CS 189/289A Introduction to Machine Learning
Spring 2022 Jonathan Shewchuk Final

- Please do not open the exam before you are instructed to do so.
- **Electronic devices are forbidden on your person**, including phones, laptops, tablet computers, headphones, and calculators. Turn your cell phone off and **leave all electronics at the front of the room**, or **risk getting a zero** on the exam.
- When you start, the **first thing you should do** is **check that you have all 11 pages and all 6 questions**. The second thing is to please **write your initials at the top right of every page after this one** (e.g., write "JS" if you are Jonathan Shewchuk).
- The exam is closed book, closed notes except your two cheat sheets.
- You have **180 minutes**. (If you are in the DSP program and have an allowance of 150% or 200% time, that comes to 270 minutes or 360 minutes, respectively.)
- Mark your answers on the exam itself in the space provided. Do **not** attach any extra sheets. If you run out of space for an answer, write a note that your answer is continued on the back of the page.
- The total number of points is 150. There are 15 multiple choice questions worth 4 points each, and 5 written questions worth a total of 90 points.
- For multiple answer questions, fill in the bubbles for **ALL correct choices:** there may be more than one correct choice, but there is always at least one correct choice. **NO partial credit** on multiple answer questions: the set of all correct answers must be checked.

First name	
Last name	
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First and last name of student to your left	
First and last name of student to your right	

Q1. [60 pts] Multiple Answer

Fill in the bubbles for **ALL correct choices**: there may be more than one correct choice, but there is always at least one correct choice. **NO partial credit**: the set of all correct answers must be checked.

(a) [4 pts] What is true of convolutional neural networks (CNNs)?

◯ A: Learned convolutional masks can act as edge detectors or line detectors.

◯ B: A convolutional layer of connections from a layer of m hidden units to a layer of m' hidden units has fewer weights than a fully-connected layer of connections from a layer of m hidden units to a layer of m' hidden units.

◯ C: Let X be a 4×4 image that is fed through an average-pooling layer with 2×2 masks, producing a 2×2 output layer Y. Then for every unit/pixel X_{ij} and every unit/pixel $Y_{k\ell}$, the partial derivative $\partial Y_{k\ell}/\partial X_{ij}$ is equal to $1/4$.

◯ D: Some research on CNNs made a strong enough impact to win the Alan M. Turing Award.

(b) [4 pts] What is true of regression algorithms?

◯ A: All regression problems can be solved by solving a system of linear equations.

◯ B: Least squares regression can be derived from maximum likelihood estimation if we assume that the sample points have a multivariate normal distribution.

◯ C: Adding a feature with no predictive value to least squares regression is unwise because it increases the bias of the method.

◯ D: *Weighted* least squares regression can be derived from maximum likelihood estimation if we assume that some points' labels are noisier than others.

(c) [4 pts] What is true of kernels?

◯ A: Kernel algorithms require you to solve a linear system with a $D \times D$ matrix, where D is the length of the lifted sample points $\Phi(X_i)$.

◯ B: Neural networks can be kernelized because there is always an optimal weight vector w that is a linear combination of the sample points.

◯ C: Fitting and evaluating a kernel ridge regression model requires access only to the kernel matrix K and not the training points X_i nor $\Phi(X_i)$.

◯ D: The kernel perceptron algorithm with a Gaussian kernel returns a classifier similar to a smoothed version of k-nearest neighbor classification.

(d) [4 pts] Which of the following statements are true of the Rayleigh quotient $Q(X, w) = w^\top X^\top X w/(w^\top w)$ for an arbitrary matrix $X \in \mathbb{R}^{n \times d}$ and vector $w \in \mathbb{R}^d$?

◯ A: $Q(X, w) \geq 0$ for all X and w.

◯ B: $Q(X, w) \leq \sigma^2_{\max}(X)$ for all X and w, where $\sigma_{\max}(X)$ is the greatest singular value of X.

◯ C: $Q(X, w)$ is maximized when w is the eigenvector of $X^\top X$ corresponding to the greatest eigenvalue.

◯ D: $Q(X, w)$ is maximized when w is the eigenvector of $X^\top X$ corresponding to the smallest eigenvalue.

