CSCI 567 Fall 2021 Quiz One

Problem	1	2	3	4	5	Total
Max	30	12	20	24	14	100
Points						

Please read the following instructions carefully:

- Use the same link for the lectures to join Zoom for the quiz (available on both the course website and the DEN website). You will be assigned to a breakout room. Each room has one proctor, and you have to **turn your camera on** during the entire quiz. If you finish early, you can submit your quiz and leave the meeting, but you cannot rejoin.
- This is an open-book/note quiz. Searching the Internet is technically not forbidden, but you are strongly encouraged to focus on solving the problems yourself. **Collaboration of any kind or consultation from others, however, is strictly prohibited.** Violation will lead to **0 score** for the entire quiz and be reported to SJACS.
- For all questions, write down your answers as you would normally do for the written assignments, and then submit a pdf/jpg/png for each of the 5 problems. Make sure that your writing is recognizable. Try to keep you solutions concise.
- Duration of the exam is 2.5 hours, which **already includes the time you need for scanning and uploading**. No extra time will be given if you fail to upload your solutions within the given 2.5 hours. Questions are **not ordered by their difficulty**, so budget your time for each question carefully.
- If you have any **clarification** questions during the quiz, make a private post on Piazza and it will be answered shortly.

1 Multiple-choice Questions (30 points)

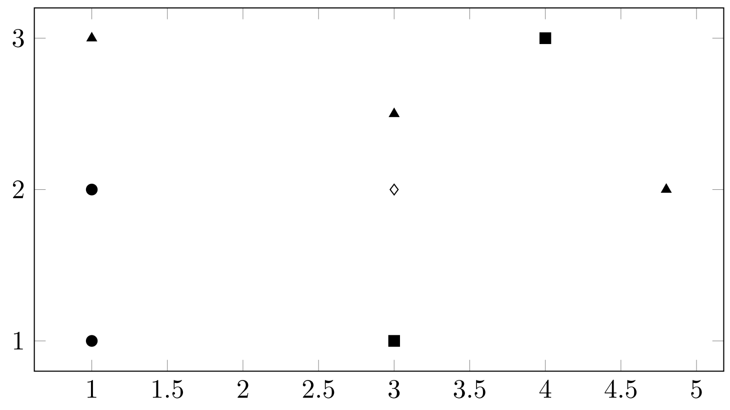
IMPORTANT: *Select ALL answers that you think are correct. You get 0.5 point for selecting each correct answer and similarly 0.5 point for not selecting each incorrect answer.*

(1) Which of the following on machine learning is correct?

(A) Cross-validation is often used to tune the hyper-parameters of a machine learning algorithm.
(B) The goal of a machine learning algorithm is to achieve zero error on a training set.
(C) Regularization is a common way to prevent overfitting.
(D) Classification and regression are two common tasks in machine learning.

Answer: ACD

(2) Consider the following two-dimensional dataset with $N = 7$ training points of three classes (triangle, square, and circle), and additionally one test point denoted by the diamond. Which of the following configuration of the K-nearest neighbor algorithm will predict triangle for the test point?



(A) $K = 1$, L2 distance
(B) $K = 3$, L1 distance
(C) $K = 3$, L2 distance.
(D) $K = 7$, any distance.

Answer: ABD

(3) Which of the following on linear regression is correct?

(A) The least square solution has a closed-form formula, even if L2 regularization is applied.
(B) The covariance matrix $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ is not invertible if and only if the number of data points N is smaller than the dimension D.
(C) When the covariance matrix $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ is not invertible, the Residual Sum of Squares (RSS) objective has no minimizers.
(D) Linear regression is a parametric method, even when it is kernelized.

Answer: A

(4) Which of the following on binary classification is correct?

(A) Similarly to the Perceptron algorithm, logistic regression can also be kernelized.
(B) The Perceptron algorithm (with $\mathbf{0}$ initialization) is an instance of SGD where the learning rate $\eta > 0$ does not matter.
(C) One can apply either SGD or the Newton method to minimize the hinge loss.

(D) Minimizing 0-1 loss is NP-hard for every dataset, even if it is linearly separable.

Answer: AB

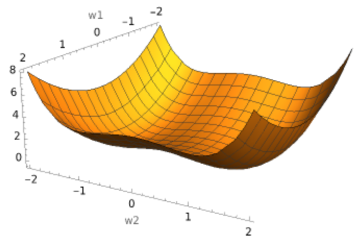
(5) Consider a training set $(\boldsymbol{x}_1, y_n), \ldots, (\boldsymbol{x}_N, y_N)$ and a probabilistic model $\mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{w})$ which specifies for each n the probability of seeing outcome y_n given feature $\boldsymbol{x}_n$ and parameter $\boldsymbol{w}$. Which of the following is the Maximum Likelihood Estimation (MLE) for $\boldsymbol{w}$?

