

机器学习半监督学习作业

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13.1

13.5

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- (1) 选用UCI数据集中的 iris 数据集
分析
- (2) 选用UCI数据集中的 wine 数据集
分析:

13.1

13.5

由高斯混合模型的定义式可知：

$$p(\mathbf{x}) = \sum_{i=1}^N \alpha_i \cdot p(\mathbf{x} \mid \boldsymbol{\mu} * i, \boldsymbol{\Sigma} * i)$$

因此：

$$\begin{aligned} p(\Theta = i \mid \mathbf{x}) &= \frac{p(\Theta = i, \mathbf{x})}{P(\mathbf{x})} \\ &= \frac{\alpha_i \cdot p(\mathbf{x} \mid \boldsymbol{\mu} * i, \boldsymbol{\Sigma} * i)}{\sum_{i=1}^N \alpha_i \cdot p(\mathbf{x} \mid \boldsymbol{\mu} * i, \boldsymbol{\Sigma} * i)} \end{aligned}$$

又因为：

$$\lambda_{ij} = P(\Theta = i \mid x)$$

所以：

$$\lambda_{ij} = \frac{\alpha_i \cdot p(\mathbf{x} \mid \boldsymbol{\mu} * i, \boldsymbol{\Sigma} * i)}{\sum_{i=1}^N \alpha_i \cdot p(\mathbf{x} \mid \boldsymbol{\mu} * i, \boldsymbol{\Sigma} * i)}$$

13.6

令

$$\frac{\partial LL(D_l \cup D_u)}{\partial \mu_i} = 0$$

其中

$$LL(D \cdot 1 \cup D \cdot u) = \sum_{(xj, yj) \in D \cdot 1} \ln \left(\sum_{i=1}^N \alpha_i \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i) \cdot p(y \cdot j \mid \Theta = i, \mathbf{x}j) \right) + \sum_{\mathbf{x} \cdot j \in D \cdot u} \ln \left(\sum_{i=1}^N \alpha_i \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i) \right)$$

将式LL (D · 1 ∪ D · u)的两项分别记为：

$$\begin{aligned} LL(D \cdot 1) &= \sum_{(xj, yj) \in D \cdot 1} \ln \left(\sum_{s=1}^N \alpha_s \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot s, \boldsymbol{\Sigma} \cdot s) \cdot p(y \cdot i \mid \Theta = s, \mathbf{x} \cdot j) \right) \\ &= \sum_{(xj, yj) \in D \cdot 1} \ln \left(\sum_{s=1}^N \alpha_{yj} \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot yj, \boldsymbol{\Sigma} \cdot y \cdot j) \right) \\ LL(D \cdot u) &= \sum_{\mathbf{x} \cdot j \in D \cdot u} \ln(\alpha_s \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot s, \boldsymbol{\Sigma} \cdot s)) \end{aligned}$$

对第一项求导

$$\begin{aligned} \frac{\partial LL(D \cdot 1)}{\partial \boldsymbol{\mu} \cdot i} &= \sum_{(xj, yj) \in D \cdot 1 \wedge yj=i} \frac{\partial \ln(\alpha_i \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i))}{\partial \boldsymbol{\mu} \cdot i} \\ &= \sum_{(xj, yj) \in D \cdot 1 \wedge yj=i} \frac{1}{p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)} \cdot \frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu}_i} \end{aligned}$$

其中

$$p(\mathbf{x} * j \mid \boldsymbol{\mu} * i, \boldsymbol{\Sigma} * i) = \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma} * i|^{\frac{1}{2}}} e^{-\frac{1}{2}(\mathbf{x} * j - \boldsymbol{\mu} * i)^{\top} \boldsymbol{\Sigma} * i^{-1} (\mathbf{x} * j - \boldsymbol{\mu} * i)}$$

$$\begin{aligned}
\frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu} \cdot i} &= \frac{\partial \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}_i|^{\frac{1}{2}}} e^{-\frac{1}{2}(\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)^\top \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)}}{\partial \boldsymbol{\mu} \cdot i} \\
&= \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}_i|^{\frac{1}{2}}} \cdot \frac{\partial e^{-\frac{1}{2}(\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)^\top \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)}}{\partial \boldsymbol{\mu} \cdot i} \\
&= \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}_i|^{\frac{1}{2}}} \cdot e^{-\frac{1}{2}(\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)^\top \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)} \cdot -\frac{1}{2} \frac{\partial (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)^\top \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)}{\partial \boldsymbol{\mu}_i}
\end{aligned}$$

