1. A Simple Neural Network

记第二层的输出为$g^{(i)}$

(a)由$w_{1,2}^{[1]}$的定义可知，我们需要先求出关于h_2的偏导数。

注意到我们有

$$o^{(i)} = f(w_0^{[2]} + w_1^{[2]} h_1^{(i)} + w_2^{[2]} h_2^{(i)} + w_3^{[2]} h_3^{(i)})$$

其中f为sigmoid函数，那么先计算l关于$h_2^{(i)}$的偏导数可得

$$\begin{aligned}\frac{\partial l}{\partial h_2^{(i)}} &= \frac{\partial l}{\partial o^{(i)}} \frac{\partial o^{(i)}}{\partial h_2^{(i)}} \\ &= \frac{1}{m}(o^{(i)} - y^{(i)}) o^{(i)} (1 - o^{(i)}) w_2^{[2]}\end{aligned}$$

接着求$h_2^{(i)}$关于$w_{1,2}^{[1]}$的偏导数，注意到我们有

$$h_2^{(i)} = f(w_{0,2}^{[1]} + w_{1,2}^{[1]} x_1^{(i)} + w_{2,2}^{[1]} x_2^{(i)})$$

其中f为sigmoid函数，那么

$$\frac{\partial h_2^{(i)}}{\partial w_{1,2}^{[1]}} = h_2^{(i)} (1 - h_2^{(i)}) x_1^{(i)}$$

$$\begin{aligned}\frac{\partial l}{\partial w_{1,2}^{[1]}} &= \sum_{i=1}^{m} \frac{\partial l}{\partial h_2^{(i)}} \frac{\partial h_2^{(i)}}{\partial w_{1,2}^{[1]}} \\ &= \frac{1}{m} \sum_{i=1}^{m} (o^{(i)} - y^{(i)}) o^{(i)} (1 - o^{(i)}) w_2^{[2]} h_2^{(i)} (1 - h_2^{(i)}) x_1^{(i)}\end{aligned}$$

(b)根据提示，中间层每个神经元应该对应于三角形区域的一条边，所以第一层的权重可以取

$$w^{[1]} = \begin{bmatrix} w_{0,1}^{[1]} & w_{1,1}^{[1]} & w_{2,1}^{[1]} \\ w_{0,2}^{[1]} & w_{1,2}^{[1]} & w_{2,2}^{[1]} \\ w_{0,3}^{[1]} & w_{1,3}^{[1]} & w_{2,3}^{[1]} \end{bmatrix} = \begin{bmatrix} -0.4 & 1 & 0 \\ -0.4 & 0 & 1 \\ 4 & -1 & -1 \end{bmatrix}$$

当点在三角形区域内时，结合激活函数可得输出结果为

$$\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

注意只有此时神经元的输出结果为1，其余7中情形输出结果都为0，所以第二层的权重可以取

$$
w^{[2]}=\begin{bmatrix} w_0^{[2]} & w_1^{[2]} & w_2^{[2]} & w_3^{[2]} \end{bmatrix}=\begin{bmatrix} -3 & 1 & 1 & 1 \end{bmatrix}
$$

(c)不存在，因为当激活函数为$f(x)=x$时，产生的边界为直线，但是图像中边界为三角形，所以不可能使得损失为0
。

2. EM for MAP estimation

对数似然函数为

$$
l=\log p(\theta)+\sum_{i=1}^{m}\log p(x^{(i)}|\theta)
$$

对每个i，令Q_i是关于z的某个分布（$\sum_z Q_i(z)=1, Q_i(z)\ge 0$），考虑下式

$$
\begin{aligned}
\log p(\theta)+\sum_{i=1}^{m}\log p(x^{(i)}|\theta) &= \log p(\theta)+\sum_{i}^{m}\log\sum_{z^{(i)}}p(x^{(i)},z^{(i)}|\theta) & (1)\\
&= \log p(\theta)+\sum_{i}^{m}\log\sum_{z^{(i)}}Q_i(z^{(i)})\frac{p(x^{(i)},z^{(i)}|\theta)}{Q_i(z^{(i)})} & (2)\\
&\ge \log p(\theta)+\sum_{i}^{m}\sum_{z^{(i)}}Q_i(z^{(i)})\log\frac{p(x^{(i)},z^{(i)}|\theta)}{Q_i(z^{(i)})} & (3)
\end{aligned}
$$

