Homework #4

CSE 446/546: Machine Learning
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Due: Friday 9 December, 2022 11:59pm
86 points(A)/25 points(B)

Please review all homework guidance posted on the website before submitting to GradeScope. Reminders:

- Make sure to read the "What to Submit" section following each question and include all items.
- Please provide succinct answers and supporting reasoning for each question. Similarly, when discussing experimental results, concisely create tables and/or figures when appropriate to organize the experimental results. All explanations, tables, and figures for any particular part of a question must be grouped together.
- For every problem involving generating plots, please include the plots as part of your PDF submission.
- When submitting to Gradescope, please link each question from the homework in Gradescope to the location of its answer in your homework PDF. Failure to do so may result in deductions of up to 10% of the points for each problem improperly tagged. For instructions, see https://www.gradescope.com/get_started#student-submission.
- If you collaborate on this homework with others, you must indicate who you worked with on your homework. Failure to do so may result in accusations of plagiarism.
- The coding problems are available in a .zip file on the course website, with some starter code. All coding questions in this class will have starter code. Before attempting these problems make sure your coding environment is working. See instructions in README file in the .zip file.
- For every problem involving code, please include the code as part of your PDF for the PDF submission in addition to submitting your code to the separate assignment on Gradescope created for code.

Not adhering to these reminders may result in point deductions.

Changelog:

- 12/5: Added Hint for B1.b
- 12/5: Fixed definition of 1 in A4
- 12/7: Remove question A1f
- 12/7: Fixed typo for B1.b Hint.

Conceptual Questions

A1. The answers to these questions should be answerable without referring to external materials. Briefly justify your answers with a few words.

- a. [2 points] True or False: Given a data matrix $X \in \mathbb{R}^{n \times d}$ where d is much smaller than n and $k = \operatorname{rank}(X)$, if we project our data onto a k-dimensional subspace using PCA, our projection will have zero reconstruction error (in other words, we find a perfect representation of our data, with no information loss).
- b. [2 points] True or False: Suppose that an $n \times n$ matrix X has a singular value decomposition of USV^{\top} , where S is a diagonal $n \times n$ matrix. Then, the rows of V are equal to the eigenvectors of $X^{\top}X$.
- c. [2 points] True or False: choosing k to minimize the k-means objective (see Equation (1) below) is a good way to find meaningful clusters.
- d. [2 points] True or False: The singular value decomposition of a matrix is unique.
- e. [2 points] True or False: The rank of a square matrix equals the number of its unique nonzero eigenvalues.

What to Submit:

• Parts a-f: 1-2 sentence explanation containing your answer.

Think before you train

A2. The first part of this problem (part a) explores how you would apply machine learning theory and techniques to a real-world problem. There is one scenario detailing a setting, a dataset, and a specific result we hope to achieve. Your job is to describe how you would handle the scenario with the tools we've learned in this class. Your response should include:

- (1) any pre-processing steps you would take (i.e., data acquisition and processing),
- (2) the specific machine learning pipeline you would use (i.e., algorithms and techniques learned in this class),
- (3) how your setup acknowledges the constraints and achieves the desired result.

You should also aim to leverage some of the theory we have covered in this class. Some things to consider may be: the nature of the data (i.e., *How hard is it to learn? Do we need more data? Are the data sources good?*), the effectiveness of the pipeline (i.e., *How strong is the model when properly trained and tuned?*), and the time needed to effectively perform the pipeline.

a. [10 points] Scenario: Disease Susceptibility Predictor

- <u>Setting</u>: You are tasked by a research institute to create an algorithm that learns the factors that contribute most to acquiring a specific disease.
- <u>Dataset</u>: A rich dataset of personal demographic information, location information, risk factors, and whether a person has the disease or not.
- Result: The company wants a system that can determine how susceptible someone is to this disease when they enter in their own personal information. The pipeline should take limited amount of personal data from a new user and infer more detailed metrics about the person.

The second part of this problem (parts b, c) focuses on exploring possible shortcomings of the model, and what real-world implications might follow from ignoring these issues.

