

XCS229 Problem Set 4

Due Sunday, July 14 at 11:59pm PT.

Guidelines

1. If you have a question about this homework, we encourage you to post your question on our Slack channel, at <http://xcs229-scpd.slack.com/>
2. Familiarize yourself with the collaboration and honor code policy before starting work.
3. For the coding problems, you must use the packages specified in the provided environment description. Since the autograder uses this environment, we will not be able to grade any submissions which import unexpected libraries.

Submission Instructions

Written Submission: Some questions in this assignment require a written response. For these questions, you should submit a PDF with your solutions online in the online student portal. As long as the PDF is legible and organized, the course staff has no preference between a handwritten and a typeset \LaTeX submission. If you wish to typeset your submission and are new to \LaTeX , you can get started with the following:

- Type responses only in `submission.tex`.
- Submit the compiled PDF, **not** `submission.tex`.
- Use the commented instructions within the `Makefile` and `README.md` to get started.

Coding Submission: Some questions in this assignment require a coding response. For these questions, you should submit only the `src/submission.py` file in the online student portal. For further details, see Writing Code and Running the Autograder below.

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 solutions independently, and without referring to written notes from the joint session. In other words, each student must understand the solution well enough in order to reconstruct it by him/herself. In addition, each student should write on the problem set the set of people with whom s/he collaborated. Further, because we occasionally reuse problem set questions from previous years, we expect students not to copy, refer to, or look at the solutions in preparing their answers. It is an honor code violation to intentionally refer to a previous year's solutions. More information regarding the Stanford honor code can be found at <https://communitystandards.stanford.edu/policies-and-guidance/honor-code>.

Writing Code and Running the Autograder

All your code should be entered into `src/submission.py`. When editing `src/submission.py`, please only make changes between the lines containing `### START_CODE_HERE ###` and `### END_CODE_HERE ###`. Do not make changes to files other than `src/submission.py`.

The unit tests in `src/grader.py` (the autograder) will be used to verify a correct submission. Run the autograder locally using the following terminal command within the `src/` subdirectory:

```
$ python grader.py
```

There are two types of unit tests used by the autograder:

- **basic:** These tests are provided to make sure that your inputs and outputs are on the right track, and that the hidden evaluation tests will be able to execute.

- **hidden:** These unit tests are the evaluated elements of the assignment, and run your code with more complex inputs and corner cases. Just because your code passed the basic local tests does not necessarily mean that they will pass all of the hidden tests. These evaluative hidden tests will be run when you submit your code to the Gradescope autograder via the online student portal, and will provide feedback on how many points you have earned.

For debugging purposes, you can run a single unit test locally. For example, you can run the test case `3a-0-basic` using the following terminal command within the `src/` subdirectory:

```
$ python grader.py 3a-0-basic
```

Before beginning this course, please walk through the [Anaconda Setup for XCS Courses](#) to familiarize yourself with the coding environment. Use the env defined in `src/environment.yml` to run your code. This is the same environment used by the online autograder.

Test Cases

The autograder is a thin wrapper over the python `unittest` framework. It can be run either locally (on your computer) or remotely (on SCPD servers). The following description demonstrates what test results will look like for both local and remote execution. For the sake of example, we will consider two generic tests: `1a-0-basic` and `1a-1-hidden`.

Local Execution - Hidden Tests

All hidden tests rely on files that are not provided to students. Therefore, the tests can only be run remotely. When a hidden test like `1a-1-hidden` is executed locally, it will produce the following result:

```
----- START 1a-1-hidden: Test multiple instances of the same word in a sentence.
----- END 1a-1-hidden [took 0:00:00.011989 (max allowed 1 seconds), ???/3 points] (hidden test ungraded)
```

Local Execution - Basic Tests

When a basic test like `1a-0-basic` passes locally, the autograder will indicate success:

```
----- START 1a-0-basic: Basic test case.
----- END 1a-0-basic [took 0:00:00.000062 (max allowed 1 seconds), 2/2 points]
```

