Intelligent Data Analysis

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Exercise sheet – week 8 – Gaussian Mixture Models (GMMs)

1. Let $X = \{x_1, \dots, x_N\}$be a set of real numbers.
    a. Show that the Maximum Likelihood estimate of the parameters m and v of a Gaussian probability density function for the set are given by:
    $m = \frac{1}{N}\sum_{n=1}^{N} x_n$, $v = \frac{1}{N}\sum_{n=1}^{N}(x_n - m)^2$. **[6 marks]**
    b. Are these values of and a local or global maximum? Justify your answer. **[4 marks]**

Solution:

a. The derivation of m was done in class. For v we want to maximise

$$P(X) = \prod_{n=1}^{N} p(x_n|m, v)$$

As a function of v. Note that

$$\log\big(P(X)\big) = \sum_{n=1}^{N} \log\big(p(x_n|m, v)\big) = \sum_{n=1}^{N} -\frac{1}{2}\log\,(2\pi v) - \frac{(x_n - m)^2}{2v}$$

Therefore,

$$\frac{d}{dv}\log\big(P(X)\big) = -\sum_{n=1}^{N} \frac{d}{dv}[-\frac{1}{2}log(2\pi v) - \frac{(x_n - m)^2}{2v}]$$

$$= -\sum_{n=1}^{N}[-\frac{1}{2} \times \frac{2\pi}{2\pi v} - \frac{2v \times 0 - 2(x_n - m)^2}{4v^2}]$$

Setting this to zero and multiplying by $2v^2$ gives

$$0 = \sum_{n=1}^{N}[v - (x_n - m)^2]$$

From which it follows that

$$v = \frac{1}{N}\sum_{n=1}^{N}(x_n - m)^2$$

b. They are a global optimum. Unlike the case with a Gaussian mixture model the solution is closed and has a unique solution. Of course, to demonstrate that the critical point is a maximum rather than a minimum you also need to look at the second derivative.

2. A 2-dimensional Gaussian PDF g has mean $m = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$ and covariance matrix $C = \begin{bmatrix} 13 & -5.2 \\ -5.2 & 7 \end{bmatrix}$.

    The matrix C has eigenvalue decomposition $\mathrm{C} = \mathrm{UDU}^{\mathrm{T}}$, where:

$$U = \begin{bmatrix} cos\left(\frac{\pi}{3}\right) & -sin\left(\frac{\pi}{3}\right) \\ sin\left(\frac{\pi}{3}\right) & cos\left(\frac{\pi}{3}\right) \end{bmatrix}, D = \begin{bmatrix} 4 & 0 \\ 0 & 16 \end{bmatrix}.$$

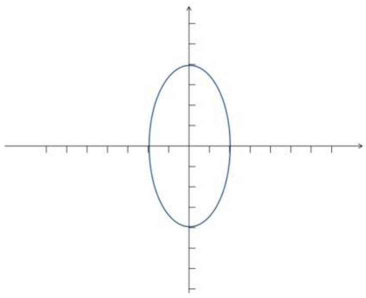
a. Sketch a 1-standard-deviation contour for g. **[4 marks].**

b. Calculate $g\left(\begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}\right)$. Show all of your calculations. **[4 marks].**

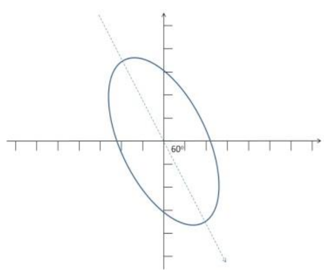
Solution:

a. First notice that the matrix U implements a rotation anti-clockwise around the origin through an angle of $\frac{\pi}{3}$.

Next use the fact that relative to the new basis (consisting of the eigenvectors of C, which are the columns of U), the covariance matrix is $D = \begin{bmatrix} 4 & 0 \\ 0 & 16 \end{bmatrix}$, and so the 1-standard deviation contour looks like figure (A) below. To get the required contour this needs to be rotated anti-clockwise though 60°, as in figure (B) below.



(A)



(B)

b. To calculate g$\left(\begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}\right)$ use the standard formula for a multivariate Gaussian PDF:

$$g(x) = \frac{1}{\sqrt{(2\pi)^d|C|}} e^{-\frac{1}{2}(x-m)^T C^{-1}(x-m)}$$

with $d = 2, m = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$ and $C = \begin{bmatrix} 13 & -5.2 \\ -5.2 & 7 \end{bmatrix}$.

