CS 229, Winter 2025
Problem Set #4

YOUR NAME HERE (`YOUR SUNET HERE`)

Due Friday, March 7 at 11:59 pm on Gradescope.

Notes: (1) These questions require thought, but do not require long answers. Please be as concise as possible.

(2) If you have a question about this homework, we encourage you to post your question on our Ed forum, at `https://edstem.org/us/courses/37893/discussion/`.

(3) If you missed the first lecture or are unfamiliar with the collaboration or honor code policy, please read the policy on the course website before starting work.

(4) For the coding problems, you may not use any libraries except those defined in the provided `environment.yml` file. In particular, ML-specific libraries such as scikit-learn are not permitted.

(5) The due date is Friday, March 7 at 11:59 pm. If you submit after Friday, March 7 at 11:59 pm, you will begin consuming your late days. The late day policy can be found in the course website: Course Logistics and FAQ.

All students must submit an electronic PDF version of the written question including plots generated from the codes. We highly recommend typesetting your solutions via LaTeX. All students must also submit a zip file of their source code to Gradescope, which should be created using the `make_zip.py` script. You should make sure to (1) restrict yourself to only using libraries included in the `environment.yml` file, and (2) make sure your code runs without errors. Your submission may be evaluated by the auto-grader using a private test set, or used for verifying the outputs reported in the writeup. Please make sure that your PDF file and zip file are submitted to the corresponding Gradescope assignments respectively. We reserve the right to not give any points to the written solutions if the associated code is not submitted.

Honor code: We strongly encourage students to form study groups. Students may discuss and work on homework problems in groups. However, each student must write down the solution independently, and without referring to written notes from the joint session. Each student must understand the solution well enough in order to reconstruct it by him/herself. It is an honor code violation to copy, refer to, or look at written or code solutions from a previous year, including but not limited to: official solutions from a previous year, solutions posted online, and solutions you or someone else may have written up in a previous year. Furthermore, it is an honor code violation to post your assignment solutions online, such as on a public git repo. We run plagiarism-detection software on your code against past solutions as well as student submissions from previous years. Please take the time to familiarize yourself with the Stanford Honor Code[1] and the Stanford Honor Code[2] as it pertains to CS courses.

[1]https://communitystandards.stanford.edu/policies-and-guidance/honor-code

[2]https://web.stanford.edu/class/archive/cs/cs106b/cs106b.1164/handouts/honor-code.pdf

1. **[15 points] PCA**

In class, we showed that PCA finds the "variance maximizing" directions onto which to project the data. In this problem, we find another interpretation of PCA.

Suppose we are given a set of points $\{x^{(1)}, \ldots, x^{(n)}\}$. Let us assume that we have as usual preprocessed the data to have zero-mean and unit variance in each coordinate. For a given unit-length vector u, let $f_u(x)$ be the projection of point x onto the direction given by u. I.e., if $\mathcal{V} = \{\alpha u : \alpha \in \mathbb{R}\}$, then

$$f_u(x) = \arg\min_{v\in\mathcal{V}} ||x - v||^2.$$

(a) [10 points] Recall that the principal component is the largest eigenvalue of $X^\top X$ for data matrix $X \in R^{n\times d}$. Show that the unit-length vector u that minimizes the mean squared error between projected points and original points corresponds to the first principal component for the data. I.e., show that

$$\arg\min_{u:u^T u=1} \sum_{i=1}^{n} \|x^{(i)} - f_u(x^{(i)})\|_2^2 \ .$$

gives the first principal component.

Remark. If we are asked to find a k-dimensional subspace onto which to project the data so as to minimize the sum of squares distance between the original data and their projections, then we should choose the k-dimensional subspace spanned by the first k principal components of the data. This problem shows that this result holds for the case of $k = 1$.
Answer:

(b) [5 points] Now we will explore the relationship between two of the most popular dimensionality reduction techniques, SVD and PCA, at a basic conceptual level. Before we proceed with the question itself, let us briefly recap the SVD and PCA techniques and a few important observations:

- **Eigenvalue Decomposition**: First, recall that the eigenvalue decomposition of a real, symmetric, and square matrix B (of size $d \times d$) can be written as the following product:

$$B = Q\Lambda Q^\top$$

where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_d)$ contains the eigenvalues of B (which are always real) along its main diagonal, and Q is an orthogonal matrix containing the eigenvectors of B as its columns.

