STA 414/2104, Spring 2014, Practice Problem Set \#2, Answers

Question 1: Suppose we model the relationship of a real-valued response variable, $y$, to a single real input, $x$, using a Gaussian process model in which the mean is zero and the covariances of the observed responses are given by

$$
\operatorname{Cov}\left(y_{i}, y_{i^{\prime}}\right)=0.5^{2} \delta_{i, i^{\prime}}+K\left(x_{i}, x_{i^{\prime}}\right)
$$

with the noise-free covariance function, $K$, defined by

$$
K\left(x, x^{\prime}\right)= \begin{cases}1-\left|x-x^{\prime}\right| & \text { if }\left|x-x^{\prime}\right|<1 \\ 0 & \text { otherwise }\end{cases}
$$

Suppose we have four training cases, as follows:

$$
\begin{array}{rr}
x & y \\
0.5 & 2.0 \\
2.8 & 3.3 \\
1.6 & 3.0 \\
3.9 & 2.7
\end{array}
$$

Recall that the conditional mean of the response in a test case with input $x_{*}$, given the responses in the training cases, is $k^{T} C^{-1} y$, where $y$ is the vector of training responses, $C$ is the covariance matrix of training responses, and $k$ is the vector of convariances of training responses with the response in the test case.

Find the predictive mean for the response in a test case in which the input is $x_{*}=1.2$.
The covariance matrix of the training responses is

$$
C=\left[\begin{array}{cccc}
1+0.5^{2} & 0 & 0 & 0 \\
0 & 1+0.5^{2} & 0 & 0 \\
0 & 0 & 1+0.5^{2} & 0 \\
0 & 0 & 0 & 1+0.5^{2}
\end{array}\right]
$$

The inverse of this is

$$
C^{-1}=\left[\begin{array}{cccc}
0.8 & 0 & 0 & 0 \\
0 & 0.8 & 0 & 0 \\
0 & 0 & 0.8 & 0 \\
0 & 0 & 0 & 0.8
\end{array}\right]
$$

The vector of covariances of the test response with the training responses is

$$
k=\left[\begin{array}{c}
1-0.7 \\
0 \\
1-0.4 \\
0
\end{array}\right]=\left[\begin{array}{c}
0.3 \\
0 \\
0.6 \\
0
\end{array}\right]
$$

So $k^{T} C^{-1}=[0.2400 .480]$, and the predictive mean for the test response is

$$
k^{T} C^{-1} y=0.24 \times 2.0+0.48 \times 3.0=1.92
$$

Question 2: Recall that for a Gaussian process model the predictive distribution for the response $y^{*}$ in a test case with inputs $x^{*}$ has mean and variance given by

$$
\begin{aligned}
E\left[y^{*} \mid x^{*}, \text { training data }\right] & =k^{T} C^{-1} y \\
\operatorname{Var}\left[y^{*} \mid x^{*}, \text { training data }\right] & =v-k^{T} C^{-1} k
\end{aligned}
$$

where $y$ is the vector of observed responses in training cases, $C$ is the matrix of covariances for the responses in training cases, $k$ is the vector of covariances of the response in the test case with the responses in training cases, and $v$ is the prior variance of the response in the test case.
a) Suppose we have just one training case, with $x_{1}=3$ and $y_{1}=4$. Suppose also that the noise-free covariance function is $K\left(x, x^{\prime}\right)=2^{-\left|x-x^{\prime}\right|}$, and the variance of the noise is $1 / 2$. Find the mean and variance of the predictive distribution for the response in a test case for which the value of the input is 5 .
The mean of the preditive distribution is

$$
K(3,5)[K(3,3)+1 / 2]^{-1}(4)=(1 / 4)[1+1 / 2]^{-1}(4)=4 / 6
$$

The variance of the predictive distribution is
$[K(5,5)+1 / 2]-K(3,5)[K(3,3)+1 / 2]^{-1} K(3,5)=[1+1 / 2]-(1 / 4)[1+1 / 2]^{-1}(1 / 4)=35 / 24$
b) Repeat the calculations for (a), but using $K\left(x, x^{\prime}\right)=2^{+\left|x-x^{\prime}\right|}$. What can you conclude from the result of this calculation?
The mean of the preditive distribution is

