## ML Written Homework 3

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## 1 Laplacian Eigenmaps

(a) The edge shown in the graph are: (1,2) (1,3) (1,4) (2,4) (2,8) (3,8) (5,6) (5,7) (7,10) (8,9) (9,10)

(b)

```
(c)
               import numpy as np
               from scipy import linalg
               import matplotlib.pyplot as plt
               from mpl_toolkits.mplot3d import Axes3D
               W = np.array([
                   [0, 1, 1, 1, 0, 0, 0, 0, 0, 0],
                                                     # x1
                   [1, 0, 0, 1, 0, 0, 0, 1, 0, 0],
                                                     # x2
                   [1, 0, 0, 0, 0, 0, 0, 1, 0, 0],
                                                     # x3
                   [1, 1, 0, 0, 0, 0, 0, 0, 0, 0],
                                                     # x4
                   [0, 0, 0, 0, 0, 1, 1, 0, 0, 0],
                                                     # x5
                   [0, 0, 0, 0, 1, 0, 0, 0, 0, 0],
                                                     # x6
                   [0, 0, 0, 0, 1, 0, 0, 0, 0, 1],
                                                     # x7
                   [0, 1, 1, 0, 0, 0, 0, 0, 1, 0],
                                                     # x8
                   [0, 0, 0, 0, 0, 0, 0, 1, 0, 1], # x9
                   [0, 0, 0, 0, 0, 0, 1, 0, 1, 0]
                                                     # x10
               ])
               degrees = W.sum(axis=1)
               D = np.diag(degrees)
               L = D - W
               try:
                   eigenvalues, eigenvectors = linalg.eigh(L, D)
               except linalg.LinAlgError:
                   print("Try use pinv")
                   safe_degrees = np.where(degrees == 0, 1e-6, degrees)
                   D_inv_sqrt = np.diag(1.0 / np.sqrt(safe_degrees))
                   L_sym = D_inv_sqrt @ L @ D_inv_sqrt
                   eigenvalues, eigenvectors_sym = linalg.eigh(L_sym)
                   eigenvectors = D_inv_sqrt @ eigenvectors_sym
               Psi = eigenvectors[:, 1:4]
               Z = Psi
               print("\n--- eigenvalues ---")
               print(eigenvalues)
               print("\n--- Psi (Z = Psi) ---")
               print(Z)
               fig = plt.figure(figsize=(10, 8))
               ax = fig.add_subplot(111, projection='3d')
               ax.scatter(Z[:, 0], Z[:, 1], Z[:, 2],
                   s=100, c=degrees, cmap='viridis', alpha=0.8)
```

#### Laplacian Eigenmaps

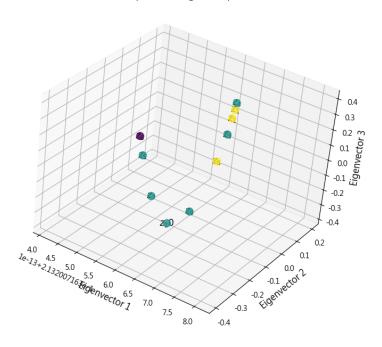


Figure 1: 3D image eigenvector 1-3

(d) This is the image of eigenvector 2-4 and the verify part

#### Laplacian Eigenmaps

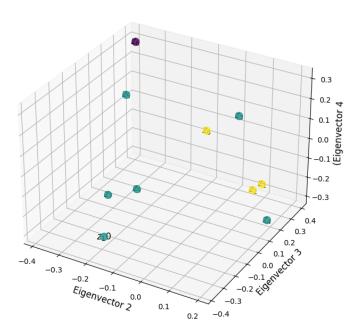


Figure 2: 3D image eigenvector 2-4

```
--- 驗證 tr(Ψ^T L Ψ) ---
tr(Ψ^T L Ψ) 的計算結果: 1.097803075120642
特徴值之和 (λ_1+λ_2+λ_3): 1.0978030751206402
此值是否約等於 1.098 (1.09779...): False
--- 驗證 Ψ^T D Ψ = I_3 ---
矩陣 Ψ^T D Ψ (應為 3x3 單位矩陣):
[[ 1.000000000e+00 -5.55111512e-17 4.16333634e-17]
  [-4.16333634e-17 1.00000000e+00 -1.28369537e-16]
  [ 4.16333634e-17 -7.28583860e-17 1.000000000e+00]]
```

Figure 3: Verify

(e) Suppose  $\mathbf{c} = [c, c, c, ..., c]^T$ , we want to show  $L\mathbf{c} = 0$  for all L.  $L\mathbf{c} = (D - W)\mathbf{c} = D\mathbf{c} - W\mathbf{c}$ 

$$(W\mathbf{c})_i = \sum_{j=1}^n W_{ij}c_j = c\sum_{j=1}^n W_{ij} = c \cdot d_i$$

$$(D\mathbf{c})_i = \sum_{j=1}^n D_{ij}c_j = c \cdot d_i$$

Hence,  $L\mathbf{c} = D\mathbf{c} - W\mathbf{c} = 0$ 

(f)

RHS = 
$$\frac{1}{2} \sum_{i,j} w_{ij} (f_i - f_j)^2$$
  
=  $\frac{1}{2} \sum_{i,j} w_{ij} (f_i^2 - 2f_i f_j + f_j^2)$   
=  $\frac{1}{2} \left( \sum_{i,j} w_{ij} f_i^2 - \sum_{i,j} w_{ij} (2f_i f_j) + \sum_{i,j} w_{ij} f_j^2 \right)$   

$$\sum_{i,j} w_{ij} f_i^2 = \sum_{i} f_i^2 \left( \sum_{j} w_{ij} \right) = \sum_{i} f_i^2 d_i$$

$$\sum_{i,j} w_{ij} f_j^2 = \sum_{j,i} w_{ji} f_i^2 = \sum_{i} f_i^2 \left( \sum_{j} w_{ij} \right) = \sum_{i} f_i^2 d_i$$
RHS =  $\frac{1}{2} \left( \left( \sum_{i} d_i f_i^2 \right) - 2 \sum_{i,j} w_{ij} f_i f_j + \left( \sum_{i} d_i f_i^2 \right) \right)$   
=  $\frac{1}{2} \left( 2 \sum_{i} d_i f_i^2 - 2 \sum_{i,j} w_{ij} f_i f_j \right)$   
=  $\sum_{i} d_i f_i^2 - \sum_{i,j} w_{ij} f_i f_j$   
LHS =  $f^T (D - W) f$   
=  $\int_{i,j} f_i D_{ij} f_j - \sum_{i,j} f_i W_{ij} f_j$   
=  $\sum_{i} d_i f_i^2 - \sum_{i,j} w_{ij} f_i f_j$ 

Hence we have LHS=RHS. QED.