- b. [5 points] Recall in Homework 2 we trained models to predict crime rates using various features. It is important to note that datasets describing crime have many shortcomings in describing the entire landscape of illegal behavior in a city, and that these shortcomings often fall disproportionately on minority communities. Some of these shortcomings include that crimes are reported at different rates in different neighborhoods, that police respond differently to the same crime reported or observed in different neighborhoods, and that police spend more time patrolling in some neighborhoods than others. What real-world implications might follow from ignoring these issues?
- c. [5 points] Briefly describe (1) some potential shortcomings of your training process from the aforementioned scenario that may result in your algorithm having different accuracy on different populations, and (2) how you may modify your procedure to address these shortcomings.

- For part (a): One clearly-written short paragraph (4-7) sentences.
- For part (b): One clearly-written short paragraph on real-world implications that may follow from ignoring dataset issues.
- For part (c): Clearly-written and well-thought-out answers addressing (1) and (2) (as described in the problem). Two short paragraphs or one medium paragraph suffice.

k-means clustering

A3. Given a dataset $\mathbf{x}_1, ..., \mathbf{x}_n \in \mathbb{R}^d$ and an integer $1 \le k \le n$, recall the following k-means objective function

$$\min_{\pi_1, \dots, \pi_k} \sum_{i=1}^k \sum_{j \in \pi_i} \|\mathbf{x}_j - \mu_i\|_2 , \quad \mu_i = \frac{1}{|\pi_i|} \sum_{j \in \pi_i} \mathbf{x}_j .$$
 (1)

Above, $\{\pi_i\}_{i=1}^k$ is a partition of $\{1, 2, ..., n\}$. The objective (1) is NP-hard¹ to find a global minimizer of. Nevertheless, Lloyd's algorithm (discussed in lecture) typically works well in practice.

- a. [5 points] Implement Lloyd's algorithm for solving the k-means objective (1). Do not use any off-the-shelf implementations, such as those found in scikit-learn. Include your code in your submission.
- b. [5 points] Run Lloyd's algorithm on the training dataset of MNIST with k=10. Show the image representing the center of each cluster, as a set of k 28 \times 28 images.

Note on Time to Run — The runtime of a good implementation for this problem should be fairly fast (a few minutes); if you find it taking upwards of one hour, please check your implementation! (Hint: For loops are costly. Can you vectorize it or use Numpy operations to make it faster in some ways? If not, is looping through data-points or through centers faster?)

- For part (a): Lloyd's algorithm code
- For part (b): 10 images of cluster centers.
- Code for parts a-b

¹To be more precise, it is both NP-hard in d when k=2 and k when d=2. See the references on the Wikipedia page for k-means for more details.

PCA

A4. Let's do PCA on MNIST dataset and reconstruct the digits in the dimensionality-reduced PCA basis. Compute your PCA basis using the training dataset only, and evaluate the quality of the basis on the test set, similar to the k-means reconstructions above. We have $n_{train} = 50,000$ training examples of size 28×28 . Begin by flattening each example to a vector to obtain $X_{train} \in \mathbb{R}^{50,000 \times d}$ and $X_{test} \in \mathbb{R}^{10,000 \times d}$ for d = 784.

Let $\mu \in \mathbb{R}^d$ denote the average of the training examples in X_{train} , i.e., $\mu = \frac{1}{n_{train}} X_{train}^{\top} \mathbf{1}$. Now let $\Sigma = (X_{train} - \mathbf{1}\mu^{\top})^{\top} (X_{train} - \mathbf{1}\mu^{\top})/50000$ denote the sample covariance matrix of the training examples, and let $\Sigma = UDU^T$ denote the eigenvalue decomposition of Σ .

- a. [2 points] If λ_i denotes the *i*th largest eigenvalue of Σ , what are the eigenvalues λ_1 , λ_2 , λ_{10} , λ_{30} , and λ_{50} ? What is the sum of eigenvalues $\sum_{i=1}^{d} \lambda_i$?
- b. [5 points] Let $x \in \mathbb{R}^d$ and $k \in 1, 2, ..., d$. Write a formula for the rank-k PCA approximation of x.
- c. [3 points] Visualize a set of reconstructed digits from the training set for different values of k. In particular, provide the reconstructions for digits 2, 6, 7 with values k = 5, 15, 40, 100 (just choose an image from each digit arbitrarily). Show the original image side-by-side with its reconstruction. Provide a brief interpretation, in terms of your perceptions of the quality of these reconstructions and the dimensionality you used.

