# Intro to Machine Learning (CS771A, Autumn 2020) Homework 1

Due Date: October 25, 2020 (11:59pm)

#### **Instructions:**

- Only electronic submissions will be accepted. Your main PDF writeup must be typeset in LaTeX (please also refer to the "Additional Instructions" below).
- The PDF writeup containing your solution has to be submitted via Gradescope https://www.gradescope.com/.
- We have created your Gradescope account (you should have received the notification). Please use your IITK CC ID (not any other email ID) to login. Use the "Forgot Password" option to set your password.

#### **Additional Instructions**

- We have provided a LaTeX template file hwlsol.tex to help typeset your PDF writeup. There is also a style file ml.sty that contain shortcuts to many of the useful LaTeX commends for doing things such as boldfaced/calligraphic fonts for letters, various mathematical/greek symbols, etc., and others. Use of these shortcuts is recommended (but not necessary).
- Your answer to every question should begin on a new page. The provided template is designed to do this automatically. However, if it fails to do so, use the \clearpage option in LaTeX before starting the answer to a new question, to *enforce* this.
- While submitting your assignment on the Gradescope website, you will have to specify on which page(s) is question 1 answered, on which page(s) is question 2 answered etc. To do this properly, first ensure that the answer to each question starts on a different page.
- Be careful to flush all your floats (figures, tables) corresponding to question n before starting the answer to question n+1 otherwise, while grading, we might miss your important parts of your answers.
- Your solutions must appear in proper order in the PDF file i.e. solution to question n must be complete in the PDF file (including all plots, tables, proofs etc) before you present a solution to question n + 1.

## Problem 1 (15 marks)

(Absolute Loss Regression with Sparsity) The absolute loss regression problem with  $\ell_1$  regularization is

$$oldsymbol{w}_{opt} = \operatorname*{argmin}_{oldsymbol{w}} \sum_{n=1}^{N} |y_n - oldsymbol{w}^{ op} oldsymbol{x}_n| + \lambda ||oldsymbol{w}||_1$$

where  $||\boldsymbol{w}||_1 = \sum_{d=1}^{D} |w_d|$ , |.| is the absolute value function, and  $\lambda > 0$  is the regularization hyperparameter.

Is the above objective function convex? You don't need to prove this formally; just a brief reasoning based on properties of other functions that are known to be convex/non-convex would be fine.

Derivate the expression for the (sub)gradient vector for this model.

## Problem 2 (15 marks)

(Feature Masking as Regularization) Consider linear regression model by minimizing the squared loss function  $\sum_{n=1}^{N} (y_n - \boldsymbol{w}^{\top} \boldsymbol{x}_n)^2$ . Suppose we decide to mask out or "drop" each feature  $x_{nd}$  of each input  $\boldsymbol{x}_n \in \mathbb{R}^D$ , independently, with probability 1-p (equivalently, retaining the feature with probability p). Masking or dropping out basically means that we will set the feature  $x_{nd}$  to 0 with probability 1-p. Essentially, it would be equivalent to replacing each input  $\boldsymbol{x}_n$  by  $\tilde{\boldsymbol{x}}_n = \boldsymbol{x}_n \circ \boldsymbol{m}_n$ , where  $\circ$  denotes elementwise product and  $\boldsymbol{m}_n$  denotes the  $D \times 1$  binary mask vector with  $m_{nd} \sim \text{Bernoulli}(p)$  ( $m_{nd} = 1$  means the feature  $x_{nd}$  was retained;  $m_{nd} = 0$  means the feature  $x_{nd}$  was masked/zeroed).

Let us now define a new loss function using these masked inputs as follows:  $\sum_{n=1}^{N} (y_n - \boldsymbol{w}^{\top} \tilde{\boldsymbol{x}}_n)^2$ . Show that minimizing the *expected* value of this new loss function (where the expectation is used since the mask vectors  $\boldsymbol{m}_n$  are random) is equivalent to minimizing a **regularized** loss function. Clearly write down the expression of this regularized loss function.

# Problem 3 (40 marks)

(Multi-output Regression with Reduced Number of Parameters) Consider the multi-output regression in which each output  $y_n \in \mathbb{R}^M$  in a real-valued vector, rather than a scalar. Assuming a linear model, we can model the outputs as  $\mathbf{Y} \approx \mathbf{X}\mathbf{W}$ , where  $\mathbf{X}$  is the  $N \times D$  feature matrix and  $\mathbf{Y}$  is  $N \times M$  response matrix with row n being  $\mathbf{y}_n^{\top}$  (note that each column of  $\mathbf{Y}$  denotes one of the M responses), and  $\mathbf{W}$  is the  $D \times M$  weight matrix, with its M columns containing the M weight vectors  $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_M$ . Let's define a squared error loss function  $\sum_{n=1}^N \sum_{m=1}^M (y_{nm} - \mathbf{w}_m^{\top} \mathbf{x}_n)^2$ , which is just the usual squared error but summed over all the M outputs. Firstly, verify that this can also be written in a more compact notation as  $\mathsf{TRACE}[(\mathbf{Y} - \mathbf{X}\mathbf{W})^{\top}(\mathbf{Y} - \mathbf{X}\mathbf{W})]$ .

