Homework 3: STA414 LEC0101, January 2018

This assignment isn't for credit; please don't submit your work. As before, you may use Piazza to compare your approaches, your answers, or useful starter code.

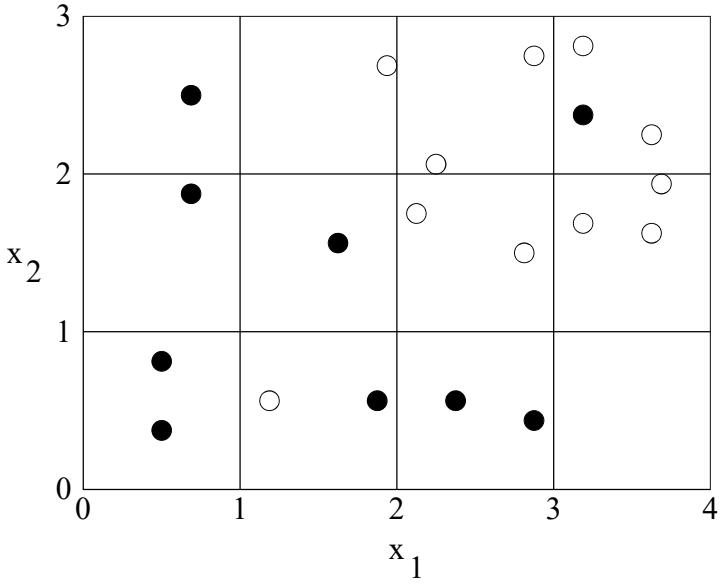
A. Examining the 10×3 data set in HW2, none of the pairs of mean vectors (cases a, b, or c) seems particularly plausible. Choose any optimization technique from Week 3 to find the maximum-likelihood estimates of the pair of mean vectors that actually produced the dataset. As before, you may use R, Python, or another language of your choice.

B. *(Bayesian warmup question, from John Rice 3rd ed. pp 94-96)* A particular coin has a probability Θ of coming up heads when flipped, and your prior knowledge about Θ can be represented by a uniform probability density on [0, 1]. Now suppose the coin is flipped n times and you observe it coming up heads x times. What is the posterior probability distribution for Θ? **Hint:** recall that the uniform distribution is a special case of the beta distribution.

C. *(From Radford Neal)* Do questions 1 to 11 on the following pages. The plan is for *a variation on at least one of these 11 questions* to appear on your test on 12 February. (Question 4 is similar to the first question on the February 2017 test, for example.)

Part C questions

Question 1: Consider a classification problem in which there are two real-valued inputs, x_1 and x_2, and a binary (0/1) target (class) variable, y. There are 20 training cases, plotted below. Cases where $y = 1$ are plotted as black dots, cases where $y = 0$ as white dots, with the location of the dot giving the inputs, x_1 and x_2, for that training case.



A) Estimate the error rate of the one-nearest-neighbor (1-NN) classifier for this problem using leave-one-out cross validation. (That is, using S-fold cross validation with S equal to the number of training cases, in which each training case is predicted using all the other training cases.)

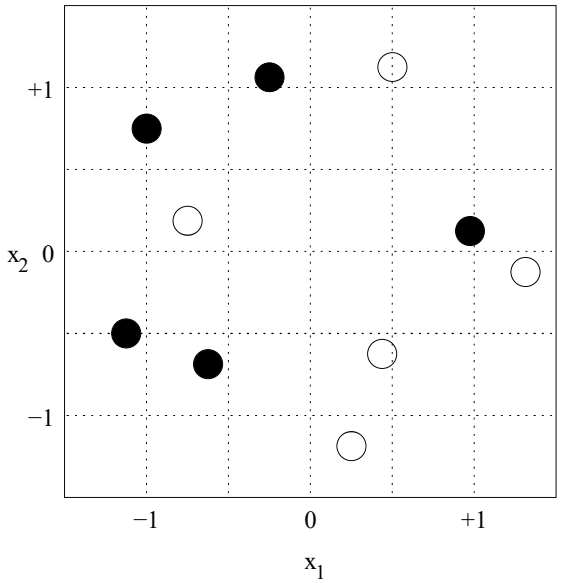
B) Suppose we use the three-nearest-neightbor (3-NN) method to estimate the probability that a test case is in class 1. For test cases with each of the following sets of input values, find the estimated probability of class 1.

