Machine Learning- Exercise 1

Python Tutorial, Probability Density, GMM, EM

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Repetition: Important Statistical Formulas

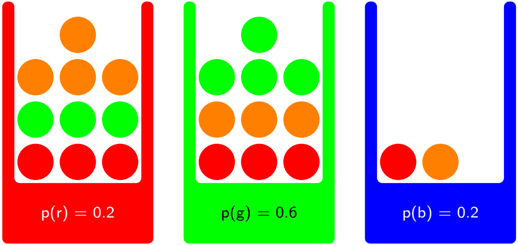
- Rules of probability

$$p(x) = \sum_y p(x, y)$$
$$p(x, y) = p(y|x)p(x)$$

- Bayes rule

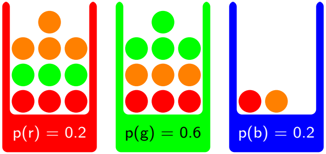
$$p(y|x) = \frac{p(x|y)p(y)}{p(x)} = \frac{p(x|y)p(y)}{\sum_{y'} p(x|y')p(y')}$$

Statement of problem



- Let $B \in \{r, g, b\}$ the random variable for the boxes.
- Let $F = \{a, o, l\}$ the random variable representing the fruits.

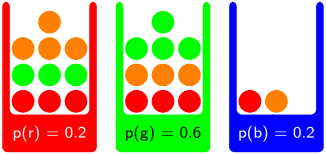
Selecting an apple



What is $p(F = a)$?

$$
\begin{aligned}
p(F = a) &= \underbrace{\sum_{b \in B} p(F = a | B = b) p(B = b)}_{\text{Law of total probability}} \\
&= p(F = a | B = r) p(B = r) + p(F = a | B = g) p(B = g) \\
&\quad + p(F = a | B = b) p(B = b) \\
&= \frac{3}{10} \cdot \frac{2}{10} + \frac{3}{10} \cdot \frac{6}{10} + \frac{1}{2} \cdot \frac{2}{10} \\
&= \frac{17}{50} = 0.34
\end{aligned}
$$

Conditional probability for orange



What is $p(B = g|F = o)$?

$$p(B = g|F = o) = \underbrace{\frac{p(F = o|B = g)p(B = g)}{p(F = o)}}_{\text{Bayes Rule}}$$

$$= \frac{p(F = o|B = g)p(B = g)}{\sum_{b \in B} p(B = b)p(F = o|B = b)}$$

$$= \frac{\frac{3}{10}\frac{6}{10}}{\frac{4}{10}\frac{2}{10} + \frac{3}{10}\frac{6}{10} + \frac{1}{2}\frac{2}{10}}$$

$$= \frac{1}{2}$$

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Minimizing the Expected Loss

- Optimal solution: Minimizing the loss by adapting decision regions
- Loss depends on true class

⇒ Minimize the **expected** loss

$$
\begin{aligned}
\mathbb{E}[L] &= \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(x, \mathcal{C}_k) dx \\
&= \sum_j \int_{\mathcal{R}_j} \sum_k L_{kj} p(x, \mathcal{C}_k) dx \\
&= \sum_j \int_{\mathcal{R}_j} \underbrace{\sum_k L_{kj} p(\mathcal{C}_k | x) p(x)}_{\to \text{min}} \, dx \to \text{min}
\end{aligned}
$$

Minimizing Expected Loss with Rejection Choice

$$\text{classify}(x) :\rightarrow \begin{cases} \mathcal{C}_j & \text{if } \forall i : p(\mathcal{C}_i|x) \leq p(\mathcal{C}_j|x) \wedge p(\mathcal{C}_j|x) \geq 1 - \frac{l_r}{l_s} \\ \mathcal{C}_{\text{rej}} & \text{otherwise} \end{cases}$$

$$\begin{aligned} \underset{j}{\operatorname{argmin}}\left\{\sum_k L_{kj} p(\mathcal{C}_k|x) p(x)\right\} &= \underset{j}{\operatorname{argmin}}\left\{\sum_k L_{kj} p(\mathcal{C}_k|x)\right\} \\ &= \underset{j}{\operatorname{argmin}}\left\{l_s \sum_{k \neq j} p(\mathcal{C}_k|x)\right\} \\ &= \underset{j}{\operatorname{argmin}}\left\{\sum_{k \neq j} p(\mathcal{C}_k|x)\right\} \\ &= \underset{j}{\operatorname{argmin}}\left\{(1 - p(\mathcal{C}_j|x))\right\} \\ &= \underset{j}{\operatorname{argmax}}\left\{p(\mathcal{C}_j|x)\right\} \end{aligned}$$