Further, we will assume that the weight matrix  $\mathbf{W}$  can be written as a product of two matrices, i.e.,  $\mathbf{W} = \mathbf{B}\mathbf{S}$  where  $\mathbf{B}$  is  $D \times K$  and  $\mathbf{S}$  is  $K \times M$  (assume  $K < \min\{D, M\}$ ). Note that there is a benefit of modeling  $\mathbf{W}$  this way, since now we need to learn only  $K \times (D+M)$  parameters as opposed to  $D \times M$  parameters and, if K is small, this can significantly reduce the number of parameters (in fact, reducing the *effective* number of parameters to be learned is another way of regularizing a machine learning model). Note (you can verify) that in this formulation, each  $\mathbf{w}_m$  can be written as a linear combination of K columns of  $\mathbf{B}$ .

With the proposed representation of W, the new objective will be  $TRACE[(Y - XBS)^{\top}(Y - XBS)]$  and you need to learn both B and S by solving the following problem:

$$\{\hat{\mathbf{B}}, \hat{\mathbf{S}}\} = \arg\min_{\mathbf{B}, \mathbf{S}} \text{trace}[(\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{S})^\top (\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{S})]$$

We will ignore regularization on B and S for brevity/simplicity.

Derive an alternating optimization (ALT-OPT) algorithm to learn **B** and **S**, clearly writing down the expressions for the updates of **B** and **S**. Are both subproblems (solving for **B** and solving for **S**) equally easy/difficult in this ALT-OPT algorithm? If yes, why? If no, why not?

Note: Since **B** and **S** are matrices, if you want, please feel free to use results for matrix derivatives (results you will need can be found in Sec. 2.5 of the Matrix Cookbook). However, the problem can be solved even without using matrix derivative results with some rearragement of terms and using vector derivatives.

## Problem 4 (10 marks)

Ridge Regression using Newton's Method Consider the ridge regression problem:

$$\hat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \frac{1}{2} \sum_{n=1}^{N} (y_n - \boldsymbol{w}^{\top} \boldsymbol{x}_n)^2 + \frac{\lambda}{2} \boldsymbol{w}^{\top} \boldsymbol{w} = \arg\min_{\boldsymbol{w}} \frac{1}{2} (\boldsymbol{y} - \mathbf{X} \boldsymbol{w})^{\top} (\boldsymbol{y} - \mathbf{X} \boldsymbol{w}) + \frac{\lambda}{2} \boldsymbol{w}^{\top} \boldsymbol{w}$$

where **X** is the  $N \times D$  feature matrix and  $\boldsymbol{y}$  is the  $N \times 1$  vector of labels of the N training examples. Note that the factor of  $\frac{1}{2}$  has been used in the above expression just for convenience of derivations required for this problem and does not change the solution to the problem.

Derive the Newton's method's update equations for each iteration. For this model, how many iterations would the Newton's method will take to converge?

## Problem 5 (20 marks)

(**Dice Roll**) You have a six-faced dice which you roll N times and record the number of times each of its six faces are observed. Suppose these numbers are  $N_1, N_2, \ldots, N_6$ , respectively. Assume that the probability of a random roll of the dice showning the  $k^{th}$  face  $(k = 1, 2, \ldots, 6)$  to be equal to  $\pi_k \in (0, 1)$ .

Assuming an appropriate conjugate prior for the probability vector  $\pi = [\pi_1, \pi_2, \dots, \pi_6]$ , derive its MAP estimate. In which situation(s), you would expect the MAP solution to be better than the MLE solution?

Also derive the full posterior distribution over  $\pi$  using the same prior that you used for MAP estimate. Given this posterior, can you get the MLE and MAP estimate without solving the MLE and MAP optimization problems? If yes, how? If no, why not?

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QUESTION

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Convex functions are bowl-shaped, have a unique minima and double derivative greater than or equal to zero wherever defined. So using basic properties of convex function, all linear and affine functions are convex, meaning if f(x) is convex then f(ax + b) is also convex. For our case, absolute function  $|y_n - \mathbf{w}^T \mathbf{x}_n|$  is a convex function and  $||\mathbf{w}||_1$  (which is  $L_1$  norm) is also a convex function, hence sum of two convex function is also convex

(Double derivative of  $|y_n - \mathbf{w}^T \mathbf{x}_n|$  and  $||\mathbf{w}||_1$  would be positive wherever defined and so would there sum be positive).

