CS 229 Midterm (Fall 2023) Solutions

Read the following points before starting the exam:

- This exam is open book (notes, homework, and solutions) but closed to the Internet.
- You have three (3) hours to complete the exam.
- You may cite (without proof) any result from lectures, lecture notes, and problem-set solutions unless otherwise stated.
- Please take a look at all of the questions before you start.

Friday, November 3rd

Question	Points
1 True/False	/20
2 Role Play!	/20
3 Negative Binomial Regression	/25
4 Implementing Naïve Bayes	/15
5 Exponential Family Discriminant Analysis	/15
6 Node-splitting via Logistic Regression	/20
Total	/115

Good luck!

1.	20	points	True	/False

For each statement, just indicate whether it is TRUE (always completely correct) or FALSE (at least some aspect is sometimes wrong). No need to provide an explanation.

Make sure to *completely* fill in the checkboxes (like this \blacksquare) corresponding to your answers. Answers with \boxtimes or \square will be marked wrong.

(a)	[2 points] Since the Expectation Maximization (EM) algorithm guarantees monotonic convergence of the likelihood function, we should only stop training if the likelihood function outputs the exact same value in successive iterations. □ True □ False Answer: False
(b)	[2 points] The M step of training a 2-class Gaussian Mixture Model (GMM) is equivalent to fitting a Gaussian Discriminant Analysis model for the current guessed labels, with the exception that only soft assignment weights are used, and each cluster has its own covariance matrix. □ True □ False Answer: True
(c)	[2 points] Suppose a K-Means model and a GMM are applied to the same dataset and suppose both of them reach their own global optima. If, for GMM, we use a "hard" cluster assignment in the final step (i.e. assign each datapoint x to the cluster with the highest $p(cluster x)$), then the clusters generated by the two models will be the same. \Box True \Box False Answer: False
(d)	[2 points] Unlike linear regression, logistic regression has a nonlinear activation, and as such, it does not have a linear decision boundary. □ True □ False

False – logistic regression also has a linear decision boundary

(e)	[2 points] Although the EM algorithm (on unlabelled data) can have multiple optima (in terms of parameters), the GDA model (on labelled data) cannot. □ True □ False
	Answer: True
(f)	[2 naints] Lat's say we're fitting a linear model to a detect with a features
(1)	[2 points] Let's say we're fitting a linear model to a dataset with n features. Suppose the last feature is replaced by the output of a random number generator. We will find that both the bias and the variance increases.
	□ True □ False
	Answer: True
(g)	convex in θ , we are guaranteed to have a unique global optimum when $\lambda > 0$. \Box True
	□ False Answer: True $-\lambda \theta _2^2$ is strictly convex (PD Hessian), so overall loss has PD Hessian, hence strictly convex
(h)	[2 points] If we use a kernel method with feature map $\phi(x)=x$, we end up with the same results as with not using a kernel method. \Box True \Box False
	Answer: True – using the identity function reducing to not using a kernel method

(i)		boosting, when adding a new model to the existing ensemble, we n unseen datapoints to avoid overfitting.
	\square True \square False	
	Answer: relabelling	False – Boosting uses the same datapoints but with reweighting o

(j)	$\sum_{i=1}^{n} x_i =$	Let $[x_1 ldots x_n]$ be samples from a mean-zero random variable, such that 0 , and $-1 < x_i < 1$. We claim that $\sum_{i=1}^n \log(1+x_i)$ must be ≥ 0 . $\log(\cdot)$ a convex function or a concave function?
	☐ True	
	\square False	
	Answer:	False – use concavity

2. [20 points] Role Play!

You are the CEO of a data consulting firm. Your VP is working with a real estate client who is trying build a house price predictor. The client's speciality is in collecting extremely detailed and high quality data about properties from a variety of sources and combining them. They have created a unique dataset of all houses in the small town they operate in.