(g) By the question we have

$$L \cdot f = \lambda \cdot f = 0 \cdot f = 0$$

so we have

$$f^T L f = f^T \cdot 0 = 0$$

(h) If f is the eigenvector of the eigenvalue 0, by f and g we can find that

$$f^{T}Lf = \frac{1}{2} \sum_{i,j} w_{ij} (f_i - f_j)^2 = 0$$

That is, for any  $w_{ij} > 0$  (means there is an edge between  $x_i$  and  $x_j$ ), we have  $f_i = f_j$ . Since the graph is connect, for any two vertex  $x_k, x_t$ , there must be a connected path  $x_k \to x_{p_1} \to \cdots \to x_{p_m} \to x_t$ , that gives us

$$f_k = f_{p_1} = \dots = f_{p_m} = f_t$$

Because the vertexes are arbitrarily chosen, the only eigenvector satisfied the above condition is  $f = [c, c, ..., c]^T$ , which means the eigenvalue 0 is only 1-dimension, then the second smallest eigenvalue  $\lambda_1$  must be greater than 0 ( $\lambda_1 > 0$ ).

## 2 Principal Component Analysis

(a) We want to maximize  $f(u) = u^T \Sigma u$  constraint  $g(u) = ||u||_2^2 = u^T u = 1$ . Suppose  $\lambda$  is a Lagrange multiplier, we have the Lagrange function

$$\mathcal{L}(u,\lambda) = f(u) - \lambda(g(u) - 1) = u^T \Sigma u - \lambda(u^T u - 1)$$

Then we compute the gradient and set it to 0

$$\nabla_u \mathcal{L}(u, \lambda) = \nabla_u (u^T \Sigma u - \lambda (u^T u - 1))$$
$$= 2\Sigma u - \lambda (2u)$$
$$= 2(\Sigma u - \lambda u) = 0$$

This gives us  $\Sigma u = \lambda u$ , so for any maximizer or minimizer u, it must satisfy the equation  $\Sigma u = \lambda u$ .

Then bring the maximizer u back to  $f(u) = u^T \Sigma u = \lambda u^T u = \lambda$ , and we have  $\lambda = \max_{\|u\|_2^2=1} u^T \Sigma u$ .

(b)  $\hat{x}_i = (u^T x_i) u$  is the orthogonal projection of  $x_i$  on u, then we have  $||x_i||_2^2 = ||\hat{x}_i||_2^2 + ||x_i - \hat{x}_i||_2^2$ . Then  $||x_i - \hat{x}_i||_2^2 = ||x_i||_2^2 - ||\hat{x}_i||_2^2$ .

Now compute  $\|\hat{x}_i\|_2^2$ 

$$\|\hat{x}_i\|_2^2 = \|(u^T x_i)u\|_2^2$$

$$= (u^T x_i)^2 \|u\|_2^2$$

$$= (u^T x_i)^2 (1)$$

$$= (u^T x_i)^2$$

So we have  $||x_i - \hat{x}_i||_2^2 = ||x_i||_2^2 - (u^T x_i)^2$ 

LHS = 
$$\left(\frac{1}{N} \sum_{i=1}^{N} \|x_i\|_2^2\right) - \left(\frac{1}{N} \sum_{i=1}^{N} (u^T x_i)^2\right)$$
  
 $\frac{1}{N} \sum_{i=1}^{N} \|x_i\|_2^2 = \frac{1}{N} \sum_{i=1}^{N} \operatorname{tr}(x_i x_i^T)$   
 $= \operatorname{tr}\left(\frac{1}{N} \sum_{i=1}^{N} x_i x_i^T\right)$   
 $= \operatorname{tr}(\Sigma)$   
 $\frac{1}{N} \sum_{i=1}^{N} (u^T x_i)^2 = \frac{1}{N} \sum_{i=1}^{N} u^T (x_i x_i^T) u$   
 $= u^T \left(\frac{1}{N} \sum_{i=1}^{N} x_i x_i^T\right) u$   
 $= u^T \Sigma u$ 

Then we get

$$\frac{1}{N} \sum_{i=1}^{N} \|x_i - \hat{x}_i\|_2^2 = \text{tr}(\Sigma) - u^T \Sigma u$$

(c)

$$\Sigma = \frac{1}{N} \sum_{i=1}^{N} \begin{pmatrix} x_{i,1}^2 & x_{i,1} x_{i,2} \\ x_{i,1} x_{i,2} & x_{i,2}^2 \end{pmatrix} = \frac{1}{N} \begin{pmatrix} \sum_{i=1}^{N} x_{i,1}^2 & \sum_{i=1}^{N} x_{i,1} x_{i,2} \\ \sum_{i=1}^{N} x_{i,1} x_{i,2} & \sum_{i=1}^{N} x_{i,2}^2 \end{pmatrix}$$

Define  $S = \sum_{i=1}^{N} x_i x_i^T$ 

$$S = \begin{pmatrix} 363 & -60 \\ -60 & 482 \end{pmatrix}$$

then  $\Sigma = \frac{1}{N}S$ 

Solve the eigenvalue of S

$$\det(S - \lambda_S I) = 0$$

$$\det\begin{pmatrix} 363 - \lambda_S & -60 \\ -60 & 482 - \lambda_S \end{pmatrix} = 0$$

$$\lambda_S^2 - 845\lambda_S + 171366 = 0$$

$$\lambda_S = \frac{845 \pm 169}{2} = 507 \text{ or } 338$$

Choose the maxima eigenvalue  $\lambda_{S,1} = 507$  and compute its eigenvector

$$\begin{pmatrix} 363 - 507 & -60 \\ -60 & 482 - 507 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$\begin{pmatrix} -144 & -60 \\ -60 & -25 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$-144a - 60b = 0 \implies -12(12a + 5b) = 0 \implies 12a = -5b$$

