

Mineria de Datos

Estudiante UNED

August 2019

Ejercicio 1

Calcule la divergencia de Kullback-Leibler entre dos gaussianas $p(x) = \mathcal{N}(x|\mu, \Sigma)$ y $q(x) = \mathcal{N}(x|m, L)$

1.30

Evaluate the Kullback-Leibler divergence (1.113) between two Gaussians $p(x) = \mathcal{N}(x|\mu, \Sigma)$ and $q(x) = \mathcal{N}(x|m, L)$

$$\begin{aligned} KL(p||q) &= - \int p(x) \ln \frac{q(x)}{p(x)} dx \\ \ln \frac{p(x)}{q(x)} &= \ln \frac{\mathcal{N}(x|m, L)}{\mathcal{N}(x|\mu, \Sigma)} = \ln \left\{ \frac{\frac{1}{(2\pi)^{D/2}} \frac{1}{|L|^{1/2}} \exp \left\{ -\frac{1}{2} (x-m)^T L^{-1} (x-m) \right\}}{\frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu) \right\}} \right\} = \\ \ln \left\{ \left(\frac{|\Sigma|}{|L|} \right)^{\frac{1}{2}} \exp \left\{ \frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu) - \frac{1}{2} (x-m)^T L^{-1} (x-m) \right\} \right\} &= \\ \frac{1}{2} \ln \left(\frac{|\Sigma|}{|L|} \right) + \frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu) - \frac{1}{2} (x-m)^T L^{-1} (x-m) &= \\ - \frac{1}{2} \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + x^T \Sigma^{-1} (x-\mu) - \mu^T \Sigma^{-1} (x-\mu) - x^T L^{-1} (x-m) + m^T L^{-1} (x-m) \right\} &= \\ - \frac{1}{2} \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + x^T \Sigma^{-1} x - \underbrace{x^T \Sigma^{-1} \mu - \mu^T \Sigma^{-1} x}_{x^T \Sigma^{-1} \mu \equiv \mu^T \Sigma^{-1} x} + \underbrace{\mu^T \Sigma^{-1} \mu - x^T L^{-1} x + x^T L^{-1} m + m^T L^{-1} x - m^T L^{-1} m}_{x^T L^{-1} m \equiv m^T L^{-1} x} \right\} &= \\ - \frac{1}{2} \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + x^T (\Sigma^{-1} - L^{-1}) x - 2\mu^T \Sigma^{-1} x + \mu^T \Sigma^{-1} \mu + 2m^T L^{-1} x - m^T L^{-1} m \right\} &= \\ - \frac{1}{2} \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + x^T (\Sigma^{-1} + L^{-1}) x - 2(\mu^T \Sigma^{-1} - m^T L^{-1}) x + \mu^T \Sigma^{-1} \mu - m^T L^{-1} m \right\} &= \\ KL(p||q) &= - \int p(x) \ln \frac{q(x)}{p(x)} dx = \\ - \int \mathcal{N}(x|\mu, \Sigma) \ln \frac{\mathcal{N}(x|m, L)}{\mathcal{N}(x|\mu, \Sigma)} dx &= - \int \mathcal{N}(x|\mu, \Sigma) dx \left(-\frac{1}{2} \right) \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + x^T (\Sigma^{-1} + L^{-1}) x - 2(\mu^T \Sigma^{-1} - m^T L^{-1}) x + \mu^T \Sigma^{-1} \mu - \right. \\ \frac{1}{2} \left\{ \underbrace{\int \ln \left(\frac{|\Sigma|}{|L|} \right) \mathcal{N}(x|\mu, \Sigma) dx}_{\int \mathcal{N}(x|\mu, \Sigma) dx = 1} + \int x^T (\Sigma^{-1} + L^{-1}) x \mathcal{N}(x|\mu, \Sigma) dx + \int -2(\mu^T \Sigma^{-1} - m^T L^{-1}) x \mathcal{N}(x|\mu, \Sigma) dx + \underbrace{\int (\mu^T \Sigma^{-1} \mu - m^T L^{-1} m) \mathcal{N}(x|\mu, \Sigma) dx}_{\int \mathcal{N}(x|\mu, \Sigma) dx = 1} \right\} &= \end{aligned}$$