- For part (a): Eigenvalues λ_1 , λ_2 , λ_{10} , λ_{30} , and λ_{50} and the sum. At least 6 leading digits.
- For part (b): The formula. If you are defining new variables/matrices, make sure their definition is stated clearly.
- For part (c): 15 total images, including 3 original and 12 reconstructed ones. Each reconstructed image corresponds to a certain digit (2, 6 or 7) and k value (5, 15, 40 or 100). In addition, provide your interpretation in a few sentences.
- Code for parts a and c from homeworks/pca/main.py

Image Classification on CIFAR-10

A5. In this problem we will explore different deep learning architectures for image classification on the CIFAR-10 dataset. Make sure that you are familiar with torch.Tensors, two-dimensional convolutions (nn.Conv2d) and fully-connected layers (nn.Linear), ReLU non-linearities (F.relu), pooling (nn.MaxPool2d), and tensor reshaping (view).

A few preliminaries:

- Each network f maps an image $x^{\text{in}} \in \mathbb{R}^{32 \times 32 \times 3}$ (3 channels for RGB) to an output $f(x^{\text{in}}) = x^{\text{out}} \in \mathbb{R}^{10}$. The class label is predicted as $\arg\max_{i=0,1,\ldots,9} x_i^{\text{out}}$. An error occurs if the predicted label differs from the true label for a given image.
- The network is trained via multiclass cross-entropy loss.
- Create a validation dataset by appropriately partitioning the train dataset. *Hint*: look at the documentation for torch.utils.data.random_split. Make sure to tune hyperparameters like network architecture and step size on the validation dataset. Do **NOT** validate your hyperparameters on the test dataset.
- At the end of each epoch (one pass over the training data), compute and print the training and validation classification accuracy.
- While one would usually train a network for hundreds of epochs to reach convergence and maximize accuracy, this can be prohibitively time-consuming, so feel free to train for just a dozen or so epochs.

For parts (a) and (b), apply a hyperparameter tuning method (e.g. random search, grid search, etc.) using the validation set, report the hyperparameter configurations you evaluated and the best set of hyperparameters from this set, and plot the training and validation classification accuracy as a function of epochs. Produce a separate line or plot for each hyperparameter configuration evaluated (top 5 configurations is sufficient to keep the plots clean). Finally, evaluate your best set of hyperparameters on the test data and report the test accuracy.

Note 1: Please refer to the Aprovided notebook with starter code for this problem, included with the code files for this assignment. That notebook provides a complete end-to-end example of loading data, training a model using a simple network with a fully-connected output and no hidden layers (this is equivalent to logistic regression), and performing evaluation using canonical Pytorch. We recommend using this as a template for your implementations of the models below.

Note 2: If you are attempting this problem and do not have access to GPU we highly recommend using Google Colab. The provided notebook includes instructions on how to use GPU in Google Colab.

Here are the network architectures you will construct and compare.

a. [18 points] Fully-connected output, 1 fully-connected hidden layer: this network has one hidden layer denoted as $x^{\text{hidden}} \in \mathbb{R}^M$ where M will be a hyperparameter you choose (M could be in the hundreds). The nonlinearity applied to the hidden layer will be the relu ($\text{relu}(x) = \max\{0, x\}$). This network can be written as

$$x^{out} = W_2 \text{relu}(W_1(x^{in}) + b_1) + b_2$$

where $W_1 \in \mathbb{R}^{M \times 3072}$, $b_1 \in \mathbb{R}^M$, $W_2 \in \mathbb{R}^{10 \times M}$, $b_2 \in \mathbb{R}^{10}$. Tune the different hyperparameters and train for a sufficient number of epochs to achieve a *validation accuracy* of at least 50%. Provide the hyperparameter configuration used to achieve this performance.