We have the eigenvector  $v_1 = \begin{pmatrix} 5 \\ -12 \end{pmatrix}$  Then we can get the unit eigenvector  $u_1$ 

$$u_1 = \frac{v_1}{\|v_1\|_2} = \frac{1}{13} \begin{pmatrix} 5\\ -12 \end{pmatrix} = \begin{pmatrix} 5/13\\ -12/13 \end{pmatrix}$$

So the eigenvalues and the unit eigenvector of the max eigenvalue are

$$\lambda_1 = \frac{507}{N}, \lambda_2 = \frac{338}{N}$$

$$u_1 = \begin{pmatrix} 5/13 \\ -12/13 \end{pmatrix}$$

Now compute the total reconstruction error, by (b)

$$\frac{1}{N} \sum_{i=1}^{N} \|x_i - \hat{x}_i\|_2^2 = \operatorname{tr}(\Sigma) - u^T \Sigma u \implies \sum_{i=1}^{N} \|x_i - \hat{x}_i\|_2^2 = N(\operatorname{tr}(\Sigma) - u^T \Sigma u)$$

$$E = N\left(\operatorname{tr}\left(\frac{1}{N}S\right) - u^T\left(\frac{1}{N}S\right)u\right)$$
$$= N\left(\frac{1}{N}\operatorname{tr}(S) - \frac{1}{N}u^TSu\right)$$
$$= \operatorname{tr}(S) - u^TSu$$

Apply 
$$S = \begin{pmatrix} 363 & -60 \\ -60 & 482 \end{pmatrix}$$
 and  $u = \begin{pmatrix} 5/13 \\ -12/13 \end{pmatrix}$  we can calculate  $tr(S) = 363 + 482 = 845$  By (a)

$$u^T S u = u^T \lambda_{S,1} u = 507 \cdot u^T u = 507$$

So 
$$E = tr(S) - \lambda_{S,1} = \lambda_{S,2} = 845 - 507 = 338$$

# 3 Gradient of the t-SNE Objective

1.

$$C = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

$$= \sum_{i \neq j} p_{ij} (\log p_{ij} - \log q_{ij})$$

$$= \sum_{i \neq j} p_{ij} \log p_{ij} - \sum_{i \neq j} p_{ij} \log q_{ij}$$

 $\sum_{i\neq j} p_{ij} \log p_{ij}: \text{ Since } p_{ij} \text{ is computed by } \{\mathbf{x}_i\}, \text{ it cannot be influenced by } \mathbf{y}_i, \text{ so for } \mathbf{y}_i, \\ \sum_{i\neq j} p_{ij} \log p_{ij} \text{ is a constant } (\text{constant}(\text{to } \mathbf{y}_i). \text{ Hence, } C = \text{constant}(\text{to } \mathbf{y}_i) - \sum_{i\neq j} p_{ij} \log q_{ij}$ 

2. We want to show  $\frac{\partial C}{\partial y_i} = 4 \sum_{j \neq i} (p_{ij} - q_{ij}) (y_i - y_j) (1 + ||y_i - y_j||^2)^{-1}$ 

$$\frac{\partial C}{\partial y_i} = \frac{\partial}{\partial y_i} \left( \text{constant} - \sum_{k \neq \ell} p_{k\ell} \log q_{k\ell} \right)$$

$$= -\frac{\partial}{\partial y_i} \left( \sum_{k \neq \ell} p_{k\ell} \log q_{k\ell} \right)$$

$$w_{ij} = (1 + ||y_i - y_j||^2)^{-1}$$

$$Z = \sum_{k \neq \ell} w_{k\ell}$$

$$q_{ij} = \frac{w_{ij}}{Z}$$

Use the above equation we can rewrite the formula

$$\sum_{k \neq \ell} p_{k\ell} \log q_{k\ell} = \sum_{k \neq \ell} p_{k\ell} \log \left(\frac{w_{k\ell}}{Z}\right)$$

$$= \sum_{k \neq \ell} p_{k\ell} (\log w_{k\ell} - \log Z)$$

$$= \sum_{k \neq \ell} p_{k\ell} \log w_{k\ell} - \left(\sum_{k \neq \ell} p_{k\ell}\right) \log Z$$

$$C = \text{const} - \left(\sum_{k \neq \ell} p_{k\ell} \log w_{k\ell} - \log Z\right)$$

Return to the derivative of C

$$\frac{\partial C}{\partial y_i} = -\frac{\partial}{\partial y_i} \left( \sum_{k \neq \ell} p_{k\ell} \log w_{k\ell} \right) + \frac{\partial}{\partial y_i} (\log Z)$$

The first term  $\frac{\partial}{\partial y_i} \left( -\sum_{k\neq \ell} p_{k\ell} \log w_{k\ell} \right)$ :

$$\frac{\partial \log w_{k\ell}}{\partial y_i} = \frac{1}{w_{k\ell}} \frac{\partial w_{k\ell}}{\partial y_i}$$
$$\frac{\partial w_{k\ell}}{\partial y_i} = \frac{\partial}{\partial y_i} (1 + \|y_k - y_\ell\|^2)^{-1}$$
$$= -1 \cdot (w_{k\ell})^2 \cdot \frac{\partial \|y_k - y_\ell\|^2}{\partial y_i}$$

If 
$$k = i$$
:  $\frac{\partial \|y_i - y_\ell\|^2}{\partial y_i} = 2(y_i - y_\ell)$   
If  $\ell = i$ :  $\frac{\partial \|y_k - y_i\|^2}{\partial y_i} = -2(y_k - y_i) = 2(y_i - y_k)$   
Else:  $\frac{\partial \|y_k - y_\ell\|^2}{\partial y_i} = 0$ 