(e) [4 pts] Given $X \in \mathbb{R}^{n \times d}$ and $y \in \mathbb{R}^n$, consider solving the normal equations $X^\top X w = X^\top y$ for $w \in \mathbb{R}^d$. Let the SVD of X be $X = UDV^\top$. Let X^+ denote the Moore–Penrose pseudoinverse of a matrix X. Which of the following statements are certain to be true, for any values of X and y?

◯ A: $w = (X^\top X)^{-1} X^\top y$ is a solution of the normal equations.

◯ B: $w = X^+ y$ is a solution of the normal equations.

◯ C: $w = VD^+ U^\top y$ is a solution of the normal equations.

◯ D: Every solution w to the normal equations is a solution to $Xw = y$.

(f) [4 pts] Which of the following would be a reasonable cost function (by the criteria discussed in lecture) for choosing splits in a decision tree for two-class classification, where p is the fraction of points in Class C in a specified treenode?

◯ A: $-p \log_2 p - (1-p) \log_2 (1-p)$

◯ B: $p \log_2 p + (1-p) \log_2 (1-p)$

◯ C: $0.5 - |p - 0.5|$

◯ D: $p(1-p)$

(g) [4 pts] Which of the following are advantages to using AdaBoost with short trees (say, depth 4) over random forests with an equal number of tall trees (refined until the leaves are pure)?

◯ A: AdaBoost is more robust against overfitting outliers in the training data.

◯ B: AdaBoost is faster to train.

◯ C: AdaBoost is better at reducing variance than a random forest.

◯ D: AdaBoost is better at reducing bias than a random forest.

(h) [4 pts] What is true of k-nearest neighbor classifiers in a Euclidean space?

◯ A: A 1-NN classifier is more likely to overfit and less likely to underfit than a 10-NN classifier.

◯ B: In the special case of a two-dimensional feature space, it is possible to preprocess a data set so that nearest neighbor queries can be answered in $O(\log n)$ time.

◯ C: Sometimes finding k approximate nearest neighbors can be done much faster than finding the k exact nearest neighbors.

◯ D: The k-d tree algorithm for nearest neighbor search can speed up 1-NN, but it doesn't work well for k-NN.

(i) [4 pts] What is true of bagging? (Note: not in a random forest; just bagging alone.)

◯ A: Bagging without replacement is more likely to overfit than bagging with replacement.

◯ B: Bagging involves using different learning algorithms on different subsamples of the training set.

◯ C: Bagging is often used with decision trees because it helps increase their training accuracy.

◯ D: Even with bagging, sometimes decision trees still end up looking very similar.

(j) [4 pts] What is true of k-means clustering?

◯ A: k-means is a supervised learning algorithm.

◯ B: k-means clustering always converges to the same solution regardless of how clusters are initialized.

◯ C: Increasing k can never increase the optimal value of the k-means cost function.

◯ D: The k-medoids algorithm with the ℓ_1 distance is less sensitive to outliers than standard k-means with the Euclidean distance.

(k) [4 pts] Which of the following statements about AdaBoost is true?

◯ A: AdaBoost is a natural good fit with the 1-nearest neighbor classifier.

◯ B: AdaBoost can give you a rough estimate of the posterior probability that a test point is in the predicted class.

◯ C: AdaBoost trains multiple weak learners that classify test points by equal majority vote.

◯ D: AdaBoost with an ensemble of soft-margin linear SVM classifiers allows the metalearner to learn nonlinear decision boundaries.

(l) [4 pts] You have n training points, each with d features. You try two different algorithms for training a decision tree.

1. The standard decision tree with single-feature (axis-aligned) splits, as covered in lecture.
2. A *randomized* decision tree—like a tree in a random forest, but there is only one tree and we don't use bagging. At each internal node of the tree, we randomly select m of the d features, and we choose the best split from among those m features.

Suppose you train both trees permitting no treenode to have depth greater than h. Upon completion, you find that in each tree, at least half its leaves are at depth h. What are the running times for training the standard decision tree and the randomized one, respectively? (Select exactly one option.)

◯ A: $\Theta(dn2^h)$; $\Theta(mn2^h)$

◯ B: $\Theta(dn2^h)$; $\Theta(dn2^h)$

◯ C: $\Theta(dnh)$; $\Theta(mnh)$

◯ D: $\Theta(dnh)$; $\Theta(dnh)$

(m) [4 pts] Suppose you have a fixed dataset and want to train a decision tree for two-class classification. If you increase the maximum depth of the decision tree, which of the following are possible effects?