Each example in the dataset corresponds to a house and has d=1000 features per house. The features are all numeric, e.g., number of floors, size in square feet, or 1 vs. 0 for the presence or absence of a pool. Yet, because this is a small town, the number of examples in the dataset is just n=100. The client is worried about this disparity and has proposed several ideas to your team.

Your VP has commented on the client's ideas. Consider each of the four ideas independently. For each of your VP's comments, say whether it is CORRECT (i.e. completely correct) or WRONG (i.e. at least some aspect is wrong), and briefly and convincingly explain your decision (in 1-2 sentences). To receive full credit for an answer of WRONG, we expect you to point out a significant issue and not, for example, an edge case that involves additional assumptions. You only need to identify a single significant issue.

Just to be clear: you only need to determine whether the VP's comments are correct. You do NOT need to comment on the quality of the client's idea.

Ideas begin on the next page...

(a) [5 points] Client's Idea: What if we just don't worry about the fact that d >> n? Keep the data as is, and use full-batch gradient descent to fit a least-squares linear regression model. Declare convergence when the L_1 norm of the weights changes by no more than a very small value like 10^{-10} .

VP's comments: Because d >> n, there may be many optimal fits, so the model will keep iterating forever and its weights will continue to get larger and larger. It will never truly converge unless we force it to do so artificially by e.g. decreasing the learning rate over time.

Your assessment of the VP's comments:

Answer:

False: modern ML runs gradient descent on data with d>>n all the time. While it is true that there may be many optimal fits, there is no reason to believe the model will not converge; this is not like the linear separability issue in Homework 2, which was for a classification problem.

(b) [5 points] Client's Idea: First, let's find the feature that has the highest correlation with the response variable (y). Now, find the other n-1 features with the *highest* correlation with that one feature. It's impossible for a rectangular matrix to be full rank, but thankfully, now, we have an $n \times n$ matrix (and hence full-rank matrix) of features that will yield the most predictive power.

VP's comments: The client is incorrect in saying that rectangular matrices cannot be full rank, and that all square matrices are full rank. However, they are correct that with the described correlation-based feature selection, they will successfully only include the features with the most predictive power, and avoid over-fitting on noise in the dataset (hence reducing variance).

Your assessment of the VP's comments:

Answer: False. We are generally looking for features to be correlated with the response variable y, and NOT with one another (this actually decreases predictive power). Of course, if the features are correlated with y, then it is likely that they may have correlations with each other. However, ideally, we would like the features to be as orthogonal as possible (in other words: each feature should provide signal that is orthogonal as possible).

This question could receive a lot of different answers, and we will be pretty permissive with awarding credit/partial credit for explanations.

(c) [5 points] Client's Idea: If the main issue is that we don't have enough data, a solution is to create more. We can use our existing datapoints to create new ones and add these copies of the originals to our dataset. If we create lots of copies of our datapoints, add random noise to them, and then include these new datapoints with the old ones, we can generate whatever amount of data we need. **VP's comments:** The client is looking to extrapolate additional datapoints from the *n* that we already have. To do so, we can take our original datapoints, add random noise to them, and then split into training and testing datasets (validation as well if desired) afterwards. Now, we won't have to deal with overfitting to too few datapoints, and we'd still have plenty of data for testing (and/or validation).

Your assessment of the VP's comments:

Answer: Wrong. If we want to generate new samples this way, which need not be as helpful as either the client or VP seem to think, then we'd need to do the splitting of data before we do the generation. Else, we risk having extremely similar datapoints in both the training and testing datasets, which means we'd essentially train on the testing data.

(d) [5 points] **Client's Idea:** Keep the data as is, and train a least-squares linear regression model, but then save only the 100 features whose weights have the largest absolute values. Then use only that subset of features to train a new model.

VP's comments: Given that the client wants to save only 100 features, the ones with the largest absolute weights are the best choice, since they should have the most explanatory power. Pruning away the remaining features could also help to reduce overfitting.

Your assessment of the VP's comments:

Answer: False. Given that these features aren't normalized, the weights cannot be compared by pure magnitude to determine their relative importance.