- b. [18 points] Convolutional layer with max-pool and fully-connected output: for a convolutional layer W_1 with filters of size $k \times k \times 3$, and M filters (reasonable choices are M = 100, k = 5), we have that $\text{Conv2d}(x^{\text{in}}, W_1) \in \mathbb{R}^{(33-k)\times(33-k)\times M}$.
 - Each convolution will have its own offset applied to each of the output pixels of the convolution; we denote this as $\operatorname{Conv2d}(x^{\operatorname{in}}, W) + b_1$ where b_1 is parameterized in \mathbb{R}^M . Apply a relu activation to the result of the convolutional layer.

- Next, use a max-pool of size $N \times N$ (a reasonable choice is N = 14 to pool to 2×2 with k = 5) we have that $\text{MaxPool}(\text{relu}(\text{Conv}2\text{d}(x^{\text{in}}, W_1) + b_1)) \in \mathbb{R}^{\lfloor \frac{33-k}{N} \rfloor \times L} \stackrel{33-k}{\sim} \cup M$.
- We will then apply a fully-connected layer to the output to get a final network given as

$$x^{output} = W_2(\text{MaxPool}(\text{relu}(\text{Conv2d}(x^{\text{input}}, W_1) + b_1))) + b_2$$

where
$$W_2 \in \mathbb{R}^{10 \times M(\lfloor \frac{33-k}{N} \rfloor)^2}$$
, $b_2 \in \mathbb{R}^{10}$.

The parameters M, k, N (in addition to the step size and momentum) are all hyperparameters, but you can choose a reasonable value. Tune the different hyperparameters (number of convolutional filters, filter sizes, dimensionality of the fully-connected layers, step size, etc.) and train for a sufficient number of epochs to achieve a *validation accuracy* of at least 65%. Provide the hyperparameter configuration used to achieve this performance. Make sure to save the best model during the hyperparameter tuning so that you can evaluate test accuracy without retraining.

The number of hyperparameters to tune, combined with the slow training times, will hopefully give you a taste of how difficult it is to construct networks with good generalization performance. State-of-the-art networks can have dozens of layers, each with their own hyperparameters to tune. Additional hyperparameters you are welcome to play with if you are so inclined, include: changing the activation function, replace max-pool with average-pool, adding more convolutional or fully connected layers, and experimenting with batch normalization or dropout.

- Parts a-b: Plot of the training and validation accuracy for the top 5 hyperparameter configurations you evaluated (x-axis is training epoch; y-axis is accuracy; plots should contain 10 lines total). If it took fewer than 5 hyperparameter configurations to pass the performance threshold, plot all hyperparameter configurations evaluated.
- Parts a-b: List the hyperparameter values you searched over, and your search method (random, grid, etc.). Provide the values of best performing hyperparameters, and accuracy of best models on test data.
- Code

Random Fourier Features

B1. Kernel methods such as Support Vector Machines are considered memory-based learners. Rather than learning a mapping from a set of input features $\mathcal{X} \subset \mathbb{R}^d$ to outputs in \mathcal{Y} , they remember all training examples $(\mathbf{x_i}, y_i)$ and learn a corresponding weight for them.

$$\hat{f}(\mathbf{x}) = \sum_{i=1}^{N} \omega_i k(\mathbf{x_i}, \mathbf{x})$$

After learning the weight vector $\mathbf{w} = [\mathbf{w}_1, ..., \mathbf{w}_N]$, we can make prediction on unseen samples using the kernel function k between all training samples and \mathbf{x} . Kernel methods are attractive because they rely on the kernel trick. Any positive definite function $k(\mathbf{x}, \mathbf{x}')$ with $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$ defines a function ψ mapping \mathbb{R}^d to a higher-dimensional space such that the inner product between datapoints can be quickly computed as $\langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle = k(\mathbf{x}, \mathbf{x}')$. In essence, the kernel trick is an efficient way to learn a linear decision boundary in a higher dimension space than that of \mathcal{X} .

The kernel trick can be prohibitively expensive for large datasets. This is because the memory-based algorithm accesses the data through evaluations of the kernel matrix k(x, x') which grows in proportion to the dataset size N.

