10-601 Machine Learning, Fall 2009: Homework 3

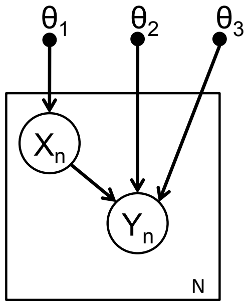
Due: Wednesday, October 7th, 10:30 am

Instructions There are 3 questions on this assignment worth the total of 140 points. Please hand in a hard copy at the beginning of the class. Refer to the webpage for policies regarding collaboration, due dates, and extensions.

1 Structured Density Estimation [40 Points]

In this problem you will have the opportunity to derive the maximum likelihood estimate (MLE) and maximum a posteriori (MAP) estimate for the parameters of a small structured model. You will also have the opportunity to derive the predictive distribution and become a better Bayesian.

Suppose you are given the simple Bayesian network in Fig. 1(a). You are told that the conditional probability tables (CPTs) for this model take the form of Table 1(b) and Table 1(c).



(a) Graphical Model

$\mathbf{P}(X=1)$	$\mathbf{P}(X=0)$
θ_1	$1-\theta_1$

(b) $\mathbf{P}(X)$

X	$\mathbf{P}(Y=1 \mid X)$	$\mathbf{P}(Y=0 \mid X)$
$X=1$	θ_2	$1-\theta_2$
$X=0$	θ_3	$1-\theta_3$

(c) $\mathbf{P}(Y \mid X)$

Figure 1: Graphical Model and Conditional Probability Tables

An expert on the study of X and Y (an XY-ologist) runs a large experiment and collects the data, $\mathcal{D} = \{(x_1, y_1), \ldots, (x_N, y_N)\}$. The marginal counts (e.g., a is the number of observations where $X = 1$ and $Y = 1$) for $\mathcal{D}$ are given by Table 1 where $a + b + c + d = N$. You will need to express your derivation using these counts.

	$Y=1$	$Y=0$
$X=1$	a	b
$X=0$	c	d

Table 1: Contingency Table

1.1 Deriving the MLE [15 Points]

We begin by deriving the MLE point estimates for $\{\theta_1, \theta_2, \theta_3\}$.

1. Show that the likelihood $\mathbf{P}(\mathcal{D} \mid \{\theta_1, \theta_2, \theta_3\})$ can be expressed as:

$$\mathbf{P}(\mathcal{D} \mid \{\theta_1, \theta_2, \theta_3\}) = \theta_1^{a+b}(1-\theta_1)^{c+d}\theta_2^{a}(1-\theta_2)^{b}\theta_3^{c}(1-\theta_3)^{d}$$

2. Take the log of the likelihood to construct the log-likelihood, $\mathcal{L}(\theta_1, \theta_2, \theta_3) = \log(\mathbf{P}(\mathcal{D} \mid \{\theta_1, \theta_2, \theta_3\}))$, as a sum of terms.

3. Why is the following expression relevant when trying to find parameters that maximize the likelihood?

$$\arg\max_x \log(f(x)) = \arg\max_x f(x)$$

4. Write the partial derivatives of the log-likelihood with respect to each parameter (i.e., $\frac{\partial \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_1}$, $\frac{\partial \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_2}$, and $\frac{\partial \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_3}$).

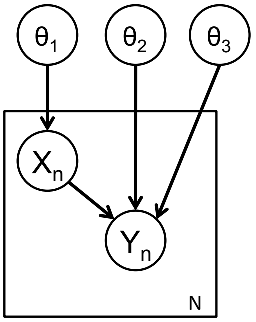
5. Do the partial derivatives with respect to each parameter depend on the other parameters? What does this say with respect to computing the maximizing joint assignment for $\{\theta_1, \theta_2, \theta_3\}$?

6. Write the second partial derivatives ($\frac{\partial^2 \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_1^2}$, $\frac{\partial^2 \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_2^2}$, and $\frac{\partial^2 \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_3^2}$) of the log-likelihood.

7. Using your answer to the previous question, argue that this function is concave with respect to each parameter in $\{\theta_1, \theta_2, \theta_3\}$ individually. How is concavity relevant to the problem of maximization?