When a basic test like `1a-0-basic` fails locally, the error is printed to the terminal, along with a stack trace indicating where the error occurred:

```
----- START 1a-0-basic: Basic test case.
<class 'AssertionError'>
{'a': 2, 'b': 1} != None ← This error caused the test to fail.
File "/Users/grinch/Local_Documents/Software/anaconda3/envs/XCS221/lib/python3.6/unittest/case.py", line 59, in testPartExecutor
yield
File "/Users/grinch/Local_Documents/Software/anaconda3/envs/XCS221/lib/python3.6/unittest/case.py", line 605, in run
testMethod()
File "/Users/grinch/Local_Documents/SCPD/XCS221/A1/src/graderUtil.py", line 54, in wrapper
result = func(*args, **kwargs)
File "/Users/grinch/Local_Documents/SCPD/XCS221/A1/src/graderUtil.py", line 83, in wrapper
result = func(*args, **kwargs)
File "/Users/grinch/Local_Documents/SCPD/XCS221/A1/src/grader.py", line 23, in test_0
submission.extractWordFeatures("a b a") ← In this case, start your debugging
in line 23 of grader.py.
File "/Users/grinch/Local_Documents/Software/anaconda3/envs/XCS221/lib/python3.6/unittest/case.py", line 829, in assertEqual
assertion_func(first, second, msg=msg)
File "/Users/grinch/Local_Documents/Software/anaconda3/envs/XCS221/lib/python3.6/unittest/case.py", line 822, in _baseAssertEqual
raise self.failureException(msg)
----- END 1a-0-basic [took 0:00:00.003809 (max allowed 1 seconds), 0/2 points]
```

Remote Execution

Basic and hidden tests are treated the same by the remote autograder. Here are screenshots of failed basic and hidden tests. Notice that the same information (error and stack trace) is provided as the in local autograder, now for both basic and hidden tests.

1a-0-basic) Basic test case. (0.0/2.0)

```
<class 'AssertionError': {'a': 2, 'b': 1} != None
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 59, in testPartExecutor
    yield
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 605, in run
    testMethod()
File "/autograder/source/graderUtil.py", line 54, in wrapper
    result = func(*args, **kwargs)
File "/autograder/source/graderUtil.py", line 83, in wrapper
    result = func(*args, **kwargs)
File "/autograder/source/grader.py", line 23, in test_0
    submission.extractWordFeatures("a b a"))
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 829, in assertEqual
    assertion_func(first, second, msg=msg)
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 822, in _baseAssertEqual
    raise self.failureException(msg)
```

Just like in the local autograder, this error caused the test to fail.

Just like in the local autograder, start your debugging in line 23 of grader.py.

1a-1-hidden) Test multiple instances of the same word in a sentence. (0.0/3.0)

```
<class 'AssertionError': {'a': 23, 'ab': 22, 'aa': 24, 'c': 16, 'b': 15} != None
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 59, in testPartExecutor
    yield
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 605, in run
    testMethod()
File "/autograder/source/graderUtil.py", line 54, in wrapper
    result = func(*args, **kwargs)
File "/autograder/source/graderUtil.py", line 83, in wrapper
    result = func(*args, **kwargs)
File "/autograder/source/grader.py", line 31, in test_1
    self.compare_with_solution_or_wait(submission, 'extractWordFeatures', lambda f: f(sentence))
File "/autograder/source/graderUtil.py", line 183, in compare_with_solution_or_wait
    self.assertEqual(ans1, ans2)
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 829, in assertEqual
    assertion_func(first, second, msg=msg)
File "/autograder/source/miniconda/envs/XCS221/lib/python3.6/unittest/case.py", line 822, in _baseAssertEqual
    raise self.failureException(msg)
```

This error caused the test to fail.

Start your debugging in line 31 of grader.py.

Finally, here is what it looks like when basic and hidden tests pass in the remote autograder.

1a-0-basic) Basic test case. (2.0/2.0)

1a-1-hidden) Test multiple instances of the same word in a sentence. (3.0/3.0)

1. 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. As we dive into the problem, [this resource](#) will help you determine more properties about KL Divergence.

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 follows¹:

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

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 $D_{KL}(P \parallel Q) = D_{KL}(P(X) \parallel Q(X))$.

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 on 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 $\{a, b, \dots, z\}$). 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 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

¹If 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.

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 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

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

If the cross entropy between P and Q is $H(P)$ (and hence $D_{KL}(P \parallel Q) = 0$) 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 $D_{KL}(Q \parallel P)$ 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 (Written)] **Nonnegativity.**

Prove the following:

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

and

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

[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.]