其中协方差矩阵的逆矩阵 $\boldsymbol{\Sigma}_i^{-1}$ 是对称阵，根据矩阵求导公式，当W为对称矩阵时，有

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

所以

$$\begin{aligned}
\frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu} \cdot i} &= \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}_i|^{\frac{1}{2}}} \cdot e^{-\frac{1}{2}(\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)^\top \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)} \cdot -\frac{1}{2} \cdot 2\boldsymbol{\Sigma} \cdot i^{-1} (\boldsymbol{\mu} \cdot i - \mathbf{x} \cdot j) \\
&= \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}_i|^{\frac{1}{2}}} \cdot e^{-\frac{1}{2}(\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)^\top \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)} \cdot \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot i - \boldsymbol{\mu} \cdot j) \\
&= p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i) \cdot \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)
\end{aligned}$$

所以

$$\begin{aligned}
\frac{\partial LL(D \cdot l)}{\partial \boldsymbol{\mu} \cdot i} &= \sum_{(\mathbf{x} \cdot j, y \cdot j) \in D \cdot l \wedge y \cdot j = i} \frac{1}{p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)} \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i) \cdot \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i) \\
&= \sum_{(\mathbf{x} \cdot j, y \cdot j) \in D \cdot l \wedge y \cdot j = i} \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu}_i)
\end{aligned}$$

对第二项求导

$$\begin{aligned}
\frac{\partial LL(D_u)}{\partial \boldsymbol{\mu} \cdot i} &= \frac{\partial LL(D \cdot u)}{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)} \cdot \frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu} \cdot i} \\
&= \frac{\partial \sum \cdot j = 1^m \ln \left(\sum_{l=1}^k \alpha_l \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot l, \boldsymbol{\Sigma} \cdot l) \right)}{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)} \cdot \frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu} \cdot i} \\
&= \sum_{j=1}^m \frac{\partial \ln \left(\sum_{l=1}^k \alpha_l \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot l, \boldsymbol{\Sigma} \cdot l) \right)}{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)} \cdot \frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu} \cdot i} \\
&= \sum_{j=1}^m \frac{\alpha_i}{\sum_{l=1}^k \alpha_l \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot l, \boldsymbol{\Sigma} \cdot l)} \cdot \frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu}_i}
\end{aligned}$$

因为

$$\frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu} \cdot i} = p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i) \cdot \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i)$$

所以

$$\begin{aligned}
\frac{\partial LL(D_u)}{\partial \boldsymbol{\mu} \cdot i} &= \sum \cdot j = 1^m \frac{\alpha_i}{\sum_{l=1}^N \alpha_l \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot l, \boldsymbol{\Sigma} \cdot l)} \cdot \frac{\partial p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\partial \boldsymbol{\mu} \cdot i} \\
&= \sum \cdot j = 1^m \frac{\alpha_i}{\sum_{l=1}^N \alpha_l \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot l, \boldsymbol{\Sigma} \cdot l)} \cdot p(\mathbf{x} \cdot j \mid \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i) \cdot \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu} \cdot i) \\
&= \sum \cdot x_j \in D \cdot u \gamma \cdot j i \cdot \boldsymbol{\Sigma} \cdot i^{-1} (\mathbf{x} \cdot j - \boldsymbol{\mu}_i)
\end{aligned}$$

因此

$$\begin{aligned}
\frac{\partial LL(D \cdot 1 \cup D \cdot u)}{\partial \boldsymbol{\mu} \cdot \mathbf{i}} &= \sum \cdot (\boldsymbol{x} \cdot \mathbf{j}, \mathbf{y} \cdot \mathbf{j}) \in D \cdot 1 \wedge \mathbf{y} \cdot \mathbf{j} = \mathbf{i} \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) + \sum \cdot \boldsymbol{x} \cdot \mathbf{j} \in D \cdot u \gamma_{\mathbf{j}\mathbf{i}} \cdot \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) \\
&= \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} \left(\sum_{(x_j, y_j) \in D \cdot 1 \wedge y_j = i} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) + \sum \cdot \boldsymbol{x} \cdot \mathbf{j} \in D \cdot u \gamma_{\mathbf{j}\mathbf{i}} \cdot (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) \right) \\
&= \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} \left(\sum \cdot (x_j, y \cdot j) \in D \cdot 1 \wedge y \cdot j = \mathbf{i} \boldsymbol{x} \cdot \mathbf{j} + \sum_{x_j \in D \cdot u} \gamma_{\mathbf{j}\mathbf{i}} \cdot \boldsymbol{x} \cdot \mathbf{j} - \sum \cdot (\boldsymbol{x} \cdot \mathbf{j}, y \cdot j) \in D \cdot 1 \wedge y \cdot j = \mathbf{i} \boldsymbol{\mu} \cdot \mathbf{i} - \sum \cdot \boldsymbol{x} \cdot \mathbf{j} \in D \cdot u \gamma_{\mathbf{j}\mathbf{i}} \cdot \boldsymbol{\mu}_i \right) \\
&= 0
\end{aligned}$$