Let

$$L(\mathbf{w}) = \sum_{n=1}^{N} |y_n - \mathbf{w}^T \mathbf{x}_n| + \lambda ||\mathbf{w}||_1$$

For subgradient vector calculation,

Case 1:  $w_i > 0$ :

$$\partial L_n(\mathbf{w}) = \begin{cases} (-x_n) + \lambda, & y_n - \mathbf{w}^T \mathbf{x}_n > 0 \\ (\mathbf{x}_n) + \lambda, & y_n - \mathbf{w}^T \mathbf{x}_n < 0 \\ -c(\mathbf{x}_n) + \lambda, & y_n - \mathbf{w}^T \mathbf{x}_n = 0 \end{cases}$$
(1)

Case 2:  $w_i < 0$ :

$$\partial L_n(\mathbf{w}) = \begin{cases} (-x_n) - \lambda, & y_n - \mathbf{w}^T \mathbf{x}_n > 0 \\ (\mathbf{x}_n) - \lambda, & y_n - \mathbf{w}^T \mathbf{x}_n < 0 \\ -c(\mathbf{x}_n) - \lambda, & y_n - \mathbf{w}^T \mathbf{x}_n = 0 \end{cases}$$
(2)

Case 3:  $w_i = 0$ :

$$\partial L_n(\mathbf{w}) = \begin{cases} (-x_n) - \lambda c_1, & y_n - \mathbf{w}^T \mathbf{x}_n > 0 \\ (\mathbf{x}_n) - \lambda c_1, & y_n - \mathbf{w}^T \mathbf{x}_n < 0 \\ -c(\mathbf{x}_n) - \lambda c_1, & y_n - \mathbf{w}^T \mathbf{x}_n = 0 \end{cases}$$
(3)

where  $c, c_1$  in range [-1, 1] in all the above three cases.

So

$$\partial L(\mathbf{w}) = \sum_{n=1}^{N} f_n \mathbf{x}_n + \lambda g_n$$

here  $f_n = \partial |y_n - \mathbf{w}^T \mathbf{x}_n|$  and  $g_n = \partial ||\mathbf{w}||_1$ 

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Instead of minimizing the squared loss function  $\sum_{n=1}^{n=N} (\mathbf{y}_n - \mathbf{w}^T \mathbf{x}_n)^2$  for the given feature matrix  $\mathbf{x}_n \in \mathbb{R}^D$ , we have to minimize  $L(w) = \mathbb{E}[\sum_{n=1}^{n=N} (\mathbf{y}_n - \mathbf{w}^T \bar{\mathbf{x}}_n)^2]$  where  $\bar{x}_n = \mathbf{x}_n$  o  $\mathbf{m}_n$  and  $\mathbf{m}_n$  is a vector and  $m_n$  is a vector  $m_n$  and  $m_n$  is a vector and  $m_n$  is a vector  $m_n$  in  $m_n$  in  $m_n$  is a vector  $m_n$  in  $m_n$  in  $m_n$  in  $m_n$  in  $m_n$  is a vector  $m_n$  in  $\mathbf{m}_n$  is a vector and  $m_{nd}$  is a Bernoulli distribution with  $\mathbb{E}[\mathbf{m}_{ij}] = \mathbf{p}$ .

(p is the probability of retaining the feature, d in scalar value  $m_{nd}$  represents  $d^{th}$  feature of  $\mathbf{m}_n$ 

So,

$$L(w) = \mathbb{E}\left[\sum_{n=1}^{n=N} (y_n - \mathbf{w}^T \bar{x}_n)^2\right] = \mathbb{E}\left[\sum_{n=1}^{n=N} (y_n^2 + (\mathbf{w}^T \bar{x}_n)^2 - 2y_n \mathbf{w}^T \bar{x}_n)\right]$$

$$= \mathbb{E}\left[\sum_{n=1}^{n=N} (y_n^2)\right] + \mathbb{E}\left[\sum_{n=1}^{n=N} (\mathbf{w}^T \bar{x}_n)^2\right] - 2\sum_{n=1}^{n=N} y_n \mathbb{E}[\mathbf{w}^T \bar{x}_n]$$

$$= \sum_{n=1}^{n=N} \mathbb{E}[(y_n^2)] + \sum_{n=1}^{n=N} \mathbb{E}[(\mathbf{w}^T \bar{x}_n)^2] - 2\sum_{n=1}^{n=N} y_n \mathbb{E}[\mathbf{w}^T \bar{x}_n]$$
(4)

$$\mathbb{E} \left[ \mathbf{w}^T \bar{x}_n \right] = \mathbb{E} \left[ \sum_{i=1}^{i=D} w_i x_{ni} m_{ni} \right] = \sum_{i=1}^{i=D} w_i x_{ni} \mathbb{E}[m_{ni}] = \sum_{i=1}^{i=D} w_i x_{ni} p$$