3. [25 points] Negative Binomial Regression

Definition: The negative binomial distribution,

$$p(y; \phi, k) = {y-1 \choose k-1} (1-\phi)^{y-k} \phi^k,$$

is a probability distribution over the number of trials until the kth success. Recall that

 $\binom{a}{b} = \frac{a!}{b!(a-b)!},$

and is also known as the "choose" operator. For the purposes of this problem, this is all you will need to know about the Negative Binomial distribution.

Background: Let's say you've been contacted by FIDE, the World Chess Federation, to construct a GLM for the number of tournaments a player needs to play until they achieve their kth big victory¹² (and hence achieve the title of Grandmaster).

In particular, you have a response variable y (the number of tournaments) and some fixed k. You decide a Negative Binomial Regression is appropriate, and so y takes on values $\{k, k+1, k+2, \ldots\}$, and its distribution (parametrized by ϕ and k) is modeled as a Negative Binomial distribution.

(a) [6 points] Show that the *negative binomial* distribution, for some fixed k, is an exponential family distribution. You should explicitly specify $b(y), \eta, T(y), a(\eta)$. Also specify what ϕ is in terms of η .

Answer:

$$p(y;\phi,k) = {y-1 \choose k-1} (1-\phi)^{y-k} \phi^k$$

$$= {y-1 \choose k-1} \exp\left((y-k)\log(1-\phi) + k\log\phi\right)$$

$$= {y-1 \choose k-1} \exp\left(y\log(1-\phi) - k\log(1-\phi) + k\log\phi\right)$$

$$= {y-1 \choose k-1} \exp\left(\log(1-\phi)y - k\log\frac{1-\phi}{\phi}\right)$$

¹(off-topic) more precisely, this is called a "norm"

²(off-topic) historically, in chess, k = 3. However, FIDE feels that there are too many grandmasters. So, they are interested in building a system that will work if they decide to raise the cut-off (and so they've contacted you).

and this is in exponential family form, as desired. Note that

$$b(y) = {y-1 \choose k-1},$$

$$\eta = \log(1-\phi),$$

$$T(y) = y,$$

$$a(\eta) = k \log \frac{1-\phi}{\phi},$$

$$\phi = 1 - e^{\eta}.$$

(b) [6 points] You're given an IID³ train set $\{(x^{(i)}, y^{(i)}) \text{ for } i = 1, ..., m\}$, and as mentioned earlier, FIDE would like you to model this using a GLM based on a negative binomial distribution. Given some fixed k, find the log-likelihood

$$\ell(\theta) := \log \prod_{i=1}^{m} p(y^{(i)}|x^{(i)};\theta)$$

defined with respect to the *entire train set*, and expressed it only in terms of $k, \theta, x^{(i)}$'s, and $y^{(i)}$'s.

Answer:

First, we calculate the log-likelihood with respect to a single example:

$$\begin{split} \log p(y^{(i)}|x^{(i)};\theta) &= \log \left(\binom{y^{(i)}-1}{k-1} (1-\phi)^{y^{(i)}-k} \phi^k \right) \\ &= \log \binom{y^{(i)}-1}{k-1} + \log (1-\phi) y^{(i)} - k \log \frac{1-\phi}{\phi} \\ &= \log \binom{y^{(i)}-1}{k-1} + y^{(i)} \log e^{\eta} - k \log \frac{e^{\eta}}{1-e^{\eta}} \\ &= \log \binom{y^{(i)}-1}{k-1} + \eta y^{(i)} - \eta k + k \log (1-e^{\eta}) \\ &= \log \binom{y^{(i)}-1}{k-1} + \theta^{\top} x^{(i)} y^{(i)} - \theta^{\top} x^{(i)} k + k \log (1-\exp(\theta^{\top} x^{(i)})) \\ &= \log \binom{y^{(i)}-1}{k-1} + \theta^{\top} x^{(i)} (y^{(i)}-k) + k \log (1-\exp(\theta^{\top} x^{(i)})). \end{split}$$