所以

$$\begin{aligned}
\sum_{x_j \in D \cdot u} \gamma \cdot \mathbf{j}\mathbf{i} \cdot \boldsymbol{\mu} \cdot \mathbf{i} + \sum \cdot (x_j, y \cdot j) \in D \cdot 1 \wedge y_j = \mathbf{i} \boldsymbol{\mu} \cdot \mathbf{i} &= \sum \cdot x_j \in D \cdot u \gamma \cdot \mathbf{j}\mathbf{i} \cdot \boldsymbol{x} \cdot \mathbf{j} + \sum \cdot (x_j, y_j) \in D \cdot 1 \wedge y_j \cdot j = \mathbf{i} \boldsymbol{x}_j \\
\left(\sum_{x_j \in D_u} \gamma_{ji} + \sum_{(x_j, y_j) \in D_1 \wedge y_j = i} 1 \right) \mu_i &= \sum_{x_j \in D_u} \gamma_{ji} \cdot x_j + \sum_{(x_j, y_j) \in D_1 \wedge y_j = i} x_j
\end{aligned}$$

因为

$$\sum_{(\mathbf{x} \cdot \mathbf{j}, y_j) \in D \cdot 1 \wedge y_j = \mathbf{i}} 1 = 1 \cdot \mathbf{i}$$

所以

$$\boldsymbol{\mu} \cdot \mathbf{i} = \frac{1}{\sum \cdot x_j \in D \cdot u \gamma \cdot \mathbf{j}\mathbf{i} + l_i} \left(\sum_{x_j \in D \cdot u} \gamma \cdot \mathbf{j}\mathbf{i} \boldsymbol{x} \cdot \mathbf{j} + \sum \cdot (\boldsymbol{x} \cdot \mathbf{j}, y_j) \in D \cdot 1 \wedge y_j = \mathbf{i} \boldsymbol{x}_j \right)$$

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$LL(D_1)$ 对 \sum_i 求偏导:

$$\begin{aligned}
\frac{\partial LL(D \cdot 1)}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} &= \sum_{(x_j, y_j) \in D \cdot 1 \wedge y_j = \mathbf{i}} \frac{\partial \ln(\alpha_i \cdot p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i}))}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} \\
&= \sum_{(x_j, y_j) \in D \cdot 1 \wedge y_j = \mathbf{i}} \frac{1}{p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i})} \cdot \frac{\partial p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i})}{\partial \boldsymbol{\Sigma}_i}
\end{aligned}$$

其中

$$\begin{aligned}
\frac{\partial p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i})}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} &= \frac{\partial}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} \left[\frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma} \cdot \mathbf{i}|^{\frac{1}{2}}} \exp \left(-\frac{1}{2} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i})^T \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) \right) \right] \\
&= \frac{\partial}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} \left\{ \exp \left[\ln \left(\frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma} \cdot \mathbf{i}|^{\frac{1}{2}}} \exp \left(-\frac{1}{2} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i})^T \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) \right) \right) \right] \right\} \\
&= p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i}) \cdot \frac{\partial}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} \left[\ln \left(\frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma} \cdot \mathbf{i}|^{\frac{1}{2}}} \exp \left(-\frac{1}{2} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i})^T \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) \right) \right) \right] \\
&= p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i}) \cdot \frac{\partial}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} \left[\ln \frac{1}{(2\pi)^{\frac{n}{2}}} - \frac{1}{2} \ln |\boldsymbol{\Sigma} \cdot \mathbf{i}| - \frac{1}{2} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i})^T \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) \right] \\
&= p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i}) \cdot \left[-\frac{1}{2} \frac{\partial (\ln |\boldsymbol{\Sigma} \cdot \mathbf{i}|)}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} - \frac{1}{2} \frac{\partial \left[(\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i})^T \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) \right]}{\partial \boldsymbol{\Sigma}_i} \right]
\end{aligned}$$