We know, 
$$(\mathbf{w}^T \bar{x}_n)^2 = \sum_{i=1}^{i=D} (w_i x_{ni} m_{ni})^2 + \sum_{i=1}^{i=D} \sum_{j>i}^{j=D} w_i w_j x_{ni} x_{nj} m_{ni} m_{nj}$$
; Hence,

$$\mathbb{E}\left[(\mathbf{w}^T \bar{x}_n)^2\right] = \sum_{i=1}^{i=D} \mathbb{E}\left[(w_i x_{ni} m_{ni})^2\right] + 2 \mathbb{E}\left[\sum_{i=1}^{i=D} \sum_{j>i}^{j=D} w_i w_j x_{ni} x_{nj} m_{ni} m_{nj}\right]$$

$$= \sum_{i=1}^{i=D} w_i^2 x_{ni}^2 \mathbb{E}[m_{ni}^2] + 2 \sum_{i=1}^{i=D} \sum_{j>i}^{j=D} w_i w_j x_{ni} x_{nj} \mathbb{E}[m_{ni} m_{nj}]$$

$$= p \sum_{i=1}^{i=D} w_i^2 x_{ni}^2 + 2p^2 \sum_{i=1}^{i=D} \sum_{j>i}^{j=D} w_i w_j x_{ni} x_{nj}$$
 (  $\mathbb{E}[m_{ni} m_{nj}] = \mathbb{E}[m_{ni}] \mathbb{E}[m_{nj}] = p^2$ )

$$= p^2 (\mathbf{w}^T x_n)^2 - p^2 \sum_{i=1}^{i=D} w_i^2 x_{ni}^2 + p \sum_{i=1}^{i=D} w_i^2 x_{ni}^2$$

= 
$$p^2 (\mathbf{w}^T x_n)^2 + (p - p^2) \sum_{i=1}^{i=D} w_i^2 x_{ni}^2$$
  
Putting the above expression in equation 4, we get

$$L(w) = y_n^2 + p^2 (\mathbf{w}^T x_n)^2 + (p - p^2) \sum_{i=1}^{i=D} w_i^2 x_{ni}^2 - 2py_n \sum_{i=1}^{i=D} w_i x_{ni}$$

$$L(w) = (y_n^2 - 2py_n \sum_{i=1}^{i=D} w_i x_{ni} + p^2 (\mathbf{w}^T x_n)^2) + (p - p^2) \sum_{i=1}^{i=D} w_i^2 x_{ni}^2$$

$$L(w) = (y_n - p\mathbf{w}^T x_n)^2 + (p - p^2) \sum_{i=1}^{i=D} w_i^2 x_{ni}^2$$

$$L(w) = (y_n - \mathbf{w}^T x_n)^2 + (\frac{1-p}{p}) \sum_{i=1}^{i=D} w_i^2 x_{ni}^2$$
 (Replaced **w** with **w**/p)

So we can say that minimizing L(w) reduces to minimizing regularized  $\sum_{n=1}^{n=N} (y_n - \mathbf{w}^T x_n)^2$  with  $(\frac{1-p}{p})$  acting as  $\lambda$  and  $\sum_{i=1}^{i=D} w_i^2 x_{ni}^2$  acting as regularised function in terms of weight vector

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QUESTION

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First verification  $\Rightarrow \sum_{n=1}^{n=N} \sum_{m=1}^{m=M} (y_{nm} - \mathbf{w}_m^T \mathbf{x}_n)^2 = \text{trace}[(\mathbf{Y} - \mathbf{X}\mathbf{W})^T (\mathbf{Y} - \mathbf{X}\mathbf{W})]$ 

$$(\mathbf{Y} - \mathbf{X}\mathbf{W})_{ij} = y_{ij} - \sum_{k=1}^{k=D} x_{ik} w_{kj}$$

$$(\mathbf{Y} - \mathbf{X}\mathbf{W})_{ij}^{T} = y_{ji} - \sum_{k=1}^{k=D} x_{jk} w_{ki}$$

$$[(\mathbf{Y} - \mathbf{X}\mathbf{W})^{T} (\mathbf{Y} - \mathbf{X}\mathbf{W})]_{ij} = \sum_{n=1}^{n=N} [(y_{ni} - \sum_{k=1}^{k=D} x_{nk} w_{kn})(y_{nj} - \sum_{k=1}^{k=D} x_{nk} w_{kj})]$$

$$trace[(\mathbf{Y} - \mathbf{X}\mathbf{W})^{T} (\mathbf{Y} - \mathbf{X}\mathbf{W})] = \sum_{m=1}^{m=M} [(\mathbf{Y} - \mathbf{X}\mathbf{W})^{T} (\mathbf{Y} - \mathbf{X}\mathbf{W})]_{mm} = \sum_{m=1}^{m=M} \sum_{n=1}^{n=N} (y_{nm} - \mathbf{w}_{m}^{T} \mathbf{x}_{n})(y_{nm} - \mathbf{w}_{m}^{T} \mathbf{x}_{n})$$

$$\Rightarrow trace[(\mathbf{Y} - \mathbf{X}\mathbf{W})^{T} (\mathbf{Y} - \mathbf{X}\mathbf{W})] = \sum_{m=1}^{m=M} \sum_{n=1}^{n=N} (y_{nm} - \mathbf{w}_{m}^{T} \mathbf{x}_{n})^{2}$$