$$\frac{1}{2} \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + \int x^T (\Sigma^{-1} + L^{-1}) x \mathcal{N}(x|\mu, \Sigma) dx - 2 (\mu^T \Sigma^{-1} - m^T L^{-1}) \underbrace{\int x \mathcal{N}(x|\mu, \Sigma) dx}_{\mu} + (\mu^T \Sigma^{-1} \mu - m^T L^{-1} m) \right\} =$$

$$\frac{1}{2} \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + \int x^T (\Sigma^{-1} + L^{-1}) x \mathcal{N}(x|\mu, \Sigma) dx - 2 (\mu^T \Sigma^{-1} - m^T L^{-1}) \mu + (\mu^T \Sigma^{-1} \mu - m^T L^{-1} m) \right\} =$$

$$\frac{1}{2} \left\{ \ln \left(\frac{|\Sigma|}{|L|} \right) + \int x^T (\Sigma^{-1} + L^{-1}) x \mathcal{N}(x|\mu, \Sigma) dx + (2m^T L^{-1} \mu - \mu^T \Sigma^{-1} \mu - m^T L^{-1} m) \right\}$$

Ejercicio 1

Considere dos variables x e y con distribución de probabilidad conjunta $p(x, y)$. Demuestre que:

- $E[x] = E_y[E_x[x|y]]$
- $var[x] = E_y[var_x[x|y]] + var_y[E_x[x|y]]$

donde $E_x[x|y]$ representa el valor esperado de x asumiendo la distribución de probabilidad condicionada $p(x|y)$, y una notación equivalente se utiliza para la varianza condicional.

2.8

Consider two variables x and y with joint distribution $p(x, y)$. Prove the following two results

- $E[x] = E_y[E_x[x|y]]$
- $var[x] = E_y[var_x[x|y]] + var_y[E_x[x|y]]$

Here $E_x[x|y]$ denotes the expectation of x under the conditional distribution $p(x|y)$, with a similar notation for the conditional variance.

$$\mathbf{E}_y[\mathbf{E}_x[\mathbf{x}|y]] = \int_y \left(\int_x x p(x|y) dx \right) p(y) dy = \int_y \int_x x p(x|y) p(y) dy dx = \int_y \int_x x p(x, y) dy dx = \int_x x \left(\int_y p(x, y) dy \right) dx = \int_x p(x) dx = \mathbf{E}[\mathbf{x}]$$

$$\mathbf{E}_y[\mathbf{var}_x[\mathbf{x}|y]] + \mathbf{var}_y[\mathbf{E}_x[\mathbf{x}|y]] =$$

$$\int_y \left(\int_x (x - E_x[x|y])^2 p(x|y) dx \right) p(y) dy + \int_y \left(\underbrace{E_y[E_x[x|y]]}_{E[x]} - E_x[x|y] \right)^2 p(y) dy =$$

$$\int_y \int_x (x^2 - 2xE_x[x|y] + E[x|y]^2) p(x|y) p(y) dy dx + \int_y (E[x]^2 - 2E[x]E_x[x|y] + E_x[x|y]^2) p(y) dy =$$

$$\int_y \int_x x^2 \underbrace{p(x|y)p(y)}_{p(x,y)=p(x|y)p(y)} dy dx - 2 \int_y \int_x x E_x[x|y] p(x|y) p(y) dy dx + \int_y \int_x E_x[x|y]^2 \underbrace{p(x|y)p(y)}_{p(x,y)=p(x|y)p(y)} dy dx + \int_y E[x]^2 p(y) dy -$$