(A) $\operatorname{argmax} \sum_{n=1}^N \mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{w})$ (B) $\operatorname{argmax} \Pi_{n=1}^N \mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{w})$
(C) $\operatorname{argmax} \sum_{n=1}^N \ln \mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{w})$ (D) $\operatorname{argmax} \Pi_{n=1}^N \ln \mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{w})$

Answer: BC

(6) Consider a two-dimensional function $F(\boldsymbol{w}) = w_1^2 - w_2^2 + \frac{1}{2}w_2^4$ (a plot is provided below). Which of the following statement is correct?

(A) F has three stationary points: $(0,0)$, $(0,-1)$, and $(0,1)$.
(B) F has three local minimizers: $(0,0)$, $(0,-1)$, and $(0,1)$.
(C) $(0,-1)$ is a local minimizer of F, so Gradient Descent always converges to this point.
(D) $(0,0)$ is a saddle point of F.



Answer: AD

(7) Machine learning objective is usually of the form $F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^N F_n(\boldsymbol{w})$ for some loss function $F_n : \mathbb{R}^D \to \mathbb{R}$ corresponding to the n-th training point. We know that $\nabla F_n(\boldsymbol{w})$ for a uniformly at random chosen n is a stochastic gradient of this objective such that $\mathbb{E}[\nabla F_n(\boldsymbol{w})] = \nabla F(\boldsymbol{w})$. Which of the following is also a stochastic gradient?

(A) $\sum_{n \in S} \nabla F_n(\boldsymbol{w})$ for a subset $S \subset \{1, \ldots, N\}$ (of some fixed size) chosen uniformly at random.
(B) $\frac{1}{|S|}\sum_{n \in S} \nabla F_n(\boldsymbol{w})$ for a subset $S \subset \{1, \ldots, N\}$ (of some fixed size) chosen uniformly at random.
(C) $\nabla F_n(\boldsymbol{w}) - \nabla F_n(\boldsymbol{w}_0) + \nabla F(\boldsymbol{w}_0)$ for an n chosen uniformly at random and some fixed point $\boldsymbol{w}_0$.
(D) $\frac{\partial F(\boldsymbol{w})}{\partial w_i} D\boldsymbol{e}_i$ for a coordinate i chosen uniformly at random ($\boldsymbol{e}_i \in \mathbb{R}^D$ is the standard basis vector with 1 in the i-th coordinate and 0 in all other coordinates).

Answer: BCD

(8) Which of the following on reduction from multiclass classification to binary classification is correct?

(A) One-versus-one is usually more robust than one-versus-all, but it is slower since it creates more binary training points.
(B) Multiclass logistic regression was invented since its binary version cannot be combined with one-versus-one or other reductions.
(C) A random code matrix is often a good choice for the Error-correcting Output Codes reduction.
(D) Tree-based reduction is especially useful when the number of possible classes is huge.

Answer: CD

(9) Which of the following about neural nets is correct?

(A) A neural net with a fixed architecture can represent any continuous function.
(B) Dropout is useful for preventing overfitting when training a nerual net.
(C) A neural net with only ReLU activation is a convex model, since ReLU is a convex function.
(D) A convolution layer is a special case of a fully connected layer.

Answer: BD

(10) Suppose a convolution layer takes a 4×6 image with 3 channels as input and outputs a $3 \times 4 \times 8$ volume. Which of the following is a possible configuration of this layer?

(A) One 2×3 filter with depth 8, stride 1, and no zero-padding.
(B) Eight 2×3 filters with depth 3, stride 1, and no zero-padding.
(C) Eight 2×2 filters with depth 3, stride 2, and 1 pixel of zero-padding.
(D) Eight 2×2 filters with depth 3, stride 2, and 2 pixels of zero-padding.

Answer: BC

(11) How many parameters do we need to learn for the following network structure? An $8 \times 8 \times 3$ image input, followed by a convolution layer with 4 filters of size 3×3 (stride 1 and 1 pixel of zero-padding), then another convolution layer with 3 filters of size 2×2 (stride 2 and no zero-padding), and finally a max-pooling layer with a 2×2 filter (stride 2 and no zero-padding). (Note: the depth of all filters are not explicitly spelled out, and we assume no bias/intercept terms used.)