(b) [4 points (Written)] 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 of 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:

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

(c) [4 points (Written)] KL and maximum likelihood.

Consider a density estimation problem, and suppose we are given a training set $\{x^{(i)}; i = 1, \dots, n\}$. 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} . I.e. prove:

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

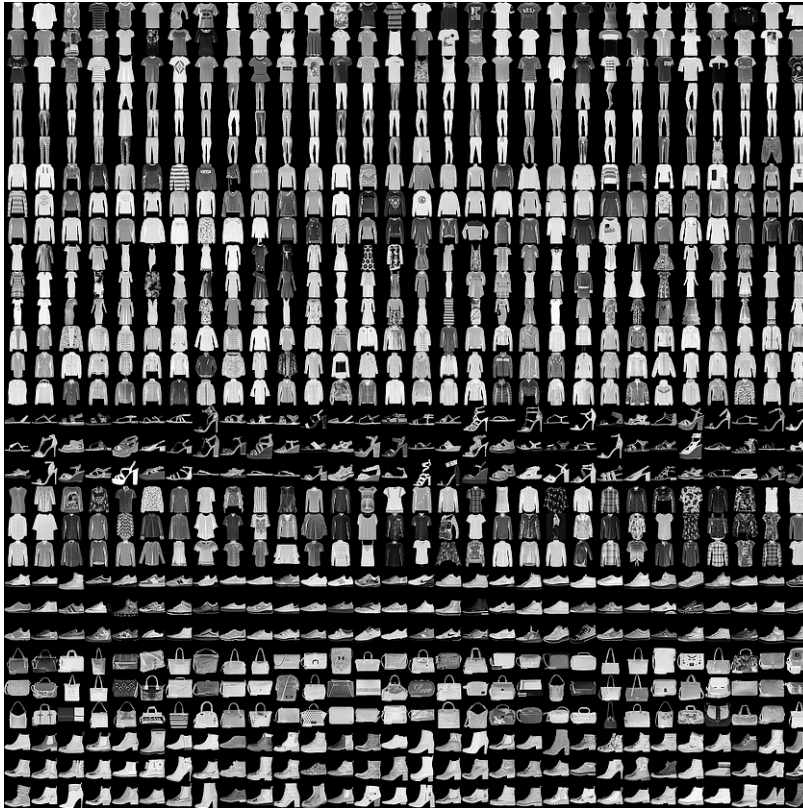
Remark. Consider the relationship between parts (b-c) and multi-variate Bernoulli Naive Bayes parameter estimation. In the Naive Bayes model we assumed P_θ is of the following form: $P_\theta(x, y) = p(y) \prod_{i=1}^d p(x_i | y)$. By the chain rule for KL divergence, we therefore have:

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

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.)

2. Neural Networks: Fashion-MNIST image classification

In this problem, you will implement a simple neural network to classify grayscale images of clothings (10 labels: T-shirts, Trouser, Pullover, Dress, Coat, Sandal, Shirt, Sneaker, Bag, Ankel boot) from the Fashion-MNIST dataset²³⁴. This is a drop-in dataset replacement for MNIST⁵. The dataset contains 60,000 training images and 10,000 testing images of clothing types, 0 - 9. Each image is 28×28 pixels in size, and is generally represented as a flat vector of 784 numbers. It also includes labels for each example, a number indicating the actual clothing types (0 - 9) that image. A sample of a few such images are shown below.



The data and starter code for this problem can be found in

- `src-mnist/submission.py`
- `src-mnist/images_train.csv` (unzip Archive.zip to access this file)
- `src-mnist/labels_train.csv` (unzip Archive.zip to access this file)
- `src-mnist/images_test.csv` (unzip Archive.zip to access this file)
- `src-mnist/labels_test.csv` (unzip Archive.zip to access this file)

The starter code splits the set of 60,000 training images and labels into a set of 50,000 examples as the training set, and 10,000 examples for dev set.