8. Set each of the first partial derivatives (i.e., $\frac{\partial \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_1}$, $\frac{\partial \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_2}$, and $\frac{\partial \mathcal{L}(\theta_1,\theta_2,\theta_3)}{\partial \theta_3}$) equal to zero and solve for the maximizing assignment. This your maximum likelihood estimate. Comment on the form of the estimate in one sentence.

1.2 Deriving the Maximum A Posteriori (MAP) Estimate [10 Points]



(a) Graphical Model

$$\begin{aligned}\theta_1 &\sim \text{Beta}(\alpha_1, \beta_1)\\ \theta_2 &\sim \text{Beta}(\alpha_2, \beta_2)\\ \theta_3 &\sim \text{Beta}(\alpha_3, \beta_3)\end{aligned}$$

(b) Priors

Figure 2: Graphical model treating $\{\theta_1, \theta_2, \theta_3\}$ as random variables with priors.

If you were a pragmatic Bayesian you would put a prior on the parameters $\{\theta_1, \theta_2, \theta_3\}$ and compute the MAP estimate instead of the MLE. You talk to the expert on X and Y and she gives you the Beta priors in Fig. 2 where α_1, β_1, α_2, β_2, α_3, and β_3 are all positive integers. Recall from class that the $\text{Beta}(\theta \mid \alpha, \beta)$ takes the form:

$$\text{Beta}(\theta \mid \alpha, \beta) = \frac{(\alpha+\beta-1)!}{(\alpha-1)!(\beta-1)!}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$

1. Write the posterior $\mathbf{P}(\{\theta_1, \theta_2, \theta_3\} \mid \mathcal{D})$. You may want to use the likelihood from the previous question.

2. Take the log of the posterior to construct the log-posterior as a sum of terms.

3. Write the partial derivatives of the log-posterior with respect to θ_1, θ_2, and θ_3.

$$\frac{\partial \log \left(\mathbf{P}\left(\{\theta_1, \theta_2, \theta_3\} \mid \mathcal{D}\right)\right)}{\partial \theta_1} =$$
$$\frac{\partial \log \left(\mathbf{P}\left(\{\theta_1, \theta_2, \theta_3\} \mid \mathcal{D}\right)\right)}{\partial \theta_2} =$$
$$\frac{\partial \log \left(\mathbf{P}\left(\{\theta_1, \theta_2, \theta_3\} \mid \mathcal{D}\right)\right)}{\partial \theta_3} =$$

4. Is $\log \left(\mathbf{P}\left(\{\theta_1, \theta_2, \theta_3\} \mid \mathcal{D}\right)\right)$ concave with respect to θ_1, θ_2, and θ_3 individually?

5. Do the partial derivatives with respect to each parameter depend on the other parameters? What does this say with respect to computing the maximizing joint assignment for $\{\theta_1, \theta_2, \theta_3\}$?

6. Set each of the partial derivatives equal to zero and solve for the maximizing assignment to each parameter $\{\theta_1, \theta_2, \theta_3\}$. This is your MAP estimate. Comment on the form of the estimate.

1.3 Deriving the Predictive Distribution [15 Points]

A proper Bayesian would not likely settle for a MAP estimate. Instead he, she, or possibly some distribution over genders would probably marginalize away the unknown parameters to construct the posterior predictive distribution. Here we will derive the posterior predictive distributions $\mathbf{P}(X \mid \mathcal{D})$, $\mathbf{P}(Y \mid X = 0, \mathcal{D})$, and $\mathbf{P}(Y \mid X = 1, \mathcal{D})$. We will use the priors on $\{\theta_1, \theta_2, \theta_3\}$ obtained from the XY-ologist in the previous question.

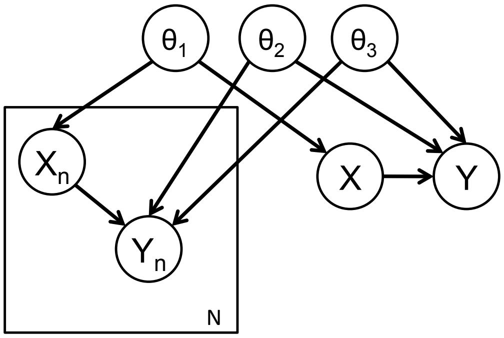


Figure 3: The model for the predictive distribution on X and Y.