(A) 48 (B) 144 (C) 156 (D) 168

Answer: C. $4 \times (3 \times 3 \times 3) + 3 \times (2 \times 2 \times 4) = 156$.

(12) What is the final output dimension of the last question?

(A) $2 \times 2 \times 3$ (B) $4 \times 4 \times 3$ (C) $2 \times 2 \times 1$ (D) $4 \times 4 \times 1$

Answer: A

(13) Which of the following on kernel is correct?

(A) A machine learning algorithm can be kernelized if it only uses the feature vectors through their inner products.
(B) A Gram/kernel matrix must be positive semidefinite.
(C) The product of two kernel functions is still a kernel function.
(D) $k(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{x} - \boldsymbol{x}'\|_1$ is not a kernel function.

Answer: ABCD

(14) Which of the following on SVM is correct?

(A) SVM tries to find a hyperplane with maximum margin, and thus it can only be applied to linearly separable data.
(B) The primal formulation of SVM minimizes L2 regularized hinge loss.
(C) A support vector must be a correctly classified point according to complementary slackness.
(D) It is possible that a support vector does not satisfy the hard-margin constraint.

Answer: BD

(15) Consider a training set of N data points $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N) \in \mathbb{R}^D \times \{-1, +1\}$ and a nonlinear mapping $\boldsymbol{\phi} : \mathbb{R}^D \to \mathbb{R}^\infty$ with a corresponding kernel function $k(\cdot, \cdot)$. Given the solution $\alpha_1^*, \ldots, \alpha_N^*$ of the SVM dual formulation for this training set (with a hyper-parameter C discussed in the lecture), which of the following is a correct way to make a prediction on a test point $\boldsymbol{x}$? (S below is the set of support vectors $\{n \in [N] : \alpha_n^* > 0\}$ and S' is a subset $\{n \in S : \alpha_n^* < C\}$.)

(A) First compute $\boldsymbol{w}^* = \sum_{m \in S} \alpha_m^* y_m \boldsymbol{\phi}(\boldsymbol{x}_m)$, then compute $b^* = y_n - \boldsymbol{w}^{*\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n)$ with any $n \in S'$, and finally predict with $\textsc{sgn}(\boldsymbol{w}^{*\mathrm{T}} \boldsymbol{x} + b^*)$.
(B) First compute $b^* = y_n - \sum_{m \in S'} \alpha_m^* y_m k(\boldsymbol{x}_m, \boldsymbol{x}_n)$ with any $n \in S'$, then predict with

$$\textsc{sgn}\left(\sum_{m \in S} \alpha_m^* y_m k(\boldsymbol{x}_m, \boldsymbol{x}) + b^*\right). \quad (1)$$

(C) First compute $b^* = y_n - \sum_{m \in S} \alpha_m^* y_m k(\boldsymbol{x}_m, \boldsymbol{x}_n)$ with any $n \in S'$, then predict with Eq. (1).
(D) First compute $b^* = \frac{1}{|S'|} \sum_{n \in S'} \left(y_n - \sum_{m \in S} \alpha_m^* y_m k(\boldsymbol{x}_m, \boldsymbol{x}_n)\right)$, then predict with Eq. (1).

Answer: CD

2 GD/SGD for Linear Regression (12 points)

(a) Least square solution is defined as $\boldsymbol{w}^* = \operatorname{argmin}_{\boldsymbol{w}\in\mathbb{R}^D} F(\boldsymbol{w})$ where

$$F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n - y_n)^2$$

for a training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N) \in \mathbb{R}^D \times \mathbb{R}$. Although we know that $\boldsymbol{w}^*$ has a closed-form, computing it requires inverting the $D\times D$ covariance matrix, which could be computationally expensive for large D. Instead, we can apply GD to approximately minimize $F(\boldsymbol{w})$. Fill in the missing details in the following implementation of this idea (no reasoning required). (3 points)

Algorithm 1: GD for minimizing RSS

```
1 Input: A training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$, learning rate $\eta$
2 Initialization: $\boldsymbol{w} = \mathbf{0} \in \mathbb{R}^D$
3 Repeat:
4     update: $\boldsymbol{w} \leftarrow \boldsymbol{w} - \frac{2\eta}{N}\sum_{n=1}^{N}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n - y_n)\boldsymbol{x}_n$.
```

(b) To speed up the algorithm further when N is large, we can instead apply SGD. Fill in the missing details in the following implementation of this idea (no reasoning required). (4 points)