$x_1 = 1,\ x_2 = 1$

$x_1 = 2,\ x_2 = 2$

$x_1 = 3,\ x_2 = 0$

Question 2: Here is a plot of 10 training cases for a binary classification problem with two input variables, x_1 and x_2, with points in class 0 in white and points in class 1 in black:



We wish to compare three variations on the K-nearest-neighbor method for this problem, using 10-fold cross validation (ie, we leave out each training case in turn and try to predict it from the other nine). We use the fraction of cases that are misclassified as the error measure. We set $K = 1$ in all methods, so we just predict the class in a test case from the class of its nearest neighbor.

A) The first method looks only at x_1, so the distance between cases with input vectors x and x' is $|x_1 - x'_1|$. What is the cross-validation error for this method?

B) The second method looks only at x_2, so the distance between cases with input vectors x and x' is $|x_2 - x'_2|$. What is the cross-validation error for this method?

C) The third method looks at both inputs, and uses Euclidean distance, so the distance between cases with input vectors x and x' is $\sqrt{(x_1 - x'_1)^2 + (x_2 - x'_2)^2}$. What is the cross-validation error for this method?

D) If we use the method (from among these three) that is best according to 10-fold cross-validation, what will be the predicted class for a test case with inputs $x = (-0.25, 0.25)$?

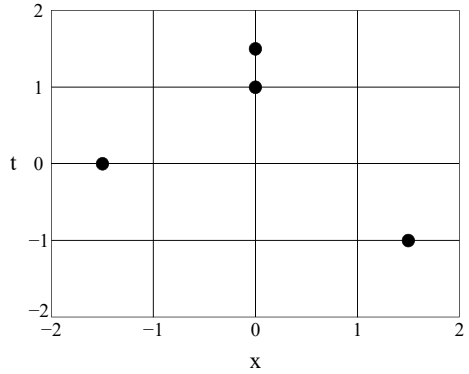
Question 3: Consider a linear basis function regression model, with one input and the following three basis functions:

$$\begin{aligned} \phi_0(x) &= 1 \\ \phi_1(x) &= x \\ \phi_2(x) &= \begin{cases} 1 - x^2 & \text{if } |x| < 1 \\ 0 & \text{if } |x| \geq 1 \end{cases} \end{aligned}$$

The model for the target variable, y, is that $P(y \mid x, \beta) = N(y \mid f(x, \beta), 1)$, where

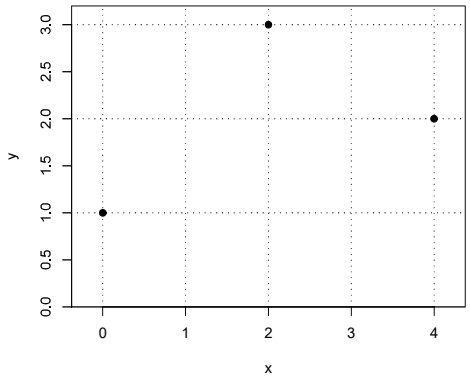
$$f(x, \beta) = \sum_{j=0}^{m-1} \beta_j \phi_j(x)$$

Suppose we have four data points, as plotted below:



What is the maximum likelihood (least squares) estimate for the parameters β_0, β_1, and β_2? Elaborate calculations should not be necessary.

Question 4: Below is a plot of a dataset of $n = 3$ observations of (x_i, y_i) pairs:

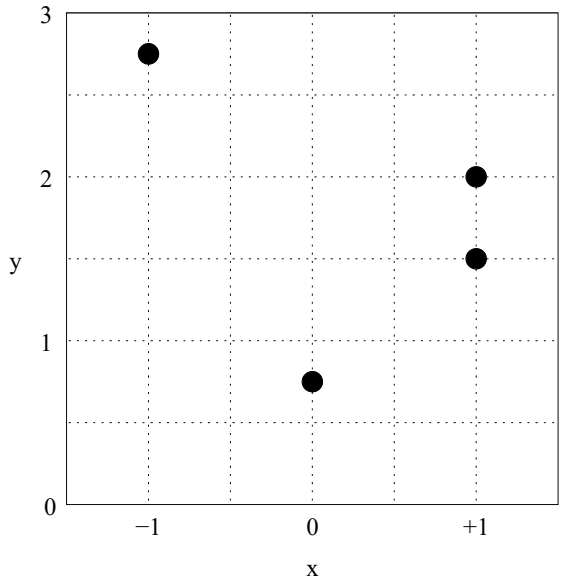


In other words, the data points are $(0, 1)$, $(2, 3)$, $(4, 2)$.

Suppose we model this data with a linear basis function model with $m = 2$ basis functions given by $\phi_0(x) = 1$ and $\phi_1(x) = x$. We use a quadratic penalty of the form $\lambda\beta_1^2$, which penalizes only the regression coefficient for $\phi_1(x)$, not that for $\phi_0(x)$.