1.3.1 Posterior Predictive Distribution for X

1. Using the equation for the posterior $\mathbf{P}\left(\{\theta_1, \theta_2, \theta_3\} \mid \mathcal{D}\right)$ show that:

$$\mathbf{P}\left(\{\theta_1, \theta_2, \theta_3\} \mid \mathcal{D}\right) = \mathbf{P}(\theta_1 \mid \mathcal{D})\, \mathbf{P}(\theta_2 \mid \mathcal{D})\, \mathbf{P}(\theta_3 \mid \mathcal{D})$$

The previous means that θ_1, θ_2, and θ_3 are conditionally independent given the data. Can you show any of these conditional independencies using only d-separation? (Consider showing (i) $\theta_1 \perp \theta_2 \mid \mathcal{D}$; (ii) $\theta_1 \perp \theta_3 \mid \mathcal{D}$; and (iii) $\theta_2 \perp \theta_3 \mid \mathcal{D}$.)

2. Using d-separation show that:

$$\mathbf{P}(X, \theta_1 \mid \mathcal{D}) = \mathbf{P}(X \mid \theta_1)\, \mathbf{P}(\theta_1 \mid \mathcal{D})$$

3. Argue that for some normalizing constant Z:

$$\begin{aligned}
\mathbf{P}(X = 1 \,|\, \mathcal{D}) &= \frac{1}{Z}\int_0^1 \theta_1 \left(\theta_1^{a+b}(1-\theta_1)^{c+d}\right)\left(\theta_1^{\alpha_1-1}(1-\theta_1)^{\beta_1-1}\right) d\theta_1 \\
\mathbf{P}(X = 0 \,|\, \mathcal{D}) &= \frac{1}{Z}\int_0^1 (1-\theta_1) \left(\theta_1^{a+b}(1-\theta_1)^{c+d}\right)\left(\theta_1^{\alpha_1-1}(1-\theta_1)^{\beta_1-1}\right) d\theta_1
\end{aligned}$$

4. Using the following identities where we assume r and q are positive integers:

$$\begin{aligned}
\int_0^1 z^{q-1}(1-z)^{r-1} dz &= \frac{(q-1)!(r-1)!}{(q+r-1)!} \\
r! &= r(r-1)!
\end{aligned}$$

derive the following expressions

$$\begin{aligned}
\mathbf{P}(X = 1 \,|\, \mathcal{D}) &= \frac{a+b+\alpha_1}{N+\alpha_1+\beta_1} \\
\mathbf{P}(X = 0 \,|\, \mathcal{D}) &= \frac{c+d+\beta_1}{N+\alpha_1+\beta_1}
\end{aligned}$$

This is your posterior predictive distribution for X. Comment on how it differs from the MAP estimate for θ_1 Which one gives you a 'smoother' prediction?

1.3.2 Posterior Predictive Distribution for Y

1. Using d-separation argue that:

$$\mathbf{P}(Y, \theta_2, \theta_3 \,|\, X, \mathcal{D}) = \mathbf{P}(Y \,|\, X, \theta_2, \theta_3)\,\mathbf{P}(\theta_2, \theta_3 \,|\, \mathcal{D})$$

2. Using the results from the previous questions argue that:

$$\mathbf{P}(Y \,|\, X, \mathcal{D}) = \int_0^1 \int_0^1 \mathbf{P}(Y \,|\, X, \theta_2, \theta_3)\,\mathbf{P}(\theta_2 \,|\, \mathcal{D})\,\mathbf{P}(\theta_3 \,|\, \mathcal{D})\, d\theta_2 d\theta_3$$

3. We can eliminate the double integral by evaluating it for each assignment to X separately. Using the definition of $\mathbf{P}(Y \,|\, X, \theta_2, \theta_3)$ show that:

$$\begin{aligned}
\mathbf{P}(Y \,|\, X = 1, \mathcal{D}) &= \int_0^1 \mathbf{P}(Y \,|\, X = 1, \theta_2)\,\mathbf{P}(\theta_2 \,|\, \mathcal{D})\, d\theta_2 \\
\mathbf{P}(Y \,|\, X = 0, \mathcal{D}) &= \int_0^1 \mathbf{P}(Y \,|\, X = 0, \theta_3)\,\mathbf{P}(\theta_3 \,|\, \mathcal{D})\, d\theta_3
\end{aligned}$$

The type of simplification we used above is called *context specific independence*, because it is facilitated through specific settings of the parents (these settings are called "contexts").