Now, with respect to the whole dataset:

$$\ell(\theta) = \log \prod_{i=1}^{m} p(y^{(i)}|x^{(i)}; \theta)$$

$$= \sum_{i=1}^{m} \log p(y^{(i)}|x^{(i)}; \theta)$$

$$= \sum_{i=1}^{m} \left(\log \binom{y^{(i)} - 1}{k - 1} + \theta^{\top} x^{(i)} (y^{(i)} - k) + k \log(1 - \exp(\theta^{\top} x^{(i)})) \right).$$

³independently and identically distributed

- (c) [8 points] Now, for this log-likelihood expression, derive
 - H the Hessian matrix,
 - $\nabla_{\theta} \ell(\theta)$ the gradient vector w.r.t.⁴ θ ,

and **state** (in terms of those two quantities) one step of Newton's method for maximizing the log-likelihood.

Answer:

$$\begin{split} \nabla_{\theta}\ell(\theta) &= \nabla_{\theta} \sum_{i=1}^{m} \left(\log \left(y^{(i)} - 1 \atop k - 1 \right) + \theta^{\intercal} x^{(i)} (y^{(i)} - k) + k \log(1 - \exp(\theta^{\intercal} x^{(i)})) \right) \\ &= \sum_{i=1}^{m} \left(x^{(i)} (y^{(i)} - k) - k \frac{x^{(i)} \exp(\theta^{\intercal} x^{(i)})}{1 - \exp(\theta^{\intercal} x^{(i)})} \right) \\ &= \sum_{i=1}^{m} \left((y^{(i)} - k) - k \frac{\exp(\theta^{\intercal} x^{(i)})}{1 - \exp(\theta^{\intercal} x^{(i)})} \right) x^{(i)} \\ &= \sum_{i=1}^{m} \left(y^{(i)} - \frac{k}{1 - \exp(\theta^{\intercal} x^{(i)})} \right) x^{(i)} \\ H &= \nabla_{\theta} \left(\nabla_{\theta} \ell(\theta) \right) \\ &= \nabla_{\theta} \left(\sum_{i=1}^{m} \left(y^{(i)} - \frac{k}{1 - \exp(\theta^{\intercal} x^{(i)})} \right) x^{(i)} \right) \\ &= -\sum_{i=1}^{m} \left(\frac{k \cdot \exp(\theta^{\intercal} x^{(i)})}{(1 - \exp(\theta^{\intercal} x^{(i)}))^{2}} \right) x^{(i)} x^{(i)\intercal}. \end{split}$$

As we learnzed in class, the Newton's method update rule is: $\theta:=\theta-H^{-1}\nabla_{\theta}\ell(\theta)$.

⁴with respect to

(d) [4 points] Show that the Hessian matrix you derived is negative semi-definite. This shows that the optimization obejctive is concave, and thus, Newton's method is indeed maximizing log-likelihood.

Answer:

$$z^{\top} H z = -\sum_{i=1}^{m} \left(\frac{k \cdot \exp(\theta^{\top} x^{(i)})}{(1 - \exp(\theta^{\top} x^{(i)}))^{2}} \right) z^{\top} x^{(i)} x^{(i) \top} z.$$

$$= -\sum_{i=1}^{m} \left(\frac{k \cdot \exp(\theta^{\top} x^{(i)})}{(1 - \exp(\theta^{\top} x^{(i)}))^{2}} \right) ||z^{\top} x^{(i)}||$$

$$< 0.$$

(e) [1 point] If we set k = 1, we find that $y|x;\theta$ is distributed according to some other member of the exponential family. What is it?

Answer: The Geometric distribution (this is in the probability reference as well).

4. [15 points] Implementing Naive Bayes

Suppose you decide to implement a Naive Bayes spam classifier from scratch, just to see what will happen. You will try to implement a **Bernoulli event model** and will not apply Laplace smoothing (for now).