$$
K(3,5)[K(3,3)+1 / 2]^{-1}(4)=(4)[1+1 / 2]^{-1}(4)=32 / 3
$$

The variance of the predictive distribution is
$[K(5,5)+1 / 2]-K(3,5)[K(3,3)+1 / 2]^{-1} K(3,5)=[1+1 / 2]-(4)[1+1 / 2]^{-1}(4)=-55 / 6$
But variances cannot be negative! We can conclude that $K\left(x, x^{\prime}\right)=2^{+\left|x-x^{\prime}\right|}$ is not a valid covariance function - it is not positive semi-definite.

Question 3: Suppose that we are fitting a Gaussian mixture model for data items consisting of a single real value, $x$, using $K=2$ components. We have $N=5$ training cases, in which the values of $x$ are as follows:

$$
5, \quad 15, \quad 25, \quad 30, \quad 40
$$

We use the EM algorithm to find the maximum likeihood estimates for the model parameters, which are the mixing proportions for the two components, $\pi_{1}$ and $\pi_{2}$, and the means for the two components, $\mu_{1}$ and $\mu_{2}$. The standard deviations for the two components are fixed at 10 .

Suppose that at some point in the EM algorithm, the E step found that the responsibilities of the two components for the five data items were as follows:

$$
\begin{array}{ll}
r_{i 1} & r_{i 2} \\
0.2 & 0.8 \\
0.2 & 0.8 \\
0.8 & 0.2 \\
0.9 & 0.1 \\
0.9 & 0.1
\end{array}
$$

What values for the parameters $\pi_{1}, \pi_{2}, \mu_{1}$, and $\mu_{2}$ will be found in the next M step of the algorithm?

The new estimates will be

$$
\begin{aligned}
& \pi_{1}=(0.2+0.2+0.8+0.9+0.9) / 5=0.6 \\
& \pi_{2}=(0.8+0.8+0.2+0.1+0.1) / 5=0.4 \\
& \mu_{1}=(0.2 \times 5+0.2 \times 15+0.8 \times 25+0.9 \times 30+0.9 \times 40) /(0.2+0.2+0.8+0.9+0.9)=29 \\
& \mu_{2}=(0.8 \times 5+0.8 \times 15+0.2 \times 25+0.1 \times 30+0.1 \times 40) /(0.8+0.8+0.2+0.1+0.1)=14
\end{aligned}
$$

Question 4: Consider a two-component Gaussian mixture model for univariate data, in which the probability density for an observation, $x$, is

$$
(1 / 2) N(x \mid \mu, 1)+(1 / 2) N\left(x \mid \mu, 2^{2}\right)
$$

Here, $N\left(x \mid \mu, \sigma^{2}\right)$ denotes the density for $x$ under a univariate normal distribution with mean $\mu$ and variance $\sigma^{2}$. Notice that mixing proportions are equal for this mixture model, that the two components have the same mean, and that the standard deviations of the two components are fixed at 1 and 2 . There is only one model parameter, $\mu$.

Suppose we wish to estimate the $\mu$ parameter by maximum likelihood using the EM algorithm. Answer the following questions regarding how the E step and $M$ step of this algorithm operate, if we have the three data points below:

$$
4.0,4.6,2.0
$$

Here is a table of standard normal probability densities that you may find useful:

$$
\begin{array}{r|ccccccccccccccccccccc}
x & 0.0 & 0.1 & 0.2 & 0.3 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.9 & 1.0 & 1.1 & 1.2 & 1.3 & 1.4 & 1.5 & 1.6 & 1.7 & 1.8 & 1.9 & 2.0 \\
\hline N(x \mid 0,1) & .40 & .40 & .39 & .38 & .37 & .35 & .33 & .31 & .29 & .27 & .24 & .22 & .19 & .17 & .15 & .13 & .11 & .09 & .08 & .07 & .05
\end{array}
$$