4. Evaluate the integrals to show that:

$$\begin{aligned}
\mathbf{P}(Y = 1 \,|\, X = 1, \mathcal{D}) &= \frac{a+\alpha_2}{a+b+\alpha_2+\beta_2} \\
\mathbf{P}(Y = 1 \,|\, X = 0, \mathcal{D}) &= \frac{c+\alpha_3}{c+d+\alpha_3+\beta_3}
\end{aligned}$$

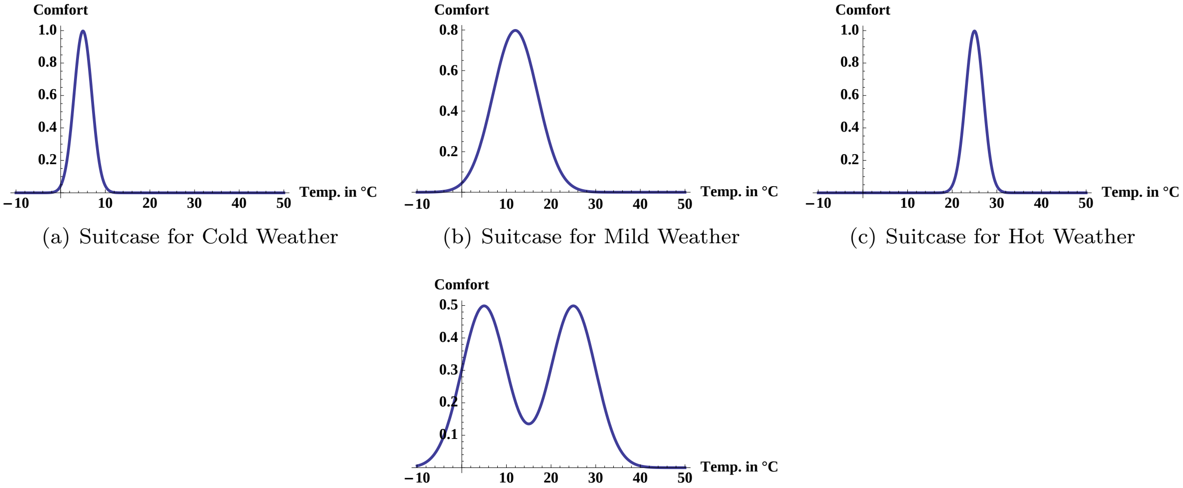
This is your predictive distribution for $Y \,|\, X$. Explain how this relates to Laplace smoothing.

5. Which parameter estimation method would likely be most robust when there is limited data: MLE, MAP, or Posterior Predictive Distribution?

2 Suitcase Packing [15 Points]

As any computer scientist will tell you, packing a suitcase is really difficult. Even if we ignore the substantial challenge of fitting everything, we are still left with the more mundane challenge of selecting the right clothing for the occasion. Naturally, we will ignore less important criteria like color and style, and focus on important characteristics like comfort with respect to temperature.

If the destination is very warm then we might want to pack clothing that will help us stay cool like swim trunks and sun-glasses. Conversely, if the destination is cold, then we would definitely want to pack gloves, a scarf, and some skis. If the destination is mild then we may want to bring pants and a light coat. What do we pack when the destination is Pittsburgh and packing for the average temperature won't suffice? To help make your life easier, we have prepared 4 prepacked suitcases at no extra charge. Naturally, we have included your utility curves for each suitcase in Fig. 4. The utility curves describe how comfortable you will be at each temperature if you select that suitcase.



