7.12

ノートのタイトル 2016/02/25

webの解答見た。
$\ln p(t|X,\alpha,\beta)$ の式変形の方向性が全く見当がつかなかったので。

(方針) 解答を見ると、$\ln p(t|X,\alpha,\beta)$ の $\ln|C|$ と $t^T C^{-1} t$ の C を Σ, m を使って表わすように変形する。

(7.85)より

$$\ln p(t|X,\alpha,\beta) = -\frac{1}{2}\left\{N\ln(2\pi) + \ln|C| + t^T C^{-1} t\right\}$$

$$C = B^{-1} + \Phi A^{-1} \Phi^T,\quad B = \beta I_N$$

これを

(7.82) $m = \Sigma \Phi^T B t$

(7.83) $\Sigma = (A + \Phi^T B \Phi)^{-1}$

を使って表わすよう努力する。

$$|B^{-1} + \Phi A^{-1} \Phi^T| = |I_N + \Phi A^{-1} \Phi^T B||B^{-1}| \leftarrow (C.12)$$

$$= |I_M + (\Phi A^{-1})^T (\Phi^T B)||B^{-1}| \leftarrow (C.14)$$

$$= |I_M + A^{-1} \Phi^T B \Phi||B^{-1}| \leftarrow A^{-1}, B \text{は対称}$$

$$= |A^{-1}||A + \Phi^T B \Phi||B^{-1}| \leftarrow (C.12)$$

$$= |A^{-1}||\Sigma^{-1}||B^{-1}| \quad \cdots ①$$

また

$$t^T (B^{-1} + \Phi A^{-1} \Phi^T)^{-1} t = t^T \{B - B\Phi(A + \Phi^T B \Phi)^{-1} \Phi^T B\} t \leftarrow (C.7)\ \text{Woodbury Identity}$$

$$= t^T (B - B\Phi \Sigma \Phi^T B) t$$

$$= t^T B t - t^T B \Phi \Sigma \Phi^T B t$$

$$= t^T B t - t^T B \Phi \Sigma \Sigma^{-1} \Sigma \Phi^T B t$$

$$= t^T B t - m^T \Sigma^{-1} m \quad \cdots ②$$

← (7.82)より、また Σ は対称なので

$(\Phi^T B \Phi)^T = \Phi^T B \Phi$ (B 対称なので)
つまり $\Phi^T B \Phi$ は対称
A も対称なので $A + \Phi^T B \Phi$ も対称
よって $(A + \Phi^T B \Phi)^{-1}$ も対称

①, ② を (7.85) に入れて

$$\ln p(t|X,\alpha,\beta) = -\frac{1}{2}\left\{N\ln(2\pi) + \ln|A^{-1}| + \ln|\Sigma^{-1}| + \ln|B^{-1}| + t^T B t - m^T \Sigma^{-1} m\right\}$$

を得る。
次にこれを α, β について偏微分し、停留条件を導く

（まず α について）

ここで

$$\frac{\partial}{\partial\alpha_i}\ln|A^{-1}| = \frac{\partial}{\partial\alpha_i}\ln\left|\begin{pmatrix}\alpha_1^{-1} & 0\\ 0 & \alpha_2^{-1}\end{pmatrix}\right| \overset{(C.47)}{=} \frac{\partial}{\partial\alpha_i}\ln\left(\prod_{i=1}^{M}\alpha_i^{-1}\right) = -\frac{1}{\alpha_i}$$

また

$$\frac{\partial}{\partial\alpha_i}\ln|\Sigma^{-1}| = \mathrm{Tr}\left(\Sigma\frac{\partial\Sigma^{-1}}{\partial\alpha_i}\right) \longleftarrow (C.22)$$

$$\frac{\partial}{\partial\alpha_2}\begin{pmatrix}\alpha_1 & 0 & 0\\ 0 & \alpha_2 & 0\\ 0 & 0 & \alpha_3\end{pmatrix} = \begin{pmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix} = \underset{\text{single entry matrix}}{J^{22}}$$

$$= \mathrm{Tr}\left(\Sigma J^{ii}\right) \longleftarrow \frac{\partial\Sigma^{-1}}{\partial\alpha_i} = \frac{\partial}{\partial\alpha_i}(A + \Phi^T B \Phi) = \frac{\partial A}{\partial\alpha_i} = J^{ii}$$

$$= \Sigma_{ii} \longleftarrow \mathrm{Tr}\begin{pmatrix}\Sigma_{11} & \Sigma_{12} & \Sigma_{13}\\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23}\\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33}\end{pmatrix}\begin{pmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix} = \mathrm{Tr}\begin{pmatrix}0 & \Sigma_{12} & 0\\ 0 & \Sigma_{22} & 0\\ 0 & \Sigma_{32} & 0\end{pmatrix} = \Sigma_{22}$$