又因为

$$\frac{\partial |\mathbf{X}|}{\partial \mathbf{X}} = |\mathbf{X}| \cdot (\mathbf{X}^{-1})^T, \frac{\partial \mathbf{a}^T \mathbf{X}^{-1} \mathbf{b}}{\partial \mathbf{X}} = -\mathbf{X}^{-T} \mathbf{a} \mathbf{b}^T \mathbf{X}^{-T}$$

$$\frac{\partial}{\partial \boldsymbol{\Sigma} \cdot \mathbf{i}} (p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i})) = p(\boldsymbol{x} \cdot \mathbf{j} \mid \boldsymbol{\mu} \cdot \mathbf{i}, \boldsymbol{\Sigma} \cdot \mathbf{i}) \cdot \left[-\frac{1}{2} \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} + \frac{1}{2} \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i}) (\boldsymbol{x} \cdot \mathbf{j} - \boldsymbol{\mu} \cdot \mathbf{i})^T \boldsymbol{\Sigma} \cdot \mathbf{i}^{-1} \right]$$

所以

$$\begin{aligned}\frac{\partial LL(D \cdot 1)}{\partial \Sigma \cdot i} &= \sum_{(x_j, y_j) \in D \cdot 1 \wedge y_j = i} \frac{1}{p(x \cdot j | \mu \cdot i, \Sigma \cdot i)} \cdot p(x \cdot j | \mu \cdot i, \Sigma \cdot i) \cdot \left(\Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top - I \right) \cdot \frac{1}{2} \Sigma \cdot i^{-1} \\ &= \sum_{(x_j, y \cdot j) \in D \cdot 1 \wedge y_j = i} \left(\Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top - I \right) \cdot \frac{1}{2} \Sigma \cdot i^{-1}\end{aligned}$$

$LL(D_u)$ 对 \sum_i 求偏导:

$$\frac{\partial LL(D_u)}{\partial \Sigma \cdot i} = \sum \cdot j = 1^m \frac{\alpha_i}{\sum_{l=1}^N \alpha_l \cdot p(x \cdot j | \mu \cdot l, \Sigma \cdot l)} \cdot \frac{\partial p(x \cdot j | \mu \cdot i, \Sigma \cdot i)}{\partial \Sigma_i}$$

因为

$$\frac{\partial}{\partial \Sigma \cdot i} (p(x \cdot j | \mu \cdot i, \Sigma \cdot i)) = p(x \cdot j | \mu \cdot i, \Sigma \cdot i) \cdot \left[-\frac{1}{2} \Sigma \cdot i^{-1} + \frac{1}{2} \Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top \Sigma \cdot i^{-1} \right]$$

所以

$$\frac{\partial LL(D_u)}{\partial \Sigma \cdot i} = \sum \cdot j = 1^m \frac{\alpha_i \cdot p(x \cdot j | \mu \cdot i, \Sigma \cdot i)}{\sum \cdot l = 1^k \alpha_l \cdot p(x \cdot j | \mu \cdot l, \Sigma \cdot l)} \cdot \left[-\frac{1}{2} \Sigma \cdot i^{-1} + \frac{1}{2} \Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top \Sigma \cdot i^{-1} \right]$$

所以

$$\frac{\partial LL(D \cdot u)}{\partial \Sigma \cdot i} = \sum_{x_j \in D \cdot u} \gamma \cdot j i \cdot \left(\Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top - I \right) \cdot \frac{1}{2} \Sigma \cdot i^{-1}$$

$$\begin{aligned}\frac{\partial LL(D \cdot 1 \cup D \cdot u)}{\partial \Sigma \cdot i} &= \sum \cdot x_i \in D \cdot u \gamma \cdot j i \cdot \left(\Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top - I \right) \cdot \frac{1}{2} \Sigma \cdot i^{-1} \\ &\quad + \sum_{(x_i, y_j) \in D \cdot i \wedge y_j = i} \left(\Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top - I \right) \cdot \frac{1}{2} \Sigma \cdot i^{-1} \\ &= \left(\sum \cdot x_j \in D \cdot u \gamma \cdot j i \cdot \left(\Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top - I \right) \right. \\ &\quad \left. + \sum \cdot (x_j, y \cdot j) \in D \setminus \wedge y \cdot i = i \left(\Sigma \cdot i^{-1} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top - I \right) \right) \cdot \frac{1}{2} \Sigma \cdot i^{-1} = 0\end{aligned}$$