In cases where more than one variable needs to be optimized, we take alternating optimization (ALT-OPT) algorithm approach to find best suitable values of  $\hat{B}$  and  $\hat{S}$  (where  $\mathbf{W} = \mathbf{BS}$ ):

$$\{\hat{B}, \hat{S}\} = argmin_{\mathbf{B}, \mathbf{S}} trace[(\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{S})^T(\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{S})]$$

Let

$$L(\mathbf{B}, \mathbf{S}) = trace[(\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{S})^T(\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{S})]$$

Now differentiating  $L(\mathbf{B}, \mathbf{S})$  wrt.  $\mathbf{B}$  keeping  $\mathbf{S}$  constant :

$$\frac{\partial L}{\partial b_{ij}} = \frac{\partial}{\partial b_{ij}} \sum_{n=1}^{n=N} \sum_{m=1}^{m=M} (y_{nm} - \mathbf{w}_m^T \mathbf{x}_n)^2$$

$$w_{mk} = \sum_{l} b_{ml} s_{lk} \Rightarrow w_{km} = \sum_{l} b_{kl} s_{lm}$$

$$\frac{\partial L}{\partial b_{ij}} = \frac{\partial}{\partial b_{ij}} \sum_{n=1}^{n=N} \sum_{m=1}^{m=M} (y_{nm} - \sum_{k=1}^{k=D} w_{km} x_{nk})^2 = \frac{\partial}{\partial b_{ij}} \sum_{n=1}^{n=N} \sum_{m=1}^{m=M} (y_{nm} - \sum_{k=1}^{k=D} \sum_{l} b_{kl} s_{lm} x_{nk})^2$$

$$\frac{\partial L}{\partial b_{ij}} = 2 \sum_{n=1}^{n=N} \sum_{m=1}^{m=M} (y_{nm} - \sum_{k=1}^{k=D} \sum_{l} b_{kl} s_{lm} x_{nk}) (-x_{ni} s_{jm})$$

$$\frac{\partial L}{\partial b_{ij}} = -2 \sum_{n=1}^{n=N} \sum_{m=1}^{m=M} x_{in}^T (y_{nm} - \sum_{k=1}^{k=D} \sum_{l} x_{nk} b_{kl} s_{lm}) (s_{mj}^T) = -2 \mathbf{X}^T (\mathbf{Y} - \mathbf{X} \mathbf{B} \mathbf{S}) \mathbf{S}^T$$

To get  $\hat{B}^p$ , where  $\hat{B}^p$  is optimum value of **B** at any iteration p:

$$-2\mathbf{X}^{T}(\mathbf{Y} - \mathbf{X}\hat{B}^{p}\mathbf{S})\mathbf{S}^{T} = 0 \Rightarrow \mathbf{X}^{T}\mathbf{Y}\mathbf{S}^{T} - \mathbf{X}^{T}\mathbf{X}\hat{B}^{p}\mathbf{S}\mathbf{S}^{T} = 0$$

$$\mathbf{X}^T \mathbf{X} \hat{B}^p \mathbf{S} \mathbf{S}^T = \mathbf{X}^T \mathbf{Y} \mathbf{S}^T \Rightarrow \hat{B}^p = [\mathbf{X}^T \mathbf{X}]^{-1} \mathbf{X}^T \mathbf{Y} \mathbf{S}^T [\mathbf{S} \mathbf{S}^T]^{-1}$$

Now differentiating  $L(\mathbf{B},\mathbf{S})$  wrt.  $\mathbf{S}$  keeping  $\mathbf{B}$  constant :

$$\frac{\partial L}{\partial s_{ij}} = 2 \sum_{n=1}^{n=N} \sum_{m=1}^{m=M} (y_{nm} - \sum_{k=1}^{k=D} \sum_{l} b_{kl} s_{lm} x_{nk}) (-\sum_{k} x_{nk} b_{ki})$$

$$\frac{\partial L}{\partial s_{ij}} = 2 \sum_{n=1}^{n=N} (-\sum_{k} b_{ik}^T x_{kn}^T) (y_{nj} - \sum_{k=1}^{k=D} \sum_{l} x_{nk} b_{kl} s_{lj}) = -2(\mathbf{X}\mathbf{B})^T (\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{S})$$