Algorithm 2: SGD for minimizing RSS

```
1 Input: A training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$, learning rate $\eta$
2 Initialization: $\boldsymbol{w} = \mathbf{0} \in \mathbb{R}^D$
3 Repeat:
4     randomly pick an example $n$.                                  (1 point)
5     update: $\boldsymbol{w} \leftarrow \boldsymbol{w} - 2\eta(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n - y_n)\boldsymbol{x}_n$.       (3 points)
```

(c) To avoid over-fitting, we consider minimizing the regularized version of F:

$$F_\lambda(\boldsymbol{w}) = \left(\sum_{n=1}^{N}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n - y_n)^2\right) + \lambda\|\boldsymbol{w}\|_2^2.$$

Fill in the missing details in the following algorithm that approximately minimizes F_λ using SGD (no reasoning required). (5 points)

Algorithm 3: SGD for minimizing regularized RSS

```
1 Input: A training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$, learning rate $\eta$, regularization coefficient $\lambda$
2 Initialization: $\boldsymbol{w} = \mathbf{0} \in \mathbb{R}^D$
3 Repeat:
4     randomly pick an example $n$.                                  (1 point)
5     update: $\boldsymbol{w} \leftarrow \boldsymbol{w} - 2\eta(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n - y_n)\boldsymbol{x}_n - 2\eta\lambda\boldsymbol{w}$.       (4 points)
```

Rubrics: Give partial credits for partially correct answers. Do not deduct points for constructing the stochastic gradient with a mini-batch or other methods.

3 Linear Classifiers (20 points)

In Lecture 3 we have seen the hinge loss $\ell(z) = \max\{0, 1-z\}$, which is non-differentiable at $z = 1$. To avoid this issue, we can consider the square of hinge loss $\ell(z)^2$, which is differentiable everywhere. More specifically, given a binary dataset $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N) \in \mathbb{R}^D \times \{-1, 1\}$, we define the following new loss function for a linear model $\boldsymbol{w} \in \mathbb{R}^D$:

$$F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N} F_n(\boldsymbol{w}), \quad \text{where } F_n(\boldsymbol{w}) = \left(\max\left\{0, 1 - y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n\right\}\right)^2. \tag{2}$$

(a) For a fixed n, write down the gradient $\nabla F_n(\boldsymbol{w})$ (show your derivation), then fill in the missing details in the repeat-loop of the algorithm below which applies SGD to minimize F. (5 points)

Algorithm 4: SGD for minimizing Eq. (2)

```
1 Input: A training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N) \in \mathbb{R}^D \times \{-1, 1\}$, learning rate $\eta > 0$
2 Initialization: $\boldsymbol{w} = \boldsymbol{0}$
3 Repeat:
4     randomly pick an example $(\boldsymbol{x}_n, y_n)$
5     compute $z = y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n$ and update $\boldsymbol{w} \leftarrow \boldsymbol{w} + 2\eta y_n \max\{0, 1-z\}\boldsymbol{x}_n$
```

When $1 - y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n < 0$, the function is a constant and thus the gradient is $\boldsymbol{0}$. On the other hand, when $1 - y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n > 0$, the function is simply $F_n(\boldsymbol{w}) = (1 - y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)^2$, and thus by chain rule we have $\nabla F_n(\boldsymbol{w}) = -2y_n(1 - y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)\boldsymbol{x}_n$, which is also $\boldsymbol{0}$ when $y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n$ approaches 1. Therefore, we have

$$\nabla F_n(\boldsymbol{w}) = -2y_n \max\{0, 1 - y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n\}\boldsymbol{x}_n.$$

Rubrics:

- 3 points for the derivation of the gradient. Technically we need some discussion for the case $y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n = 1$ as the solution above shows, but for simplicity it is okay if such discussion is missing as long as the final gradient is correct.
- 2 points for the SGD implementation. Do not deduct more points for wrong gradient from the earlier wrong derivation.

