1 Relative entropy for Gaussians II

1. Let $M \in \mathbb{R}^{N\times N}$ and X_1 and X_2 the normal random variables with respectively probability density functions p and q. Define the change of variable $Y_i = MX_i$, $i = 1,2$.

i) A linear transformation of a normally distributed random variable is another normally distributed random variable. Using the property of the expected value one can show that

$$\begin{aligned} E[MX_i] &= ME[X_i] = M\widehat{x}_i \\ E\left[(MX_i - E[MX_i])(MX_i - E[MX_i])^T\right] &= ME\left[(X_i-\widehat{x}_i)(X_i-\widehat{x}_i)^T\right]M^T = MK_i^{-1}M^T. \end{aligned}$$

for $i = 1,2$.

ii) A direct computation gives:

$$\begin{aligned} D(\tilde{p},\tilde{q}) &= \frac{1}{2}\left[\mathrm{tr}(M^{-T}K_2M^{-1}MK_1^{-1}M^T) - \ln\frac{\det M{-}TK_2M{-}1}{\det M{-}TK_2M{-}1}\right] \\ &+ \frac{1}{2}M(\widehat{x}_1-\widehat{x}_2)\cdot M^{-T}K_2M^{-1}M(\widehat{x}_1-\widehat{x}_2) \\ &= \frac{1}{2}\left[\mathrm{tr}(M^{-T}K_2K_1^{-1}M^T) - \ln\frac{\det K_2}{\det K_2}\right] \\ &+ \frac{1}{2}(\widehat{x}_1-\widehat{x}_2)\cdot M^{-T}M^{-T}K_2M^{-1}M(\widehat{x}_1-\widehat{x}_2) \\ &= \frac{1}{2}\left[\mathrm{tr}(K_2K_1^{-1}M^TM^{-T}) - \ln\frac{\det K_2}{\det K_2}\right] + \frac{1}{2}(\widehat{x}_1-\widehat{x}_2)\cdot K_2(\widehat{x}_1-\widehat{x}_2) \\ &= \frac{1}{2}\left[\mathrm{tr}(K_2K_1^{-1}) - \ln\frac{\det K_2}{\det K_2}\right] + \frac{1}{2}(\widehat{x}_1-\widehat{x}_2)\cdot K_2(\widehat{x}_1-\widehat{x}_2) \\ &= D(p,q). \end{aligned}$$

2. The generalised eigenvalue problem can be rewritten as

$$K_2v_i = \mu_iK_1v_i \Rightarrow K_2K_1^{-1}v_i = \mu_i\mathbf{I}v_i \Rightarrow K_2K_1^{-1} = \mu_i\mathbf{I}, i = 1,\dots N. \tag{1}$$

We can also rewrite the definition of $D^\dagger$ as

$$D^\dagger(K_1,K_2) = \frac{1}{2}\left[\mathrm{tr}\left(K_2K_1^{-1}\right) - \ln\det K_2K_1^{-1} - N\right]. \tag{2}$$

Fix now the value of the index i and use the relation (1) into (2):

$$D^\dagger(K_1,K_2) = \frac{1}{2}\left(N\mu_i - N\ln\mu_i - N\right) = \frac{N}{2}\left(\mu_i - \ln\mu_i - 1\right), \tag{3}$$

The latter equation is true for all $i = 1,\dots,N$. Thus,

$$ND^\dagger(K_1,K_2) = \frac{N}{2}\sum_{i=1}^{N}\left(\mu_i - \ln\mu_i - 1\right) \Rightarrow D^\dagger(K_1,K_2) = \frac{1}{2}\sum_{i=1}^{N}\left(\mu_i - \ln\mu_i - 1\right). \tag{4}$$