Instead of relying on the implicit feature mapping ψ provided by the kernel trick, suppose we can approximate the kernel function k as the inner product of two vectors in \mathbb{R}^D . Mathematically, we would like to find a mapping \mathbf{z} :

$$\mathbf{z}: \mathbb{R}^d \to \mathbb{R}^D$$
 such that $k_p(\mathbf{x}, \mathbf{x}') = \langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle \approx \langle \mathbf{z}(\mathbf{x}), \mathbf{z}(\mathbf{x}') \rangle$

With this approximation, we no longer require the kernel trick to express $\langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle$ as $k(\mathbf{x}, \mathbf{x}')$. Rather, we can approximate it by directly computing the tractable inner product $\langle \mathbf{z}(\mathbf{x}), \mathbf{z}(\mathbf{x}') \rangle$.

$$\hat{f}(\mathbf{x}) = \sum_{i=1}^{N} \omega_i k(\mathbf{x}_i, \mathbf{x}) = \sum_{i=1}^{N} \omega_i \langle \psi(\mathbf{x}_i), \psi(\mathbf{x}) \rangle \approx \sum_{i=1}^{N} \omega_i \langle \mathbf{z}(\mathbf{x}), \mathbf{z}(\mathbf{x}) \rangle = \left(\sum_{i=1}^{N} \omega_i \mathbf{z}(\mathbf{x}_i)^T\right) \mathbf{z}(\mathbf{x}) = \beta^T \mathbf{z}(\mathbf{x})$$

Assuming $\mathbf{z}(\mathbf{x}) = \sigma(M\mathbf{x} + b)$ for some nonlinear function σ , this "approximate" SVM can potentially be evaluated much quicker than the kernel SVM. To see why, note that the left-hand-side requires evaluating $k(\mathbf{x_i}, \mathbf{x})$ for all $i \in \{1, ..., N\}$, in general, if ω_i is not sparse. On the other hand, the right-hand-side just requires computing $\mathbf{z}(\mathbf{x}) = \sigma(M\mathbf{x} + b)$ which is dominated by the time to compute a $D \times d$ matrix-vector product, and then inner product with β which is \mathbb{R}^D . Thus, the total computation time for the left-hand-side scales linearly with N, and the right-hand-side scales with just d and D, independent of N! When training the approximate SVM we also get similar computational savings if $N \gg \max\{d, D\}$.

a. [15 points] **Deriving Random Fourier Features**: Bochner's theorem states that a continuous kernel $k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x} - \mathbf{x}')$ on \mathbb{R}^d is positive definite if and only if k is the Fourier transform of a non-negative measure. While we won't delve into the logic of Fourier transforms here, this theorem lets us express the kernel as follows: for any probability distribution $p(\mathbf{w})$ define

$$k_p(\mathbf{x}, \mathbf{x}') := \int_{\mathbb{R}^d} p(\mathbf{w}) e^{i\mathbf{w}^T(\mathbf{x} - \mathbf{x}')} dw = \mathbb{E}_{\mathbf{w}} \left[e^{i\mathbf{w}^T(\mathbf{x} - \mathbf{x}')} \right]$$

where $i = \sqrt{-1}$, the imaginary unit. While any choice of $p(\mathbf{w})$ induces a valid kernel, in this problem we'll be focusing on the Gaussian distribution, namely

$$p(\mathbf{w}) = (2\pi\sigma^2)^{-\frac{D}{2}} e^{-\frac{1}{2\sigma^2}||\mathbf{w}||_2^2} = (2\pi/\gamma^2)^{-\frac{D}{2}} e^{-\gamma^2||\mathbf{w}||_2^2/2} \quad \text{where } \gamma = \frac{1}{\sigma}$$

In this sub-problem, we'll use this Fourier-transform interpretation of k to derive a randomized mapping $\mathbf{z} : \mathbb{R}^d \to \mathbb{R}^D$ which is an unbiased estimate of the kernel function i.e.

$$\mathbb{E}_{\mathbf{w}}[\mathbf{z}(\mathbf{x})^T \mathbf{z}(\mathbf{x}')] = k_p(\mathbf{x}, \mathbf{x}')$$

If $\mathbf{z}(x)^T \mathbf{z}(x')$ serves as a good approximation to the kernel matrix, we can apply the aforementioned approximation algorithm.

i Use Euler's formula $e^{iy} = \cos(y) + i\sin(y)$ to show that $k_p(\mathbf{x}, \mathbf{x}') = E_{\mathbf{w}} \left[\cos(\mathbf{w}^T(\mathbf{x} - \mathbf{x}')) \right]$.