(b) Now kernelize Algorithm 4 using a kernel function $k(\cdot, \cdot)$ (with a corresponding feature mapping $\boldsymbol{\phi}$). Specifically, fill in the missing details in the repeat-loop of the algorithm below which maintains and updates weights $\alpha_1, \ldots, \alpha_N$ such that $\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_n)$ is always the same as what one would get by running Algorithm 4 with $\boldsymbol{x}_n$ replaced by $\boldsymbol{\phi}(\boldsymbol{x}_n)$ for all n. (No reasoning is required.) (5 points)

Algorithm 5: Kernelized version of Algorithm 4

```
1 Input: A training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N) \in \mathbb{R}^D \times \{-1, 1\}$, learning rate $\eta > 0$, kernel $k(\cdot, \cdot)$
2 Initialization: $\alpha_1 = \cdots = \alpha_N = 0$
3 Repeat:
4     randomly pick an example $(\boldsymbol{x}_n, y_n)$                                        (1 point)
5     compute $z = y_n \sum_{m=1}^{N} \alpha_m k(\boldsymbol{x}_m, \boldsymbol{x}_n)$ and update $\alpha_n \leftarrow \alpha_n + 2\eta y_n \max\{0, 1-z\}$    (4 points)
```

(c) Continuing from Question (a) (and forgetting about kernel from Question (b)), we now want to generalize the method to multiclass classification with C classes. Instead of coming up with a multiclass version of Eq. (2), we will apply the one-versus-all approach to learn C weight vectors $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_C$, each obtained by properly running Algorithm 4 for T iterations. Based on this information, fill in the missing details in the repeat-loop of the algorithm below. (No reasoning is required.) (6 points)

```
Algorithm 6: One-versus-all applied to Algorithm 4
1 Input: A training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N) \in \mathbb{R}^D \times [C]$, learning rate $\eta > 0$, iteration number $T$
2 Initialization: $\boldsymbol{w}_1 = \cdots = \boldsymbol{w}_C = \mathbf{0}$
3 for $c = 1, \ldots, C$ do
4     Repeat for $T$ iterations:                                   ▷ a loop to update $\boldsymbol{w}_c$
5         randomly pick an example $(\boldsymbol{x}_n, y_n)$
6         set $y = \begin{cases} +1, \text{if } y_n = c \\ -1, \text{else} \end{cases}$
7         compute $z = y\boldsymbol{w}_c^{\mathrm{T}}\boldsymbol{x}_n$ and update $\boldsymbol{w}_c \leftarrow \boldsymbol{w}_c + 2\eta y \max\{0, 1 - z\}\boldsymbol{x}_n$
```

Rubrics: Give partial credits for partially correct answer. Flipping 1 and -1 in Line 6 is okay.

(d) After running Algorithm 6, state how you would make a prediction for a test point $\boldsymbol{x}$ based on what we discussed in the lecture for one-versus-all. (2 points)

First compute $\text{SGN}(\boldsymbol{w}_c^{\mathrm{T}}\boldsymbol{x})$ for all $c = 1, \ldots, C$. Among all c such that $\text{SGN}(\boldsymbol{w}_c^{\mathrm{T}}\boldsymbol{x}) = 1$, randomly pick one of them as the final prediction.

Rubrics: If 1 and -1 are flipped in the last question, then here 1 must be -1.

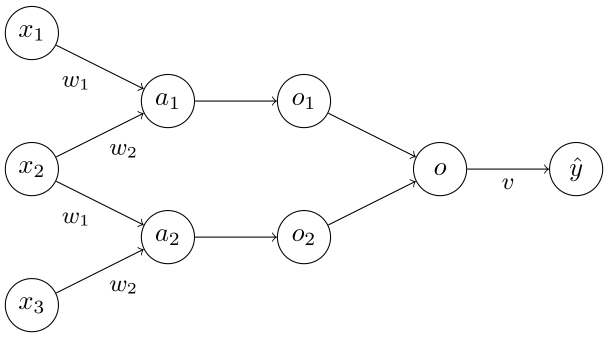
(e) Continuing from Question (d), can you propose another reasonable (and potentially better) way to make a prediction? Simply write down your proposal with no reasoning needed. (2 points)

Similarly to what we discussed in Lecture 4, a reasonable way is to predict $y = \operatorname{argmax}_{c \in [C]} \boldsymbol{w}_c^{\top}\boldsymbol{x}$ (where we treat $\boldsymbol{w}_c^{\top}\boldsymbol{x}$ as the "score" for class c).

Rubrics: Similarly, if 1 and -1 are flipped in last questions, then here argmax must be argmin. There are other acceptable proposals, such as randomly predicting c with probability proportional to $e^{\boldsymbol{w}_c^{\top}\boldsymbol{x}}$ (also discussed in Lecture 4).

4 Backpropagation for CNN (24 points)

Consider the following mini convolutional neural net, where (x_1, x_2, x_3) is the input, followed by a convolution layer with a filter (w_1, w_2), a ReLU layer, an average-pooling layer, and finally a fully connected layer with weight v.