等号成立当且仅当对某个不依赖的$z^{(i)}$的常数c，下式成立

$$
\frac{p(x^{(i)},z^{(i)}|\theta)}{Q_i(z^{(i)})}=c
$$

结合$\sum_i Q_i(z^{(i)})=1$，我们有

$$
\begin{aligned}
Q_i(z^{(i)}) &= \frac{p(x^{(i)},z^{(i)}|\theta)}{\sum_z p(x^{(i)},z|\theta)}\\
&= \frac{p(x^{(i)},z^{(i)}|\theta)}{p(x^{(i)}|\theta)}\\
&= p(z^{(i)}|x^{(i)},\theta)
\end{aligned}
$$

所以E步骤我们选择$Q_i(z^{(i)})=p(z^{(i)}|x^{(i)},\theta)$，那么M步骤中，我们需要选择$\theta$为

$$
\theta:=\arg\max_\theta\Big(\log p(\theta)+\sum_{i}^{m}\sum_{z^{(i)}}Q_i(z^{(i)})\log\frac{p(x^{(i)},z^{(i)}|\theta)}{Q_i(z^{(i)})}\Big)
$$

最后证明上述算法会让$\prod_{i=1}^m p(x^{(i)}|\theta)p(\theta)$单调递增。假设$\theta^{(t)}$和$\theta^{(t+1)}$是两次成功迭代得到的参数那么

$$
\begin{aligned}
l(\theta^{(t+1)}) &\geq \log p(\theta^{(t+1)}) + \sum_{i}^{m}\sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}|\theta^{(t+1)})}{Q_i(z^{(i)})} && (4)\\
&\geq \ \log p(\theta^{(t)}) + \sum_{i}^{m}\sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}|\theta^{(t)})}{Q_i(z^{(i)})} && (5)\\
&= l(\theta^{(t)}) && (6)
\end{aligned}
$$

第一个不等号成立是因为如下不等式对任意Q_i和θ都成立

$$
l(\theta) \geq \log p(\theta) + \sum_{i}^{m}\sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}|\theta)}{Q_i(z^{(i)})}
$$

特别地，上式对$Q_i = Q_i^{(t)}, \theta = \theta^{(t+1)}$成立。第二个不等号成立是因为我们选择$\theta^{(t+1)}$为

$$
\arg\max_{\theta}\Big(\log p(\theta) + \sum_{i}^{m}\sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}|\theta)}{Q_i(z^{(i)})}\Big)
$$

因此这个式子在$\theta^{(t+1)}$的取值必然大于等于在$\theta^{(t)}$的取值。最后一个等号成立是在选择$Q_i^{(t)}$时我们就是要保证不等号取等号。

3. EM application

(a)

(i)因为$y^{(pr)}, z^{(pr)}, \epsilon^{(pr)}$服从正态分布且相互独立，所以$(y^{(pr)}, z^{(pr)}, \epsilon^{(pr)})^T$服从多元正态分布，因为

$$
\left[\begin{array}{c} y^{(pr)} \\ z^{(pr)} \\ x^{(pr)} \end{array}\right] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \left[\begin{array}{c} y^{(pr)} \\ z^{(pr)} \\ \epsilon^{(pr)} \end{array}\right]
$$

所以$(y^{(pr)}, z^{(pr)}, x^{(pr)})^T$服从多元正态分布，因此只要分别计算期望和协方差矩阵即可。

首先求期望：

$$
\begin{gathered}
\mathbb{E}[y^{(pr)}] = \mu_p \\
\mathbb{E}[z^{(pr)}] = \nu_r \\
\mathbb{E}[x^{(pr)}] = \mathbb{E}[y^{(pr)}] + \mathbb{E}[z^{(pr)}] + \mathbb{E}[\epsilon^{(pr)}] = \mu_p + \nu_r
\end{gathered}
$$

接着求协方差矩阵，首先求方差：

$$
\begin{gathered}
\mathrm{Var}[y^{(pr)}] = \sigma_p^2 \\
\mathrm{Var}[z^{(pr)}] = \tau_r^2 \\
\mathrm{Var}(x^{(pr)}) = \mathrm{Var}[y^{(pr)}] + \mathrm{Var}[z^{(pr)}] + \mathrm{Var}[\epsilon^{(pr)}] = \sigma_p^2 + \tau_r^2 + \sigma^2
\end{gathered}
$$