To start, you will implement a neural network with a single hidden layer and cross entropy loss, and train it with the provided data set. Use the sigmoid function as activation for the hidden layer, and softmax function for the output layer. Recall that for a single example (x, y) , the cross entropy loss is:

$$CE(y, \hat{y}) = - \sum_{k=1}^K y_k \log \hat{y}_k,$$

²<https://github.com/zalandoresearch/fashion-mnist>

³This dataset is newly introduced from this cohort, which replaces MNIST, which is considered to be too easy nowadays.

⁴The original Fashion-MNIST dataset is converted to the format for PS4 using this code <https://github.com/insop/Fashion-MNIST-csv>

⁵https://en.wikipedia.org/wiki/MNIST_database

where $\hat{y} \in \mathbb{R}^K$ is the vector of softmax outputs from the model for the training example x , and $y \in \mathbb{R}^K$ is the ground-truth vector for the training example x such that $y = [0, \dots, 0, 1, 0, \dots, 0]^\top$ contains a single 1 at the position of the correct class (also called a “one-hot” representation).

For n training examples, we average the cross entropy loss over the n examples.

$$J(W^{[1]}, W^{[2]}, b^{[1]}, b^{[2]}) = \frac{1}{n} \sum_{i=1}^n CE(y^{(i)}, \hat{y}^{(i)}) = -\frac{1}{n} \sum_{i=1}^n \sum_{k=1}^K y_k^{(i)} \log \hat{y}_k^{(i)}.$$

The starter code already converts labels into one hot representations for you.

Instead of batch gradient descent or stochastic gradient descent, the common practice is to use mini-batch gradient descent for deep learning tasks. In this case, the cost function is defined as follows:

$$J_{MB} = \frac{1}{B} \sum_{i=1}^B CE(y^{(i)}, \hat{y}^{(i)})$$

where B is the batch size, i.e. the number of training example in each mini-batch.

(a) [9 points (Coding)]

Implement both forward-propagation and back-propagation for the above loss function. More specifically you will implement the `softmax`, `sigmoid`, `get_initial_params`, `forward_prop`, `backward_prop`, and `gradient_descent_epoch` functions inside `src-mnist/submission.py`.

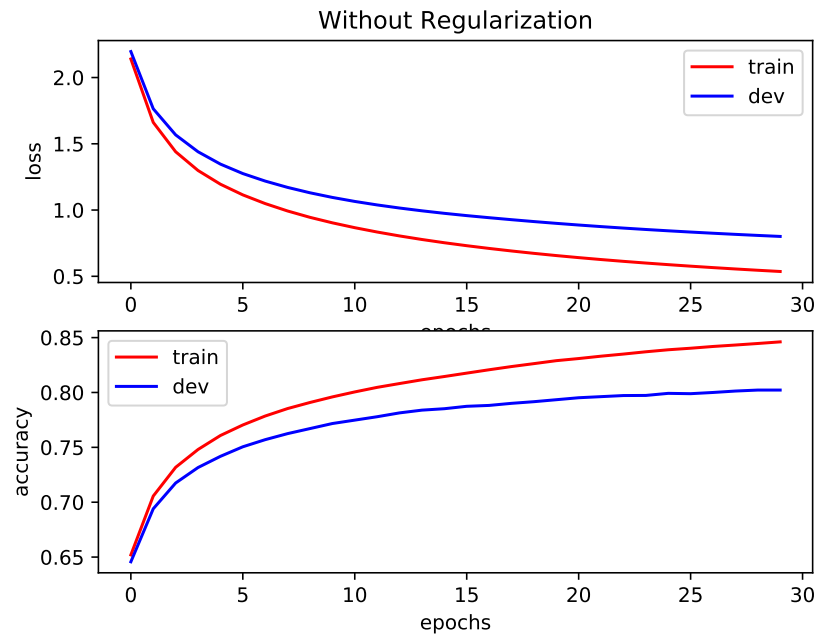
Initialize the weights of the network by sampling values from a standard normal distribution. Initialize the bias/intercept term to 0. Set the number of hidden units to be 300, and learning rate to be 0.4. Set $B = 1,000$ (mini batch size). This means that we train with 1,000 examples in each iteration. Therefore, for each epoch, we need 50 iterations to cover the entire training data. The images are pre-shuffled. So you don't need to randomly sample the data, and can just create mini-batches sequentially.