所以

$$\begin{aligned}\sum_{x_j \in D_u} \gamma_{ji} \cdot \Sigma_i^{-1} (x_j - \mu_i) (x_j - \mu_i)^\top &+ \sum_{(x_j, y_j) \in D_l \wedge y_j = i} \Sigma_i^{-1} (x_j - \mu_i) (x_j - \mu_i)^\top \\ &= \sum_{x_j \in D_u} \gamma_{ji} \cdot I + \sum_{(x_j, y_j) \in D_1 \wedge y_j = i} I \\ &= \left(\sum_{x_j \in D_u} \gamma_{ji} + l_i \right) I \\ \sum_{x_j \in D_u} \gamma_{ji} \cdot (x_j - \mu_i) (x_j - \mu_i)^\top &+ \sum_{(x_j, y_j) \in D_1 \wedge y_j = i} (x_j - \mu_i) (x_j - \mu_i)^\top = \left(\sum_{x_j \in D_u} \gamma_{ji} + l_i \right) \Sigma_i\end{aligned}$$

所以

$$\Sigma \cdot i = \frac{1}{\sum \cdot x_j \in D_u \gamma_{ji} + 1 \cdot i} \left(\sum \cdot x_j \in D \cdot u \gamma \cdot j i \cdot (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top + \sum_{(x_i, y_j) \in D \cdot 1 \wedge y_j = i} (x \cdot j - \mu \cdot i) (x \cdot j - \mu \cdot i)^\top \right)$$

13.8

$LL(D_l \cup D_u)$ 的拉格朗日形式

$$\mathcal{L}(D \cdot 1 \cup D \cdot u, \lambda) = LL(D \cdot 1 \cup D \cdot u) + \lambda \left(\sum_{s=1}^N \alpha_s - 1 \right) = LL(D \cdot 1) + LL(D \cdot u) + \lambda \left(\sum_{s=1}^N \alpha_s - 1 \right)$$

$LL(D_u)$ 对 α_i 求偏导

$$\frac{\partial LL(D \cdot u)}{\partial \alpha \cdot i} = \sum_{x_j \in D \cdot u} \frac{1}{\sum \cdot s = 1^N \alpha_s \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot s, \boldsymbol{\Sigma} \cdot s)} \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)$$

$LL(D_l)$ 对 α_i 求偏导

$$\begin{aligned} \frac{\partial LL(D \cdot l)}{\partial \alpha \cdot i} &= \sum_{(x \cdot j, y \cdot j) \in D \cdot 1 \wedge y \cdot j = i} \frac{\partial \ln(\alpha_i \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i))}{\partial \alpha \cdot i} \\ &= \sum_{(x \cdot j, y \cdot j) \in D \cdot 1 \wedge y \cdot j = i} \frac{1}{\alpha \cdot i \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)} \cdot \frac{\partial (\alpha \cdot i \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i))}{\partial \alpha \cdot i} \\ &= \sum_{(x \cdot j, y \cdot j) \in D \cdot 1 \wedge y \cdot j = i} \frac{1}{\alpha_i \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)} \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i) \\ &= \sum_{(x \cdot j, y \cdot j) \in D \cdot 1 \wedge y \cdot j = i} \frac{1}{\alpha_i} = \frac{1}{\alpha_i} \cdot \sum_{(x \cdot j, y \cdot j) \in D \cdot 1 \wedge y \cdot j = i} 1 = \frac{1 \cdot i}{\alpha \cdot i} \end{aligned}$$

$\alpha_i, p(x_j | \mu_i, \Sigma_i)$ 是常量, 所以

$$\frac{\partial \mathcal{L}(D \cdot 1 \cup D \cdot u, \lambda)}{\partial \alpha_i} = \frac{1 \cdot i}{\alpha \cdot i} + \sum_{x_j \in D \cdot u} \frac{p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\sum_{s=1}^N \alpha_s \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot s, \boldsymbol{\Sigma} \cdot s)} + \lambda = 0$$

两边同乘以 α_i

$$\begin{aligned} \alpha_i \cdot \frac{1 \cdot i}{\alpha \cdot i} + \sum_{x_j \in D \cdot u} \frac{\alpha \cdot i \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot i, \boldsymbol{\Sigma} \cdot i)}{\sum \cdot s = 1^N \alpha_s \cdot p(\mathbf{x} \cdot j | \boldsymbol{\mu} \cdot s, \boldsymbol{\Sigma} \cdot s)} + \lambda \cdot \alpha \cdot i &= 0 \\ 1 \cdot i + \sum \cdot x \cdot i \in D \cdot u \gamma_{ji} + \lambda \alpha_i &= 0 \end{aligned}$$

对所有混合成分求和

$$\sum_{i=1}^N l_i + \sum_{i=1}^N \sum_{x_i \in D_u} \gamma_{ji} + \sum_{i=1}^N \lambda \alpha_i = 0$$

