[\Sigma_1^{-1}\left(x-\mu_1\right)\left(x-\mu_1\right)^T\right]\right)+\frac{1}{2}tr\left(E_p\left[\Sigma_2^{-1}\left(x-\mu_2\right)\left(x-\mu_2\right)^T\right]\right) && (8)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{1}{2}tr\left(\Sigma_1^{-1}E_p\left[\left(x-\mu_1\right)\left(x-\mu_1\right)^T\right]\right)+\frac{1}{2}tr\left(\Sigma_2^{-1}E_p\left[\left(x-\mu_2\right)\left(x-\mu_2\right)^T\right]\right) && (9)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{1}{2}tr\left(\Sigma_1^{-1}\Sigma_1\right)+\frac{1}{2}tr\left(\Sigma_2^{-1}E_p\left[xx^T-x\mu_2^T-\mu_2x^T+\mu_2\mu_2^T\right]\right) && (10)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{n}{2}+\frac{1}{2}tr\left(\Sigma_2^{-1}\left(\Sigma_1+\mu_1\mu_1^T-\mu_1\mu_2^T-\mu_2\mu_1^T+\mu_2\mu_2^T\right)\right) && (11)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{n}{2}+\frac{1}{2}tr\left(\Sigma_2^{-1}\Sigma_1+\Sigma_2^{-1}\left(\mu_1\mu_1^T-\mu_1\mu_2^T-\mu_2\mu_1^T+\mu_2\mu_2^T\right)\right) && (12)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{n}{2}+\frac{1}{2}tr\left(\Sigma_2^{-1}\Sigma_1+\Sigma_2^{-1}\left(\mu_1-\mu_2\right)\left(\mu_1-\mu_2\right)^T\right) && (13)\\
&= \frac{1}{2}\ln\frac{|\Sigma_1|}{|\Sigma_2|}-\frac{n}{2}+\frac{1}{2}tr\left(\Sigma_2^{-1}\Sigma_1\right)+\frac{1}{2}tr\left(\Sigma_2^{-1}\left(\mu_1-\mu_2\right)\left(\mu_1-\mu_2\right)^T\right) && (14)\\
&= \frac{1}{2}\left(\ln\frac{|\Sigma_1|}{|\Sigma_2|}-n+tr\left(\Sigma_2^{-1}\Sigma_1\right)+tr\left(\Sigma_2^{-1}\left(\mu_1-\mu_2\right)\left(\mu_1-\mu_2\right)^T\right)\right) && (15)\\
&= \frac{1}{2}\left(\ln\frac{|\Sigma_1|}{|\Sigma_2|}-n+tr\left(\Sigma_2^{-1}\Sigma_1\right)+\left(\mu_1-\mu_2\right)^T\Sigma_2^{-1}\left(\mu_1-\mu_2\right)\right) && (16)
\end{aligned}$$

(1) $Kullback$-$Leibler$距离的定义

(6) 满足期望的形式

$$\boxed{E\left(g(x)\right) = \int_x p(x)g(x)\,dx}$$

(7) $\left(x-\mu_2\right)^T \Sigma_2^{-1}\left(x-\mu_2\right) = tr\left(\Sigma_1^{-1}\left(x-\mu_1\right)\left(x-\mu_1\right)^T\right)$
为方便,简记为$A^TBA = tr(BAA^T)$

$$A^TBA = \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix} \begin{bmatrix} b_{11} & \cdots & b_{1n} \\ \vdots & b_{ij} & \vdots \\ b_{n1} & \cdots & b_{nn} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \tag{17}$$

$$= \begin{bmatrix} \sum_{i=1}^n a_i b_{i1} & \cdots & \sum_{i=j}^n a_i b_{ij} & \cdots \sum_{i=j}^n a_i b_{in} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \tag{18}$$

$$= \sum_{j=1}^n a_j \sum_{i=1}^n a_i b_{ij} \tag{19}$$

$$= \sum_{j=1}^n \sum_{i=1}^n a_j a_i b_{ij} \tag{20}$$

$$= \sum_{i=1}^n \sum_{j=1}^n \left(a_i a_j\right) b_{ji} \tag{21}$$

$$= \sum_{i=1}^n \sum_{j=1}^n \left(AA^T\right)_{ij} B_{ji} \tag{22}$$

$$= tr\left(B\left(AA^T\right)\right) \tag{23}$$

$$= tr\left(BAA^T\right) \tag{24}$$

(8) $\boxed{tr\left(E\left[x\right]\right) = E\left[tr\left(x\right)\right]}$

(9) $\boxed{E_p\left[\left(x-\mu_1\right)\left(x-\mu_1\right)^T\right] = \Sigma_1}$
协方差的定义,注意后面的$E_p\left[\left(x-\mu_2\right)\left(x-\mu_2\right)^T\right] \neq \Sigma_2$

(10) $\boxed{E(xx^T) = \Sigma + \mu\mu_T}$

(16) 同(7)

(24)

$$\boxed{tr\left(AB\right) = \sum_{i=1}^n (AB)_{ii} = \sum_{i=1}^n \sum_{j=1}^n A_{ij} B_{ji}}$$