◯ A: The test accuracy goes up.

◯ B: The training accuracy goes down.

◯ C: The number of pure leaves is reduced.

◯ D: The time to classify a test point increases.

(n) [4 pts] What is true of the shatter function $\Pi_H(n)$, where n is the number of training points?

◯ A: It either grows polynomially with n or is 2^n for all n, but it can never be in between those extremes.

◯ B: We use it to compute an estimate of how many training points we need to ensure we choose a hypothesis with nearly optimal risk with high probability.

◯ C: For a linear classifier in $\mathbb{R}^d$, the shatter function grows polynomially with n.

◯ D: For a power set classifier, the shatter function grows polynomially with n.

(o) [4 pts] What is true of human neurology?

◯ A: The output of a unit in an artificial neural network is roughly analogous to the voltage of an axon at the synapse.

◯ B: A connection in an artificial neural network is roughly analogous to a synapse in the brain.

◯ C: The brain is made of general-purpose neurons, each of which could be trained to do any job that neurons do.

◯ D: The visual cortex has neurons primarily devoted to detecting lines or edges.

Q2. [20 pts] Decision Tree Construction

You want to figure out what makes people click on online advertisements, so you try a variety of different advertisements, and record user behavior in the following table, which is our training set.

Advertisement	Animated?	Popup?	Colorful?	Clicked
1	Yes	Yes	No	No
2	No	Yes	Yes	No
3	No	Yes	No	No
4	No	No	Yes	Yes
5	Yes	No	Yes	Yes
6	Yes	No	No	Yes
7	No	No	Yes	Yes
8	No	No	No	No

The middle three columns ("Animated," "Popup," "Colorful") are the features of each advertisement. The last column, "Clicked," is the label, specifying whether or not a user clicked on the advertisement. You want to predict the "Clicked" label for other advertisements not in this training set.

(a) [8 pts] **Which feature** should you split on at the root of the decision tree to maximize the information gain? **Write an expression for the information gain** of the best split. (Your expression can contain logarithms and fractions.)

(b) [8 pts] **Draw the decision tree** that maximizes information gain at each split. Your drawing should include the leaves and the training points they store. (Do not include entropies or information gains.) Stop splitting at pure nodes.

(c) [4 pts] Suppose you are using AdaBoost with stumps, which are trees with just one split. In the first iteration, AdaBoost assigns each advertisement a weight of $1/8$, and it constructs a one-split tree with the split you specified in part (a). **What weights does AdaBoost assign** to the eight advertisements for the **second iteration**? Show your work.

Q3. [12 pts] Review of k-means Clustering

Let's see how well you remember k-means clustering, also known as Lloyd's Algorithm. As usual, the input is a set of n sample points $X_1, X_2, \ldots, X_n \in \mathbb{R}^d$ and an integer k. There are no input labels; we want to assign each sample point X_j a label $y_j \in \{1, 2, \ldots, k\}$, which can be interpreted as "X_j is assigned to cluster y_j." The means of the clusters are written $\mu_1, \mu_2, \ldots, \mu_k$.

(a) [4 pts] **What is the cost function** that k-means clustering tries to minimize? Write it in terms of the X_j's, the y_j's, and the μ_i's. (Not the formula for the within-cluster variation, please; a formula that uses the means. We are flexible about what notation you use to sum the terms in the cost function; please explain it if it's not obvious.)