Use autograder test case `2aii-6-basic` to train the model with mini-batch gradient descent as described above. Before running this test case, edit line 186 of `src-mnist/grader.py` to state `skip = False` (model plotting/training is disabled by default to run the autograder faster). This will run the training for 30 epochs. At the end of each epoch, it will calculate the value of loss function averaged over the entire training set. It will then plot the average loss (y-axis) against the number of epochs (x-axis). In the same image, it will also plot the value of the loss function averaged over the dev set, and against the number of epochs.

This will also plot the accuracy (on y-axis) over the training set, measured as the fraction of correctly classified examples, versus the number of epochs (x-axis). In the same image, it will plot the accuracy over the dev set versus number of epochs.

Hint: Be sure to vectorize your code as much as possible! Training can be very slow otherwise.

You plots should look similar to the following (You are not required to submit any plots. These are for your own verification.):

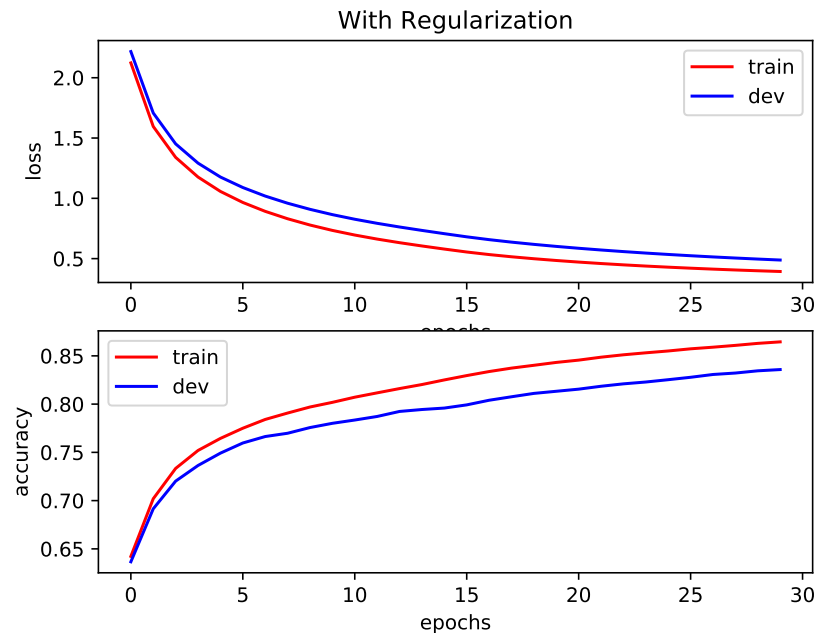


- (b) [4 points (Coding)] Now add a regularization term to your cross entropy loss by implementing `backward_prop_regularized()`. The loss function will become

$$J_{MB} = \left(\frac{1}{B} \sum_{i=1}^B CE(y^{(i)}, \hat{y}^{(i)}) \right) + \frac{1}{2} \lambda \left(\|W^{[1]}\|^2 + \|W^{[2]}\|^2 \right)$$

Autograder test case `2b-2-basic` will perform the same as `2a1-6-basic` (described earlier), except that it utilizes your new regularized backprop function. Before running this test case, edit line 285 of `src-mnist/grader.py` to state `skip = False` (model plotting/training is disabled by default to run the autograder faster). It will also plot the same figures as part (a). Note that it does NOT include the regularization term to measure the loss value for plotting (i.e., regularization should only be used for gradient calculation for the purpose of training).

After creating the plots from the previous part, they should look similar to the following (You are not required to submit any plots. These are for your own verification.):



- (c) **[2 points (Coding)]** All this while the test cases have avoided the test data completely. Now that you have convinced yourself that the model is working as expected (i.e, the observations you made in the previous part matches what you learnt in class about regularization), it is finally time to measure the model performance on the test set. Once we measure the test set performance, we report it (whatever value it may be), and NOT go back and refine the model any further.

Autograder test case `2c-1-basic` will train your model and then evaluate its performance on the test data for both the regularized and non-regularized training strategies. Before running this test case, edit line 361 of `src-mnist/grader.py` to state `skip = False` (model plotting/training is disabled by default to run the autograder faster).

You should have accuracy close to 0.7855 without regularization, and 0.819 with regularization.

Note: Even if you do not have precisely these numbers, you should observe better test accuracy with regularization than without.