3. i) By using the fact that $\ln \frac{\det K_2}{\det K_1} = \ln\det K_2 - \ln\det K_1$, we get that the symmetrized version of the stiffness part of the relative entropy between two Gaussians is :

$$D^{\dagger}_{sym} = \frac{1}{4}\operatorname{tr}\left(K_2K_1^{-1} + K_1K_2^{-1}\right) - \frac{N}{2}. \tag{5}$$

ii) By using the same argument used in part 2 of this exercise we find that

$$D^{\dagger}_{sym} = \frac{1}{4}\sum_{i=1}^{N}\left(\sqrt{\mu_i} - \frac{1}{\sqrt{\mu_i}}\right)^2. \tag{6}$$

2 Maximum entropy fit for the stiffness matrix

Recall that the matrix C is the following partitioned matrix:

$$C = \begin{bmatrix} a & e & \mathrm{x} \\ e^T & b & d \\ \mathrm{x}^T & d^T & c \end{bmatrix},\ a = a^T,\ b = b^T,\ c = c^T,$$

where we have assumed $C > 0$. We want to show that if $\mathrm{x} = eb^{-1}d$, then $K := C^{-1}$ has zeros blocks in the $(1,3)$ and $(3,1)$ entries. For that we will prove the following statements:

1. By direct computation we have

$$\begin{aligned}
\begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & \Psi & I \end{bmatrix}\begin{bmatrix} a & e & 0 \\ e^T & b & 0 \\ 0 & 0 & H \end{bmatrix}\begin{bmatrix} I & 0 & 0 \\ 0 & I & \Omega \\ 0 & 0 & I \end{bmatrix}
&= \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & \Psi & I \end{bmatrix}\begin{bmatrix} a & e & e\Omega \\ e^T & b & b\Omega \\ 0 & 0 & H \end{bmatrix} \\
&= \begin{bmatrix} a & e & e\Omega \\ e^T & b & b\Omega \\ \Psi e^T & \Psi b & \Psi b\Omega + H \end{bmatrix}
\end{aligned}$$

Now by using the definition of x, Ψ, Ω, and H we can conclude that

$$C = \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & \Psi & I \end{bmatrix}\begin{bmatrix} a & e & 0 \\ e^T & b & 0 \\ 0 & 0 & H \end{bmatrix}\begin{bmatrix} I & 0 & 0 \\ 0 & I & \Omega \\ 0 & 0 & I \end{bmatrix}, \tag{7}$$

2. In order to compute the inverse of C using the decomposition (7), one have to check that the two following matrices

$$\begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & -\Psi & I \end{bmatrix},\ \begin{bmatrix} I & 0 & 0 \\ 0 & I & -\Omega \\ 0 & 0 & I \end{bmatrix}$$

are actually the inverses of

$$\begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & \Psi & I \end{bmatrix} \text{ and } \begin{bmatrix} I & 0 & 0 \\ 0 & I & \Omega \\ 0 & 0 & I \end{bmatrix},$$

Moreover, the inverse of a block diagonal matrix (without overlaps) is the inverse of each block. Thus, we obtain that $C^{-1} := K$ is

$$K = \begin{bmatrix} I & 0 & 0 \\ 0 & I & -\Omega \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \alpha & \varepsilon & 0 \\ \varepsilon^T & \beta & 0 \\ 0 & 0 & H^{-1} \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & -\Psi & I \end{bmatrix},$$

where $\begin{bmatrix} \alpha & \varepsilon \\ \varepsilon^T & \beta \end{bmatrix} = \begin{bmatrix} a & e \\ e^T & b \end{bmatrix}^{-1}$

3.

$$\begin{aligned} K &= \begin{bmatrix} I & 0 & 0 \\ 0 & I & -\Omega \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \alpha & \varepsilon & 0 \\ \varepsilon^T & \beta & 0 \\ 0 & 0 & H^{-1} \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & -\Psi & I \end{bmatrix} \\ &= \begin{bmatrix} \alpha & \varepsilon & 0 \\ \varepsilon^T & \beta + \Omega H^{-1}\Psi & -\Omega H^{-1} \\ 0 & H^{-1}\Psi & H^{-1} \end{bmatrix}. \end{aligned} \tag{8}$$

Thus, the blocks outside the stencil are zero.