最后求协方差：

$$
\begin{aligned}
\mathrm{Cov}(x^{(pr)}, y^{(pr)}) &= \mathrm{Cov}(y^{(pr)} + z^{(pr)} + \epsilon^{(pr)}, y^{(pr)}) \\
&= \mathrm{Cov}(y^{(pr)}, y^{(pr)}) \\
&= \sigma_p^2 \\
\mathrm{Cov}(x^{(pr)}, z^{(pr)}) &= \mathrm{Cov}(y^{(pr)} + z^{(pr)} + \epsilon^{(pr)}, z^{(pr)}) \\
&= \mathrm{Cov}(z^{(pr)}, z^{(pr)}) \\
&= \tau_r^2 \\
\mathrm{Cov}(y^{(pr)}, z^{(pr)}) &= 0
\end{aligned}
$$

所以期望方差分别为

$$
\mu = \begin{bmatrix} \mu_p \\ \nu_r \\ \mu_p + \nu_r \end{bmatrix}, \Sigma = \begin{bmatrix} \sigma_p^2 & 0 & \sigma_p^2 \\ 0 & \tau_r^2 & \tau_r^2 \\ \sigma_p^2 & \tau_r^2 & \sigma_p^2 + \tau_r^2 + \sigma^2 \end{bmatrix}
$$

(ii)在求解该问题之前，介绍如下结论：

假设我们有一个向量值随机变量

$$
x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix},
$$

其中$x_1 \in \mathbb{R}^r, x_2 \in \mathbb{R}^s$，因此$x \in \mathbb{R}^{r+s}$。假设$x \sim \mathcal{N}(\mu, \Sigma)$，其中

$$
\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}
$$

其中，$\mu_1 \in \mathbb{R}^r$，$\mu_2 \in \mathbb{R}^s$，$\Sigma_{11} = \mathbb{R}^{r\times r}$，$\Sigma_{12} \in \mathbb{R}^{r\times s}$，以此类推。注意到因为协方差矩阵对称，所以$\Sigma_{12} = \Sigma_{21}^T$。

对上述随机变量，我们有

$$
\begin{gathered}
x_1 | x_2 \sim \mathcal{N}(\mu_{1|2}, \Sigma_{1|2}) \\
\text{其中} \, \mu_{1|2} = \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \\
\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}
\end{gathered}
$$

对于此题，我们有

$$
\begin{gathered}
\mu_1 = \begin{bmatrix} \mu_p \\ \nu_r \end{bmatrix}, \mu_2 = [\, \mu_p + \nu_r \,] \\
\Sigma_{11} = \begin{bmatrix} \sigma_p^2 & 0 \\ 0 & \tau_r^2 \end{bmatrix}, \Sigma_{12} = \begin{bmatrix} \sigma_p^2 \\ \tau_r^2 \end{bmatrix}, \Sigma_{22} = [\, \sigma_p^2 + \tau_r^2 + \sigma^2 \,]
\end{gathered}
$$

所以

$$
y^{(pr)}, z^{(pr)} | x^{(pr)} \sim \mathcal{N}(\mu_{1|2}, \Sigma_{1|2})
$$

其中

$$
\begin{aligned}
\mu_{1|2} &= \begin{bmatrix} \mu_p \\ \nu_r \end{bmatrix} + \begin{bmatrix} \sigma_p^2 \\ \tau_r^2 \end{bmatrix} (\sigma_p^2 + \tau_r^2 + \sigma^2)^{-1} (x^{(pr)} - \mu_p - \nu_r) \\
&= \begin{bmatrix} \mu_p + \frac{\sigma_p^2}{\sigma_p^2+\tau_r^2+\sigma^2} (x^{(pr)} - \mu_p - \nu_r) \\ \nu_r + \frac{\tau_r^2}{\sigma_p^2+\tau_r^2+\sigma^2} (x^{(pr)} - \mu_p - \nu_r) \end{bmatrix} \\
&\triangleq \begin{bmatrix} (\mu_{pr})_y \\ (\mu_{pr})_z \end{bmatrix} \\
\Sigma_{1|2} &= \begin{bmatrix} \sigma_p^2 & 0 \\ 0 & \tau_r^2 \end{bmatrix} - \begin{bmatrix} \sigma_p^2 \\ \tau_r^2 \end{bmatrix} (\sigma_p^2 + \tau_r^2 + \sigma^2)^{-1} \begin{bmatrix} \sigma_p^2 & \tau_r^2 \end{bmatrix} \\
&= \frac{1}{\sigma_p^2 + \tau_r^2 + \sigma^2} \begin{bmatrix} \sigma_p^2(\sigma_p^2 + \tau_r^2 + \sigma^2) - \sigma_p^4 & -\sigma_p^2\tau_r^2 \\ -\sigma_p^2\tau_r^2 & \tau_r^2(\sigma_p^2 + \tau_r^2 + \sigma^2) - \tau_r^4 \end{bmatrix} \\
&= \frac{1}{\sigma_p^2 + \tau_r^2 + \sigma^2} \begin{bmatrix} \sigma_p^2(\tau_r^2 + \sigma^2) & -\sigma_p^2\tau_r^2 \\ -\sigma_p^2\tau_r^2 & \tau_r^2(\sigma_p^2 + \sigma^2) \end{bmatrix} \\
&\triangleq \begin{bmatrix} (\Sigma_{pr})_{yy} & (\Sigma_{pr})_{yz} \\ (\Sigma_{pr})_{yz} & (\Sigma_{pr})_{zz} \end{bmatrix}
\end{aligned}
$$