Fashion-MNIST is challenging dataset compared to MNIST. With the similar hyperparameters, the accuracy of regularized model was 0.96 for MNIST dataset. Once you finished the assignment with given network specification, we encourage you to improve the accuracy by modifying the neural network model on your environment, such as adding more hidden layers, changing the hidden layer size, or using a different initialization. Once you do, please share your accuracy and model on the slack PS4 channel!

3. Spam classification

In this problem, we will use the Naive Bayes algorithm and an SVM to build a spam classifier.

In recent years, spam on electronic media has been a growing concern. Here, we'll build a classifier to distinguish between real messages, and spam messages. For this class, we will be building a classifier to detect SMS spam messages. We will be using an SMS spam dataset developed by Tiago A. Almeida and José María Gómez Hidalgo which is publicly available on <http://www.dt.fee.unicamp.br/~tiago/smsspamcollection>⁶

We have split this dataset into training and testing sets and have included them in this assignment as:

- `src-spam/spam_train.tsv`
- `src-spam/spam_test.tsv`

See `src-spam/spam_readme.txt` for more details about this dataset. Please refrain from redistributing these dataset files. The goal of this assignment is to build a classifier from scratch that can tell the difference the spam and non-spam messages using the text of the SMS message.

- (a) **[7 points (Coding)]** Implement code for processing the spam messages into numpy arrays that can be fed into machine learning models. Do this by completing the `get_words()`, `create_dictionary()`, and `transform_text()` functions within our provided `src-spam/submission.py`. Do note the corresponding comments for each function for instructions on what specific processing is required.

The autograder test case `3a-4-basic` will then run your functions and save the resulting dictionary into `spam_dictionary` and a sample of the resulting training matrix into `spam_sample_train_matrix(soln)`.

- (b) **[2 points (Coding)]** In this question you are going to implement a Naive Bayes classifier for spam classification with **multinomial event model** and Laplace smoothing.

Code your implementation by completing the `fit_naive_bayes_model()` and `predict_from_naive_bayes_model()` functions in `src-spam/submission.py`.

Now the functions in `src-spam/submission.py` should be able to train a Naive Bayes model. Use autograder test case `3b-1-basic` to compute your prediction accuracy and then save your resulting predictions to `spam_naive_bayes_predictions(soln)`.

Remark. If you implement Naive Bayes the straightforward way, you will find that the computed $p(x|y) = \prod_i p(x_i|y)$ often equals zero. This is because $p(x|y)$, which is the product of many numbers less than one, is a very small number. The standard computer representation of real numbers cannot handle numbers that are too small, and instead rounds them off to zero. (This is called “underflow.”) You'll have to find a way to compute Naive Bayes' predicted class labels without explicitly representing very small numbers such as $p(x|y)$. **[Hint:** Think about using logarithms.]

- (c) **[2 points (Coding)]** Intuitively, some tokens may be particularly indicative of an SMS being in a particular class. We can try to get an informal sense of how indicative token i is for the SPAM class by looking at:

$$\log \frac{p(x_j = i|y = 1)}{p(x_j = i|y = 0)} = \log \left(\frac{P(\text{token } i|\text{email is SPAM})}{P(\text{token } i|\text{email is NOTSPAM})} \right).$$

Complete the `get_top_five_naive_bayes_words()` function within the provided code using the above formula. Run autograder test case `3c-1-basic` to obtain the 5 most indicative tokens.

- (d) **[4 points (Coding)]** Support vector machines (SVMs) are an alternative machine learning model that we discussed in class. We have provided you an SVM implementation (using a radial basis function (RBF) kernel) within `src-spam/svm.py` (You should not need to modify that code).

One important part of training an SVM parameterized by an RBF kernel (a.k.a Gaussian kernel) is choosing an appropriate kernel radius parameter.

Complete the `compute_best_svm_radius()` by writing code to compute the best SVM radius which maximizes accuracy on the validation dataset.

⁶Almeida, T.A., Gómez Hidalgo, J.M., Yamakami, A. Contributions to the Study of SMS Spam Filtering: New Collection and Results. Proceedings of the 2011 ACM Symposium on Document Engineering (DOCENG'11), Mountain View, CA, USA, 2011.