(a) [4 points] Being the machine learning whiz you are, both your math and your code are perfected. However, when running this model (on your training dataset), the prediction almost always gives a division-by-zero error.

When checking through your code, you realize that the error occurs because your code is making predictions by following these steps:

i. Calculate p(y = 1|x) and p(y = 0|x) by equations

$$p(y=1|x) = \frac{\left(\prod_{j=1}^{d} p(x_j|y=1)\right) p(y=1)}{\left(\prod_{j=1}^{d} p(x_j|y=1)\right) p(y=1) + \left(\prod_{j=1}^{d} p(x_j|y=0)\right) p(y=0)}$$
$$p(y=0|x) = 1 - p(y=1|x)$$

ii. Select the y with the higher posterior probability as the predicted label.

Why is this problematic? Explain your answer in 1-2 sentences. (**Hint**: this is **not** due to not applying Laplace smoothing.)

Answer: A correct answer would explain underflow of the terms $\prod_{j=k}^d p(x_j|y=k)$. i.e. multiplying a large number of terms close to 0 would lead to a term evaluated to 0 by the computer.

Note that answers related to "terms within $\prod_{j=k}^d p(x_j|y=k)$ equal to 0 due to unseen words" will be given partial credit. However, based on the **Hint** the answer is technically incorrect, as Laplace smoothing solves the 0-term problem.

(b) [4 points] Come up with a way of avoiding this error and write out the new steps for prediction. Explain why the new method will be able to produce the same predicted label as the process in (a).

Answer: A standard answer here would be using log probability $\sum_{j=k}^{d} \log p(x_j|y=k)$ to replace $\prod_{j=k}^{d} p(x_j|y=k)$. The equation can be

$$p(y=1|x) = \frac{\left(\sum_{j=1}^{d} \log p(x_j|y=1)\right) + \log p(y=1)}{\left(\sum_{j=1}^{d} \log p(x_j|y=1)\right) + \log p(y=1) + \left(\sum_{j=0}^{d} \log p(x_j|y=0)\right) + \log p(y=0)}$$
$$p(y=0|x) = 1 - p(y=1|x)$$

but other reasonable answers, such as directly comparing the value of $\sum_{j=1}^d \log p(x_j|y=1) \log p(y=1)$ and $\sum_{j=0}^d \log p(x_j|y=0) \log p(y=0)$, should also be accepted.

The explanation needs to touch on the monotonicity of log.

(c) [4 points] After implementing the solution in (b), your model runs smoothly for the training data. However, you still need to deal with unseen words to make predictions over the test dataset. To save yourself from the headache of implementing Laplace smoothing, you come up with another way of treating unseen words:

- If the model encountered a word in both spam and regular emails in the training dataset, we use its ϕ values from training.
- If the model did not encounter a word j in any spam emails, we consider it equally likely that j will appear or not appear in any given spam email. Therefore, we set its $\phi_{j|y=1} = \frac{1}{2}$ and use its $\phi_{j|y=0}$ from training as usual.
- Conversely, if the model did not encounter j in any regular email, we set its $\phi_{j|y=0} = \frac{1}{2}$ and use the $\phi_{j|y=1}$ from training.
- Based on this logic, if j is never encountered in any email during training, we let $\phi_{j|y=1} = \phi_{j|y=0} = \frac{1}{2}$.

Recall that without Laplace smoothing:

$$p(x_j|y=1) = \phi_{j|y=1} = \frac{\sum_{i=1}^n \mathbf{1}\{x_j^{(i)} = 1 \land y^{(i)} = 1\}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = 1\}}$$
$$p(x_j|y=0) = \phi_{j|y=0} = \frac{\sum_{i=1}^n \mathbf{1}\{x_j^{(i)} = 1 \land y^{(i)} = 0\}}{\sum_{i=1}^n \mathbf{1}\{y^{(i)} = 0\}}$$

Please provide a one-sentence answer to each of the following questions.