$$2 \int_y E[x] E_x[x|y] p(y) dy + \int_y E_x[x|y]^2 p(y) dy =$$

$$\int_x x^2 \underbrace{\left(\int_y p(x, y) dy \right)}_{p(x)} dx - 2 \int_y E_x[x|y] \underbrace{\left(\int_x x p(x|y) dx \right)}_{E_x[x|y]} p(y) dy + \int_y E_x[x|y]^2 \underbrace{\left(\int_x p(x, y) dx \right)}_{p(y)} dy + E[x]^2 \int_y p(y) dy -$$

$$\begin{aligned}
& 2E[x] \underbrace{\int_y E_x[x|y] p(y) dy}_{E_y[E_x[x|y]]} + \int_y E_x[x|y]^2 p(y) dy = \\
& \int_x x^2 p(x) dx - 2 \int_y E_x[x|y] E_x[x|y] p(y) dy + \int_y E_x[x|y]^2 p(y) dy + E[x]^2 \int_y p(y) dy - 2E[x] \underbrace{E_y[E_x[x|y]]}_{E[x]} + \int_y E_x[x|y]^2 p(y) dy = \\
& E[x^2] - 2 \int_y E_x[x|y]^2 p(y) dy + \int_y E_x[x|y]^2 p(y) dy + E[x]^2 - 2E[x] E[x] + \int_y E_x[x|y]^2 p(y) dy = \\
& E[x^2] - E[x]^2 = \text{var}[x]
\end{aligned}$$

Ejercicio 1

Sabiendo que en un problema de clasificación con dos clases

$$p(C_1|x) = \frac{1}{1 + \exp\left(-\ln \frac{p(x|c_1)p(c_1)}{p(x|c_2)p(c_2)}\right)} = \frac{1}{1 + \exp(-a)} = \sigma(a)$$

y suponiendo un modelo generativo en el que las verosimilitudes (likelihoods) de las dos clases vienen dadas por dos gaussianas de medias μ_1 y μ_2 , pero la misma varianza Σ , demuestre que

$$p(c_1|x) = \sigma(w^T x + w_0)$$

con $w = \Sigma^{-1}(\mu_1 - \mu_2)$

$$w_0 = -\frac{1}{2}\mu_1^T \Sigma^{-1} \mu_1 + \frac{1}{2}\mu_2^T \Sigma^{-1} \mu_2 + \ln \frac{c_1}{c_2}$$

4.8

Using (4.57) and (4.58), derive the result (4.65) for the posterior class probability in the two-class generative model with Gaussian densities, and verify the results (4.66) and (4.67) for the parameters w and w_0 .

$$p(c_1|x) = \frac{p(x|c_1)p(c_1)}{p(x|c_1)p(c_1) + p(x|c_2)p(c_2)} = \frac{1}{1 + \exp(-a)} = \sigma(a)$$

$$a = \ln \frac{p(x|c_1)p(c_1)}{p(x|c_2)p(c_2)}$$

$$p(c_1|x) = \sigma(w^T x + w_0)$$

$$w = \Sigma^{-1}(\mu_1 - \mu_2)$$

$$w_0 = -\frac{1}{2}\mu_1^T \Sigma^{-1} \mu_1 + \frac{1}{2}\mu_2^T \Sigma^{-1} \mu_2 + \ln \frac{c_1}{c_2}$$

Entonces

$$\ln \frac{p(x|c_1)p(c_1)}{p(x|c_2)p(c_2)} = w^T x + w_0$$

Teniendo en cuenta que:

$$p(x|c_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1} (x - \mu_k)\right\}$$