a) Find the responsibilities that will be computed in the E step if the model parameter estimates from the previous M step are $\mu=4, \sigma_{1}=1$, and $\sigma_{2}=2$. Since the responsibilities for the two components must add to one, it is enough to give $r_{i 1}=P$ (component $1 \mid x_{i}$ ) for $i=1,2,3$.
First, note that the normal density function with mean $\mu$ and variance $\sigma^{2}$ is $N\left(x \mid \mu, \sigma^{2}\right)=$ $(1 / \sigma) N((x-\mu) / \sigma \mid 0,1)$. Also $N(-x \mid 0,1)=N(x \mid 0,1)$.
Using Bayes' Rule, we get that

$$
P(\text { component } 1 \mid x)=\frac{(1 / 2) N(x \mid \mu, 1)}{(1 / 2) N(x \mid \mu, 1)+(1 / 2) N\left(x \mid \mu, 2^{2}\right)}
$$

Applying this the three observations, we get

$$
\begin{aligned}
& r_{1} 1=\frac{(1 / 2) 0.40}{(1 / 2) 0.40+(1 / 2)(1 / 2) 0.40}=2 / 3 \\
& r_{2} 1=\frac{(1 / 2) 0.33}{(1 / 2) 0.33+(1 / 2)(1 / 2) 0.38}=33 / 52 \\
& r_{3} 1=\frac{(1 / 2) 0.05}{(1 / 2) 0.05+(1 / 2)(1 / 2) 0.24}=5 / 17
\end{aligned}
$$

b) Using the responsibilities that you computed in part (a), find the estimate for $\mu$ that will be found in the next $M$ step. Recall that the M step maximizes the expected value of the log of the probability density for $x_{1}, x_{2}, x_{3}$ and the unknown component indicators, with the expectation taken with respect to the distribution for the component indicators found in the previous E step.
The expected log likelihood is

$$
\sum_{i=1}^{3}\left[r_{i 1}\left(-(1 / 2)\left(x_{i}-\mu\right)^{2}\right)+\left(1-r_{i 1}\right)\left(-(1 / 2)\left(x_{i}-\mu\right) / 2^{2}\right)\right]
$$

To find the maximum of this with respect to $\mu$, we take the derivative with respect to $\mu$, which is

$$
\sum_{i=1}^{3}\left[r_{i 1}\left(x_{i}-\mu\right)+\left(1-r_{i 1}\right)\left(x_{i}-\mu\right) / 4\right]
$$

Setting this to zero and solving for $\mu$ gives

$$
\hat{\mu}=\frac{\sum_{i=1}^{3}\left(r_{i 1}+\left(1-r_{i 1}\right) / 4\right) x_{i}}{\sum_{i=1}^{3}\left(r_{i 1}+\left(1-r_{i 1}\right) / 4\right)}=\frac{(3 / 4) 4.0+(151 / 208) 4.6+(25 / 68) 2.0}{(3 / 4)+(151 / 208)+(25 / 68)}
$$

Question 5: Consider a binary classification task in which a $0 / 1$ response, $y$, is to be predicted from three binary covariates, $x_{1}, x_{2}, x_{3}$. We have six training cases, as follows:

| $y$ | $x_{1}$ | $x_{2}$ | $x_{3}$ |
| :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 1 |
| 0 | 0 | 1 | 0 |
| 1 | 1 | 0 | 1 |
| 1 | 1 | 1 | 0 |
| 1 | 0 | 0 | 1 |
| 1 | 1 | 0 | 0 |