- **Principal Component Analysis (PCA)**: Given a data matrix M (of size $p \times q$), we showed in part (a) that PCA involves finding eigenvectors of the matrix $M^\top M$. The matrix of these eigenvectors can be thought of as a rigid rotation in a high-dimensional space. PCA then projects each row of M onto the top k principal components to produce a lower dimensional version of each data point (where $k << q$).

Now we turn to the question! Let us define a real matrix M (of size $p \times q$) and let us assume this matrix corresponds to a dataset with p data points and q dimensions.

i. [2 points] Prove that $M^\top M$ is real, symmetric, and square. Write its eigenvalue decomposition in terms of Q, Λ, Q^T.

ii. [2 points] SVD involves the decomposition of a data matrix $M \in \mathbb{R}^{p\times q}$ into a product $M = U\Sigma V^\top$ where $U \in \mathbb{R}^{p\times p}$ and $V \in \mathbb{R}^{q\times q}$ are column-orthonormal matrices and

$\Sigma \in \mathbb{R}^{p \times q}$ is a diagonal matrix. The entries along the diagonal of Σ are referred to as the singular values of M. Write a simplified expression for $M^\top M$ in terms of V, V^T, and Σ.
Hint: A matrix A is column-orthonormal if and only if $A^T A = I$

iii. [1 points] What is the relationship (if any) between the eigenvalues of $M^\top M$ and the singular values of M?

Answer:

2. **[20 points] K-means for compression**

In this problem, we will apply the K-means algorithm to lossy image compression, by reducing the number of colors used in an image.

We will be using the files `src/k_means/peppers-small.tiff` and `src/k_means/peppers-large.tiff`.

The `peppers-large.tiff` file contains a 512×512 image of peppers represented in 24-bit color. This means that, for each of the 262,144 pixels in the image, there are three 8-bit numbers (each ranging from 0 to 255) that represent the red, green, and blue intensity values for that pixel. The straightforward representation of this image therefore takes about $262144 \times 3 = 786432$ bytes (a byte being 8 bits). To compress the image, we will use K-means to reduce the image to $k = 16$ colors. More specifically, each pixel in the image is considered a point in the three-dimensional (r, g, b)-space. To compress the image, we will cluster these points in color-space into 16 clusters, and replace each pixel with the closest cluster centroid.

Follow the instructions below. Be warned that some of these operations can take a while (several minutes even on a fast computer)!

(a) [15 points] **[Coding Problem] K-Means Compression Implementation.** First let us *look* at our data. From the `src/k_means/` directory, open an interactive Python prompt, and type

```
from matplotlib.image import imread; import matplotlib.pyplot as plt;
```

and run `A = imread('peppers-large.tiff')`. Now, `A` is a "three dimensional matrix," and `A[:,:,0]`, `A[:,:,1]` and `A[:,:,2]` are 512×512 arrays that respectively contain the red, green, and blue values for each pixel. Enter `plt.imshow(A); plt.show()` to display the image.

Since the large image has 262,144 pixels and would take a while to cluster, we will instead run vector quantization on a smaller image. Repeat (a) with `peppers-small.tiff`.

Next we will implement image compression in the file `src/k_means/k_means.py` which has some starter code. Treating each pixel's (r, g, b) values as an element of $\mathbb{R}^3$, implement K-means with 16 clusters on the pixel data from this smaller image, iterating (preferably) to convergence, but in no case for less than 30 iterations. For initialization, set each cluster centroid to the (r, g, b)-values of a randomly chosen pixel in the image.