$$\ln \frac{p(x|c_1)p(c_1)}{p(x|c_2)p(c_2)} =$$

$$\begin{aligned}
& \ln \left\{ \frac{\frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_1)^T \Sigma^{-1} (x - \mu_1) \right\}}{\frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_2)^T \Sigma^{-1} (x - \mu_2) \right\}} \right\} + \ln \frac{p(c_1)}{p(c_2)} = \\
& \ln \left\{ \exp \left\{ -\frac{1}{2} (x - \mu_1)^T \Sigma^{-1} (x - \mu_1) + \frac{1}{2} (x - \mu_2)^T \Sigma^{-1} (x - \mu_2) \right\} \right\} + \ln \frac{p(c_1)}{p(c_2)} = \\
& -\frac{1}{2} \{ x^T \Sigma^{-1} (x - \mu_1) - \mu_1^T \Sigma^{-1} (x - \mu_1) - x^T \Sigma^{-1} (x - \mu_2) + \mu_2^T \Sigma^{-1} (x - \mu_2) \} + \ln \frac{p(c_1)}{p(c_2)} = \\
& -\frac{1}{2} \{ x^T \Sigma^{-1} x - x^T \Sigma^{-1} \mu_1 - \mu_1^T \Sigma^{-1} x + \mu_1^T \Sigma^{-1} \mu_1 - x^T \Sigma^{-1} x + x^T \Sigma^{-1} \mu_2 + \mu_2^T \Sigma^{-1} x - \mu_2^T \Sigma^{-1} \mu_2 \} + \ln \frac{p(c_1)}{p(c_2)} = \\
& -\frac{1}{2} \{ -x^T \Sigma^{-1} (\mu_1 - \mu_2) - (\mu_1 - \mu_2)^T \Sigma^{-1} x + \mu_1^T \Sigma^{-1} \mu_1 - \mu_2^T \Sigma^{-1} \mu_2 \} + \ln \frac{p(c_1)}{p(c_2)} = \\
& -\frac{1}{2} \{ -2(\mu_1 - \mu_2)^T \Sigma^{-1} x + \mu_1^T \Sigma^{-1} \mu_1 - \mu_2^T \Sigma^{-1} \mu_2 \} + \ln \frac{p(c_1)}{p(c_2)} = (\mu_1 - \mu_2)^T \Sigma^{-1} x - \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^T \Sigma^{-1} \mu_2 + \\
& \ln \frac{p(c_1)}{p(c_2)} = \\
& \underbrace{(\Sigma^{-1} (\mu_1 - \mu_2))^T x}_{w^T} - \underbrace{\frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^T \Sigma^{-1} \mu_2 + \ln \frac{p(c_1)}{p(c_2)}}_{w_0} = \\
& w^T x + w_0
\end{aligned}$$

Ejercicio 1

Considere un modelo generativo de clasificación de K clases definido por K probabilidades a priori $p(C_k) = \pi_k$ y densidades de probabilidad del vector de características de entrada Φ condicionadas a la clase $p(\Phi|C_k)$ dadas por distribuciones normales multi-variantes con la misma covarianza:

$$p(\phi_n|C_k) = \mathcal{N}(\phi_n|\mu, \Sigma)$$

Suponga que se nos proporciona un conjunto de entrenamiento Φ_m, t_n donde el subíndice n toma valores $n = 1, \dots, N$ y t_n es un vector binario de longitud K que utiliza la codificación uno-de- K (es decir, que sus componentes son $t_{n,j} = I_{j,k}$ si el patrón t_n pertenece a la clase C_k). Si asumimos que el conjunto de entrenamiento constituye una muestra independiente de datos de este modelo, entonces el estimador máximo-verosímil de las probabilidades a priori viene dado por

$$\pi_k = \frac{N_k}{N}$$

donde N_k es el número de patrones asignados a la clase C_k .

Demuestre que el estimador máximo-verosímil de la media de la distribución de la clase C_k viene dado por

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^N t_{n,k} \phi_n$$

y de la matriz de covarianza, viene dado por

$$\Sigma = \sum_{k=1}^K \frac{N_k}{N} S_k$$

con

$$S_k = \frac{1}{N_k} \sum_{n=1}^N t_{n,k} (\phi_n - \mu_k) (\phi_n - \mu_k)^T$$

4.10

Consider the classification model of Exercise 4.9 and now suppose that the class-conditional densities are given by Gaussian distributions with a shared covariance matrix, so that

$$p(\phi_n|C_k) = \mathcal{N}(\phi_n|\mu, \Sigma)$$

Show that the maximum likelihood solution for the mean of the Gaussian distribution for class C_k is given by