因为

$$\begin{aligned} \sum_{i=1}^N \gamma_{ji} &= \sum_{i=1}^N \frac{\alpha_i \cdot p(x_j | \mu_i, \Sigma_i)}{\sum_{s=1}^N \alpha_s \cdot p(x_j | \mu_s, \Sigma_s)} = \frac{\sum_{i=1}^N \alpha_i \cdot p(x_j | \mu_i, \Sigma_i)}{\sum_{s=1}^N \alpha_s \cdot p(x_j | \mu_s, \Sigma_s)} = 1 \\ \Rightarrow \sum_{i=1}^N \sum_{x_i \in D_u} \gamma_{ji} &= \sum_{x_i \in D_u} \sum_{i=1}^N \gamma_{ji} = \sum_{x_i \in D_u} 1 = u \end{aligned}$$

因为 $\sum_{x_j \in D_u}$ 形式与 $\sum_{j=1}^u$ 等价, $\sum_{i=1}^N l_i = l$ 其中 l 为有标记样本集的样本个数; 代入

$$\sum_{i=1}^N l_i + \sum_{i=1}^N \sum_{x_i \in D_u} \gamma_{ji} + \sum_{i=1}^N \lambda \alpha_i = 0$$

解得

$$\begin{aligned} &\begin{cases} l + u + \lambda = 0 \\ l + u = m \end{cases} \\ \Rightarrow 1 \cdot i + \sum \cdot x \cdot j \in D \cdot u \gamma_{ji} - \lambda \alpha_i &= 0 \end{aligned}$$

所以

$$\alpha_i = \frac{1}{m} \left(\sum_{x \cdot j \in D \cdot u} \gamma_{ji} + l_i \right)$$

13.5

具体代码见“半监督学习.py”，在此仅列出部分代码

```
# 定义TSVM函数
def TSVM(test_feature, test_label, x1, y1, x2, x3):
    # 调用sklearn中的SVM
    clf_svm = svm.SVC(C=1, kernel='linear')
    clf_svm.fit(x1, y1)
    y3_svm = clf_svm.predict(x3)

    clf_TSVM = svm.SVC(C=1, kernel='linear')
    clf_TSVM.fit(x1, y1)

    # 用训练好的 SVM对Du进行预测
    y2 = clf_TSVM.predict(x2)

    # 初始化cu, c1
    cu = 0.001
    c1 = 1

    # 样本权重， 直接让有标签数据的权重为c1, 无标签数据的权重为cu
    sample_weight = np.ones(len(x1) + len(x2))
    sample_weight[len(x1):] = cu

    # 初始化 id 数组
    id_set = np.arange(len(x2))

    while cu < c1:
        y3 = np.concatenate((y1, y2)) # 合并有标签样本和无标签样本
        clf_TSVM.fit(x3, y3, sample_weight=sample_weight) # 对TSVM模型进行训练
        while True:
            y2 = clf_TSVM.predict(x2)
            x2_dist = clf_TSVM.decision_function(x2) # 计算无标签样本的距离
            norm_weight = np.linalg.norm(clf_TSVM.coef_) # 进行标准化
            epsilon = 1 - x2_dist * y2 * norm_weight

            plus_set, plus_id = epsilon[y2 > 0], id_set[y2 > 0] # 正标记 (1) 样本
            minus_set, minus_id = epsilon[y2 < 0], id_set[y2 < 0] # 负标记 (-1) 样本

            # 找到最大、最小值的索引
            plus_max_id, minus_max_id = plus_id[np.argmax(plus_set)],
            minus_id[np.argmax(minus_set)]
            a, b = epsilon[plus_max_id], epsilon[minus_max_id]

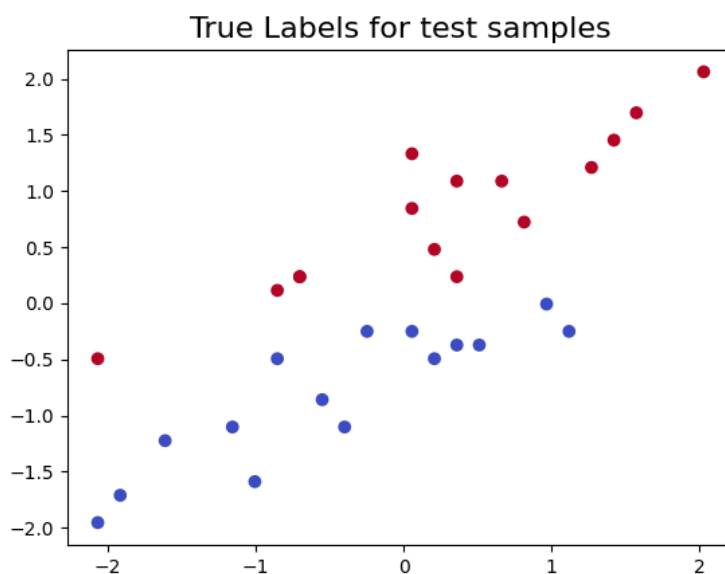
            if a > 0 and b > 0 and a + b > 2:
                # 将无标签样本的预测值进行翻转
                y2[plus_max_id], y2[minus_max_id] = -y2[plus_max_id], -
                y2[minus_max_id]
                y3 = np.concatenate((y1, y2)) # 合并有标签样本和无标签样本的预测值
                clf_TSVM.fit(x3, y3, sample_weight=sample_weight) # 对TSVM模型进
                行训练
            else:
                break
        cu = min(cu * 2, c1)
        sample_weight[len(y1):] = cu
```