Suppose we use squared error from three-fold cross-validation (ie, with each validation set having only one case) to choose the value of λ. Suppose we consider only two values for λ — one very close to zero, and one very large. For the data above, will we choose λ near zero, or λ that is very big?

Question 5: Consider a linear basis function model for a regression problem with response y and a single scalar input, x, in which the basis functions are $\phi_0(x) = 1$, $\phi_1(x) = x$, and $\phi_2(x) = |x|$. Below is a plot of four training cases to be fit with this model:



A) Suppose we fit this linear basis function model by least squares. What will be the estimated coefficients for the three basis functions, $\widehat{\beta}_0$, $\widehat{\beta}_1$, and $\widehat{\beta}_2$?

B) Suppose we fit this linear basis function model by penalized least squares, with a penalty of $\lambda|\beta_1|$ (note that the penalty does not depend on β_0 and β_2). What will be the estimated coefficients for the three basis functions, $\widehat{\beta}_0$, $\widehat{\beta}_1$, and $\widehat{\beta}_2$ in the limit as λ goes to infinity?

C) Suppose we use the form of the penalty as in part (B), but with $\lambda = 1$. Will the penalized least squares estimate for β_1 be exactly zero? Show why or why not.

Question 6: Suppose that we observe a binary (0/1) variable, Y_1. We do not know the probability, θ, that Y_1 will be 1, but we have a prior distribution for θ, that has the following density function on the interval $(0, 1)$:

$$P(\theta) \;\; = \;\; 12\left(\theta - \frac{1}{2}\right)^2$$

A) Find as simple a formula as you can for the density function of the posterior distribution of θ given that we observe $Y_1 = 1$. Your formula should give the correcty normalized density.

B) Suppose that Y_2 is a future observation, that is independent of Y_1 given θ. Find the predictive probability that $Y_2 = 1$ given that $Y_1 = 1$ — ie, find $P(Y_2 = 1 \,|\, Y_1 = 1)$.

Question 7: Let X_1, X_2, X_3, ... for a sequence of binary (0/1) random variables. Given a value for θ, these random variables are independent, and $P(X_i = 1) = \theta$ for all i. Suppose that we are sure that θ is at least $1/2$, and that our prior distribution for θ for values $1/2$ and above is uniform on the interval $[1/2, 1]$. We have observed that $X_1 = 0$, but don't know the values of any other X_i.

A) Write down the likelihood function for θ, based on the observation $X_1 = 0$.

B) Find an expression for the posterior probability density function of θ given $X_1 = 0$, simplified as much as possible, with the correct normalizing constant included.

C) Find the predictive probability that $X_2 = 1$ given that $X_1 = 0$.

D) Find the probability that $X_2 = X_3$ given that $X_1 = 0$.

Question 8: Consider a binary classification problem in which the probability that the class, y, of an item is 1 depends on a single real-valued input, x, with the classes for different cases being independent, given a parameter ϕ and x. We use the following model for this class probability in terms of the unknown parameter ϕ:

$$P(y = 1 \mid x, \phi) \;\; = \;\; \begin{cases} 1/2 & \text{if } x \le \phi \\ 1 & \text{if } x > \phi \end{cases}$$

We have a training set consisting of the following six (x, y) pairs:

$$(0.1,\, 0),\;\; (0.3,\, 1),\;\; (0.4,\, 0),\;\; (0.6,\, 1),\;\; (0.7,\, 1),\;\; (0.8,\, 1)$$

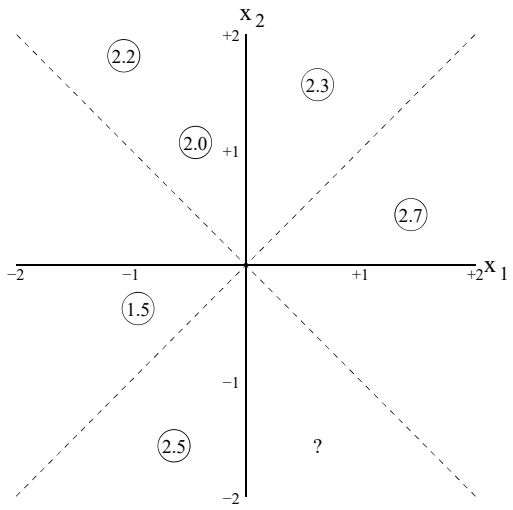
A) Draw a graph of the likelihood function for ϕ based on the six training cases above.

B) Compute the marginal likelihood for this model with this data (ie, the prior probability of the observed training data with this model and prior distribution), assuming that the prior distribution of ϕ is uniform on the interval [0.5, 1]

C) Find the posterior distribution of ϕ given the six training cases above, and the prior from part (B) Display this posterior distribution by drawing a graph of its probability density function.