Take the image of `peppers-large.tiff`, and replace each pixel's (r, g, b) values with the value of the closest cluster centroid from the set of centroids computed with `peppers-small.tiff`. Visually compare it to the original image to verify that your implementation is reasonable. **Include in your write-up a copy of this compressed image alongside the original image.**

Answer:

(b) [5 points] **Compression Factor.**

If we represent the image with these reduced (16) colors, by (approximately) what factor have we compressed the image?

Answer:

3. **[15 points] KL divergence and Maximum Likelihood**

The Kullback-Leibler (KL) divergence is a measure of how much one probability distribution is different from a second one. It is a concept that originated in Information Theory, but has made its way into several other fields, including Statistics, Machine Learning, Information Geometry, and many more. In Machine Learning, the KL divergence plays a crucial role, connecting various concepts that might otherwise seem unrelated.

In this problem, we will introduce KL divergence over discrete distributions, practice some simple manipulations, and see its connection to Maximum Likelihood Estimation.

The *KL divergence* between two discrete-valued distributions $P(X), Q(X)$ over the outcome space $\mathcal{X}$ is defined as follows[3]:

$$D_{KL}(P\|Q) = \sum_{x\in\mathcal{X}} P(x)\log\frac{P(x)}{Q(x)}.$$

For notational convenience, we assume $P(x) > 0, \forall x$. (One other standard thing to do is to adopt the convention that "$0\log 0 = 0$.") Sometimes, we also write the KL divergence more explicitly as $D_{KL}(P||Q) = D_{KL}(P(X)||Q(X))$.

Background on Information Theory

Before we dive deeper, we give a brief (optional) Information Theoretic background on KL divergence. While this introduction is not necessary to answer the assignment question, it may help you better understand and appreciate why we study KL divergence, and how Information Theory can be relevant to Machine Learning.

We start with the *entropy* $H(P)$ of a probability distribution $P(X)$, which is defined as

$$H(P) = -\sum_{x\in\mathcal{X}} P(x)\log P(x).$$

Intuitively, entropy measures how dispersed a probability distribution is. For example, a uniform distribution is considered to have very high entropy (i.e., a lot of uncertainty), whereas a distribution that assigns all its mass to a single point is considered to have zero entropy (i.e., no uncertainty). Notably, it can be shown that among continuous distributions over $\mathbb{R}$, the Gaussian distribution $\mathcal{N}(\mu,\sigma^2)$ has the highest entropy (highest uncertainty) among all possible distributions that have the given mean μ and variance σ^2.

To further solidify our intuition, we present motivation from communication theory. Suppose we want to communicate from a source to a destination, and our messages are always (a sequence of) discrete symbols over space $\mathcal{X}$ (for example, $\mathcal{X}$ could be letters $\{\mathrm{a}, \mathrm{b}, \dots, \mathrm{z}\}$). We want to construct an encoding scheme for our symbols in the form of sequences of binary bits that are transmitted over the channel. Further, suppose that in the long run the frequency of occurrence of symbols follow a probability distribution $P(X)$. This means, in the long run, the fraction of times the symbol x gets transmitted is $P(x)$.

A common desire is to construct an encoding scheme such that the average number of bits per symbol transmitted remains as small as possible. Intuitively, this means we want very frequent symbols to be assigned to a bit pattern having a small number of bits. Likewise, because we are

[3]If P and Q are densities for continuous-valued random variables, then the sum is replaced by an integral, and everything stated in this problem works fine as well. But for the sake of simplicity, in this problem we'll just work with this form of KL divergence for probability mass functions/discrete-valued distributions.

interested in reducing the average number of bits per symbol in the long term, it is tolerable for infrequent words to be assigned to bit patterns having a large number of bits, since their low frequency has little effect on the long term average. The encoding scheme can be as complex as we desire, for example, a single bit could possibly represent a long sequence of multiple symbols (if that specific pattern of symbols is very common). The entropy of a probability distribution $P(X)$ is its optimal bit rate, i.e., the lowest average bits per message that can possibly be achieved if the symbols $x \in \mathcal{X}$ occur according to $P(X)$. It does not specifically tell us *how* to construct that optimal encoding scheme. It only tells us that no encoding can possibly give us a lower long term bits per message than $H(P)$.