因此

$$
Q_{pr}(y^{(pr)}, z^{(pr)}) = \frac{1}{2\pi|\Sigma_{1|2}|^{\frac{1}{2}}} \exp\Big(- \frac{1}{2}\Big(\begin{bmatrix} y^{(pr)} \\ z^{(pr)} \end{bmatrix} - \mu_{1|2}\Big)^T \Sigma_{1|2}^{-1} \Big(\begin{bmatrix} y^{(pr)} \\ z^{(pr)} \end{bmatrix} - \mu_{1|2}\Big)\Big)
$$

为了后续计算，这里再计算如下几个量：

$$
\begin{aligned}
\mathbb{E}_{(y^{(pr)}, z^{(pr)}) \sim Q_{pr}}[y^{(pr)}] &= (\mu_{pr})_y & (1) \\
\mathbb{E}_{(y^{(pr)}, z^{(pr)}) \sim Q_{pr}}[z^{(pr)}] &= (\mu_{pr})_z & (2) \\
\mathbb{E}_{(y^{(pr)}, z^{(pr)}) \sim Q_{pr}}[(y^{(pr)})^2] &= (\Sigma_{pr})_{yy} + (\mu_{pr})_y^2 & (3) \\
\mathbb{E}_{(y^{(pr)}, z^{(pr)}) \sim Q_{pr}}[(z^{(pr)})^2] &= (\Sigma_{pr})_{zz} + (\mu_{pr})_z^2 & (4)
\end{aligned}
$$

(b)接下来我们需要最大化下式

$$
\sum_{p=1}^P \sum_{r=1}^R \int_{(y^{(pr)}, z^{(pr)})} Q_{pr}(y^{(pr)}, z^{(pr)}) \log \frac{p(y^{(pr)}, z^{(pr)}, x^{(pr)})}{Q_{pr}(y^{(pr)}, z^{(pr)})} dy^{(pr)} dz^{(pr)}
$$

注意到在迭代过程中我们视$Q_{pr}(y^{(pr)}, z^{(pr)})$为常数，因此我们需要最大化

$$
\sum_{p=1}^P \sum_{r=1}^R \int_{(y^{(pr)}, z^{(pr)})} Q_{pr}(y^{(pr)}, z^{(pr)}) \log p(y^{(pr)}, z^{(pr)}, x^{(pr)}) dy^{(pr)} dz^{(pr)}
$$

上式可以记为

$$
\sum_{p=1}^P \sum_{r=1}^R \mathbb{E}_{(y^{(pr)}, z^{(pr)}) \sim Q_{pr}} \Big[\log p(y^{(pr)}, z^{(pr)}, x^{(pr)}) \Big]
$$