(a) Suitcase for Cold Weather

(b) Suitcase for Mild Weather

(c) Suitcase for Hot Weather

(d) Suitcase for Mixed Conditions

Figure 4: The comfort zones for each suitcase. Notice that the suitcase for mixed conditions is not quite as comfortable when its hot or cold as the respective suitcases for hot and cold weather.

In this question we will investigate the disadvantages of point estimates and try to illustrate the importance of working with the posterior distribution. For this question you will not need to do any calculations or derive equations; instead, we ask you to provide concise explanations for your decisions.

2.1 The Average Temperature

As part of your preliminary planning phase you check the weather at your destination and discover that the average temperature is $15°C$. Which suitcase do you choose and why?

2.2 The Most Common Temperature

You call a friend who frequently visits your destination and he says that it is usually $25°C$. Which suitcase do you choose and why?

2.3 Working with Distributions

Feeling slightly Bayesian, you contact the National Weather Service and obtain the distribution over temperatures plotted in Fig. 5.

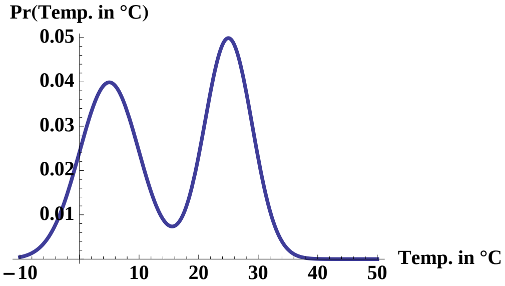


Figure 5: Temperature Distribution

1. Is the distribution in Fig. 5 consistent with the average temperature information and your friend's testimony? Explain.
2. Given the utility function u(Temperature) and the distribution $\mathbf{P}$ (Temperature) write down the integral you would need to evaluate to obtain the expected comfort.
3. Which suitcase maximizes your expected comfort and why?

3 Linear Regression [85 Points]

The linear regression method is widely used in the medical domain. In this question you will work on a prostate cancer data from a study by Stamey et al.[1] You can download the data from http://www.cs.cmu.edu/~ggordon/10601/hws/hw3/prostatecancer.csv.

Your task is to predict the level of prostate-specific antigen (PSA) using a set of medical test results. PSA is a protein produced by the cells of the prostate gland. High levels of PSA often indicate the presence of prostate cancer or other prostate disorders.

The attributes are several clinical measurements on men who have prostate cancer. There are 8 attributes: log cancer volume `lcavol`, log prostate weight (`lweight`), log of the amount of benign prostatic hyperplasia (`lbph`), seminal vesicle invasion (`svi`), `age`, log of capsular penetration (`lcp`), Gleason score (`gleason`), and percent of Gleason scores of 4 or 5 (`pgg45`). `svi` and `gleason` are categorical, that is they take values either 1 or 0; others are real-valued. We will refer to these attributes as $A_1 = \text{lcavol}, A_2 = \text{lweight}, A_3 = \text{age}, A_4 = \text{lbph}, A_5 = \text{svi}, A_6 = \text{lcp}, A_7 = \text{gleason}, A_8 = \text{pgg45}$.

Each row of the input file describes one data point: the first column is the index of the data point, the following eight columns are attributes, and the tenth column gives the log PSA level `lpsa`, the response variable we are interested in. We already randomized the data and split it into three parts corresponding to training, validation and test sets. The last column of the file indicates whether the data point belongs to the training set, validation set or test set, indicated by '1' for training, '2' for validation and '3' for testing. The training data includes 57 examples; validation and test sets contain 20 examples each.

3.1 Inspecting the Data [10 points]

1. Calculate the correlation matrix of the 8 attributes and report it in a table. The table should be 8-by-8. You can use matlab functions.
2. Report the top 2 pairs of attributes that show the highest pairwise positive correlation and the top 2 pairs of attributes that show the highest pairwise negative correlation.

[1] Stamey TA, Kabalin JN, McNeal JE et al. Prostate specific antigen in the diagnosis and treatment of the prostate. II. Radical prostatectomy treated patients. J Urol 1989;141:107683.