To see a concrete example, suppose our messages have a vocabulary of $K = 32$ symbols, and each symbol has an equal probability of transmission in the long term (i.e, uniform probability distribution). An encoding scheme that would work well for this scenario would be to have $\log_2 K$ bits per symbol, and assign each symbol some unique combination of the $\log_2 K$ bits. In fact, it turns out that this is the most efficient encoding one can come up with for the uniform distribution scenario.

It may have occurred to you by now that the long term average number of bits per message depends only on the frequency of occurrence of symbols. The encoding scheme of scenario A can in theory be reused in scenario B with a different set of symbols (assume equal vocabulary size for simplicity), with the same long term efficiency, as long as the symbols of scenario B follow the same probability distribution as the symbols of scenario A. It might also have occurred to you, that reusing the encoding scheme designed to be optimal for scenario A, for messages in scenario B having a *different probability* of symbols, will always be suboptimal for scenario B. To be clear, we do not need to know *what* the specific optimal schemes are in either scenarios. As long as we know the distributions of their symbols, we can say that the optimal scheme designed for scenario A will be suboptimal for scenario B if the distributions are different.

Concretely, if we reuse the optimal scheme designed for a scenario having symbol distribution $Q(X)$, into a scenario that has symbol distribution $P(X)$, the long term average number of bits per symbol achieved is called the *cross entropy*, denoted by $H(P, Q)$:

$$H(P, Q) = -\sum_{x \in \mathcal{X}} P(x) \log Q(x).$$

To recap, the entropy $H(P)$ is the best possible long term average bits per message (optimal) that can be achieved under a symbol distribution $P(X)$ by using an encoding scheme (possibly unknown) specifically designed for $P(X)$. The cross entropy $H(P, Q)$ is the long term average bits per message (suboptimal) that results under a symbol distribution $P(X)$, by reusing an encoding scheme (possibly unknown) designed to be optimal for a scenario with symbol distribution $Q(X)$.

Now, KL divergence is the penalty we pay, as measured in average number of bits, for using the optimal scheme for $Q(X)$, under the scenario where symbols are actually distributed as $P(X)$. It is straightforward to see this

$$\begin{aligned} D_{KL}(P \| Q) &= \sum_{x \in \mathcal{X}} P(x) \log \frac{P(x)}{Q(x)} \\ &= -\sum_{x \in \mathcal{X}} P(x) \log Q(x) + \sum_{x \in \mathcal{X}} P(x) \log P(x) \\ &= H(P, Q) - H(P). \quad \text{(difference in average number of bits.)} \end{aligned}$$

If the cross entropy between P and Q is $H(P)$ (and hence $D_{KL}(P||Q) = 0$) then it necessarily means $P = Q$. In Machine Learning, it is a common task to find a distribution Q that is "close" to another distribution P. To achieve this, it is common to use $D_{KL}(Q||P)$ as the loss function to be optimized. As we will see in this question below, Maximum Likelihood Estimation, which is a commonly used optimization objective, turns out to be equivalent to minimizing the KL divergence between the training data (i.e., the empirical distribution over the data) and the model.

Now, we get back to showing some simple properties of KL divergence.

(a) [5 points] **Nonnegativity.**
Prove the following:

$$\forall P, Q. \quad D_{KL}(P\|Q) \geq 0$$

and

$$D_{KL}(P\|Q) = 0 \qquad \text{if and only if} \qquad P = Q.$$

[Hint: You may use the following result, called **Jensen's inequality**. If f is a convex function, and X is a random variable, then $E[f(X)] \geq f(E[X])$. Moreover, if f is strictly convex (f is convex if its Hessian satisfies $H \geq 0$; it is *strictly* convex if $H > 0$; for instance $f(x) = -\log x$ is strictly convex), then $E[f(X)] = f(E[X])$ implies that $X = E[X]$ with probability 1; i.e., X is actually a constant.]