利用题目中的条件化简可得

$$
\begin{aligned}
&\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[\log p(y^{(pr)},z^{(pr)},x^{(pr)})\Big]\\
&=\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[\log\Big(p(x^{(pr)}|y^{(pr)},z^{(pr)})p(y^{(pr)})p(z^{(pr)})\Big)\Big]\\
&=\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[\log\Big(\frac{1}{\sqrt{2\pi}\sigma}\exp\Big(-\frac{1}{2\sigma^2}(x^{(pr)}-y^{(pr)}-z^{(pr)})^2\Big)\times\frac{1}{\sqrt{2\pi}\sigma_p}\exp\Big(-\frac{1}{2\sigma_p^2}(y^{(pr)}-\mu_p)^2\Big)\times\frac{1}{\sqrt{2\pi}\tau_r}\exp\Big(-\frac{1}{2\tau_r^2}(z^{(pr)}-\nu_r)^2\Big)\Big)\Big]\\
&=\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[-\frac{3}{2}\log(2\pi)-\frac{1}{2}\log\sigma^2-\frac{1}{2}\log\sigma_p^2-\frac{1}{2}\log\tau_r^2-\frac{1}{2\sigma^2}(x^{(pr)}-y^{(pr)}-z^{(pr)})^2-\frac{1}{2\sigma_p^2}(y^{(pr)}-\mu_p)^2-\frac{1}{2\tau_r^2}(z^{(pr)}-\nu_r)^2\Big]
\end{aligned}
$$

将和参数无关的项丢弃，我们需要最大化：

$$
\begin{aligned}
&\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[-\frac{1}{2}\log\sigma_p^2-\frac{1}{2}\log\tau_r^2-\frac{1}{2\sigma_p^2}(y^{(pr)}-\mu_p)^2-\frac{1}{2\tau_r^2}(z^{(pr)}-\nu_r)^2\Big]\\
&=\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[-\frac{1}{2}\log\sigma_p^2-\frac{1}{2}\log\tau_r^2-\frac{1}{2\sigma_p^2}(y^{(pr)}-\mu_p)^2-\frac{1}{2\tau_r^2}(z^{(pr)}-\nu_r)^2\Big]\\
&=\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[-\frac{1}{2}\log\sigma_p^2-\frac{1}{2}\log\tau_r^2-\frac{1}{2\sigma_p^2}\big((y^{(pr)})^2-2y^{(pr)}\mu_p+\mu_p^2\big)-\frac{1}{2\tau_r^2}\big((z^{(pr)})^2-2z^{(pr)}\nu_r+\nu_r^2\big)\Big]
\end{aligned}
$$

代入(1)(2)(3)(4)，得到：

$$
\begin{aligned}
L&=\sum_{p=1}^{P}\sum_{r=1}^{R}\mathbb{E}_{(y^{(pr)},z^{(pr)})\sim Q_{pr}}\Big[-\frac{1}{2}\log\sigma_p^2-\frac{1}{2}\log\tau_r^2-\frac{1}{2\sigma_p^2}\big((y^{(pr)})^2-2y^{(pr)}\mu_p+\mu_p^2\big)-\frac{1}{2\tau_r^2}\big((z^{(pr)})^2-2z^{(pr)}\nu_r+\nu_r^2\big)\Big]\\
&=\sum_{p=1}^{P}\sum_{r=1}^{R}\Big[-\frac{1}{2}\log\sigma_p^2-\frac{1}{2}\log\tau_r^2-\frac{1}{2\sigma_p^2}\big((\Sigma_{pr})_{yy}^2+(\mu_{pr})_y^2-2(\mu_{pr})_y\mu_p+\mu_p^2\big)-\frac{1}{2\tau_r^2}\big((\Sigma_{pr})_{zz}^2+(\mu_{pr})_z^2-2(\mu_{pr})_z\nu_r+\nu_r^2\big)\Big]
\end{aligned}
$$