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^N t_{n,k} \phi_n$$

which represents the mean of those feature vectors assigned to class C_k . Similarly, show that the maximum likelihood solution for the shared covariance matrix is given by

$$\Sigma = \sum_{k=1}^K \frac{N_k}{N} S_k$$

where

$$S_k = \frac{1}{N_k} \sum_{n=1}^N t_{n,k} (\phi_n - \mu_k) (\phi_n - \mu_k)^T$$

Thus Σ is given by a weighted average of the covariances of the data associated with each class, in which the weighting coefficients are given by the prior probabilities of the classes.

$$p(\{\phi_n, t_n\} | \{\pi_k\}) = \prod_{n=1}^N \prod_{k=1}^K \{p(\phi_n | C_k) p(C_k)\}^{t_{n,k}}$$

$$\begin{aligned} p(C_k) &= \pi_k \\ p(\phi_n | C_k) &= \mathcal{N}(\phi_n | \mu, \Sigma) \end{aligned}$$

$$\ln p(\{\phi_n, t_n\} | \{\pi_k\}) = \ln \prod_{n=1}^N \prod_{k=1}^K \{\mathcal{N}(\phi_n | \mu, \Sigma) \pi_k\}^{t_{n,k}}$$

$$\begin{aligned} \ln \prod_{m=1}^M a_m &= \ln \sum_{m=1}^M a_m \\ \ln a^n &= n \ln a \end{aligned}$$

$$\ln p(\{\phi_n, t_n\} | \{\pi_k\}) = \sum_{n=1}^N \sum_{k=1}^K t_{n,k} \ln \{\mathcal{N}(\phi_n | \mu, \Sigma) \pi_k\}$$

$$\ln \mathcal{N}(\phi_n | \mu, \Sigma) = \ln(2\pi |\Sigma|)^{-1/2} - \frac{1}{2} (\phi_n - \mu_k)^T \Sigma^{-1} (\phi_n - \mu_k)$$

$$\ln p(\{\phi_n, t_n\} | \{\pi_k\}) = \sum_{n=1}^N \sum_{k=1}^K t_{n,k} \left\{ -\frac{1}{2} \ln(|\Sigma|) - \frac{1}{2} (\phi_n - \mu_k)^T \Sigma^{-1} (\phi_n - \mu_k) - \frac{1}{2} \ln(2\pi) + \ln \pi_k \right\}$$

$$\frac{\partial}{\partial \mu_m} \left\{ \sum_{m=1}^m F(x_m) \right\} = \frac{\partial F(x_m)}{\partial \mu_m}$$

$$\frac{\partial}{\partial \mu_k} \{\ln p(\{\phi_n, t_n\} | \{\pi_k\})\} = \frac{\partial}{\partial \mu_k} \left\{ \sum_{n=1}^N t_{n,k} \left\{ -\frac{1}{2} (\phi_n - \mu_k)^T \Sigma^{-1} (\phi_n - \mu_k) \right\} \right\} = 0$$

$$\frac{\partial}{\partial s} (x-s)^T W (x-s) = 2W (x-s)$$

$$\sum_{n=1}^N t_{n,k} \{-\Sigma^{-1}(\phi_n - \mu_k)\} = 0 \implies -\sum_{n=1}^N t_{n,k} \Sigma^{-1} \phi_n - t_{n,k} \Sigma^{-1} \mu_k = 0$$

$$\sum a - b = \sum a - \sum b$$

$$\sum_{n=1}^N t_{n,k} \Sigma^{-1} \mu_k - \sum_{n=1}^N t_{n,k} \Sigma^{-1} \phi_n = 0 \implies \sum_{n=1}^N t_{n,k} \Sigma^{-1} \mu_k = \sum_{n=1}^N t_{n,k} \Sigma^{-1} \phi_n$$