Answer:

(b) [5 points] **Chain rule for KL divergence.**
The KL divergence between 2 conditional distributions $P(X|Y), Q(X|Y)$ is defined as follows:

$$D_{KL}(P(X|Y)\|Q(X|Y)) = \sum_y P(y) \left(\sum_x P(x|y) \log \frac{P(x|y)}{Q(x|y)} \right)$$

This can be thought as the expected KL divergence between the corresponding conditional distributions on x (that is, between $P(X|Y = y)$ and $Q(X|Y = y)$), where the expectation is taken over the random y.

Prove the following chain rule for KL divergence:

$$D_{KL}(P(X,Y)\|Q(X,Y)) = D_{KL}(P(X)\|Q(X)) + D_{KL}(P(Y|X)\|Q(Y|X)).$$

Answer:

(c) [5 points] **KL and maximum likelihood.**
Consider a density estimation problem, and suppose we are given a training set $\{x^{(i)}; i = 1, \ldots, n\}$. Let the empirical distribution be $\hat{P}(x) = \frac{1}{n}\sum_{i=1}^{n} 1\{x^{(i)} = x\}$. ($\hat{P}$ is just the uniform distribution over the training set; i.e., sampling from the empirical distribution is the same as picking a random example from the training set.)

Suppose we have some family of distributions P_θ parameterized by θ. (If you like, think of $P_\theta(x)$ as an alternative notation for $P(x; \theta)$.) Prove that finding the maximum likelihood estimate for the parameter θ is equivalent to finding P_θ with minimal KL divergence from $\hat{P}$, that is, prove:

$$\arg\min_\theta D_{KL}(\hat{P}\|P_\theta) = \arg\max_\theta \sum_{i=1}^{n} \log P_\theta(x^{(i)})$$

Remark. Consider the relationship between parts (b-c) and multi-variate Bernoulli Naive Bayes parameter estimation. In the Naive Bayes model we assumed P_θ is of the following form: $P_\theta(x, y) = p(y) \prod_{i=1}^{d} p(x_i|y)$. By the chain rule for KL divergence, we therefore have:

$$D_{KL}(\hat{P}\|P_\theta) = D_{KL}(\hat{P}(y)\|p(y)) + \sum_{i=1}^{d} D_{KL}(\hat{P}(x_i|y)\|p(x_i|y)).$$

This shows that finding the maximum likelihood/minimum KL-divergence estimate of the parameters decomposes into $2n + 1$ independent optimization problems: One for the class priors $p(y)$, and one for each of the conditional distributions $p(x_i|y)$ for each feature x_i given each of the two possible labels for y. Specifically, finding the maximum likelihood estimates for each of these problems individually results in also maximizing the likelihood of the joint distribution. (If you know what Bayesian networks are, a similar remark applies to parameter estimation for them.)

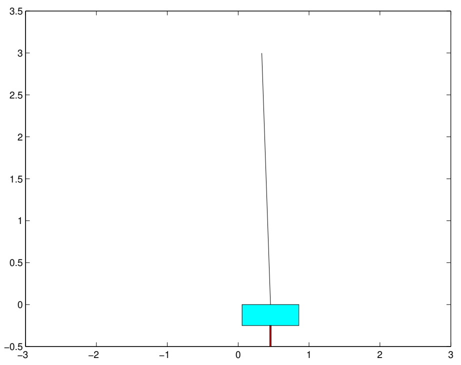
Answer:

4. **[25 points] Reinforcement Learning: The inverted pendulum**

In this problem, you will apply reinforcement learning to automatically design a policy for a difficult control task, without ever using any explicit knowledge of the dynamics of the underlying system.

The problem we will consider is the inverted pendulum or the pole-balancing problem.[4]

Consider the figure shown. A thin pole is connected via a free hinge to a cart, which can move laterally on a smooth table surface. The controller is said to have failed if either the angle of the pole deviates by more than a certain amount from the vertical position (i.e., if the pole falls over), or if the cart's position goes out of bounds (i.e., if it falls off the end of the table). Our objective is to develop a controller to balance the pole with these constraints, by appropriately having the cart accelerate left and right.