More concretely, the computation is specified by

$$\begin{aligned}
a_1 &= x_1 w_1 + x_2 w_2 \\
a_2 &= x_2 w_1 + x_3 w_2 \\
o_1 &= \max\{0, a_1\} \\
o_2 &= \max\{0, a_2\} \\
o &= (o_1 + o_2)/2 \\
\hat{y} &= ov
\end{aligned}$$

For an example $(\boldsymbol{x}, y) \in \mathbb{R}^3 \times \{-1, +1\}$, the logistic loss of the CNN is

$$\ell = \ln(1 + \exp(-y\hat{y})),$$

which is a function of the parameters of the network: w_1, w_2, v.

(a) Write down $\frac{\partial \ell}{\partial v}$ (show the intermediate steps that use chain rule). You can use the sigmoid function $\sigma(z) = \frac{1}{1+e^{-z}}$ to simplify your notation. (4 points)

$$\frac{\partial \ell}{\partial v} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial v} \qquad \text{(2 points)}$$

$$= \frac{-ye^{-y\hat{y}}}{1+e^{-y\hat{y}}} o = -\sigma(-y\hat{y})yo = (\sigma(y\hat{y}) - 1)yo \qquad \text{(2 points)}$$

Either one of the last three expressions is acceptable.

(b) Write down $\frac{\partial \ell}{\partial w_1}$ and $\frac{\partial \ell}{\partial w_2}$ (show the intermediate steps that use chain rule). The derivative of the ReLU function is $H(a) = \mathbb{I}[a > 0]$, which you can use directly in your answer. (12 points)

$$\begin{aligned}
\frac{\partial \ell}{\partial w_1} &= \frac{\partial \ell}{\partial a_1}\frac{\partial a_1}{\partial w_1} + \frac{\partial \ell}{\partial a_2}\frac{\partial a_2}{\partial w_1} && \text{(2 points)}\\
&= \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial o}\frac{\partial o}{\partial o_1}\frac{\partial o_1}{\partial a_1}\frac{\partial a_1}{\partial w_1} + \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial o}\frac{\partial o}{\partial o_2}\frac{\partial o_2}{\partial a_2}\frac{\partial a_2}{\partial w_1} && \text{(2 points)}\\
&= (\sigma(y\hat{y}) - 1)y \cdot v \cdot \tfrac{1}{2} \cdot H(a_1) \cdot x_1 + (\sigma(y\hat{y}) - 1)y \cdot v \cdot \tfrac{1}{2} \cdot H(a_2) \cdot x_2 && \text{(2 points)}\\
&= \tfrac{1}{2}(\sigma(y\hat{y}) - 1)yv(H(a_1)x_1 + H(a_2)x_2)
\end{aligned}$$

Similarly

$$\begin{aligned}
\frac{\partial \ell}{\partial w_2} &= \frac{\partial \ell}{\partial a_1}\frac{\partial a_1}{\partial w_2} + \frac{\partial \ell}{\partial a_2}\frac{\partial a_2}{\partial w_2} && \text{(2 points)}\\
&= \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial o}\frac{\partial o}{\partial o_1}\frac{\partial o_1}{\partial a_1}\frac{\partial a_1}{\partial w_2} + \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial o}\frac{\partial o}{\partial o_2}\frac{\partial o_2}{\partial a_2}\frac{\partial a_2}{\partial w_2} && \text{(2 points)}\\
&= (\sigma(y\hat{y}) - 1)y \cdot v \cdot \tfrac{1}{2} \cdot H(a_1) \cdot x_2 + (\sigma(y\hat{y}) - 1)y \cdot v \cdot \tfrac{1}{2} \cdot H(a_2) \cdot x_3 && \text{(2 points)}\\
&= \tfrac{1}{2}(\sigma(y\hat{y}) - 1)yv(H(a_1)x_2 + H(a_2)x_3)
\end{aligned}$$

Again, other equivalent expressions are acceptable.