To get  $\hat{S}^p$ , where  $\hat{S}^p$  is optimum value of **S** at any iteration p:

$$-2(\mathbf{X}\mathbf{B})^{T}(\mathbf{Y} - \mathbf{X}\mathbf{B}\hat{S}^{p}) = 0 \Rightarrow (\mathbf{X}\mathbf{B})^{T}\mathbf{Y} - (\mathbf{X}\mathbf{B})^{T}\mathbf{X}\mathbf{B}\hat{S}^{p} = 0$$

$$(\mathbf{X}\mathbf{B})^T\mathbf{X}\mathbf{B}\hat{S}^p = (\mathbf{X}\mathbf{B})^T\mathbf{Y} \Rightarrow \hat{S}^p = [(\mathbf{X}\mathbf{B})^T\mathbf{X}\mathbf{B}]^{-1}(\mathbf{X}\mathbf{B})^T\mathbf{Y}$$

Lets write the algorithm for iteration part now:

**Step 1**: Initialize  $\hat{B}^{(p)}$ ,  $\hat{S}^{(p)}$  at p=0

Step 2: 
$$\hat{B}^{(p+1)} = [\mathbf{X}^T \mathbf{X}]^{-1} \mathbf{X}^T \mathbf{Y} \hat{S}^{(p)T} [\hat{S}^{(p)} \hat{S}^{(p)T}]^{-1}$$

**Step 3**: 
$$\hat{S}^{(p+1)} = [(\mathbf{X}\hat{B}^{(p+1)})^T\mathbf{X}\hat{B}^{(p+1)}]^{-1}(\mathbf{X}\hat{B}^{(p+1)})^T\mathbf{Y}$$

Step 4: Repeat Step 2 and Step 3 until both converge

Finally we get optimum  $\hat{B}$  and  $\hat{S}$ 

Both the sub-problems (solving for  $\hat{B}$  and  $\hat{S}$ ) are **not** equally easy as we can see in the case for  $\hat{B}$ , there are more inversions and different multiplications need to be calculated as compared to that for  $\hat{S}$ .

QUESTION

4

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Date: October 30, 2020

Given 
$$L(w) = \frac{1}{2} \sum_{n=1}^{n=N} (y_n - \mathbf{w}^T \mathbf{x}_n)^2 + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w} = \frac{1}{2} (\mathbf{y} - \mathbf{X} \mathbf{w})^T (\mathbf{y} - \mathbf{X} \mathbf{w}) + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w}$$

$$\nabla L(w) = -\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X} \mathbf{w} + \lambda \mathbf{w}$$

$$\nabla^2 L(w) = \mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}$$

For Newton's method we know that

$$\mathbf{w}^{(t+1)} = \arg\min_{w} \left[ L(\mathbf{w}^{(t)}) + \nabla L(\mathbf{w}^{(t)})^{T} (\mathbf{w} - \mathbf{w}^{(t)}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}^{(t)})^{T} \nabla^{2} L(w) (\mathbf{w} - \mathbf{w}^{(t)}) \right]$$

The below expression will give  $\mathbf{w}^{(t+1)}$ 

$$\nabla [L(\mathbf{w}^{(t)}) + \nabla L(\mathbf{w}^{(t)})^T (\mathbf{w} - \mathbf{w}^{(t)}) + \frac{1}{2} (\mathbf{w} - \mathbf{w}^{(t)})^T \nabla^2 L(w) (\mathbf{w} - \mathbf{w}^{(t)})] = 0$$

$$\Rightarrow 0 + \nabla L(\mathbf{w}^{(t)}) + (\mathbf{w}^{(t+1)} - \mathbf{w}^{(t)})\nabla^2 L(w) = 0$$

$$\Rightarrow \mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - (\nabla^2 L(w^{(t)}))^{-1} \nabla L(w^{(t)})$$

After Equating values of  $\nabla L(w)$  and  $\nabla^2 L(w)$  from above, we get

$$\Rightarrow \mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{X} \mathbf{w}^{(t)} + \lambda \mathbf{w}^{(t)} - \mathbf{X}^T \mathbf{y})$$

$$\Rightarrow \mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{X} \mathbf{w}^{(t)} + \lambda \mathbf{w}^{(t)}) + (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{y})$$

$$\Rightarrow \mathbf{w}^{(t+1)} = (\mathbf{X}^T \mathbf{X} - \lambda \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{y})$$

We can see that  $\mathbf{w}^{(t+1)}$  is not dependent on  $\mathbf{w}^{(t)}$  and is a constant for a given feature matrix  $\mathbf{X}$  and vector  $\mathbf{y}$  and hence it takes only one iteration to converge.