所以

$$
\begin{aligned}
\nabla_{\mu_p} L &= \sum_{r=1}^{R}\Big[-\frac{1}{2\sigma_p^2}\big(-2(\mu_{pr})_y + 2\mu_p\big)\Big] \\
&= \frac{R}{\sigma_p^2}\sum_{r=1}^{R}\Big[(\mu_{pr})_y - \mu_p\Big] \\
&= \frac{R}{\sigma_p^2}\Big(\sum_{r=1}^{R}(\mu_{pr})_y - R\mu_p\Big) \\
\nabla_{\nu_r} L &= \sum_{p=1}^{P}\Big[-\frac{1}{2\tau_r^2}\big(-2(\mu_{pr})_z + 2\nu_r\big)\Big] \\
&= \frac{P}{\tau_r^2}\sum_{p=1}^{P}\Big[(\mu_{pr})_z - \nu_r\Big] \\
&= \frac{P}{\tau_r^2}\Big(\sum_{p=1}^{P}(\mu_{pr})_z - P\nu_r\Big) \\
\nabla_{\sigma_p^2} L &= \sum_{r=1}^{R}\Big[-\frac{1}{2\sigma_p^2} + \frac{1}{2(\sigma_p^2)^2}\big((\Sigma_{pr})_{yy}^2 + (\mu_{pr})_y^2 - 2(\mu_{pr})_y\mu_p + \mu_p^2\big)\Big] \\
&= -\frac{R}{2\sigma_p^2} + \frac{1}{2(\sigma_p^2)^2}\sum_{r=1}^{R}\Big[(\Sigma_{pr})_{yy}^2 + (\mu_{pr})_y^2 - 2(\mu_{pr})_y\mu_p + \mu_p^2\Big] \\
\nabla_{\tau_r^2} L &= \sum_{p=1}^{P}\Big[-\frac{1}{2\tau_r^2} + \frac{1}{2(\tau_r^2)^2}\big((\Sigma_{pr})_{zz}^2 + (\mu_{pr})_z^2 - 2(\mu_{pr})_z\nu_r + \nu_r^2\big)\Big] \\
&= -\frac{P}{2\tau_r^2} + \frac{1}{2(\tau_r^2)^2}\sum_{p=1}^{P}\Big[(\Sigma_{pr})_{zz}^2 + (\mu_{pr})_z^2 - 2(\mu_{pr})_z\nu_r + \nu_r^2\Big]
\end{aligned}
$$

令上述梯度为0，求解得到：

$$
\begin{aligned}
\mu_p &= \frac{1}{R}\sum_{r=1}^{R}(\mu_{pr})_y \\
\nu_r &= \frac{1}{P}\sum_{p=1}^{P}(\mu_{pr})_z \\
\sigma_p^2 &= \frac{1}{R}\sum_{r=1}^{R}\Big[(\Sigma_{pr})_{yy}^2 + (\mu_{pr})_y^2 - 2(\mu_{pr})_y\mu_p + \mu_p^2\Big] \\
\tau_r^2 &= \frac{1}{P}\sum_{p=1}^{P}\Big[(\Sigma_{pr})_{zz}^2 + (\mu_{pr})_z^2 - 2(\mu_{pr})_z\nu_r + \nu_r^2\Big]
\end{aligned}
$$

4. KL divergence and Maximum Likelihood

(a)我们知道$f(x) = -\log x$是凸函数，所以

$$
\begin{aligned}
KL(P||Q) &= \sum_x P(x) f(\frac{Q(x)}{P(x)}) \\
&\geq f(\sum_x P(x) \frac{Q(x)}{P(x)}) \\
&= -\log 1 \\
&= 0
\end{aligned}
$$

当且仅当存在与x无关的c，使得下式成立时等号成立

$$
\frac{Q(x)}{P(x)} = c
$$

所以

$$
1 = \sum_x Q(x) = c \sum_x P(x) = c
$$

所以当且仅当$Q(x) = P(x)$时等号成立。

(b)

$$
\begin{aligned}
KL(P(X,Y)||Q(X,Y)) &= \sum_y \sum_x P(x,y) \log \frac{P(x,y)}{Q(x,y)} \\
&= \sum_y \sum_x P(x|y)P(y) \log \frac{P(x|y)P(y)}{Q(x|y)Q(y)} \\
&= \sum_y \sum_x P(x|y)P(y) \log \frac{P(x|y)}{Q(x|y)} + \sum_y \sum_x P(x|y)P(y) \log \frac{P(y)}{Q(y)} \\
&= \sum_y P(y) \Big(\sum_x P(x|y) \log \frac{P(x|y)}{Q(x|y)} \Big) + \sum_y P(y) \log \frac{P(y)}{Q(y)} \\
&= KL(P(Y|X)||Q(Y|X)) + KL(P||Q)
\end{aligned}
$$

(c)不妨设对应的离散分布取值于$\{x_1, \ldots, x_N\}$

$$
\begin{aligned}
KL(\hat{P}||P_\theta) &= KL(\hat{P}(x)||P_\theta(x)) \\
&= \sum_{i=1}^m \hat{P}(x^{(i)}) \log \frac{\hat{P}(x^{(i)})}{P_\theta(x^{(i)})} \\
&= \sum_{i=1}^m \frac{1}{m}(\sum_{j=1}^m 1\{x^{(j)}=x^{(i)}\}) \log \frac{\frac{1}{m}(\sum_{j=1}^m 1\{x^{(j)}=x^{(i)}\})}{P_\theta(x^{(i)})} \\
&= \sum_{i=1}^m \frac{1}{m} \log \frac{\frac{1}{m}}{P_\theta(x^{(i)})} \\
&= \frac{1}{m}\sum_{i=1}^m (-\log m - \log P_\theta(x^{(i)})) \\
&= -\log m - \frac{1}{m}\sum_{i=1}^m \log P_\theta(x^{(i)})
\end{aligned}
$$