(1) 选用UCI数据集中的 iris 数据集

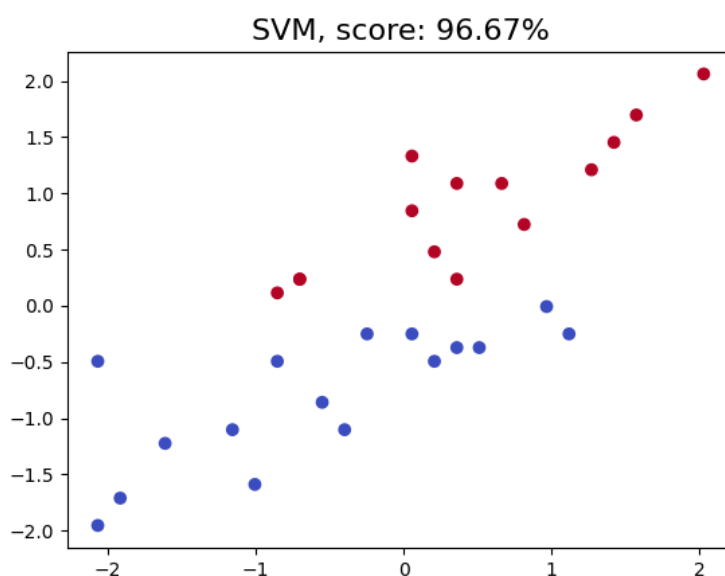
```
from sklearn.datasets import load_iris
iris = load_iris()
# 取iris数据集后100数据，即分类为2, 3的数据集，构成一个二分类问题
feature, label = iris.data[50:, :], iris.target[50:] * 2 - 3
# 按题目要求分成测试集，有标签样本，无标签样本
# 特征均已归一化
```