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QUESTION

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Given problem has 6 classes. So unlike in 2 classes case where we use Beta Distribution, here we would use Dirichlet prior for multinomial likelihood which would give us Dirichlet posterior. We know for i.i.d data, likelihood can be expressed as

$$p(\mathbf{y}|\pi) = \prod_{n=1}^{n=N} p(y_n|\pi) = \prod_{n=1}^{n=N} \pi_n^{N_n}$$

Dirichlet prior  $p(\pi|\alpha)$  with  $\alpha$  as hyperparameter is given as below, where  $\sum_{n=1}^{n=N} \pi_n = 1$ 

$$p(\pi|\alpha) = \frac{\Gamma(\sum_{n=1}^{n=N} \alpha_n)}{\prod_{n=1}^{n=N} \Gamma(\alpha_n)} \prod_{n=1}^{n=N} \pi_n^{\alpha_n - 1}$$

Also for pdf

$$\int p(\pi|\alpha)d\pi = 1 \Rightarrow \int \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}{\prod_{n=1}^{n=N}\Gamma(\alpha_n)} \Pi_{n=1}^{n=N}\pi_n^{\alpha_n - 1} = 1$$

$$\Rightarrow \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}{\prod_{n=1}^{n=N}\Gamma(\alpha_n)} \int \Pi_{n=1}^{n=N}\pi_n^{\alpha_n - 1}d\pi = 1 \Rightarrow \int \Pi_{n=1}^{n=N}\pi_n^{\alpha_n - 1}d\pi = \frac{\prod_{n=1}^{n=N}\Gamma(\alpha_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}$$

We know,

$$p(\pi|y) = \frac{p(\pi|\alpha)p(y|\pi)}{p(y)}$$

Taking N.L.L of above expression:

$$\begin{split} -\log(p(\pi|y)) &= -\log(p(\pi|\alpha)) - \log(p(y|\pi)) + \log(p(y)) \\ -\log(p(\pi|y)) &= -\log(\frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}{\Pi_{n=1}^{n=N}\Gamma(\alpha_n)}\Pi_{n=1}^{n=N}\pi_n^{\alpha_n-1}) - \log(\Pi_{n=1}^{n=N}\pi_n^{N_n}) + \log(p(y)) \\ -\log(p(\pi|y)) &= -\log(\frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}{\Pi_{n=1}^{n=N}\Gamma(\alpha_n)}) - \log(\Pi_{n=1}^{n=N}\pi_n^{N_n-1}) - \log(\Pi_{n=1}^{n=N}\pi_n^{N_n}) + \log(p(y)) \end{split}$$

To find MAP estimate, we know  $\hat{\pi}_{MAP} = \arg\max_{\pi} p(\pi|y)$  or effectively  $\hat{\pi}_{MAP} = \arg\min_{\pi} \log(p(\pi|y))$ 

To find the minimum of some function f(x) constrained to g(x) = 0, the Lagrangian function can formulated as :  $L(x, \lambda) = f(x) + \lambda g(x)$ 

So the constraint we have is  $\sum_{n=1}^{n=N} \pi_n = 1$  and hence we can replace g(x) with  $(\sum_{n=1}^{n=N} \pi_n - 1)$  and f(x) with  $[-\log(\Pi_{n=1}^{n=N} \pi_n^{\alpha_n - 1}) - \log(\Pi_{n=1}^{n=N} \pi_n^{N_n})]$  as rest of the terms from  $-\log(p(\pi|y))$  expression are not dependent on  $\pi$ . So now we have to minimize  $L(\pi, \lambda)$  given as,

$$L(\pi, \lambda) = \left[ -\log(\Pi_{n=1}^{n=N} \pi_n^{\alpha_n - 1}) - \log(\Pi_{n=1}^{n=N} \pi_n^{N_n}) \right] + \lambda \left( \sum_{n=1}^{n=N} \pi_n - 1 \right)$$

$$L(\pi, \lambda) = \left[ -\sum_{n=1}^{n=N} (\alpha_n - 1) \log(\pi_n) - \sum_{n=1}^{n=N} N_n \log(\pi_n) \right] + \lambda \left( \sum_{n=1}^{n=N} \pi_n - 1 \right)$$
$$L(\pi, \lambda) = -\sum_{n=1}^{n=N} (\alpha_n + N_n - 1) \log(\pi_n) + \lambda \left( \sum_{n=1}^{n=N} \pi_n - 1 \right)$$

Now apply

$$\begin{split} \frac{\partial L(\pi,\lambda)}{\partial \pi_n} &= 0 \\ -(\frac{\alpha_n + N_n - 1}{\pi_n}) + \lambda &= 0 \Rightarrow \pi_n = \frac{\alpha_n + N_n - 1}{\lambda} \end{split}$$

To find  $\lambda$ , we know that  $\sum_{n=1}^{n=N} \pi = 1 \Rightarrow \sum_{n=1}^{n=N} \frac{(\alpha_n + N_n - 1)}{\lambda} = 1 \Rightarrow \lambda = \sum_{n=1}^{n=N} (\alpha_n + N_n - 1)$ 

$$\hat{\pi}_{MAP} = \frac{\alpha_n + N_n - 1}{\sum_{n=1}^{n=N} (\alpha_n + N_n - 1)}$$

The MAP solution would be better than MLE solution in cases where we have data of very few experiments which can result in skewed distribution of classes or observations from some classes will not appear which in general is not true. MAP estimate helps us in such cases by giving a prior knowledge of distribution over distinct classes.