所以最小化$KL(\hat{P}||P_\theta)$等于最大化$\sum_{i=1}^n \log P_\theta(x^{(i)})$，因此

$$
\arg\min_\theta KL(\hat{P}||P_\theta) = \arg\max_\theta \sum_{i=1}^m \log P_\theta(x^{(i)})
$$

5. K-means for compression

本题有一个注意点，图片的数据格式为整型，运行聚类前需要将其转换为浮点型，否则会报错。另外，本题使用向量化的方法加快计算速度，介绍如下：

假设

$$
X = \begin{bmatrix} —(x^{(1)})^T— \\ —(x^{(2)})^T— \\ \vdots \\ —(x^{(m)})^T— \end{bmatrix} \in \mathbb{R}^{m\times d}, Y = \begin{bmatrix} —(y^{(1)})^T— \\ —(y^{(2)})^T— \\ \vdots \\ —(y^{(n)})^T— \end{bmatrix} \in \mathbb{R}^{n\times d}
$$

其中$x^{(i)}, y^{(i)} \in \mathbb{R}^d$，现在的问题是如何高效计算矩阵$D \in \mathbb{R}^{m\times n}$，其中

$$
D_{i,j} = ||x^{(i)} - y^{(j)}||^2
$$

首先对$D_{i,j}$进行处理

$$
\begin{aligned}
D_{i,j} &= ||x^{(i)} - y^{(j)}||^2 \\
&= (x^{(i)} - y^{(j)})^T (x^{(i)} - y^{(j)}) \\
&= (x^{(i)})^T x^{(i)} - 2(x^{(i)})^T y^{(j)} + (y^{(j)})^T y^{(j)}
\end{aligned}
$$

那么

$$
\begin{aligned}
D &= \begin{bmatrix} D_{1,1} & \dots & D_{1,n} \\ \dots & \dots & \dots \\ D_{m,1} & \dots & D_{m,n} \end{bmatrix} \\
&= \begin{bmatrix} (x^{(1)})^T x^{(1)} - 2(x^{(1)})^T y^{(1)} + (y^{(1)})^T y^{(1)} & \dots & (x^{(1)})^T x^{(1)} - 2(x^{(1)})^T y^{(n)} + (y^{(n)})^T y^{(n)} \\ \dots & \dots & \dots \\ (x^{(m)})^T x^{(m)} - 2(x^{(m)})^T y^{(1)} + (y^{(1)})^T y^{(1)} & \dots & (x^{(m)})^T x^{(m)} - 2(x^{(m)})^T y^{(n)} + (y^{(n)})^T y^{(n)} \end{bmatrix} \\
&= \begin{bmatrix} (x^{(1)})^T x^{(1)} & \dots & (x^{(1)})^T x^{(1)} \\ \dots & \dots & \dots \\ (x^{(m)})^T x^{(m)} & \dots & (x^{(m)})^T x^{(m)} \end{bmatrix} + \begin{bmatrix} (y^{(1)})^T y^{(1)} & \dots & (y^{(n)})^T y^{(n)} \\ \dots & \dots & \dots \\ (y^{(1)})^T y^{(1)} & \dots & (y^{(n)})^T y^{(n)} \end{bmatrix} - 2 \begin{bmatrix} (x^{(1)})^T y^{(1)} & \dots & (x^{(1)})^T y^{(n)} \\ \dots & \dots & \dots \\ (x^{(m)})^T y^{(1)} & \dots & (x^{(m)})^T y^{(n)} \end{bmatrix} \\
&= \begin{bmatrix} (x^{(1)})^T x^{(1)} \\ \dots \\ (x^{(m)})^T x^{(m)} \end{bmatrix} \underbrace{\begin{bmatrix} 1 & \dots & 1 \end{bmatrix}}_{1\times n\text{矩阵}} + \underbrace{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}_{m\times 1\text{矩阵}} \begin{bmatrix} (y^{(1)})^T y^{(1)} & \dots & (y^{(n)})^T y^{(n)} \end{bmatrix} - 2XY^T
\end{aligned}
$$