(c) Using the derivations above, fill in the missing details of the repeat-loop of the Backpropagation algorithm below that is used to train this mini CNN. (8 points)

Algorithm 7: Backpropagation for the above mini CNN

```
1 Input: A training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$, learning rate $\eta$
2 Initialize: set $w_1, w_2, v$ randomly
3 Repeat:
4     randomly pick an example $(\boldsymbol{x}_n, y_n)$
5     Forward propagation: compute                                   (4 points)
          $a_1 = x_{n1}w_1 + x_{n2}w_2,\ a_2 = x_{n2}w_1 + x_{n3}w_2$
          $o_1 = \max\{0, a_1\},\ o_2 = \max\{0, a_2\},\ o = (o_1 + o_2)/2,\ \hat{y} = ov$
6     Backward propagation: update                                   (4 points)
          $w_1 \leftarrow w_1 - \frac{1}{2}\eta(\sigma(y_n\hat{y}) - 1)y_n v(H(a_1)x_{n1} + H(a_2)x_{n2})$
          $w_2 \leftarrow w_2 - \frac{1}{2}\eta(\sigma(y_n\hat{y}) - 1)y_n v(H(a_1)x_{n2} + H(a_2)x_{n3})$
          $v \leftarrow v - \eta(\sigma(y_n\hat{y}) - 1)y_n o$
```

Rubrics:

- Deduct 1 point for writing x_1, x_2, x_3 instead of x_{n1}, x_{n2}, x_{n3} in the forward propagation.
- Deduct 1 point for writing x_1, x_2, x_3, y instead of $x_{n1}, x_{n2}, x_{n3}, y_n$ in the backward propagation.
- Deduct 2 points if updating w_1/w_2 with the updated value of v.
- Do not deduct points for using the wrong gradients solely due to mistakes from previous questions.

5 Nonlinear Mappings and Kernel Methods (14 points)

Consider the following Gaussian/RBF kernel

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(\frac{-\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{2}\right). \tag{3}$$

It is known that there exists an infinite-dimensional nonlinear mapping $\boldsymbol{\phi}_{\mathrm{RBF}}$ such that

$$\boldsymbol{\phi}_{\mathrm{RBF}}(\boldsymbol{x})^{\mathrm{T}} \boldsymbol{\phi}_{\mathrm{RBF}}(\boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}') \tag{4}$$

for any $\boldsymbol{x}$ and $\boldsymbol{x}'$. In this problem, you will investigate a way to approximate this nonlinear mapping $\boldsymbol{\phi}_{\mathrm{RBF}}$.

(a) Consider a nonlinear mapping $\phi_{\boldsymbol{v},b} : \mathbb{R}^D \to \mathbb{R}$ constructed as follows: randomly draw a vector $\boldsymbol{v} \in \mathbb{R}^D$ from the standard Gaussian and a scalar b from the uniform distribution over $[0, \pi]$, then define $\phi_{\boldsymbol{v},b}(\boldsymbol{x}) = \sqrt{2}\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x} + b)$ for any input feature vector $\boldsymbol{x} \in \mathbb{R}^D$.

For any two feature vectors $\boldsymbol{x}$ and $\boldsymbol{x}'$, prove the following

$$\mathbb{E}\left[\phi_{\boldsymbol{v},b}(\boldsymbol{x})\phi_{\boldsymbol{v},b}(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}') \tag{5}$$

where the expectation is over the randomness of $\boldsymbol{v}$ and b, and $k(\cdot,\cdot)$ is defined in Eq. (3). You can directly use the following two identities in your proof:

- trigonometric identity: $2\cos(\alpha)\cos(\beta) = \cos(\alpha - \beta) + \cos(\alpha + \beta)$;
- integral identity: $\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{z})\right] = \exp\left(\frac{-\|\boldsymbol{z}\|_2^2}{2}\right)$ where the expectation is with respect to $\boldsymbol{v}$ randomly drawn from the standard Gaussian. (With this, you do not even need to know what the standard Gaussian is to solve this problem.)

(5 points)

Plugging in the definition of $\phi_{\boldsymbol{v},b}$, we first have

$$\mathbb{E}\left[\phi_{\boldsymbol{v},b}(\boldsymbol{x})\phi_{\boldsymbol{v},b}(\boldsymbol{x}')\right] = 2\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x} + b)\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}' + b)\right]. \qquad \text{(1 point)}$$

Using the given trigonometric identity, the above is equal to

$$\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{x}')) + \cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}' + 2b)\right]. \qquad \text{(1 point)}$$

For the first term above, directly applying the given integral identity gives

$$\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{x}'))\right] = k(\boldsymbol{x}, \boldsymbol{x}'). \qquad \text{(1 point)}$$

For the second term, fixing $\boldsymbol{v}$ and taking the expectation over b shows

$$\begin{aligned}\mathbb{E}\left[\cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}' + 2b)\right] &= \frac{1}{\pi}\int_0^{\pi} \cos(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}' + 2b)db \\ &= \frac{1}{2\pi}\sin(\boldsymbol{v}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{x}' + 2b)\Big|_0^{\pi} = 0. \qquad \text{(2 points)}\end{aligned}$$

This finishes the proof. (The last step can also be argued by symmetry without writing down the integral explicitly.)