Hence, the first term can be represented as

$$\frac{\partial}{\partial y_i} \left( -\sum_{k \neq \ell} p_{k\ell} \log w_{k\ell} \right) = \sum_{j \neq i} p_{ij} \frac{1}{w_{ij}} \underbrace{\left( -w_{ij}^2 \cdot 2(y_i - y_j) \right)}_{\frac{\partial w_{ij}}{\partial y_i}} - \sum_{j \neq i} p_{ji} \frac{1}{w_{ji}} \underbrace{\left( -w_{ji}^2 \cdot 2(y_i - y_j) \right)}_{\frac{\partial w_{ji}}{\partial y_i}}$$

$$= \sum_{j \neq i} p_{ij} w_{ij} \cdot 2(y_i - y_j) + \sum_{j \neq i} p_{ji} w_{ji} \cdot 2(y_i - y_j)$$

$$= 4 \sum_{j \neq i} p_{ij} w_{ij} (y_i - y_j)$$

Now deal with the second term  $\frac{\partial}{\partial u_i}(\log Z)$ :

$$\frac{\partial \log Z}{\partial y_i} = \frac{1}{Z} \frac{\partial Z}{\partial y_i}$$
$$\frac{\partial Z}{\partial y_i} = \frac{\partial}{\partial y_i} \left( \sum_{k \neq \ell} w_{k\ell} \right)$$
$$= \sum_{k \neq \ell} \frac{\partial w_{k\ell}}{\partial y_i}$$

It is same as the first term, only when k = i or  $\ell = i$ , the value is not 0.

$$\frac{\partial Z}{\partial y_i} = \sum_{j \neq i} \frac{\partial w_{ij}}{\partial y_i} + \sum_{j \neq i} \frac{\partial w_{ji}}{\partial y_i}$$

$$= \sum_{j \neq i} -w_{ij}^2 \cdot 2(y_i - y_j) + \sum_{j \neq i} -w_{ji}^2 \cdot 2(y_i - y_j)$$

$$= -4 \sum_{j \neq i} w_{ij}^2(y_i - y_j)$$

$$\frac{\partial}{\partial y_i} (\log Z) = \frac{1}{Z} \left( -4 \sum_{j \neq i} w_{ij}^2(y_i - y_j) \right)$$

$$= -4 \sum_{j \neq i} \frac{w_{ij}}{Z} w_{ij}(y_i - y_j)$$

$$= -4 \sum_{j \neq i} q_{ij} w_{ij}(y_i - y_j)$$

Combined those two terms:

$$\frac{\partial C}{\partial y_i} = 4 \sum_{j \neq i} p_{ij} w_{ij} (y_i - y_j) - 4 \sum_{j \neq i} q_{ij} w_{ij} (y_i - y_j) 
= 4 \sum_{j \neq i} (p_{ij} - q_{ij}) w_{ij} (y_i - y_j) 
= 4 \sum_{j \neq i} (p_{ij} - q_{ij}) (y_i - y_j) (1 + ||y_i - y_j||^2)^{-1}$$

#### 4 EM for Mixture of Multivariate t-Distributions

1. Observe the log-likelihood function  $L(\theta) = \log p(Y|\theta)$ , let  $Z = \{z_i\}_{i=1}^N$  be the one-hot vector to show which component  $y_i$  belongs to. Then we have the relation  $L(\theta) = \log p(Y|\theta) = \log \left(\frac{p(Y,Z|\theta)}{p(Z|Y,\theta)}\right)$ .

$$\begin{split} L(\theta) &= E_{Z|Y,\theta^{(t)}}[\log p(Y|\theta)] \\ L(\theta) &= E_{Z|Y,\theta^{(t)}}\left[\log\left(\frac{p(Y,Z|\theta)}{p(Z|Y,\theta)}\right)\right] \\ L(\theta) &= E_{Z|Y,\theta^{(t)}}[\log p(Y,Z|\theta)] - E_{Z|Y,\theta^{(t)}}[\log p(Z|Y,\theta)] \end{split}$$

According to the question, we separate L to two parts Q, H

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = E_{Z|Y,\boldsymbol{\theta}^{(t)}}[\log p(Y,Z|\boldsymbol{\theta})]$$

$$H(\theta|\theta^{(t)}) = -E_{Z|Y,\theta^{(t)}}[\log p(Z|Y,\theta)]$$

We deal with Q first, we have

$$p(Y, Z|\theta) = \prod_{i=1}^{N} p(y_i, z_i|\theta) = \prod_{i=1}^{N} p(z_i|\theta) p(y_i|z_i, \theta)$$

Use  $z_{ik}$  (if  $y_i$  belongs to k - th component then  $z_{ik} = 1$  else 0):

$$p(y_i, z_i | \theta) = \prod_{k=1}^{K} [\pi_k \cdot tp(y_i; \mu_k, \Sigma_k, \nu_k)]^{z_{ik}}$$

So we can rewrite  $p(Y, Z|\theta)$ :

$$p(Y, Z|\theta) = \prod_{i=1}^{N} \prod_{k=1}^{K} [\pi_k \cdot tp(y_i; \mu_k, \Sigma_k, \nu_k)]^{z_{ik}}$$

$$\log p(Y, Z|\theta) = \sum_{i=1}^{N} \sum_{k=1}^{K} z_{ik} (\log \pi_k + \log t p(y_i; \mu_k, \Sigma_k, \nu_k))$$

Define  $\delta_{i,k}^{(t)} := E[z_{ik}|y_i, \theta^{(t)}] = P(z_i = k|y_i, \theta^{(t)})$  to be the posterior expected value of  $z_{ik}$ , then by Bayes' theorem

$$\delta_{i,k}^{(t)} = \frac{P(z_i = k | \theta^{(t)}) p(y_i | z_i = k, \theta^{(t)})}{\sum_{\ell=1}^K P(z_i = \ell | \theta^{(t)}) p(y_i | z_i = \ell, \theta^{(t)})}$$

$$= \frac{\pi_k^{(t)} t p(y_i; \mu_k^{(t)}, \sum_k^{(t)}, \nu_k^{(t)})}{\sum_{\ell=1}^K \pi_\ell^{(t)} t p(y_i; \mu_\ell^{(t)}, \sum_\ell^{(t)}, \nu_\ell^{(t)})}$$

$$Q(\theta | \theta^{(t)}) = E\left[\sum_{i=1}^N \sum_{k=1}^K z_{ik} (\log \pi_k + \log t p(y_i; \mu_k, \sum_k, \nu_k))\right]$$

$$= \sum_{i=1}^N \sum_{k=1}^K E[z_{ik} | y_i, \theta^{(t)}] (\log \pi_k + \log t p(y_i; \mu_k, \sum_k, \nu_k))$$

$$= \sum_{i=1}^N \sum_{k=1}^K \delta_{i,k}^{(t)} (\log \pi_k + \log t p(y_i; \mu_k, \sum_k, \nu_k))$$