- i. What critical assumption are we making when using this method?
- ii. What is wrong with this assumption?

Answer: The method is wrong because it is based on the assumption that it is equally likely for an unseen word to appear or not appear in an email, given that it is a spam or regular email.

In fact, if a word never appears in spam/regular emails in the training dataset, we should reasonably assume that the probability for the word to appear in that type of email should be very low.

This is the assumption Laplace smoothing is making; Laplace smoothing essentially delegates a very small portion of the conditional probability to the event that the unseen word appears in the spam/regular email.

(d) [3 points] Hooray! After implementing everything (including Laplace smoothing) based on the previous questions, you have created a spam classifier that, for a test dataset, achieves a prediction accuracy of 95%. However, when you use this classifier for your own inbox, the model performs quite poorly. In fact, it does not block any spam email.

Suppose the model implementation and the adaptation to your inbox are all done perfectly, and suppose there is no significant difference between the new spam/regular emails you are receiving and the emails in the dataset. What is a possible explanation for the high accuracy and the poor performance? (Hint: in your answer, we are looking for a particular characteristic of the dataset that the model trained on.)

Answer: The problem is that accuracy is not a good indicator of whether the classifier does a great job in the test dataset. If there are a lot more regular emails than spam emails in the test dataset, based on our prediction method, it is possible that the model can achieve a high accuracy score by simply predicting all emails as regular emails.

5. [15 points] Exponential Family Discriminant Analysis

In class, we have seen Gaussian Discriminant Analysis. In this problem we generalize the approach to work with abstract exponential families.

Consider the model

$$y \sim \text{Bernoulli}(\phi)$$
 (1)

$$x \mid y = 0 \sim \text{EF}(\eta_0) \tag{2}$$

$$x \mid y = 1 \sim \mathrm{EF}(\eta_1) \tag{3}$$

where $\mathrm{EF}(\eta)$ denotes the exponential family distribution parameterized by η , which has density

$$p(x;\eta) = b(x) \exp\left(\eta^{\top} T(x) - a(\eta)\right) \tag{4}$$

(a) [5 points] We are given data $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})$, where $x^{(i)} \in \mathbb{R}^d$ and $y^{(i)} \in \{0, 1\}$. Let $n_j = \sum_{i=1}^n 1[y^{(i)} = j]$ i.e. the number of examples with label j. Given that T(x) = x, show that the maximum likelihood estimate of η_j , denoted $\hat{\eta}_j$, must satisfy

$$\mathbb{E}[X; \hat{\eta}_j] = \frac{1}{n_j} \sum_{i=1}^n 1[y^{(i)} = j] T(x^{(i)})$$
 (5)

You may use any result from class or problem sets without proof.

Answer: The log-likelihood writes

$$\sum_{i=1}^{n} \log p(y^{(i)}; \phi) + p(x^{(i)} | y^{(i)}; \eta_0, \eta_1)$$

Let $S_j = \{i : y^{(i)} = j\}$ i.e. the set of examples with the label j. We drop the terms that don't depend on η_i :

$$\sum_{i \in S_j} \log p(x^{(i)} | y^{(i)} = j; \eta_j) = \sum_{i \in S_j} \left(\log b(x^{(i)}) + \eta^\top T(x^{(i)}) - a(\eta) \right)$$

For optimality, the gradient, which is

$$\sum_{i \in S_i} \left(T(x^{(i)}) - \nabla a(\eta) \right) = -n_j \nabla a(\eta) + \sum_{i \in S_i} T(x^{(i)})$$

must vanish, so necessarily

$$\nabla a(\hat{\eta}_j) = \frac{1}{n_j} \sum_{i \in S_j} T(x^{(i)})$$

Recalling from Problem Set 1 that $\nabla a(\eta) = \mathbb{E}[X \mid \eta]$ proves the result.