Minimizing Expected Loss with Rejection Choice

$$\text{classify}(x) :\rightarrow \begin{cases} \mathcal{C}_j & \text{if } \forall i : p(\mathcal{C}_i|x) \le p(\mathcal{C}_j|x) \wedge p(\mathcal{C}_j|x) \ge 1 - \frac{l_r}{l_s} \\ \mathcal{C}_{\text{rej}} & \text{otherwise} \end{cases}$$

$$\begin{aligned} & & l_s \sum_{k \neq j} p(\mathcal{C}_k|x) &\le l_r \\ &\Leftrightarrow & l_s \Big(1 - p(\mathcal{C}_j|x)\Big) &\le l_r \\ &\Leftrightarrow & 1 - p(\mathcal{C}_j|x) &\le \frac{l_r}{l_s} \\ &\Leftrightarrow & -p(\mathcal{C}_j|x) &\le \frac{l_r}{l_s} - 1 \\ &\Leftrightarrow & p(\mathcal{C}_j|x) &\ge 1 - \frac{l_r}{l_s} \end{aligned}$$

Minimizing the Expected Loss

(b) Unless the $p(\mathcal{C}_i|x) = 1$ always reject.

(c) Never reject.

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Maximum Likelihood

- Single data point

$$p(x_n|\theta)$$

- IID assumption: Likelihood

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

- Log-likelihood

$$E(\theta) = \ln L(\theta) = \ln\left(\prod_{n=1}^{N} p(x_n|\theta)\right) = \sum_{n=1}^{N} \ln p(x_n|\theta)$$

- Maximize Log-likelihood

$$\frac{\partial}{\partial\theta} E(\theta) = \frac{\partial}{\partial\theta} \sum_{n=1}^{N} \ln p(x_n|\theta) = \sum_{n=1}^{N} \frac{\frac{\partial}{\partial\theta} p(x_n|\theta)}{p(x_n|\theta)} \stackrel{!}{=} 0$$

Maximum Likelihood

$$p(x|\theta) = \theta^2 x \exp(-\theta x) g(x) = \theta^2 x \exp(-\theta x) \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned}
\frac{\partial}{\partial\theta} E(\theta) &= \sum_{n=1}^{N} \frac{\frac{\partial}{\partial\theta} p(x_n|\theta)}{p(x_n|\theta)} \\
&= \sum_{n=1}^{N} \frac{x_n g(x_n) \cdot \left[2\theta \exp(-\theta x_n) - \theta^2 x_n \exp(-\theta x_n)\right]}{\theta^2 x_n \exp(-\theta x_n) g(x_n)} \\
&= \sum_{n=1}^{N} \left(\frac{2}{\theta} - x_n\right) \\
&= -\sum_{n=1}^{N} x_n + \frac{2N}{\theta} \stackrel{!}{=} 0
\end{aligned}$$

$$\Rightarrow \hat{\theta} = \frac{2N}{\sum_{n=1}^{N} x_n}$$

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Kernel Density Estimation with Gaussian Kernel

- Kernel function

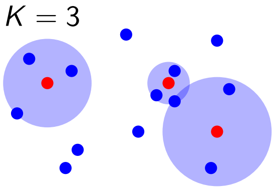
$$k(u) = \frac{1}{(2\pi)^{D/2}h} \exp\left(-\frac{u}{2h^2}\right)$$

$$K = \sum_{n=1}^{N} k(\|x - x_n\|) \qquad V = \int_{-\infty}^{\infty} k(u)du = 1$$

- Probability density estimate

$$p(x) = \frac{K}{NV} = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi)^{D/2}h} \exp\left(-\frac{\|x - x_n\|}{2h^2}\right)$$

K-Nearest Neighbor Density Estimation



- Fix K, estimate V from data
- Consider a hypersphere centered at x and let it grow to volume V^* that includes K of the given N data points
- Then

$$p(x) = \frac{K}{NV^*}$$

- Strictly speaking, the model produced by K-NN is not a true density model, because the integral over all spaces may diverge
- E.g. consider $K = 1$ and a sample exactly on a data point $x = x_j$