Now deal with H

$$p(Z|Y,\theta) = \prod_{i=1}^{N} p(z_i|y_i,\theta) = \prod_{i=1}^{N} \prod_{k=1}^{K} [P(z_i = k|y_i,\theta)]^{z_{ik}}$$

$$\log p(Z|Y,\theta) = \sum_{i=1}^{N} \sum_{k=1}^{K} z_{ik} \log P(z_i = k|y_i, \theta)$$

where  $E[z_{ik}|y_i, \theta^{(t)}] = P(z_i = k|y_i, \theta^{(t)}) = \delta_{i,k}^{(t)}$ 

$$E[\log p(Z|Y,\theta)] = E\left[\sum_{i=1}^{N} \sum_{k=1}^{K} z_{ik} \log P(z_i = k|y_i, \theta)\right]$$

$$= \sum_{i=1}^{N} \sum_{k=1}^{K} E[z_{ik}|y_i, \theta^{(t)}] \log P(z_i = k|y_i, \theta)$$

$$= \sum_{i=1}^{N} \sum_{k=1}^{K} \delta_{i,k}^{(t)} \log P(z_i = k|y_i, \theta)$$

Hence, we get H

$$H(\theta|\theta^{(t)}) = -\sum_{i=1}^{N} \sum_{k=1}^{K} \delta_{i,k}^{(t)} \log \left( \frac{\pi_k t p(y_i; \mu_k, \Sigma_k, \nu_k)}{\sum_{\ell=1}^{K} \pi_\ell t p(y_i; \mu_\ell, \Sigma_\ell, \nu_\ell)} \right)$$

2. In this question, we are asked to find the posterior probability  $p(u_{i,k}|y_i, z_i = k)$ . From Bayes' theorem

$$p(u_{i,k}|y_i, z_i = k) \propto p(y_i|u_{i,k}, z_i = k) \cdot p(u_{i,k}|z_i = k)$$

(a) Likelihood: p(y|u, z = k) For given  $(u, y \sim N_p(\mu, \Sigma/u))$ , its PDF can be computed by

$$p(y|u) = \frac{1}{(2\pi)^{p/2} |\Sigma/u|^{1/2}} \exp\left(-\frac{1}{2}(y-\mu)^T (\Sigma/u)^{-1} (y-\mu)\right)$$

$$p(y|u) = \frac{|\Sigma|^{-1/2} u^{p/2}}{(2\pi)^{p/2}} \exp\left(-\frac{u}{2} (y - \mu)^T \Sigma^{-1} (y - \mu)\right)$$

Define Mahalanobis distance  $d = (y - \mu)^T \Sigma^{-1} (y - \mu)$ 

$$p(y|u) \propto u^{p/2} \exp\left(-\frac{d}{2}u\right)$$

(b) Prior probability: p(u|z=k) Given  $z=k, u \sim \text{Gamma}(\nu/2, \nu/2)$ , the PDF is:

$$p(u) = \frac{(\nu/2)^{\nu/2}}{\Gamma(\nu/2)} u^{\nu/2-1} \exp\left(-\frac{\nu}{2}u\right)$$

$$p(u) \propto u^{\nu/2-1} \exp\left(-\frac{\nu}{2}u\right)$$

(c) Posterior probability: p(u|y, z = k)

$$p(u|y) \propto \left[ u^{p/2} \exp\left(-\frac{d}{2}u\right) \right] \cdot \left[ u^{\nu/2-1} \exp\left(-\frac{\nu}{2}u\right) \right]$$
$$p(u|y) \propto u^{p/2+\nu/2-1} \cdot \exp\left(-\frac{d}{2}u - \frac{\nu}{2}u\right)$$
$$p(u|y) \propto u^{\frac{\nu+p}{2}-1} \cdot \exp\left(-\left[\frac{\nu+d}{2}\right]u\right)$$

From the relation we can find that u|y is a Gamma distribution with  $\alpha_{\text{new}} = \frac{\nu+p}{2}$ ,  $\beta_{\text{new}} = \frac{\nu+d}{2}$ Now put i, k, t back to the relation, we have

$$u_{i,k}|(y_i, z_i = k; \theta^{(t)}) \sim \text{Gamma}\left(\frac{\nu_k^{(t)} + p}{2}, \frac{\nu_k^{(t)} + d_{i,k}^{(t)}}{2}\right)$$

where 
$$d_{i,k}^{(t)} = (y_i - \mu_k^{(t)})^T (\Sigma_k^{(t)})^{-1} (y_i - \mu_k^{(t)})$$

3. We need to compute the moments of  $X \sim \text{Gamma}(\alpha, \beta) : E[X]$  and  $E[\log X]$ . The standard expected value E(X) of the Gamma distribution is  $E[X] = \frac{\alpha}{\beta}$ . And for the expected value  $E[\log X]$  can be calculated by

$$E[\log X] = \psi(\alpha) - \log(\beta)$$

with  $\psi(\alpha) = \frac{d}{d\alpha} \log \Gamma(\alpha)$ ,  $\alpha = \frac{\nu_k^{(t)} + p}{2}$ ,  $\beta = \frac{\nu_k^{(t)} + d_{i,k}^{(t)}}{2}$ 

So we can rewrite the moments  $w_{i,k}^{(t)} := E[u_{i,k}|y_i, z_i = k; \theta^{(t)}]$  and  $\ell_{i,k}^{(t)} := E[\log u_{i,k}|y_i, z_i = k; \theta^{(t)}]$ 

$$\begin{split} w_{i,k}^{(t)} &= \frac{\alpha}{\beta} \\ &= \frac{(\nu_k^{(t)} + p)/2}{(\nu_k^{(t)} + d_{i,k}^{(t)})/2} \\ &= \frac{\nu_k^{(t)} + p}{\nu_k^{(t)} + d_{i,k}^{(t)}} \end{split}$$

$$\ell_{i,k}^{(t)} = \psi(\alpha) - \log(\beta)$$

$$= \psi\left(\frac{\nu_k^{(t)} + p}{2}\right) - \log\left(\frac{\nu_k^{(t)} + d_{i,k}^{(t)}}{2}\right)$$