さらに

$$\frac{\partial}{\partial\alpha_i} m^T\Sigma^{-1}m = \frac{\partial m^T}{\partial\alpha_i}\Sigma^{-1}m + m^T\frac{\partial\Sigma^{-1}}{\partial\alpha_i}m + m^T\Sigma^{-1}\frac{\partial m}{\partial\alpha_i}$$

$$= -t^T B\Phi\Sigma J^{ii}\Sigma\Sigma^{-1}m + m^T J^{ii} m + m^T\Sigma^{-1}(-\Sigma J^{ii}\Sigma\Phi^T B t) \longleftarrow$$

$$\left\{\begin{aligned} &\frac{\partial m^T}{\partial\alpha_i} = \frac{\partial}{\partial\alpha_i}t^T B\Phi\Sigma \overset{\Sigma^T=\Sigma}{=} t^T B\Phi\frac{\partial\Sigma}{\partial\alpha_i} \overset{(C.21)}{=} t^T B\Phi(-\Sigma)\frac{\partial\Sigma^{-1}}{\partial\alpha_i}\Sigma = -t^T B\Phi\Sigma J^{ii}\Sigma \\ &\text{同様に} \\ &\frac{\partial m}{\partial\alpha_i} = \frac{\partial}{\partial\alpha_i}\Sigma\Phi^T B t = -\Sigma J^{ii}\Sigma\Phi^T B t \end{aligned}\right.$$

$$= -mJ^{ii}m + m^T J^{ii} m - m^T J^{ii} m$$

$$= -mJ^{ii}m = -m_i^2 \longleftarrow (m_1\ m_2\ m_3)\begin{pmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}m_1\\ m_2\\ m_3\end{pmatrix} = (m_1\ m_2\ m_3)\begin{pmatrix}0\\ m_2\\ 0\end{pmatrix} = m_2^2$$

よって

$$\frac{\partial}{\partial\alpha_i}\ln p(t|X,\alpha,\beta) = -\frac{1}{2}\left\{-\frac{1}{\alpha_i} + \Sigma_{ii} - (-m_i^2)\right\}$$

を得る。これより停留条件は

$$-\frac{1}{2}\left\{-\frac{1}{\alpha_i} + \Sigma_{ii} - (-m_i^2)\right\} = 0$$

$$\therefore\ -\frac{1}{\alpha_i} + \Sigma_{ii} + m_i^2 = 0$$

$$\therefore\ -1 + \alpha_i\Sigma_{ii} + \alpha_i m_i^2 = 0$$

$$\therefore\ \alpha_i = \frac{1 - \alpha_i\Sigma_{ii}}{m_i^2} \overset{(7.87)}{=} \frac{\gamma_i}{m_i^2},\quad \gamma_i = 1 - \alpha_i\Sigma_{ii}$$

となり、(7.87)を得る。

(次にβについて)

$$\frac{\partial}{\partial \beta}\ln|\Sigma^{-1}| = \mathrm{Tr}\left(\Sigma \frac{\partial \Sigma^{-1}}{\partial \beta}\right) \leftarrow (C.22)$$

$$\frac{\partial \Sigma^{-1}}{\partial \beta} = \Phi^T\Phi$$

$$= \mathrm{Tr}\left(\Sigma \Phi^T \Phi\right)$$

$\Sigma^{-1} = A + \beta\Phi^T\Phi$ なので $\Phi^T\Phi = \frac{1}{\beta}(\Sigma^{-1} - A)$

$$= \frac{1}{\beta}\mathrm{Tr}\left(\Sigma(\Sigma^{-1} - A)\right)$$

$$\mathrm{Tr}(kX) = k\,\mathrm{Tr}(X)$$

$$= \frac{1}{\beta}\mathrm{Tr}\left(I_M - \Sigma A\right)$$

$$\mathrm{Tr}(A+B) = \mathrm{Tr}(A) + \mathrm{Tr}(B)$$

$$= \frac{1}{\beta}\left(M - \sum_{i=1}^{M}\alpha_i\Sigma_{ii}\right)$$

$$\mathrm{Tr}(\Sigma A) = \mathrm{Tr}\begin{pmatrix}\Sigma_{11} & \Sigma_{12}\\ \Sigma_{21} & \Sigma_{22}\end{pmatrix}\begin{pmatrix}\alpha_1 & 0\\ 0 & \alpha_2\end{pmatrix} = \mathrm{Tr}\begin{pmatrix}\Sigma_{11}\alpha_1 & \Sigma_{12}\alpha_2\\ \Sigma_{21}\alpha_1 & \Sigma_{22}\alpha_2\end{pmatrix} = \sum_i \alpha_i\Sigma_{ii}$$