4. In order to derive the algorithm we first decompose (8) in the following manner:

$$\begin{bmatrix} \alpha & \varepsilon & 0 \\ \varepsilon^T & \beta + \Omega H^{-1}\Psi & -\Omega H^{-1} \\ 0 & -H^{-1}\Psi & H^{-1} \end{bmatrix} = \begin{bmatrix} \alpha & \varepsilon & 0 \\ \varepsilon^T & \beta & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & -b^{-1} & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & b^{-1} + \Omega H^{-1}\Psi & -\Omega H^{-1} \\ 0 & -H^{-1}\Psi & H^{-1} \end{bmatrix},$$

where the first term of the right hand side is the inverse of $\begin{bmatrix} a & e \\ e^T & b \end{bmatrix}$, the second term is minus the inverse of b and the last term is the inverse of $\begin{bmatrix} b & d \\ d^T & c \end{bmatrix}$. The algorithm then is easy:

Step 1: Create an empty (only zero entries) matrix K of the same size as C,

Step 2: Invert each block of C inside the stencil and add them to K in the same position as they appear in C,

Step 3: Invert each overlap in the stencil and subtract them to the overlaps of K, again the position of the overlap must stay the same.

Remark: We recall that the inverse of a partitioned matrix $\begin{bmatrix} A & B \\ C & D \end{bmatrix}$ is

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix}$$

5. No, it is not possible to capture the five block a, b, c, d, and e from the non zeros blocks of K.

3 Principle of maximum entropy parameter estimation for banded stiffness matrices

According to the maximum entropy principle, the distribution $\rho_{ME}(x)$ can be defined as

$$\rho_{ME} = \text{argmin}_{\rho \in C} S[\rho] \text{ where } S[\rho] = \int_\Omega \rho(x) \ln \rho(x) dx.$$

The Lagrange multiplier method allows to write the distribution $\rho_{ME}(x) \in C$ as the solution of

$$\int_\Omega \{(1 + \ln \rho_{ME}(x)) - \lambda_0 - \lambda_1 \cdot x - [[\lambda_2]] : (x \otimes x)\} \, \delta\rho(x) dx = 0 \quad (*)$$

for any $\delta\rho \in \mathrm{L}^1(\Omega)$ and for some Lagrange multipliers $\lambda_0 \in \mathbb{R}$, $\lambda_1 \in \mathbb{R}^{12n-6}$ and $\lambda_2 \in \mathbb{R}^{(12n-6)\times(12n-6)}$. Note that we have used that the first variation of the functional $S[\rho]$ can be written as

$$\delta S[\rho]\delta\rho = \int_\Omega (1 + \ln \rho(x))\delta\rho(x) dx$$

for any $\rho, \delta\rho \in \mathrm{L}^1(\Omega)$ and that

$$\delta \left\{ \int_\Omega \phi(x)\rho(x)dx \right\} \delta\rho = \int_\Omega \phi(x)\delta\rho(x)dx$$

for any $\phi \in \mathrm{L}^1(\Omega)$ to deduce $(*)$. A sufficient condition is then that the distribution $\rho_{ME}(x)$ is normal, i.e. that it is of the form

$$\rho_{ME}(x) = \frac{1}{Z} \exp\left\{ -\frac{1}{2}(x - a) \cdot A(x - a) \right\}$$

with

$$(\lambda_0 - 1) + \lambda_1 \cdot x + [[\lambda_2]] : (x \otimes x) = -\frac{1}{2}(x - a) \cdot A(x - a) - \ln Z \quad (**)$$

for all $x \in \Omega$. Moreover, since we have the constraints $\rho_{ME}(x) \in C$, we can directly deduce that we have to define

$$a = \mu, A = K_{ME} \text{ and } Z = \sqrt{\det(2\pi K_{ME})}$$

according the identities regarding the first and second moment of a normal distribution. We note that the equality $(**)$ allows then to compute explicitly the values of the Lagrange multipliers λ_0, λ_1 and λ_2.