4. Double Descent on Linear Models

In this problem, you will empirically observe the sample-wise double descent phenomenon. That is, the validation losses of some learning algorithms or estimators do not monotonically decrease as we have more training examples, but instead have a curve with two U-shaped parts. The double descent phenomenon can be observed even for simple linear models. In this question, we consider the following setup. Let $\{(x^{(i)}, y^{(i)})\}_{i=1}^n$ be the training dataset. Let $X \in \mathbb{R}^{n \times d}$ be the matrix representing the inputs (i.e., the i -th row of X corresponds to $x^{(i)}$), and $\vec{y} \in \mathbb{R}^n$ the vector representing the labels (i.e., the i -th row of \vec{y} corresponds to $y^{(i)}$):

$$X = \begin{bmatrix} - & x^{(1)} & - \\ - & x^{(2)} & - \\ \vdots & \vdots & \vdots \\ - & x^{(n)} & - \end{bmatrix}, \quad \vec{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}.$$

Similarly, we use $X_v \in \mathbb{R}^{m \times d}$, $\vec{y}_v \in \mathbb{R}^m$ to represent the validation dataset, where m is the size of the validation dataset. We assume that the data are generated with $d = 500$.

In this question, we consider *regularized* linear regression. For a regularization level $\lambda \geq 0$, define the regularized cost function

$$J_\lambda(\beta) = \frac{1}{2} \|X\beta - \vec{y}\|_2^2 + \frac{\lambda}{2} \|\beta\|_2^2,$$

and its minimizer $\hat{\beta}_\lambda = \arg \min_{\beta \in \mathbb{R}^d} J_\lambda(\beta)$.

(a) [3 points (Written)] **Derive closed-form solution.**

In this question, we derive the closed-form solution of $\hat{\beta}_\lambda$. **Prove** that when $\lambda > 0$,

$$\hat{\beta}_\lambda = (X^\top X + \lambda I_{d \times d})^{-1} X^\top \vec{y} \quad (1)$$

(recall that $I_{d \times d} \in \mathbb{R}^{d \times d}$ is the identity matrix.)

Note: $\lambda = 0$ is a special case here. When $\lambda = 0$, $(X^\top X + \lambda I_{d \times d})$ could be singular. Therefore, there might be more than one solutions that minimize $J_0(\beta)$. In this case, we define $\hat{\beta}_0$ in the following way:

$$\hat{\beta}_0 = (X^\top X)^+ X^\top \vec{y}. \quad (2)$$

where $(X^\top X)^+$ denotes the [Moore-Penrose pseudo-inverse](#) of $X^\top X$. You don't need to prove the case when $\lambda = 0$, but this definition is useful in the following sub-questions.

(b) [2 points (Coding)] **The double descent phenomenon for unregularized models**

In this question, you will empirically observe the double descent phenomenon. You are given 13 training datasets of sample sizes $n = 200, 250, \dots, 750$, and 800, and a validation dataset, located at

- `src-doubledescent/train200.csv`, `train250.csv`, etc.
- `src-doubledescent/validation.csv`

For each training dataset (X, \vec{y}) , compute the corresponding $\hat{\beta}_0$, and evaluate the mean squared error (MSE) of $\hat{\beta}_0$ on the validation dataset. The MSE for your estimators $\hat{\beta}$ on a validation dataset (X_v, \vec{y}_v) of size m is defined as:

$$\text{MSE}(\hat{\beta}) = \frac{1}{2m} \|X_v \hat{\beta} - \vec{y}_v\|_2^2.$$

Complete the `regression` method of `src-doubledescent/submission.py` which takes in a training file and a validation file, and computes $\hat{\beta}_0$. You can use `numpy.linalg.pinv` to compute the pseudo-inverse.