(b) [6 points] Show that the posterior $p(y=1\,|\,x,\phi,\eta_0,\eta_1)$ can be written in the familiar form $\sigma(\tilde{\eta}^\top T(x)+c)$, where σ is the sigmoid function $\sigma(t)=\frac{1}{1+\exp(-t)}$, and $\tilde{\eta}$ and c are expressed in terms of the parameters $\{\phi,\eta_0,\eta_1\}$ and possibly the functions a and/or b. Your answer should specify these expressions.

Answer: Using Bayes rule, we have

$$p(y = 1 \mid x; \phi, \eta_0, \eta_1) = \frac{p(y = 1; \phi)p(x \mid y = 1; \eta_1)}{p(y = 0; \phi)p(x \mid y = 0; \eta_0) + p(y = 1; \phi)p(x \mid y = 1; \eta_1)}$$

$$= \frac{1}{1 + \frac{p(y = 0; \phi)}{p(y = 1; \phi)} \frac{p(x \mid y = 0; \eta_0)}{p(x \mid y = 1; \eta_1)}}$$

$$= \frac{1}{1 + \frac{1 - \phi}{\phi} \cdot \frac{b(x) \exp(\eta_0^\top T(x) - a(\eta_0))}{b(x) \exp(\eta_1^\top T(x) - a(\eta_1))}}$$

$$= \frac{1}{1 + \exp\left(\log \frac{1 - \phi}{\phi} + (\eta_0 - \eta_1)^\top T(x) + a(\eta_1) - a(\eta_0)\right)}$$

which is the stated form with

$$\tilde{\eta} = \eta_1 - \eta_0$$

$$c = a(\eta_0) - a(\eta_1) - \log \frac{1 - \phi}{\phi}$$

(c) [4 points] Under what condition(s) is the decision boundary linear in x? Be as general as possible.

Answer: The decision boundary is the set $p(y=1 \mid x, \phi, \eta_0, \eta_1) = \frac{1}{2}$. Based on the previous part, this is the same as $\tilde{\eta}^{\top}T(x) + c = 0$. For this to be linear in x, T must be affine in x, i.e. T(x) = Ax + v for some matrix A and vector v.

6. [20 points] Node-splitting via logistic regression

Let's revisit our use of the decision tree model on the binary classification task with d-dimensional real-valued datapoints. That is, we have $x^{(i)} \in \mathbb{R}^d$ and $y^{(i)} \in \{0,1\}$ for each datapoint. We learned a greedy algorithm in class for fitting a decision tree to a training set of real-valued data. In this algorithm, to determine how to split a node, we iterate over all feature-value pairs to find a threshold that yields the best split, leaving us with two new nodes in the tree (in this problem, we'll consider "best" to mean that the split yields the highest classification accuracy). We'll refer to this node splitting practice as "threshold split selection".

In this problem, we'll also consider an alternative method of node-splitting where we train a logistic regression classifier on the data in a node and use the resulting model to determine the split. Concretely, the two resulting nodes from the logistic regression split will contain the datapoints classified as 0 and 1 by the model, respectively. We'll refer to this as "logistic regression split selection".

Overall note: While we make plenty of assumptions throughout this problem, the solutions that received full credit made no assumptions beyond those made explicit in the problem statements. Strong assumptions about the number of splits in each tree (e.g., $j \approx k$), relationships between m, w, and d (e.g., m >> w), and certain values of m, w, and d (e.g., $d \approx 1$) were not necessary to answer the questions correctly and thus did not receive full credit.

(a) [4 points] Suppose we have m datapoints for training. What is the (asymptotic) running time for training a logistic regression model on these datapoints via stochastic gradient descent? Assume that the model converges to an optimum after exactly w epochs. Express your final answer for this and future running time complexity questions using Big O notation (e.g., $O(x + y^3 \log z)$).

Answer: Each stochastic gradient descent update is dominated by O(d) calculations for the inner product between the model parameters and the training datapoint. Since there are m training datapoints and w epochs of training, we have O(dmw) as our overall runtime.