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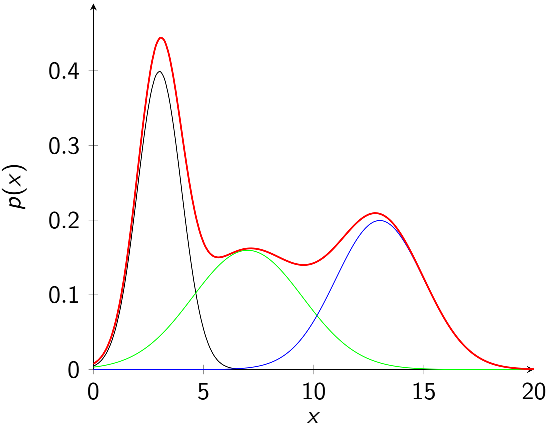
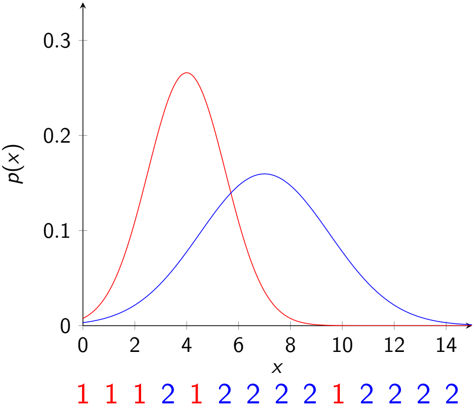
Expectation Maximization Algorithm for GMM

- Generative model

$$p(x|\theta) = \sum_{k=1}^{K} p(k)p(x|\theta_k, k)$$



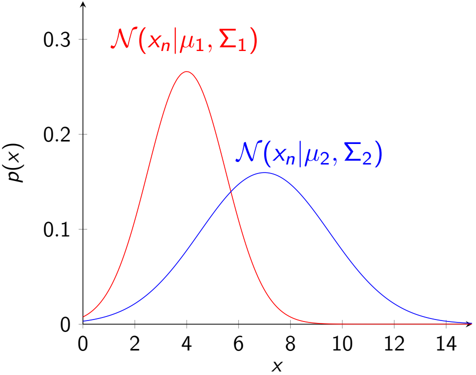
Maximum Likelihood - known assignments



If assignment $h(k|x)$ is known, we can estimate parameters:

$$\mu_1 = \frac{\sum_{n=1}^{N} h(k=1|x_n)x_n}{\sum_{n=1}^{N} h(k=1|x_n)} \qquad \mu_2 = \frac{\sum_{n=1}^{N} h(k=2|x_n)x_n}{\sum_{n=1}^{N} h(k=2|x_n)}$$

Maximum Likelihood - known mixtures



If parameters μ_k, Σ_k are known, we can estimate $\mathcal{N}(x_n|\mu_k, \Sigma_k)$ for each mixture component and sample x_n.

Iterative Optimization: Expectation Maximization (EM)

- E-Step: **softly** assign samples to mixture components

$$\gamma_k(x_n) = \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}(x_n|\mu_{k'}, \Sigma_{k'})}$$

- M-Step: re-estimate mixture parameters based on soft assignment

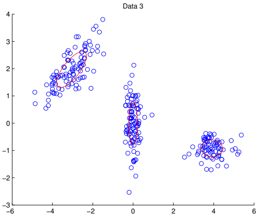
$$\hat{N}_k = \sum_{n=1}^{N} \gamma_k(x_n) \qquad \hat{\pi}_k = \frac{\hat{N}_k}{N}$$

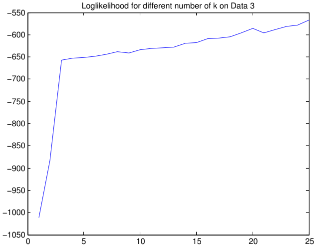
$$\hat{\mu}_k = \frac{1}{\hat{N}_k} \sum_{n=1}^{N} \gamma_k(x_n) x_n$$

$$\widehat{\Sigma}_k = \frac{1}{\hat{N}_k} \sum_{n=1}^{N} \gamma_k(x_n)(x_n - \hat{\mu}_k)(x_n - \hat{\mu}_k)^T$$

Optimal number of clusters k

- What is the optimal number of clusters?





- You can NOT use the log-likelihood!
  - Potentially each point forms it own cluster: $\mathcal{L}(\theta) = 0$
- There is no "good" evaluation of clustering.