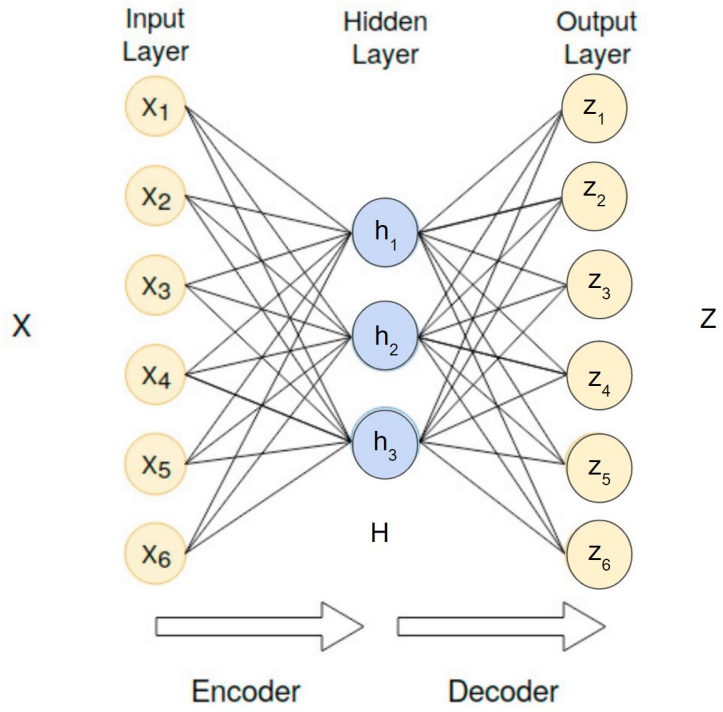
(b) [5 pts] Consider the step of the algorithm where the labels y_j are held fixed while the cluster means μ_i are updated. I asserted in lecture that it is easy to show with calculus that if we want to minimize the cost function, we should **choose each μ_i to be the mean (centroid) of the sample points assigned to cluster i**. Please do that calculus and **show that this claim is correct**. (Make sure you explain your notation for counting the points in a cluster.) **Show your work and don't skip any steps of the derivation.**

(c) [3 pts] Consider the step of the algorithm where the cluster means μ_i are held fixed while the labels y_j are updated. Sometimes a sample point X_j has several cluster means that are equally close. In class I said, "If there's a tie, and one of the choices is for X_j to stay in the same cluster as the previous iteration, always take that choice." **What could conceivably go wrong** if you don't follow that advice?

Q4. [20 pts] Backpropagation through an Autoencoder

An autoencoder is a type of neural network used to learn efficient encodings of data. We present a vector $x \in \mathbb{R}^d$ at the network's input units. A fully connected layer of edges produces a lower-dimensional vector of hidden units $h \in \mathbb{R}^m$, where $m < d$. Another fully connected layer produces an output vector $z \in \mathbb{R}^d$. Usually, the output label associated with x is x—in other words, the goal of training is simply to reproduce the input vector at the output. What makes this difficult is that there are so few hidden units. The network has to learn how to compress the information in the training set so it can be represented in a lower-dimensional space without losing much information. This is not always possible; it depends on the data. If successful, the hidden units are considered to be a *latent representation* of the input data.

We will use sigmoid/logistic units and a notation similar to that used in lecture, but we will break out the bias terms into separate vectors. Specifically, $h = s(Vx + p)$ where $V \in \mathbb{R}^{m \times d}$ is a matrix of weights connecting x to h, $p \in \mathbb{R}^m$ is a vector of bias terms, and $s(\cdot)$ denotes the logistic (sigmoid) function $s(\gamma) = 1/(1 + e^{-\gamma})$ applied element-wise to a vector. Similary, $z = s(Wh + q)$ where $W \in \mathbb{R}^{d \times m}$ and $q \in \mathbb{R}^d$. As the goal of training is to make the output vector z match the input vector x very tightly, we use the loss function $L(z, x) = \|z - x\|_2^4$.



(a) [6 pts] See the list of gradients below. **Draw a directed graph** whose vertices are the gradients (from this list) that are calculated during backpropagation to train our autoencoder. Do not include gradients that are not computed as part of backpropagation. If a gradient G is used by backpropagation to speed up the calculation of another gradient G', draw an arrow from G pointing to G'. (In other words, $G \rightarrow G'$ means G must be computed before G' if you want all the speed advantages of backpropagation. The graph will show us a partial ordering of the gradient computations.)

$$\nabla_x L, \nabla_h L, \nabla_z L, \nabla_V L, \nabla_p L, \nabla_W L, \nabla_q L$$

(b) [4 pts] **Derive an expression for** $\nabla_z L$ in terms of z and x (or components of z and x).

(c) [5 pts] **Derive an expression for** $\frac{\partial z_j}{\partial h_i}$ (the jth unit of z with respect to the ith unit of h). Express your final answer in terms of W and z (or components of W and z; if you need a notation for a column or row of W, explain your notation). **Show every step in the derivation** (i.e., include the steps that were skipped in lecture, except the derivation that $s' = s(1 - s)$, which you may take for granted).