利用numpy的广播机制上式可以简写如下：

```
#计算距离矩阵
d1 = np.sum(X ** 2, axis=1).reshape(-1, 1)
d2 = np.sum(centroids ** 2, axis=1).reshape(1, -1)

dist = d1 + d2 - 2 * X.dot(centroids.T)
```

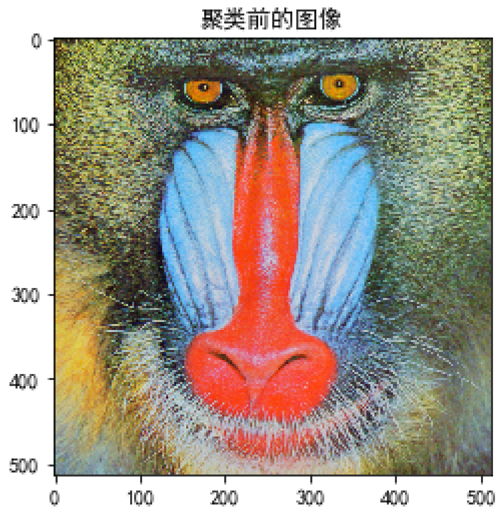
全部代码如下：

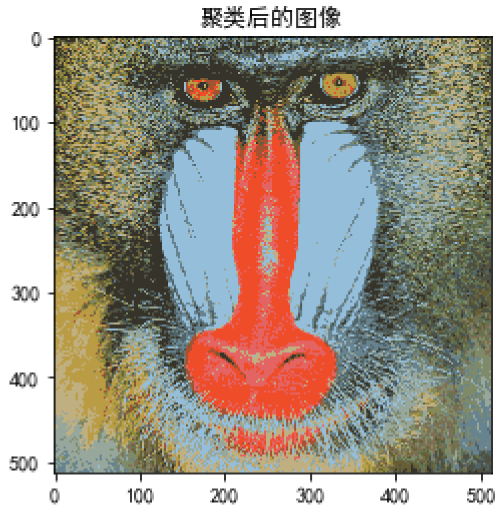
```
from matplotlib.image import imread
import matplotlib.pyplot as plt
import numpy as np
plt.rcParams['font.sans-serif']=['SimHei'] #用来正常显示中文标签
plt.rcParams['axes.unicode_minus']=False #用来正常显示负号

def k_means(X, k, D=1e-5):
    """
    X数据，k为聚类数量，D为阈值
    """
    #数据数量
    n = X.shape[0]
    #聚类标签
    clusters = np.zeros(n, dtype=int)
    #初始中心点
    index = np.random.randint(0, n, k)
    centroids = X[index]
    #记录上一轮迭代的聚类中心
    centroids_pre = np.copy(centroids)

    while True:
        #计算距离矩阵
        d1 = np.sum(X ** 2, axis=1).reshape(-1, 1)
        d2 = np.sum(centroids ** 2, axis=1).reshape(1, -1)
```

```
        dist = d1 + d2 - 2 * X.dot(centroids.T)
        #STEP1:找到最近的中心
        clusters = np.argmin(dist, axis=1)

        #STEP2:重新计算中心
        for i in range(k):
            index = X[clusters==i]
            #判断是否有点和某聚类中心在一类
            if len(index) != 0:
                centroids[i] = np.mean(index, axis=0)
        #计算误差
        delta = np.linalg.norm(centroids - centroids_pre)

        #判断是否超过阈值
        if delta < D:
            break

        centroids_pre = np.copy(centroids)

    return clusters, centroids
```

运行结果如下:

```
#读取图片并展示图片
A = imread('mandrill-large.tiff')
plt.imshow(A)
plt.title("聚类前的图像")
plt.show()

#将图片转化为矩阵
A_proceed = A.reshape(-1, 3)
#转换为浮点型，否则会报错
A_proceed = A_proceed.astype(np.float32)
#运行聚类
clusters, centroids = k_means(A_proceed, 16, 30)
#变成图片的形状
A_compressed = np.reshape(centroids[clusters], A.shape)
#转换为整型
A_compressed = A_compressed.astype(np.uint8)
#显示图像
plt.imshow(A_compressed)
plt.title("聚类后的图像")
plt.show()
```





总体来说图像效果还不错。