また

$$\frac{\partial}{\partial \beta}\ln|\beta^{-1}| = \frac{\partial}{\partial \beta}\ln\prod_{i=1}^{N}\beta^{-1} = \frac{\partial}{\partial \beta}\ln\beta^{-N} = \frac{\partial}{\partial \beta}(-N\ln\beta) = -\frac{N}{\beta}$$

$$|A| = \prod_i \lambda_i \quad (C.47)$$

さらに

$$\frac{\partial}{\partial \beta}t^T\beta t = \frac{\partial}{\partial \beta}\beta t^T t = t^T t$$

$$\frac{\partial \Sigma^{-1}}{\partial \beta} = \Phi^T\Phi$$

$$\frac{\partial \Sigma}{\partial \beta} = (-\Sigma)\frac{\partial \Sigma^{-1}}{\partial \beta}\Sigma = -\Sigma\Phi^T\Phi\Sigma$$

$$\begin{cases}\dfrac{\partial m^T}{\partial \beta} = \dfrac{\partial}{\partial \beta}\beta t^T\Phi\Sigma = t^T\Phi\Sigma + \beta t^T\Phi\dfrac{\partial \Sigma}{\partial \beta} = t^T\Phi\Sigma - \beta t^T\Phi\Sigma\Phi^T\Phi\Sigma = t^T\Phi\Sigma - m^T\Phi^T\Phi\Sigma \\ \dfrac{\partial m}{\partial \beta} = \dfrac{\partial}{\partial \beta}\beta\Sigma\Phi^T t = \Sigma\Phi^T t + \beta\dfrac{\partial \Sigma}{\partial \beta}\Phi^T t = \Sigma\Phi^T t - \beta\Sigma\Phi^T\Phi\Sigma\Phi^T t = \Sigma\Phi^T t - \Sigma\Phi^T\Phi m\end{cases}$$

また

$$\frac{\partial}{\partial \beta}m^T\Sigma^{-1}m$$

$$= \frac{\partial m^T}{\partial \beta}\Sigma^{-1}m + m^T\frac{\partial \Sigma^{-1}}{\partial \beta}m + m^T\Sigma^{-1}\frac{\partial m}{\partial \beta}$$

$$= (t^T\Phi\Sigma - m^T\Phi^T\Phi\Sigma)\Sigma^{-1}m + m^T\Phi^T\Phi m + m^T\Sigma^{-1}(\Sigma\Phi^T t - \Sigma\Phi^T\Phi m)$$

$$= t^T\Phi m - m^T\Phi^T\Phi m + m^T\Phi^T\Phi m + m^T\Phi^T t - m^T\Phi^T\Phi m$$

$$= t^T\Phi m + m^T\Phi^T t - m^T\Phi^T\Phi m$$

これらより

$$\frac{\partial}{\partial \beta}\ln p(t|X,\alpha,\beta) = -\frac{1}{2}\left\{\frac{1}{\beta}\left(M - \sum_{i=1}^{M}\alpha_i\Sigma_{ii}\right) - \frac{N}{\beta} + t^T t - \left(t^T\Phi m + m^T\Phi^T t - m^T\Phi^T\Phi m\right)\right\}$$

$$= -\frac{1}{2}\left[\frac{1}{\beta}\left\{\left(M - \sum_{i=1}^{M}\alpha_i\Sigma_{ii}\right) - N\right\} + t^T t - t^T\Phi m + m^T\Phi^T t + m^T\Phi^T\Phi m\right]$$

$$= -\frac{1}{2}\left[\frac{1}{\beta}\left\{\left(M - \sum_{i=1}^{M}\alpha_i\Sigma_{ii}\right) - N\right\} + (t - \Phi m)^T(t - \Phi m)\right]$$

$$= -\frac{1}{2}\left[\frac{1}{\beta}\left\{\left(M - \sum_{i=1}^{M}\alpha_i\Sigma_{ii}\right) - N\right\} + \|t - \Phi m\|^2\right]$$

を得る。

これよりβについての停留条件は、

$$-\frac{1}{2}\left[\frac{1}{\beta}\left\{\left(M - \sum_{i=1}^{M}\alpha_i\Sigma_{ii}\right) - N\right\} + \|t - \Phi m\|^2\right] = 0$$

$$\therefore\ \beta^{-1} = \frac{\|t - \Phi m\|^2}{N - \left(M - \sum_{i=1}^{M}\alpha_i\Sigma_{ii}\right)} = \frac{\|t - \Phi m\|^2}{N - \sum_{i=1}^{M}(1 - \alpha_i\Sigma_{ii})} = \frac{\|t - \Phi m\|^2}{N - \sum_{i=1}^{M}\gamma_i}, \quad \gamma_i = 1 - \alpha_i\Sigma_{ii} \quad (7.88)$$

となり、(7.88)を得る。