3.2 Solving the Linear Regression Problem [45 points]

You will now try to find several models in order to predict the `lpsa` levels. The linear regression model is

$$Y = f(X) + \epsilon$$

where ϵ is a Gaussian noise variable and

$$f(X) = \sum_{j=0}^{p} w_j \phi_j(X)$$

where p is the number of basis functions (features), ϕ_j is the jth basis function, and w_j is the weight we wish to learn for the j^{th} basis function. In the models below, we will always assume that $\phi_0(X) = 1$ represents the intercept term.

1. Write a matlab function that takes the data matrix Φ and the column vector of responses y as an input and produces the least squares fit w as the output (refer to the lecture notes for the calculation of w).

2. You will create the following three models. Note that before solving each regression problem below, you should scale each feature vector to have a zero mean and unit variance. Don't forget to include the intercept column, $\phi_0(X) = 1$, after scaling the other features. Notice that since you shifted the attributes to have zero mean, in your solutions, the intercept term will be the mean of the response variable.

   - **Model1** Features are equal to input attributes, with the addition of a constant feature ϕ_0. That is, $\phi_0(X) = 1,\ \phi_1(X) = A_1,\ \ldots,\ \phi_8(X) = A_8$. Solve the linear regression problem and report the resulting feature weights. Discuss what it means for a feature to have a large negative weight, a large positive weight, or a small weight. Would you be able to comment on the weights, if you had not scaled the predictors to have the same variance? Report mean squared error (MSE) on the training and validation data.
   - **Model2** Include additional features corresponding to pairwise products of the first six of the original attributes[2], i.e., $\phi_9(X) = A_1A_2,\ \ldots,\ \phi_{13}(X) = A_1A_6,\ \phi_{15}(X) = A_2A_3,\ \ldots,\ \phi_{23}(X) = A_5A_6$. First compute the features according to the formulas above using the unnormalized values, then shift and scale the new features to have zero mean and unit variance and add the column for the intercept term $\phi_0(X) = 1$. Report the five features whose weights achieved the largest absolute values.
   - **Model3** Starting with the results of Model1, drop the four features with the lowest weights (in absolute values). Build a new model using only the remaining features. Report the resulting weights.

3. Make two bar charts, the first to compare the *training* errors of the three models, the second to compare the *validation* errors of the three models. Which model achieves the best performance on the training data? Which model achieves the best performance on the validation data? Comment on differences between training and validation errors for individual models.

4. Which of the models would you use for predicting the response variable? Explain.

3.3 Ridge Regression [20 points]

For this question you will start with Model2 and employ regularization on it.

1. Write a matlab function to solve ridge regression. The function should take the data matrix Φ, the column vector of responses y, and the regularization parameter λ as the inputs and produce the least squares fit w as the output (refer to the lecture notes for the calculation of w). Do not penalize the intercept term. (You can achieve this by replacing the first column of the λI matrix with zeros.)

[2] These features are also called 'interactions', because they attempt to account for the effect of two attributes being simultaneously high or simultaneously low.

2. You will create a plot exploring the effect of the regularization parameter on training and validation errors. The x-axis is the regularization parameter (on a log scale) and the y-axis is the mean squared error. Show two curves in the same graph, one for the training error and one for the validation error. Starting with $\lambda = 2^{-30}$, try 50 values: at each iteration increase λ by a factor of 2, so that for example the second iteration uses $\lambda = 2^{-29}$. For each λ, you need to train a new model.

3. What happens to the training error as the regularization parameter increases? What about the validation error? Explain the curve in terms of overfitting, bias and variance.

4. What is the λ that achieves the lowest validation error and what is the validation error at that point? Compare this validation error to the Model2 validation error when no regularization was applied (you solved this in part 3.2). How does w differ in the regularized and unregularized versions, i.e., what effect did regularization have on the weights?

5. Is this validation error lower or higher than the validation error of the model you chose in 3.2.4? Which one should be your final model?

3.4 Building the Final Model [10 points]

Now that you have decided on your model (features and possibly the regularization parameter), combine your training and validation data to make a combined training set, train your model on this combined training set, and test it on the test set. Report the training and test errors.