Hint: If both x and A are real, then $A = \int f(x) + ig(x)dx = \int f(x)dx$.

ii We begin by defining $z_{\mathbf{w}}: \mathbb{R}^d \to \mathbb{R}$ as

$$z_{\mathbf{w}}(\mathbf{x}) = \sqrt{2}\cos(\mathbf{w}^T\mathbf{x} + b)$$
 where $\mathbf{w} \sim p(\mathbf{w}), \ b \sim \text{Uniform}(0, 2\pi)$

Note that this is not yet the mapping vector \mathbf{z} , but rather a mapping to \mathbb{R} . Use part (i) to show that the expected product of $z_{\mathbf{w}}(\mathbf{x})$ s is an unbiased estimate of the kernel function i.e.

$$E_{\mathbf{w},b}\left[z_{\mathbf{w}}(\mathbf{x})z_{\mathbf{w}}(\mathbf{x}')\right] = k_{p}(\mathbf{x},\mathbf{x}')$$

Hint: For this problem you may use the following identity: $2\cos(\alpha)\cos(\beta) = \cos(\alpha+\beta) + \cos(\alpha-\beta)$.

iii Now we're ready to define our random Fourier features $\mathbf{z} : \mathbb{R}^d \to \mathbb{R}^D$. Let \mathbf{z} be the d-dimensional concatenation of $z_{\mathbf{w}}(\mathbf{x})$ s:

$$\mathbf{z}(\mathbf{x}) = \left[\frac{1}{\sqrt{D}} z_{\mathbf{w}_1}(\mathbf{x}), \ \frac{1}{\sqrt{D}} z_{\mathbf{w}_2}(\mathbf{x}), \ \dots, \ \frac{1}{\sqrt{D}} z_{\mathbf{w}_D}(\mathbf{x}) \right]^T$$

Use parts (i) and (ii) to show that the expected inner product of the mapping z is an unbiased estimate of the kernel function i.e.

$$E_{\mathbf{w}}[\mathbf{z}(\mathbf{x})^T\mathbf{z}(\mathbf{x}')] = k_p(\mathbf{x}, \mathbf{x}')$$

b. [5 points] Random Fourier Features and the RBF Kernel. As mentioned in part (b), using different distributions $p(\mathbf{w})$ induces different valid kernels. Using the $p(\mathbf{w})$ given in part (a), show that expected value of the inner product between random Fourier features is the RBF kernel i.e.

$$E_{\mathbf{w}}[\mathbf{z}(\mathbf{x})^T \mathbf{z}(\mathbf{x}')] = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||_2^2}{2\gamma^2}\right)$$

Hint: The PDF for a variable $X \in \mathbb{R}^d$ following normal distribution with mean μ and covariance matrix Σ is as follows:

$$P(X = x) = ((2\pi)^d |\Sigma|)^{-1/2} \exp\left(-\frac{1}{2}(x - \mu)^\top \Sigma^{-1}(x - \mu)\right)$$

where $|\Sigma| = \det(\Sigma)$ denote the determinant of matrix Σ . In addition, if $\Sigma = \operatorname{diag}(\sigma^2, \dots, \sigma^2)$, then $|\Sigma| = \sigma^{2d}$, and $\Sigma^{-1} = \operatorname{diag}(\sigma^{-2}, \dots, \sigma^{-2})$.

c. [5 points] Concentration Bounds In part (a) we derived our function **z** which serve as a good approximation to the kernel function. Our results let us get an upper bound our approximation error for the kernel function. Explain why we can apply Hoeffding's inequality to obtain

$$p(|\mathbf{z}(\mathbf{x})^T\mathbf{z}(\mathbf{x}') - k(\mathbf{x}, \mathbf{x}')| \ge \epsilon) \le 2 \exp(-D\epsilon^2/8)$$

- Part a: Separate proofs for subproblems (i), (ii) and (iii)
- Part b: proof
- Part c: proof, 1-2 sentence explanation about which conditions are met that allow us to apply Hoeffding's inequality e.g. "B is bounded by [...]".