4. We use lagrange multiplier  $\lambda$  to find  $\pi_k^{(t+1)}$ 

$$\mathcal{L}(\pi, \lambda) = Q(\pi) + \lambda \left( 1 - \sum_{k=1}^{K} \pi_k \right) = \sum_{i=1}^{N} \sum_{k=1}^{K} \delta_{i,k}^{(t)} \log \pi_k + \lambda \left( 1 - \sum_{k=1}^{K} \pi_k \right)$$

Let  $N_k = \sum_{i=1}^N \delta_{i,k}^{(t)}$ 

$$\mathcal{L}(\pi, \lambda) = \sum_{k=1}^{K} N_k \log \pi_k + \lambda \left( 1 - \sum_{k=1}^{K} \pi_k \right)$$

Set its derivative to 0

$$\frac{\partial \mathcal{L}}{\partial \pi_k} = \frac{N_k}{\pi_k} - \lambda = 0 \implies \pi_k = \frac{N_k}{\lambda}$$

$$\sum_{k=1}^K \frac{N_k}{\lambda} = 1 \implies \frac{1}{\lambda} \sum_{k=1}^K N_k = 1$$

$$\sum_{k=1}^K N_k = \sum_{k=1}^K \sum_{i=1}^N \delta_{i,k}^{(t)} = \sum_{i=1}^N \sum_{k=1}^K \delta_{i,k}^{(t)} = \sum_{i=1}^N 1 = N$$

$$\pi_k^{(t+1)} = \frac{N_k}{N} = \frac{1}{N} \sum_{i=1}^N \delta_{i,k}^{(t)}$$

Then we set the partial derivative of  $\mu$  to 0 to find  $\mu_k^{(t+1)}$ 

$$Q(\mu_k) = \sum_{i=1}^{N} \delta_{i,k}^{(t)} \left( -\frac{w_{i,k}^{(t)}}{2} (y_i - \mu_k)^T \Sigma_k^{-1} (y_i - \mu_k) \right)$$

$$\frac{\partial Q(\mu_k)}{\partial \mu_k} = \sum_{i=1}^N \delta_{i,k}^{(t)} \left( -\frac{w_{i,k}^{(t)}}{2} \cdot 2\Sigma_k^{-1} (\mu_k - y_i) \right) = 0$$
$$\sum_{i=1}^N \delta_{i,k}^{(t)} w_{i,k}^{(t)} \Sigma_k^{-1} (y_i - \mu_k) = 0$$

Since  $\Sigma^{-1}$  is invertible, we can remove it from the equation

$$\sum_{i=1}^{N} \delta_{i,k}^{(t)} w_{i,k}^{(t)} (y_i - \mu_k) = 0$$

$$\sum_{i=1}^{N} \delta_{i,k}^{(t)} w_{i,k}^{(t)} y_i - \sum_{i=1}^{N} \delta_{i,k}^{(t)} w_{i,k}^{(t)} \mu_k = 0$$

$$\left(\sum_{i=1}^{N} \delta_{i,k}^{(t)} w_{i,k}^{(t)}\right) \mu_k = \sum_{i=1}^{N} \delta_{i,k}^{(t)} w_{i,k}^{(t)} y_i$$

$$\mu_k^{(t+1)} = \frac{\sum_{i=1}^{N} \delta_{i,k}^{(t)} w_{i,k}^{(t)} y_i}{\sum_{i=1}^{N} \delta_{i,k}^{(t)} w_{i,k}^{(t)}}$$

Last, we use the new  $\mu_k^{(t+1)}$  and  $S_k = \Sigma_k^{-1}$  to find  $\Sigma_k^{(t+1)}$ 

$$Q(S_k) = \sum_{i=1}^{N} \delta_{i,k}^{(t)} \left( -\frac{1}{2} \log |\Sigma_k| - \frac{w_{i,k}^{(t)}}{2} (y_i - \mu_k^{(t+1)})^T S_k (y_i - \mu_k^{(t+1)}) \right)$$

Note that  $\log |\Sigma_k| = -\log |\Sigma_k^{-1}| = -\log |S_k|$  and let  $N_k = \sum_{i=1}^N \delta_{i,k}^{(t)}$  again, so we can rewrite  $Q(S_k)$ 

$$Q(S_k) = \frac{N_k}{2} \log |S_k| - \sum_{i=1}^N \frac{\delta_{i,k}^{(t)} w_{i,k}^{(t)}}{2} (y_i - \mu_k^{(t+1)})^T S_k (y_i - \mu_k^{(t+1)})$$

For a scalar a, we have Tr(a) = a, so we can write  $\frac{\delta_{i,k}^{(t)}w_{i,k}^{(t)}}{2}(y_i - \mu_k^{(t+1)})^T S_k(y_i - \mu_k^{(t+1)}) = \text{its trace}$ , and for the trace, we have the property  $\text{Tr}(u^T S u) = \text{Tr}(S u u^T)$ .

$$Q(S_k) = \frac{N_k}{2} \log |S_k| - \frac{1}{2} \operatorname{Tr} \left( S_k \cdot \sum_{i=1}^N \delta_{i,k}^{(t)} w_{i,k}^{(t)} (y_i - \mu_k^{(t+1)}) (y_i - \mu_k^{(t+1)})^T \right)$$

Let  $A_k = \sum_{i=1}^N \delta_{i,k}^{(t)} w_{i,k}^{(t)} (y_i - \mu_k^{(t+1)}) (y_i - \mu_k^{(t+1)})^T$ 

$$Q(S_{-}k) = \frac{N_k}{2} \log |S_k| - \frac{1}{2} \operatorname{Tr}(S_k A_k)$$

Set the derivative to 0

$$\frac{\partial Q(S_k)}{\partial S_k} = \frac{N_k}{2} (S_k^{-1})^T - \frac{1}{2} A_k^T = 0$$

$$\frac{N_k}{2} S_k^{-1} - \frac{1}{2} A_k = 0 \implies N_k S_k^{-1} = A_k \implies S_k^{-1} = \frac{A_k}{N_k} = \Sigma_k$$

$$\Sigma_k^{(t+1)} = \frac{A_k}{N_k} = \frac{\sum_{i=1}^N \delta_{i,k}^{(t)} w_{i,k}^{(t)} (y_i - \mu_k^{(t+1)}) (y_i - \mu_k^{(t+1)})^T}{\sum_{i=1}^N \delta_{i,k}^{(t)}}$$