We decide to use a naive Bayes model for this task, in which the three covariates are modeled as being independent within each class. The distribution for covariate $j$ within class $k$ is modeled as $\operatorname{Bernoulli}\left(\theta_{k j}\right)$. We estimate the probabilities of the classes and $\theta_{k j}$ for $k=0,1$ and $j=1,2,3$ from the training data, by maximum likelihood.
a) Based on the training data above, what will be the estimates for the class probabilities and for the $\theta_{k j}$ parameters?
The class probabilities will be estimated from the frequencies in the training data as $P(y=$ $0)=2 / 6=1 / 3$ and $P(y=1)=4 / 6=2 / 3$.
The probabilities for the $x_{i}$ given $y=0$ will be estimated from the two training cases with $y=0$ as $\theta_{01}=\theta_{02}=\theta_{03}=1 / 2$.
The probabilities for the $x_{i}$ given $y=1$ will be estimated from the four training cases with $y=0$ as $\theta_{11}=3 / 4, \theta_{12}=1 / 4$, and $\theta_{13}=2 / 4=1 / 2$.
b) According to this naive Bayes model, using the training data above, what is that probability that $y=1$ for each of the test cases below?

- $x_{1}=1, x_{2}=1, x_{3}=0$

Answer:

$$
\begin{aligned}
P(y & \left.=1 \mid x_{1}=1, x_{2}=1, x_{3}=0\right) \\
& =\frac{P(y=1) P\left(x_{1}=1, x_{2}=1, x_{3}=0 \mid y=1\right)}{P(y=0) P\left(x_{1}=1, x_{2}=1, x_{3}=0 \mid y=0\right)+P(y=1) P\left(x_{1}=1, x_{2}=1, x_{3}=0 \mid y=1\right)} \\
& =\frac{(2 / 3)(3 / 4)(1 / 4)(1 / 2)}{(1 / 3)(1 / 2)(1 / 2)(1 / 2)+(2 / 3)(3 / 4)(1 / 4)(1 / 2)} \\
& =3 / 5
\end{aligned}
$$

- $x_{1}=1, x_{2}=0, x_{3}=1$

Answer:

$$
\begin{aligned}
P(y & \left.=1 \mid x_{1}=0, x_{2}=0, x_{3}=1\right) \\
& =\frac{P(y=1) P\left(x_{1}=1, x_{2}=0, x_{3}=1 \mid y=1\right)}{P(y=0) P\left(x_{1}=1, x_{2}=0, x_{3}=1 \mid y=0\right)+P(y=1) P\left(x_{1}=1, x_{2}=0, x_{3}=1 \mid y=1\right)} \\
& =\frac{(2 / 3)(3 / 4)(3 / 4)(1 / 2)}{(1 / 3)(1 / 2)(1 / 2)(1 / 2)+(2 / 3)(3 / 4)(3 / 4)(1 / 2)} \\
& =9 / 11
\end{aligned}
$$

c) Suppose that the loss from classifying an item as being in class 1 when it is really in class 0 is twice as large as the loss from classifying an item as being in class 0 when it is really in class 1 . How should you classify each of the following test cases?

- $x_{1}=1, x_{2}=1, x_{3}=0$

Let the loss classifying as class 1 when really class 0 be 2, and the loss classifying as class 0 when really class 1 be 1 .
Expected loss if you classify as class 0 is $1 \times P\left(y=1 \mid x_{1}=1, x_{2}=1, x_{3}=0\right)=3 / 5$.
Expected loss if you classify as class 1 is $2 \times P\left(y=0 \mid x_{1}=1, x_{2}=1, x_{3}=0\right)=4 / 5$.
So you should classify as class 0 .

- $x_{1}=1, x_{2}=0, x_{3}=1$

Expected loss if you classify as class 0 is $1 \times P\left(y=1 \mid x_{1}=1, x_{2}=0, x_{3}=1\right)=9 / 11$. Expected loss if you classify as class 1 is $2 \times P\left(y=0 \mid x_{1}=1, x_{2}=0, x_{3}=1\right)=4 / 11$. So you should classify as class 1.