(b) Comparing Eq. (4) and Eq. (5), we see that $\phi_{\boldsymbol{v},b}$ can be used as an approximation for $\boldsymbol{\phi}_{\text{RBF}}$. However, using only one sample $(\boldsymbol{v}, b)$ leads to large variance for this approximation. Based on this information, for any given dimension $M > 1$, can you come up with a random nonlinear mapping $\boldsymbol{\phi} : \mathbb{R}^D \to \mathbb{R}^M$, such that it is a better approximation of $\boldsymbol{\phi}_{\text{RBF}}$ satisfying $\mathbb{E}\left[\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}')$? Write down your proposal, prove $\mathbb{E}\left[\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}')$, and finally explain why it is a better approximation (in one concise sentence). (5 points)

Proposal: $\boldsymbol{\phi}(\boldsymbol{x}) = \left(\frac{1}{\sqrt{M}}\phi_{\boldsymbol{v}_1,b_1}(\boldsymbol{x}), \ldots, \frac{1}{\sqrt{M}}\phi_{\boldsymbol{v}_M,b_M}(\boldsymbol{x})\right)$ where each $(\boldsymbol{v}_j, b_j)$ is an independent sample drawn from the distribution described in the last question.

It satisfies the claimed equality since

$$\mathbb{E}\left[\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')\right] = \mathbb{E}\left[\frac{1}{M}\sum_{j=1}^{M}\phi_{\boldsymbol{v}_j,b_j}(\boldsymbol{x})\phi_{\boldsymbol{v}_j,b_j}(\boldsymbol{x}')\right] = \frac{1}{M}\sum_{j=1}^{M}k(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}'),$$

where the second step is by Eq. (5). It is a better approximation since using multiple independent samples reduces the variance (by a factor of $1/M$ precisely).

Rubrics:

- 2 points for the definition of $\boldsymbol{\phi}$: one for "independent samples", and another one for the correct scaling $1/\sqrt{M}$.
- 2 points for the proof $\mathbb{E}\left[\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')\right] = k(\boldsymbol{x}, \boldsymbol{x}')$.
- 1 point for the explanation (okay as long as "reducing variance" is mentioned).

(c) As discussed in Lecture 5, in RBF-kernelized linear regression with training set $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$, we maintain a weight vector $\boldsymbol{\alpha} = (\boldsymbol{K} + \lambda\boldsymbol{I})^{-1}\boldsymbol{y} \in \mathbb{R}^N$, where $\boldsymbol{K} \in \mathbb{R}^{N\times N}$ is the Gram matrix (such that $K_{n,m} = k(\boldsymbol{x}_n, \boldsymbol{x}_m)$), $\lambda > 0$ is the regularization coefficient, and $\boldsymbol{y} = (y_1, \ldots, y_N)^{\mathrm{T}}$ is the response vector. For a test point $\boldsymbol{x}$, we make a prediction via $\sum_{n=1}^{N}\alpha_n k(\boldsymbol{x}_n, \boldsymbol{x})$. While powerful, this method can be computationally expensive when N is huge.

Based on the nonlinear mapping you proposed in the last question for M much smaller than N, describe how you can approximate the kernelized linear regression described above with a much better time and space complexity. You only need to describe what quantities your method maintains, and how it makes a prediction for a test point. (4 points)

The method is simply what we discussed in Lectures 2 and 5: maintain a weight vector $\boldsymbol{w}^* \in \mathbb{R}^M$ as:

$$\boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y},$$

where the n-th row of $\boldsymbol{\Phi} \in \mathbb{R}^{N\times M}$ is $\boldsymbol{\phi}(\boldsymbol{x}_n)^{\mathrm{T}}$. To make a prediction for a test point $\boldsymbol{x}$, simply compute ${\boldsymbol{w}^*}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$.

Reasoning (NOT required): First, this has better time and space complexity since M is assumed to be much smaller than N. Second, based on the discussion in Lecture 5, this is equivalent to kernelized linear regression with Gram matrix $\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}}$, which is a good approximation of $\boldsymbol{K}$ according to the last question.

Rubrics:

- 2 points for what the method maintains, and another 2 points for how to make a prediction.
- using SGD or other methods in the primal space to find $\boldsymbol{w}^*$ is also okay.
- do not deduct points for mistake in the form of $\boldsymbol{\phi}$ inherited from the last question.