D) Find the predictive probability that $y = 1$ for each of three test cases in which x has the values 0.2, 0.6, and 0.7, based on the posterior distribution you found in part (C).

Question 9: Below is a plot of six training cases for a regression problem with two inputs. The location of the circle for a training case gives the values of the two inputs, x_1 and x_2, for that case, and the number in the circle is the value of the response, y, for that case.



Suppose we use a linear basis function model for this data, with the following basis functions:

$$\phi_0(x) = 1$$

$$\phi_1(x) = \begin{cases} 1 & \text{if } x_1 > 0 \\ 0 & \text{if } x_1 \leq 0 \end{cases}$$

$$\phi_2(x) = \begin{cases} 1 & \text{if } x_1 + x_2 > 0 \\ 0 & \text{if } x_1 + x_2 \leq 0 \end{cases}$$

A) What will be the least squares estimates of the regression coefficients, β_0, β_1, and β_2, based on these six training cases (ignore the question mark in the lower right for now)? No elaborate matrix computations should be needed to answer this.

B) Based on the least squares estimates for part (A), what will be the prediction for the value of the response in a test case whose x_1 and x_2 values are given by the location of the question mark in the plot above?

C) For this training set, find and estimate of the average squared error of prediction using least squares estimates, by applying leave-one-out cross-validation (which is the same as six-fold cross validation here, since there are six training cases).

D) What will be the prediction for the test case at the question mark based on penalized least squares estimates, if the penalty has the form $\lambda(\beta_1^2 + \beta_2^2)$, and λ is very large?

Question 10: Let Y_1, Y_2, Y_3, ... be random quantities that are independent given a parameter θ, with each Y_t having the value 1, 2, or 3, with probabilities

$$P(Y_t = y \mid \theta) \;=\; \begin{cases} \theta & \text{if } y = 1 \\ 2\theta & \text{if } y = 2 \\ 1-3\theta & \text{if } y = 3 \end{cases}$$

The prior distribution for the model parameter θ is uniform on the interval $[0, 1/3]$.

For the questions below, suppose we observe that $Y_1 = 1$ and $Y_2 = 3$, but do not observe Y_3, Y_4 ....

A) Find the marginal likelihood for this data (that is, the probability that $Y_1 = 1$ and $Y_2 = 3$, integrating over the prior distribution of θ).

B) Find the posterior probability density function for θ (that is, the density for θ given $Y_1 = 1$ and $Y_2 = 3$), with the correct normalizing constant.

C) Find the predictive distribution for Y_3 given the observed data (that is, give a table of $P(Y_3 = y \,|\, Y_1 = 1,\, Y_2 = 3)$ for $y = 1, 2, 3$).

Question 11: Answer the following questions about Bayesian inference for linear basis function models. Recall that if the noise variance is σ^2, and the prior distribution for β is Gaussian with mean zero and covariance matrix S_0, the posterior distribution for β is Gaussian with mean m_n and covariance matrix S_n that can be written as follows:

$$S_n \;=\; \left[S_0^{-1} \,+\, (1/\sigma^2)\Phi^T\Phi\right]^{-1}, \qquad m_n \;=\; S_n\Phi^T y/\sigma^2$$

and the log of the marginal likelihood for the model is

$$-\frac{n}{2}\log(2\pi) \;-\; \frac{n}{2}\log(\sigma^2) \;-\; \frac{1}{2}\log\Big(\frac{|S_0|}{|S_n|}\Big) \;-\; \frac{1}{2}||y - \Phi m_n)||^2/\sigma^2 \;-\; \frac{1}{2}m_n^T S_0^{-1} m_n$$

For the questions below, assume that $S_0 = \omega^2 I$, for some positive ω.

A) Suppose we set the noise variance, σ^2, to be bigger and bigger, while fixing other aspects of the model. What will be the limiting values of the the posterior mean and covariance matrix?

B) Suppose we set ω^2, the prior variance of the β_j, to be bigger and bigger, while fixing other aspects of the model. What will be the limiting values of the the posterior mean, m_n, and covariance matrix, S_n?

C) Suppose we set ω^2 to be bigger and bigger while fixing other aspects of the model. What will be the limiting value of the marginal likelihood?

D) Suppose there is only one input (so x is a scalar), and the basis functions are $\phi_j(x) = x^j$, for $j = 0, \ldots, m-1$. The Bayesian mean prediction for the value of y in a test case with input x is found by integrating the prediction based on β (ie, the expected value of y given x and β) with respect to the posterior distribution of β. Will this final mean prediction be a polynomial function of x?