The output plot should look similar to the following (no plot submission is required):

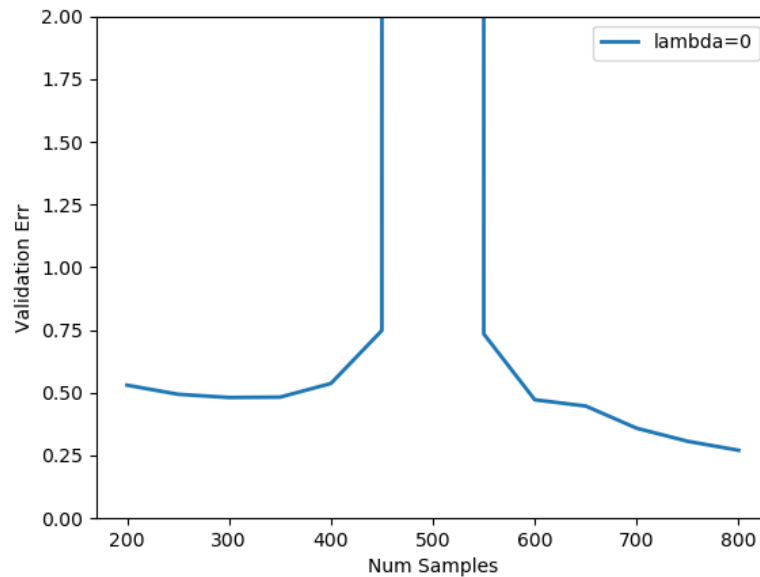


Figure 1: Num of samples vs. validation error.

The x-axis is the size of the training dataset (from 200 to 800); the y-axis is the MSE on the validation dataset. You should observe that the validation error increases and then decreases as we increase the sample size.

Note: When $n \approx d$, the test MSE could be very large. For better visualization, we let the if the test MSE goes out of scope in the plot for some points.

(c) [2 points (Coding)] **Duble descent phenomenon and the effect of regularization.**

In this question, we will show that regularization mitigates the double descent phenomenon for linear regression. We will use the same datasets as specified in sub-question (b). Now consider using various regularization strengths. For $\lambda \in \{0, 1, 5, 10, 50, 250, 500, 1000\}$, you will compute the minimizer of $J_\lambda(\beta)$.

Complete the `ridge_regression` method of `src-doubledescent/submission.py` which takes in a training file and a validation file, computes the $\hat{\beta}_\lambda$ that minimizes the training objective under different regularization strengths, and returns a list of validation errors (one for each choice of λ).

The output plot should look similar to the following (no plot submission is required):

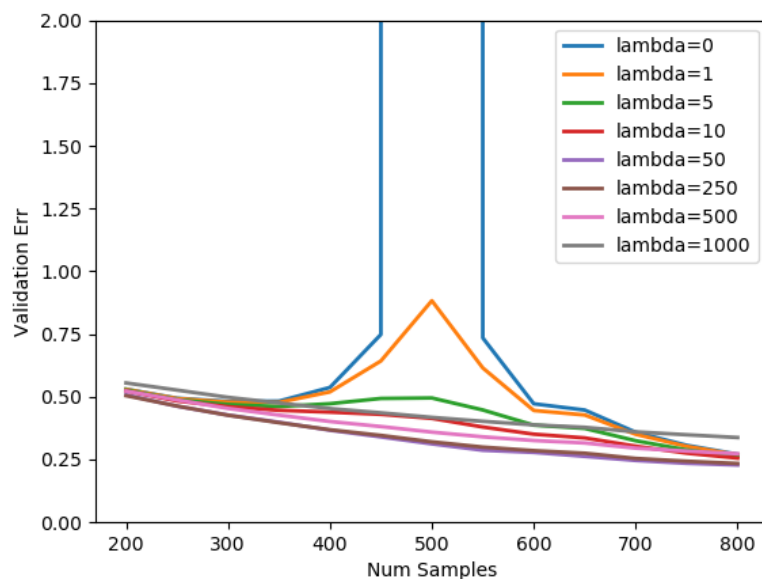


Figure 2: Num of samples vs. validation error for different regularization strengths

The x-axis is the size of the training dataset (from 200 to 800); the y-axis is the MSE on the validation dataset. You should observe that for some small λ 's, the validation error may increase and then decrease as we increase the sample size. However, double descent does not occur for a relatively large λ .

Remark: If you want to learn more about the double descent phenomenon and the effect of regularization, you can start with this paper [Nakkiran, et al. 2020](#).

This handout includes space for every question that requires a written response. Please feel free to use it to handwrite your solutions (legibly, please). If you choose to typeset your solutions, the `README.md` for this assignment includes instructions to regenerate this handout with your typeset L^AT_EX solutions.

1.a

1.b

1.c

4.a