经训练后，在测试集上得到如下结果：

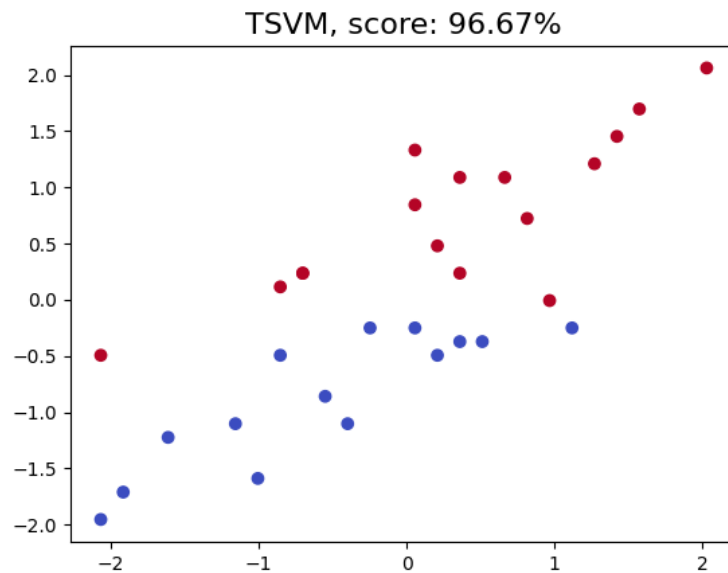
测试集样本：



在SVM上的结果：



在TSVM上的结果：



分析

二者的模型精度一致，可能是因为样测试样本较少的缘故；

在坐标 (-2, -0.5) 和 (1.2, -0.2) 两处SVM与TSVM的预测结果不一致，并且都与真实情况相差一例；

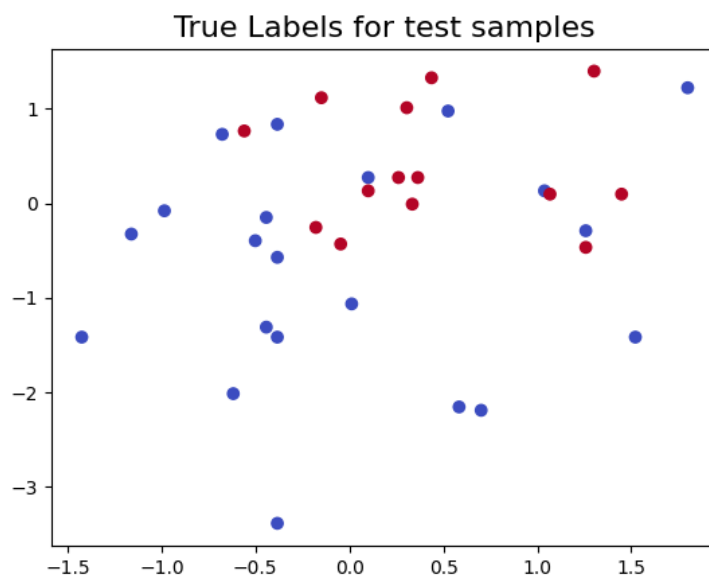
对基本训练模型svm采用高斯核效果一致。

(2) 选用UCI数据集中的 wine 数据集

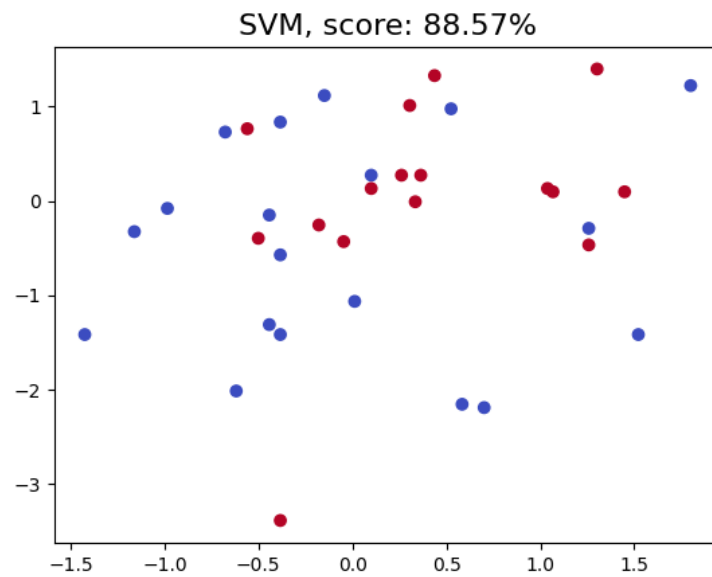
```
from sklearn.datasets import load_wine
iris = load_wine()
# 取wine数据集后119个数据，即分类为2, 3的数据集，构成一个二分类问题
feature, label = wine.data[59:, :], wine.target[59:] * 2 - 3
# 按题目要求分成测试集，有标签样本，无标签样本
# 特征均已归一化
```

经训练后，在测试集上得到如下结果：

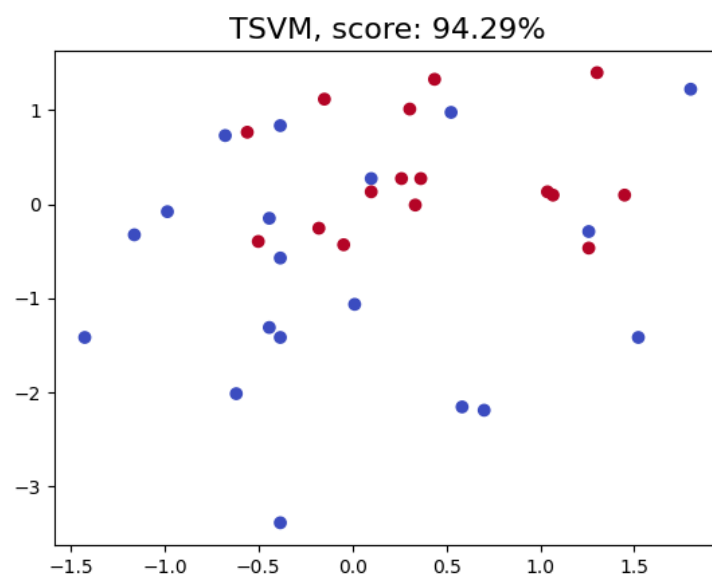
测试集样本：



在SVM上的结果：



在TSVM上的结果：



分析：

与普通SVM相比，TSVM的模型精度较高；

SVM与TSVM容易将正类模型预测为负，SVM预测为负的数量较多；

对基本训练模型svm采用高斯核效果略有提升。