(d) [5 pts] **Derive an expression for** $\frac{\partial L}{\partial x_k}$**.** Express your final answer in terms of V, h, and $\nabla_h L$ (or components of V, h, and $\nabla_h L$). **Show every step in the derivation** (i.e., include the steps that were skipped in lecture, except $s' = s(1 - s)$).

Q5. [18 pts] Musings

(a) [4 pts] It's well known that a memory in the brain may be "distributed" rather than "localized." What this means is that there is no one small portion of the brain where the memory is located. **What evidence do we have of that?**

(b) [4 pts] Memories in neural networks can also be "distributed." **What technique** we have learned in lecture that actively forces a neural net to distribute its memories? **How does it achieve this?**

(c) [4 pts] However, not every memory in every neural network is distributed. If a neural network has only two layers of units—input and output, with no hidden units—then the memories it stores are entirely local, not distributed. **Explain why.**

(d) [6 pts] Recall that in the lecture on principal components analysis, we saw a projection of the genetics (single nucleotide polymorphisms, abbreviated to SNPs, to be specific) of various old-stock Europeans onto a two-dimensional subspace, and we saw that it bore some resemblance to the geography of Europe. A skeptic might claim that distinct European ethnicities (e.g., French, Norwegian, Italian) do not exist, as "There is no single SNP that can identify the ethnicity of a European." The latter half of that sentence is true; probably there are no 10 SNPs that can do it.

Explain how we, as machine learning researchers, might generate evidence in favor of the existence of distinct ethnicities, despite the lack of a single SNP that distinguishes them, and despite the fact that some people cannot be classified unambiguously (because of multiple ancestry). **Also, explain** what insights random projections give us about the dimensions of the spaces we can use to answer such questions.

Q6. [20 pts] Boosting with a Squared Loss Function

Recall that AdaBoost trains T classifiers $G_1, ..., G_T$ iteratively with the training points re-weighted in each iteration. Given a test point z, the final metalearner's output is a linear combination of these learners,

$$M_T(z) = \sum_{t=1}^{T} \beta_t G_t(z).$$

AdaBoost trains the metalearner with an exponential loss function. In this problem, we explore another common boosting algorithm known as *Gradient Boosting*. Let $\rho = M_T(z)$ be a prediction made by the metalearner, and let $\ell \in \{+1, -1\}$ be the real-world label for the same point z. Gradient Boosting replaces the exponential loss function with the squared error loss,

$$L(\rho, \ell) = (\rho - \ell)^2.$$

We will do classification with two classes. As usual, assume we are given n training points $X_1, X_2, \ldots, X_n \in \mathbb{R}^d$ and a vector $y \in \mathbb{R}^n$ of labels, with $y_i = \pm 1$.

(a) [6 pts] **Write down the total empirical risk** of the Gradient Boosting metalearner with a squared error loss function. Express your answer in terms of the β_t's, G_t's, and y_i's.

(b) [8 pts] Suppose Gradient Boosting is in iteration T, and it has just trained a weak learner G_T but it has not yet determined the optimal coefficient β_T. (We assume that $\beta_1, \ldots, \beta_{T-1}$ are already fixed constants that can't be changed during iteration T.) **Derive an expression for β_T that minimizes the metalearner's empirical risk.** Show your work and simplify your answer as much as possible. *Hint:* Rewrite the risk in terms of M_{T-1}, the metalearner from iteration $T - 1$. (That way you don't have to write a summation repeatedly. Note that there's more space to write on the next page.)

(You may continue part (b) here.)

(c) [6 pts] In iteration T, before we compute β_T, Gradient Boosting has to train a weak learner G_T. Recall that the metalearner output $M_T(X_i)$ is a continously-valued real number, but the output of a weak learner $G_T(X_i)$ can only be $+1$ or -1. A paradoxical outcome of the squared error loss function is that if you truly want to minimize the empirical risk, the metalearner should provide the wrong label for some of the training points to the weak learner G_T during training! **Which training points should be given the wrong label when G_T is trained?** (Note: we'll accept an answer written in plain English, but we'll also accept an answer written in the form of a mathematical set. Your choice.)