For full posterior,

$$p(\pi|y) = \frac{p(\pi|\alpha)p(y|\pi)}{p(y)} = \frac{p(\pi|\alpha)p(y|\pi)}{\int p(\pi|\alpha)p(y|\pi)d\pi}$$

And.

$$\int p(\pi|\alpha)p(y|\pi)d\pi = \int \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}{\prod_{n=1}^{n=N}\Gamma(\alpha_n)} \prod_{n=1}^{n=N}\pi_n^{\alpha_n-1} \prod_{n=1}^{n=N}\pi_n^{N_n}d\pi = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}{\prod_{n=1}^{n=N}\Gamma(\alpha_n)} \int \prod_{n=1}^{n=N}\pi_n^{\alpha_n+N_n-1}d\pi$$

We know that,

$$\int \Pi_{n=1}^{n=N} \pi_n^{\alpha_n - 1} d\pi = \frac{\Pi_{n=1}^{n=N} \Gamma(\alpha_n)}{\Gamma(\sum_{n=1}^{n=N} \alpha_n)} \Leftrightarrow \int \Pi_{n=1}^{n=N} \pi_n^{\alpha_n + N_n - 1} d\pi = \frac{\Pi_{n=1}^{n=N} \Gamma(\alpha_n + N_n)}{\Gamma(\sum_{n=1}^{n=N} (\alpha_n + N_n))}$$

Hence,

$$\int p(\pi|\alpha)p(y|\pi)d\pi = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)}{\prod_{n=1}^{n=N}\Gamma(\alpha_n)} \frac{\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}(\alpha_n+N_n))\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\Gamma(\sum_{n=1}^{n=N}(\alpha_n+N_n))\prod_{n=1}^{n=N}\Gamma(\alpha_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)\prod_{n=1}^{n=N}\Gamma(\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)} = \frac{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)}{\Gamma(\sum_{n=1}^{n=N}\alpha_n+N_n)} = \frac{\Gamma(\sum_{n$$

$$p(\pi|y) = \frac{\Gamma(\sum_{n=1}^{n=N} (\alpha_n + N_n)}{\prod_{n=1}^{n=N} \Gamma(\alpha_n + N_n)} \prod_{n=1}^{n=N} \pi_n^{\alpha_n + N_n - 1}$$

To get MAP estimate from posterior, we have  $\hat{\pi}_{MAP} = argmax_{\pi}(\log(p(\pi|y)))$  with constraint  $\sum_{n=1}^{N} \pi_n = 1$  and to solve it without optimization, we will calculate its mode. Let  $x \in 1, 2, ...N$  such that  $\sum_{n \neq x}^{N} \pi_n + \pi_x = 1$ , where x is the most frequent class. Then,

$$\log(p(\pi|y) = (\alpha_n + N_n - 1) \sum_{n \neq x}^{N} \log(\pi_n) + (\alpha_x + N_x - 1) \log(\pi_x)$$

$$\log(p(\pi|y) = (\alpha_n + N_n - 1) \sum_{n \neq x}^{N} \log(\pi_n) + (\alpha_x + N_x - 1) \log(1 - \sum_{n \neq x}^{N} \pi_n)$$

Now differentiate  $\log(p(\pi|y))$  and set it to zero.

$$\frac{(\alpha_n+N_n-1)}{\pi_n}-\frac{(\alpha_x+N_x-1)}{1-\sum_{n\neq x}^N\pi_n}=0\Rightarrow \pi_n=\frac{\alpha_n+N_n-1}{\alpha_x+N_x-1}\pi_x$$

Also,

$$\sum_{n \neq x}^{N} \pi_n + \pi_x = 1 \Rightarrow \sum_{n \neq x}^{N} \frac{\alpha_n + N_n - 1}{\alpha_x + N_x - 1} \pi_x + \pi_x = 1 \Rightarrow \sum_{n = 1}^{N} (\alpha_n + N_n - 1) \pi_x = (\alpha_x + N_x - 1)$$

$$\pi_x = \frac{(\alpha_x + N_x - 1)}{\sum_{n=1}^{N} (\alpha_n + N_n - 1)}$$

For MLE, since there is no assumed prior  $\Rightarrow \hat{\pi}_{MLE} = \hat{\pi}_{MAP}$ , this can be done with  $\alpha_n = 1$ 

$$\pi_n = \frac{N_n}{N_x} \pi_x$$

and hence for MLE,  $\pi_x = \frac{N_x}{\sum_{n=1}^{N} N_n}$