5. Write Q with the parameter  $\nu_k$ 

$$Q(\nu_k) = \sum_{i=1}^N \delta_{i,k}^{(t)} \left( \frac{\nu_k}{2} \log(\frac{\nu_k}{2}) - \log \Gamma(\frac{\nu_k}{2}) + (\frac{\nu_k}{2} - 1) \ell_{i,k}^{(t)} - \frac{\nu_k}{2} w_{i,k}^{(t)} + \frac{p}{2} \ell_{i,k}^{(t)} \right)$$

$$Q(\nu_k) = N_k \left( \frac{\nu_k}{2} \log(\frac{\nu_k}{2}) - \log \Gamma(\frac{\nu_k}{2}) \right) + \frac{\nu_k}{2} \sum_{i=1}^N \delta_{i,k}^{(t)} (\ell_{i,k}^{(t)} - w_{i,k}^{(t)}) + \text{const}$$

$$\frac{\partial}{\partial \nu_k} \left( \frac{\nu_k}{2} \log(\frac{\nu_k}{2}) \right) = \frac{\partial}{\partial (\nu_k/2)} \left( \frac{\nu_k}{2} \log(\frac{\nu_k}{2}) \right) \cdot \frac{\partial (\nu_k/2)}{\partial \nu_k} = \left[ \log(\frac{\nu_k}{2}) + 1 \right] \cdot \frac{1}{2}$$

$$\frac{\partial}{\partial \nu_k} \left( \log \Gamma(\frac{\nu_k}{2}) \right) = \psi(\frac{\nu_k}{2}) \cdot \frac{1}{2}$$

Now compute the derivative and set it to 0

$$\frac{\partial Q(\nu_k)}{\partial \nu_k} = N_k \left[ \frac{1}{2} \left( \log(\frac{\nu_k}{2}) + 1 \right) - \frac{1}{2} \psi(\frac{\nu_k}{2}) \right] + \frac{1}{2} \sum_{i=1}^N \delta_{i,k}^{(t)}(\ell_{i,k}^{(t)} - w_{i,k}^{(t)}) = 0$$

$$N_k \left( \log(\frac{\nu_k}{2}) + 1 - \psi(\frac{\nu_k}{2}) \right) + \sum_{i=1}^N \delta_{i,k}^{(t)}(\ell_{i,k}^{(t)} - w_{i,k}^{(t)}) = 0$$

$$\log(\frac{\nu_k}{2}) + 1 - \psi(\frac{\nu_k}{2}) + \frac{1}{N_k} \sum_{i=1}^N \delta_{i,k}^{(t)}(\ell_{i,k}^{(t)} - w_{i,k}^{(t)}) = 0$$

$$\log(\frac{\nu_k}{2}) - \psi(\frac{\nu_k}{2}) + 1 + \frac{1}{\sum_{i=1}^N \delta_{i,k}^{(t)}} \sum_{i=1}^N \delta_{i,k}^{(t)}(\ell_{i,k}^{(t)} - w_{i,k}^{(t)}) = 0$$

6. From the result we get from last question, let  $f(\nu_k) = \log(\frac{\nu_k}{2}) - \psi(\frac{\nu_k}{2}) + 1 + C_k$  with  $C_k = \frac{1}{\sum_{i=1}^N \delta_{i,k}^{(t)}} \sum_{i=1}^N \delta_{i,k}^{(t)} (\ell_{i,k}^{(t)} - w_{i,k}^{(t)})$ . Find the derivative of f

$$f'(\nu_k) = \frac{d}{d\nu_k} \left( \log(\frac{\nu_k}{2}) - \psi(\frac{\nu_k}{2}) + 1 + C_k \right)$$
$$= \frac{1}{\nu_k} - \frac{1}{2} \psi'(\frac{\nu_k}{2})$$

Then we find the one step update

$$\nu_k^{\text{new}} \leftarrow \nu_k - \frac{\log(\frac{\nu_k}{2}) - \psi(\frac{\nu_k}{2}) + 1 + C_k}{\frac{1}{\nu_k} - \frac{1}{2}\psi'(\frac{\nu_k}{2})}$$

## 5 Gradient Descent Convergence

1. Observe the log-likelihood function  $L(\theta) = \log \prod_{i=1}^N p(x_i|y_i,\theta) = \sum_{i=1}^N \log p(x_i|y_i,\theta)$ . Consider two set  $L = \{i|y_i \neq 0\}$  and  $U = \{i|y_i = 0\}$  to represent the labeled and unlabeled data. Then  $L(\theta)$  can be rewritten as

$$L_{obs}(\theta) = \sum_{i \in L} \log p(x_i|y_i, \theta) + \sum_{i \in U} \log p(x_i|y_i = 0, \theta)$$
$$= \sum_{i:y_i \neq 0} \log \mathcal{N}(x_i|\mu_{y_i}, \Sigma_{y_i}) + \sum_{i:y_i = 0} \log \sum_{k=1}^{N} \pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)$$

Let  $z_i$  be the one-hot label for unlabeled  $x_i$ , that is,  $z_{i,k} = 1$  if  $x_i$  is from the component k.

$$L_c(\theta) = \sum_{i \in L} \log p(x_i|y_i, \theta) + \sum_{i \in U} \log p(x_i, z_i|\theta)$$

$$= \sum_{i \in L} \log p(x_i|y_i, \theta) + \sum_{i \in U} \log \prod_{k=1}^{K} [\pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)]^{z_{i,k}}$$

$$= \sum_{i \in L} \log p(x_i|y_i, \theta) + \sum_{i \in U} \sum_{k=1}^{K} z_{i,k} (\log \pi_k + \log \mathcal{N}(x_i|\mu_k, \Sigma_k))$$

Compute Q

$$Q(\theta|\theta^{(t)}) = E_{Z|D_{obs},\theta^{(t)}}[L_c(\theta)]$$

$$= \sum_{i \in L} \log p(x_i|y_i,\theta) + \sum_{i \in U} \sum_{k=1}^K E[z_{i,k}|x_i,\theta^{(t)}](\log \pi_k + \log \mathcal{N}(x_i|\mu_k,\Sigma_k))$$