$$\Sigma \cdot \Sigma^{-1} = I$$

$$\Sigma^{-1} \mu_k \sum_{n=1}^N t_{n,k} = \Sigma^{-1} \sum_{n=1}^N t_{n,k} \phi_n \implies \Sigma \left\{ \Sigma^{-1} \mu_k \sum_{n=1}^N t_{n,k} \right\} = \Sigma \left\{ \Sigma^{-1} \sum_{n=1}^N t_{n,k} \phi_n \right\}$$

$$N_k = \sum_{n=1}^N t_{n,k}$$

$$\mu_k N_k = \sum_{n=1}^N t_{n,k} \phi_n \implies \mu_k = \frac{1}{N_k} \sum_{n=1}^N t_{n,k} \phi_n$$

$$\frac{\partial}{\partial \Sigma} \{ \ln p(\{\phi_n, t_n\} | \{\pi_k\}) \} = \frac{\partial}{\partial \Sigma} \left\{ \sum_{n=1}^N \sum_{k=1}^K t_{n,k} \left\{ -\frac{1}{2} \ln(|\Sigma|) - \frac{1}{2} (\phi_n - \mu_k)^T \Sigma^{-1} (\phi_n - \mu_k) \right\} \right\}$$

$$\sum a + b = \sum a + \sum b$$

$$D(a + b) = Da + Db$$

$$-\frac{1}{2} \frac{\partial}{\partial \Sigma} \left\{ \sum_{n=1}^N \sum_{k=1}^K t_{n,k} \ln(|\Sigma|) \right\} - \frac{1}{2} \frac{\partial}{\partial \Sigma} \left\{ \sum_{n=1}^N \sum_{k=1}^K t_{n,k} (\phi_n - \mu_k)^T \Sigma^{-1} (\phi_n - \mu_k) \right\} = 0$$

$$S_k = \frac{1}{N_k} \sum_{n=1}^N t_{n,k} (\phi_n - \mu_k) (\phi_n - \mu_k)^T$$

$$-\frac{1}{2} \left\{ \sum_{n=1}^N \sum_{k=1}^K t_{n,k} \frac{\partial \ln(|\Sigma|)}{\partial \Sigma} \right\} = \frac{1}{2} \left\{ \sum_{k=1}^K \frac{\partial}{\partial \Sigma} \underbrace{\sum_{n=1}^N t_{n,k} (\phi_n - \mu_k)^T \Sigma^{-1} (\phi_n - \mu_k)}_{N_k \text{ Tr}(\Sigma^{-1} S_k)} \right\}$$

$$\frac{\partial \ln(|A|)}{\partial \Sigma} = (A^{-1})^T$$

$$-\sum_{n=1}^N \sum_{k=1}^K t_{n,k} \underbrace{(\Sigma^{-1})^T}_{\Sigma^{-1}} = \sum_{k=1}^K \frac{\partial \{N_k \text{ Tr}(\Sigma^{-1} S_k)\}}{\partial \Sigma}$$

$$\frac{\partial \{ \text{Tr}(AX^{-1}B) \}}{\partial X} = (X^{-1}B A X^{-1})^T$$

$$-\sum_{n=1}^N \sum_{k=1}^K t_{n,k} \Sigma^{-1} = -\sum_{k=1}^K N_k (\Sigma^{-1} S_k \Sigma^{-1})^T$$

$$(A B C)^T = C^T B^T A^T \quad N = \sum_{n=1}^N \sum_{k=1}^K t_{n,k}$$

$$\Sigma^{-1} \underbrace{\sum_{n=1}^N \sum_{k=1}^K t_{n,k}}_N = \sum_{k=1}^K N_k (\Sigma^{-1} S_k \Sigma^{-1})^T$$

Multiplicando por Σ tanto por la izquierda como por la derecha ambos miembros de la ecuaci3n

$$\Sigma (\Sigma^{-1} N) \Sigma = \Sigma \left(\sum_{k=1}^K N_k \Sigma^{-1} S_k \Sigma^{-1} \right) \Sigma N \Sigma = \sum_{k=1}^K N_k S_k \implies \Sigma = \sum_{k=1}^K \frac{N_k}{N} S_k$$