We have written a simple simulator for this problem. The simulation proceeds in discrete time cycles (steps). The state of the cart and pole at any time is completely characterized by 4 parameters: the cart position x, the cart velocity $\dot{x}$, the angle of the pole θ measured as its deviation from the vertical position, and the angular velocity of the pole $\dot{\theta}$. Since it would be simpler to consider reinforcement learning in a discrete state space, we have approximated the state space by a discretization that maps a state vector $(x, \dot{x}, \theta, \dot{\theta})$ into a number from 0 to `NUM_STATES-1`. Your learning algorithm will need to deal only with this discretized representation of the states.

At every time step, the controller must choose one of two actions - push (accelerate) the cart right, or push the cart left. (To keep the problem simple, there is no *do-nothing* action.) These are represented as actions 0 and 1 respectively in the code. When the action choice is made, the simulator updates the state parameters according to the underlying dynamics, and provides a new discretized state.

We will assume that the reward $R(s)$ is a function of the current state only. When the pole angle goes beyond a certain limit or when the cart goes too far out, a negative reward is given, and the system is reinitialized randomly. At all other times, the reward is zero. Your program must learn to balance the pole using only the state transitions and rewards observed.

To solve the inverted pendulum problem, you will estimate a model (i.e., transition probabilities and rewards) for the underlying MDP, solve Bellman's equations for this estimated MDP to obtain a value function, and act greedily with respect to this value function.

[4]The dynamics are adapted from `http://www-anw.cs.umass.edu/rlr/domains.html`

Briefly, you will maintain a current model of the MDP and a current estimate of the value function. Initially, each state has estimated reward zero, and the estimated transition probabilities are uniform (equally likely to end up in any other state).

During the simulation, you must choose actions at each time step according to some current policy. As the program goes along taking actions, it will gather observations on transitions and rewards, which it can use to get a better estimate of the MDP model. Since it is inefficient to update the whole estimated MDP after every observation, we will store the state transitions and reward observations each time, and update the model and value function/policy only periodically. Thus, you must maintain counts of the total number of times the transition from state s_i to state s_j using action a has been observed (similarly for the rewards). Note that the rewards at any state are deterministic, but the state transitions are not because of the discretization of the state space (several different but close configurations may map onto the same discretized state).

Each time a failure occurs (such as if the pole falls over), you should re-estimate the transition probabilities and rewards as the average of the observed values (if any). Your program must then use value iteration to solve Bellman's equations on the estimated MDP, to get the value function and new optimal policy for the new model. For value iteration, use a convergence criterion that checks if the maximum absolute change in the value function on an iteration exceeds some specified tolerance.

Finally, assume that the whole learning procedure has converged once several consecutive attempts (defined by the parameter `NO_LEARNING_THRESHOLD`) to solve Bellman's equation all converge in the first iteration. Intuitively, this indicates that the estimated model has stopped changing significantly.

(a) [20 points] **Implementation**

Follow the instructions in `src/cartpole/cartpole.py` to implement the algorithm. Use a discount factor of $\gamma = 0.995$. **In particular, implement the following functions:**

i. `choose_action(state, mdp_data)`. We recommend you incorporate the helper function `sample_random_action`
ii. `update_mdp_transition_counts_reward_counts(mdp_data, state, action, new_state, reward)`
iii. `update_mdp_transition_probs_reward(mdp_data)`
iv. `update_mdp_value(mdp_data, tolerance, gamma)`

Once you've finished implementing the above functions, run the experiment via `python cartpole.py`. Plot a learning curve showing the number of time-steps for which the pole was balanced on each trial (the starter code already includes the code to plot). Include it in your write-up.

Answer:

(b) [5 points] **Convergence**

i. How many trials (how many times did the pole fall over or the cart fall off) did it take before the algorithm converged? This is equivalent to the number on the last printed line that says "[INFO] Failure number ###".
Note: Different random action sampling methods in NumPy can cause significant differences in the number of iterations and other metrics.
ii. Find the line of code that says np.random.seed, and rerun the code with the seed set to 1, 2, and 3. What do you observe?

Answer:

If you got here and finished all the above problems, you are done with the final PSet of CS 229! We know these assignments are not easy, so well done :)