Define  $\delta_{i,k}^{(t)} = E[z_{i,k}|x_i,\theta^{(t)}]$ , then we have

$$Q(\theta|\theta^{(t)}) = \sum_{i \in L} \log p(x_i|y_i, \theta) + \sum_{i \in U} \sum_{k=1}^K \delta_{i,k}^{(t)} (\log \pi_k + \log \mathcal{N}(x_i|\mu_k, \Sigma_k))$$

First we use lagrange multiplier  $\lambda$  to find  $\pi_k$ 

$$Q_{\pi}(\pi) = \sum_{i \in U} \sum_{k=1}^{K} \delta_{i,k}^{(t)} \log \pi_{k}$$

$$\mathcal{L}(\pi, \lambda) = \sum_{k=1}^{K} \sum_{i \in U} \delta_{i,k}^{(t)} \log \pi_{k} + \lambda \left(\sum_{k=1}^{N} \pi_{k} - 1\right)$$

$$\frac{\partial \mathcal{L}}{\partial \pi_{k}} = \frac{\sum_{i \in U} \delta_{i,k}^{(t)}}{\pi_{k}} + \lambda = 0 \implies \pi_{k} = -\frac{\sum_{i \in U} \delta_{i,k}^{(t)}}{\lambda}$$

$$\sum_{k=1}^{N} \pi_{k} = 1 \implies \sum_{k=1}^{N} -\frac{\sum_{i \in U} \delta_{i,k}^{(t)}}{\lambda} = 1$$

Since  $\sum_{k=1}^{K} \delta_{i,k}^{(t)} = 1$  we have

$$-\frac{\sum_{i \in U} \sum_{k=1}^{N} \delta_{i,k}^{(t)}}{\lambda} = 1 \implies \lambda = -\sum_{i \in U} 1 = -\sum_{i:y_i=0} 1$$
$$\pi_k^{(t+1)} = \frac{\sum_{i \in U} \delta_{i,k}^{(t)}}{\sum_{i:y_i=0} 1}$$

Then calculate  $\mu$ 

$$Q_k(\mu_k, \Sigma_k) = \sum_{i:u_i=k} \log \mathcal{N}(x_i | \mu_k, \Sigma_k) + \sum_{i:u_i=0} \sum_{k=1}^K \delta_{i,k}^{(t)} \log \mathcal{N}(x_i | \mu_k, \Sigma_k)$$

We only need the term with  $\mu$ 

$$L(\mu_k) = \sum_{i:y_i=k} (x_i - \mu_k)^T \Sigma_k^{-1} (x_i - \mu_k) + \sum_{i:y_i=0} \sum_{k=1}^K \delta_{i,k}^{(t)} (x_i - \mu_k)^T \Sigma_k^{-1} (x_i - \mu_k)$$

$$\nabla_{\mu_k} L = \sum_{i:y_i=k} -2\Sigma_k^{-1} (x_i - \mu_k) + \sum_{i:y_i=0} -2\delta_{i,k}^{(t)} \Sigma_k^{-1} (x_i - \mu_k) = 0$$

Since  $\Sigma$  is invertible, we have

$$\sum_{i:y_i=k} (x_i - \mu_k) + \sum_{i:y_i=0} \delta_{i,k}^{(t)}(x_i - \mu_k) = 0$$

$$\sum_{i:y_i=k} x_i + \sum_{i:y_i=0} \delta_{i,k}^{(t)} x_i = \left(\sum_{i:y_i=k} 1 + \sum_{i:y_i=0} \delta_{i,k}^{(t)}\right) \mu_k$$

$$\mu = \frac{\sum_{i:y_i=k} x_i + \sum_{i:y_i=0}}{\sum_{i:y_i=k} 1 + \sum_{i:y_i=0} \delta_{i,k}^{(t)}} = \frac{\sum_{i:y_i=k} x_i + \sum_{i:y_i=0}}{N_k + \sum_{i:y_i=0} \delta_{i,k}^{(t)}}$$

Last we can use the result from the last problem

$$\Sigma_k^{(t+1)} == \frac{\sum_{i=1}^N \text{weight}_i (y_i - \mu_k^{(t+1)}) (y_i - \mu_k^{(t+1)})^T}{\sum_{i=1}^N \text{weight}_i}$$

In this equation, weight<sub>i</sub> = 1 if  $y_i = k$  else  $\delta_{i,k}^{(t)}$ , so we have

$$\Sigma_k^{(t+1)} = \frac{\sum_{i:y_i=k} (y_i - \mu_k^{(t+1)}) (y_i - \mu_k^{(t+1)})^T + \sum_{i:y_i=0} \delta_{i,k}^{(t)} (y_i - \mu_k^{(t+1)}) (y_i - \mu_k^{(t+1)})^T}{N_k + \sum_{i:y_i=0} \delta_{i,k}^{(t)}}$$

2. Compute  $\delta_{i,k}^{(t)}$ 

$$\delta_{i,k}^{(t)} = E[z_{i,k}|x_i, y_i = 0, \theta^{(t)}] = P(z_{i,k} = 1|x_i, y_i = 0, \theta^{(t)})$$

$$P(z_{i,k} = 1|x_i, y_i = 0, \theta^{(t)}) = \frac{P(z_{i,k} = 1|y_i = 0, \theta^{(t)}) \cdot P(x_i|z_{i,k} = 1, y_i = 0, \theta^{(t)})}{P(x_i|y_i = 0, \theta^{(t)})}$$

We have

$$P(z_{i,k} = 1 | y_i = 0, \theta^{(t)}) = \pi_k^t$$

$$P(x_i | z_{i,k} = 1, y_i = 0, \theta^{(t)}) = \mathcal{N}(x_i; \mu_k, \Sigma_k)$$

$$P(x_i | y_i = 0, \theta^{(t)}) = \sum_{j=1}^K P(z_{i,j} = 1 | y_i = 0, \theta^{(t)}) \cdot P(x_i | z_{i,j} = 1, y_i = 0, \theta^{(t)}) = \sum_{j=1}^K \pi_j^{(t)} \mathcal{N}(x_i; \mu_j, \Sigma_j)$$

Hence, we get  $\delta_{i,k}^{(t)}$ 

$$\delta_{i,k}^{(t)} = \frac{\pi_k^t \mathcal{N}(x_i; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j^t \mathcal{N}(x_i; \mu_j, \Sigma_j)}$$