(b) [3 points] Supposing again that we have m datapoints, what is the running time for choosing the best threshold via the threshold split selection algorithm from lecture? Assume that evaluating the classification error of a certain split is O(1) (this is a result of an common amortization technique—no need to think about/explain why this assumption holds).

Hint: The running time associated with sorting a list of z values is $O(z \log z)$. **Answer:** We can sort the m datapoints according to their values on a single feature in $O(m \log m)$ time according to the hint, so doing this sorting for every feature takes $O(dm \log m)$ time. We then can iterate over the $d \times (m-1)$ unique thresholds to generate splits, each of which takes O(1) time to evaluate by assumption, so we have overall cost of only O(dm) for this search. Thus, we have $O(dm \log m)$ as the runtime.

(c) [5 points] Suppose that we want to create two decision trees T_1 and T_2 to fit to a training set of size m, where T_1 uses logistic regression split selection and T_2 uses threshold split selection.

Provide brief explanations (1–2 sentences) for each of the following questions:

- i. Can any split achieved via threshold split selection be achieved via logistic regression split selection? And can any split via logistic regression split selection be achieved via a threshold split selection?
- ii. Assume that on any individual node, the split that results from logistic regression split selection achieves a classification accuracy no worse than that of threshold split selection. If we allow both trees to perfectly fit the data, which of T_1 and T_2 would you expect to be smaller (have fewer nodes)?

Answer:

- i. The split from any threshold corresponds to using some axis-aligned separating hyperplane in \mathbb{R}^d . Because logistic regression can output any separating hyperplane in \mathbb{R}^d , it follows that the possible splits via threshold are a subset of those via logistic regression.
- ii. Since logistic regression is a better classifier than a threshold split by our assumption, we would require fewer splits to perfectly fit to the training set. Therefore, we'd expect fewer nodes in T_1 than T_2 .

(d) [4 points]

We will now evaluate total running time for training each of these models. To do so, we'll make the following simplifying assumptions:

- i. We will restrict the training of T_1 to involve exactly j splits.
- ii. We will restrict the training of T_2 to involve exactly k splits.
- iii. We will assume that there are O(m) datapoints present at any node we want to split.

With these assumptions in place, what is the running time for T_1 and for T_2 ? State once in **mathematical notation** and once in **plain language** what condition would make the running times for training (asymptotically) equal for T_1 and T_2 .

Hint: You've already done part of the work here in parts (a) and (b).

Answer: Since we have j and k splits for the logistic regression- and threshold-based models, respectively, and we have by assumption the same number of datapoints in each split, our runtimes are O(jdmw) for T_1 and $O(kdm\log m)$ for T_2 . These are asymptotically equivalent when $jw \approx k\log m$, i.e., the total number of epochs required to train T_1 is roughly equal to the product of the number of splits in T_2 and the logarithm of the number of datapoints in the training set.

(e) [4 points] What is the running time of prediction for both T_1 and T_2 (where by prediction we mean evaluating $T_t(x)$ for some datapoint $x \in \mathbb{R}^d$)? State once in **mathematical notation** and once in **plain language** what condition would make the running times for prediction (asymptotically) equal for T_1 and T_2 . The restrictions from part (d) still apply, namely that we have exactly j splits in T_1 and k splits in T_2 .

Hint: If we have z splits in a tree, then the tree's depth is O(z) in the worst case.

Answer: For T_1 , we must predict via our learned logistic regression model at a given node to decide which child to descend to. Each of these predictions is dominated by the inner product between parameters and the datapoint, which is O(d), so overall runtime is O(jd) since there are O(j) splits to evaluate at most. For T_2 , since feature-wise comparisons are O(1), we have that prediction runtime is O(k) for similar reasoning as with T_1 . So we seek $dj \approx k$, i.e., when T_1 has roughly one split for every d splits in T_2 , we have approximately similar prediction time.

That's all! Congratulations on completing the exam!