We have: $|C| = 64, C^{-1} = \begin{bmatrix} 0.109 & 0.081 \\ 0.081 & 0.203 \end{bmatrix}$, so

$$g\left(\begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}\right) = \frac{1}{\sqrt{(2\pi)^2 \times 64}} e^{-\frac{1}{2}\left(\begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \end{bmatrix}\right)^T \begin{bmatrix} 0.109 & 0.081 \\ 0.081 & 0.203 \end{bmatrix}\left(\begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \end{bmatrix}\right)} = 0.0188$$

3. What are the similarities and differences between using a Mcomponent GMM to model a set of data points in N dimensional space compared to using a set of M centroids obtained through clustering?

[4 marks].

Solution:

Similarities:

a. Both methods model the data using a small set of carefully positioned data points. In clustering these are the M centroids $c_1, \dots, c_M$and in a GMM these are the M component means $\mu_1, \dots, \mu_M$.

Differences:

a. In clustering there is no further information. In a GMM, as well as the component means $\mu_1, \dots, \mu_M$ we have the component variances $\vartheta_1, \dots, \vartheta_M$, which indicate the spread of the data around the mean, and the component weights $w_1, \dots, w_M$ which indicate the proportion of the data that is modelled by the m^{th} component.
b. During training, in clustering a data point x is associated with its closest centroid c_x and only contributes to the re-estimation of the centroid c_x, so

$$c_{new} = \frac{1}{N_c} \sum_{\substack{c \text{ is closest} \\ \text{centroid to } x_n}} x_n$$

where N_c is the number of data points that have c as their closest centroid. In the E-M algorithm all of the data points contribute to the re-estimation of all of the centroids, but the extent to which x contributes to the reestimate of the m^{th} component depends on the posterior probability of the m^{th} component given x:

$$\mu_m^{new} = \frac{1}{P_m} \sum_{n=1}^{N} P(m|x_n) x_n$$

where $P(m|x_n)$ is the probability of the m^{th} GMM component given the data point x_n and $P_m = \sum_{n=1}^{N} P(m|x_n)$.

4. Let $X = \{x_1, x_2, x_3, x_4\}$, where $x_1 = 1$, $x_2 = 7$, $x_3 = 5$, $x_4 = 4$. Suppose that:

- g_1 is a Gaussian PDF with mean $m_1 = 2$ and variance $v_1 = 2$, and
- g_2 is a Gaussian PDF with mean $m_2 = 3$ and variance $v_2 = 2$, and
- g is the Gaussian Mixture Model $g(x) = 0.3 \times g_1(x) + 0.7 \times g_2(x)$.

Calculate the new values of the means m_1 and m_2 after the application of one iteration of the E-M algorithm with the samples X. **[8 marks].**

Solution:
We need to calculate the (posterior) probabilities $P(1|x_n)$ and $P(2|x_n)$ for each data point x_n, where $P(m|x_n)$ is the posterior probability of the m^{th} component given the data point x_n.

First note that, for example:

$$g_1(x_n) = \frac{1}{\sqrt{2\pi v_1}} e^{-\frac{(x_n - m_1)^2}{2v_1}}$$

So,

$$g_1(x_1) = g_1(1) = \frac{1}{\sqrt{2\pi \times 2}} e^{-\frac{(1-2)^2}{2\times 2}} = \frac{1}{2\sqrt{\pi}} e^{-\frac{1}{4}} = 0.22$$

Similarly,

$$g_1(x_2) = 0.0005, g_1(x_3) = 0.03, g_1(x_4) = 0.104$$
$$g_2(x_1) = 0.04, g_2(x_2) = 0.03, g_2(x_3) = 0.03, g_2(x_4) = 0.035$$

Now apply Bayes' rule to obtain the posterior probabilities:

$$P(1|x_1) = \frac{g_1(x_1)w_1}{g_1(x_1)w_1 + g_2(x_1)w_2} = \frac{0.22 \times 0.3}{0.22 \times 0.3 + 0.04 \times 0.7} = 0.7$$

Similarly,

$$P(1|x_2) = 0.008, P(1|x_3) = 0.3, P(1|x_4) = 0.56$$
$$P(2|x_1) = 0.3, P(2|x_2) = 0.99, P(2|x_3) = 0.7, P(2|x_4) = 0.44$$

Therefore,

$$\overline{m_1} = \frac{P(1|x_1)x_1 + P(1|x_2)x_2 + P(1|x_3)x_3 + P(1|x_4)x_4}{P(1|x_1) + P(1|x_2) + P(1|x_3) + P(1|x_4)}$$
$$= \frac{0.7 \times 1 + 0.008 \times 7 + 0.3 \times 5 + 0.56 \times 4}{0.7 + 0.008 + 0.3 + 0.56} = 2.86$$

Similarly, $\overline{m_2} = 5.14$.

[Total marks 30]