CS-475/675 Machine Learning (Fall 2023): Assignment 5

Due on December 10th, 2023 at 8:00 PM ET

Instructions: Please read these instructions carefully and follow them precisely. Feel free to ask the instructor if anything is unclear!

1. Please submit your solutions electronically via Gradescope.
2. Please submit a PDF file for the written component of your solution including derivations, explanations, etc. You can create this PDF in any way you want: typeset the solution in LATEX (recommended), type it in Word or a similar program and convert/export to PDF. We recommend that you restrict your solutions to the space allocated for each problem; you may need to adjust the white space by tweaking the argument to `\vspace{xpt}` command.
3. Submit the empirical component of the solution (Python code and the documentation of the experiments you are asked to run, including figures) in a Jupyter notebook file.
4. In addition, you will need to submit your predictions on digit recognition and sentiment classification tasks to `Kaggle`, as described below, according to the competition rules. Please report kaggle scores in the pdf submission or in the Jupyter notebook.
5. You have a total of 96 late hours for the entire semester that you may use as you deem fit. After you have used up your quota, there will be a penalty of 50% of your grade on a late homework if submitted within 48 hours of the deadline and a penalty of 100% of your grade on the homework for submissions that are later than 48 hours past the deadline.
6. **What is the required level of detail?** When asked to derive something, please clearly state the assumptions, if any, and strive for balance: justify any non-obvious steps, but try to avoid superfluous explanations. When asked to plot something, please include the figure as well as the code used to plot it. If multiple entities appear on a plot, make sure that they are clearly distinguishable (by color or style of lines and markers). When asked to provide a brief explanation or description, try to make your answers concise, but do not omit anything you believe is important. When submitting code, please make sure it's reasonably documented, and describe succinctly in the written component of the solution what is done in each `py`-file.

Name: _____

I. Generative Models

Here we will consider the Gaussian generative model for $\mathbf{x} \in \mathbb{R}^d$ which assumes equal, isotropic covariance matrices for each class:

$$\mathbf{\Sigma}_c \;=\; \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & \sigma_d^2 \end{bmatrix}. \tag{1}$$

The classes of course have separate means. That is, the conditional density of the j-th coordinate of $\mathbf{x}$ given class c is a Gaussian $\mathcal{N}(\mu_{c,j}, \sigma_j)$, with these densities independent (given class) for different values of j.

For simplicity, let's consider a two-class problem, with $y \in \{0, 1\}$. As we discussed in class, when training the generative model, we simply fit $p(\mathbf{x} \,|\, y)$ and $p(y)$ to the training data, and use the resulting discriminant analysis to produce a decision rule which predicts

$$\widehat{y}(\mathbf{x}) \;=\; \operatorname*{argmax}_c \left\{ p(\mathbf{x} \,|\, y = c)\, p(y = c) \right\}. \tag{2}$$

However, this model does also produce an (implicit) estimate for the posterior $p(y = c \,|\, \mathbf{x})$.

Problem 1 [15 points] Show that the posterior $p(y = c \,|\, \mathbf{x})$ resulting from the generative model above has the same form as the posterior in logistic regression model,

$$p(y = c \,|\, \mathbf{x}) \;=\; \frac{1}{1 + \exp\left(w_0 + \mathbf{w} \cdot \mathbf{x}\right)}, \tag{3}$$

for appropriate values of $w_0 \in \mathbb{R}, \mathbf{w} \in \mathbb{R}^d$. (*Advice: Start with Bayes rule, and use the simplifying assumptions in* (1) *to derive the posterior.)*

Problem 2 [10 points] The previous problem established that the two models – logistic regression and the linear discriminant analysis based on the isotropic Gaussian model (1) – have the same form of the posterior $p(y \mid \mathbf{x})$. Will the two models produce the same classifier when applied to a given training set? Why or why not?

II. Regularization due to Dropout

Dropout is a popular algorithmic heuristic for training deep neural networks. In this question, we seek to understand Dropout by describing the explicit form of the regularizer induced by Dropout.

We revisit the well-studied problem of least-squares linear regression problem. We are given a dataset, $S = \{(\mathrm{x}_i, y_i)\}_{i=1}^n$, of n labeled examples sampled i.i.d. from some underlying (unknown) distribution $\mathcal{D}$ over $\mathbb{R}^d \times \mathbb{R}$. We assume that the data has been normalized so that each feature is zero mean and has unit variance, i.e.,

$$\widehat{\mu}_j := \frac{1}{n}\sum_{i=1}^{n} x_{ij} = 0, \text{ for } j = 1, \ldots, d,$$

and

$$\widehat{\sigma}_j^2 := \frac{1}{n}\sum_{i=1}^{n} (x_{ij} - \widehat{\mu}_j)^2 = 1, \text{ for } j = 1, \ldots, d.$$

We seek $\mathrm{w} \in \mathbb{R}^d$ that minimizes the following empirical risk:

$$\widehat{L}_{\mathrm{ERM}}(\mathrm{w}) := \frac{1}{n}\sum_{i=1}^{n} \left(y_i - \mathrm{w}^\top \mathrm{x}_i\right)^2. \tag{4}$$

We represent linear predictors as single-layer linear networks with d input nodes, a single output linear node with weights w_i on the edge connecting the i^{th} input node to the output node.

We train the network using SGD with Dropout on the input nodes, i.e., at each iteration of SGD, each input node, independently, is left `ON` (i.e., it contributes to the forward pass) with probability

p and is turned `OFF` with probability $1-p$; furthermore, to ensure that the output of the function is at the same level we scale the input of each node by $1/p$. Formally, consider i.i.d. Bernoulli random variable ϵ_j, $j = 1, \ldots, d$, such that

$$\epsilon_j = \begin{cases} \frac{1}{p}, & \text{with probability } p \\ 0, & \text{with probability } 1-p \end{cases}.$$

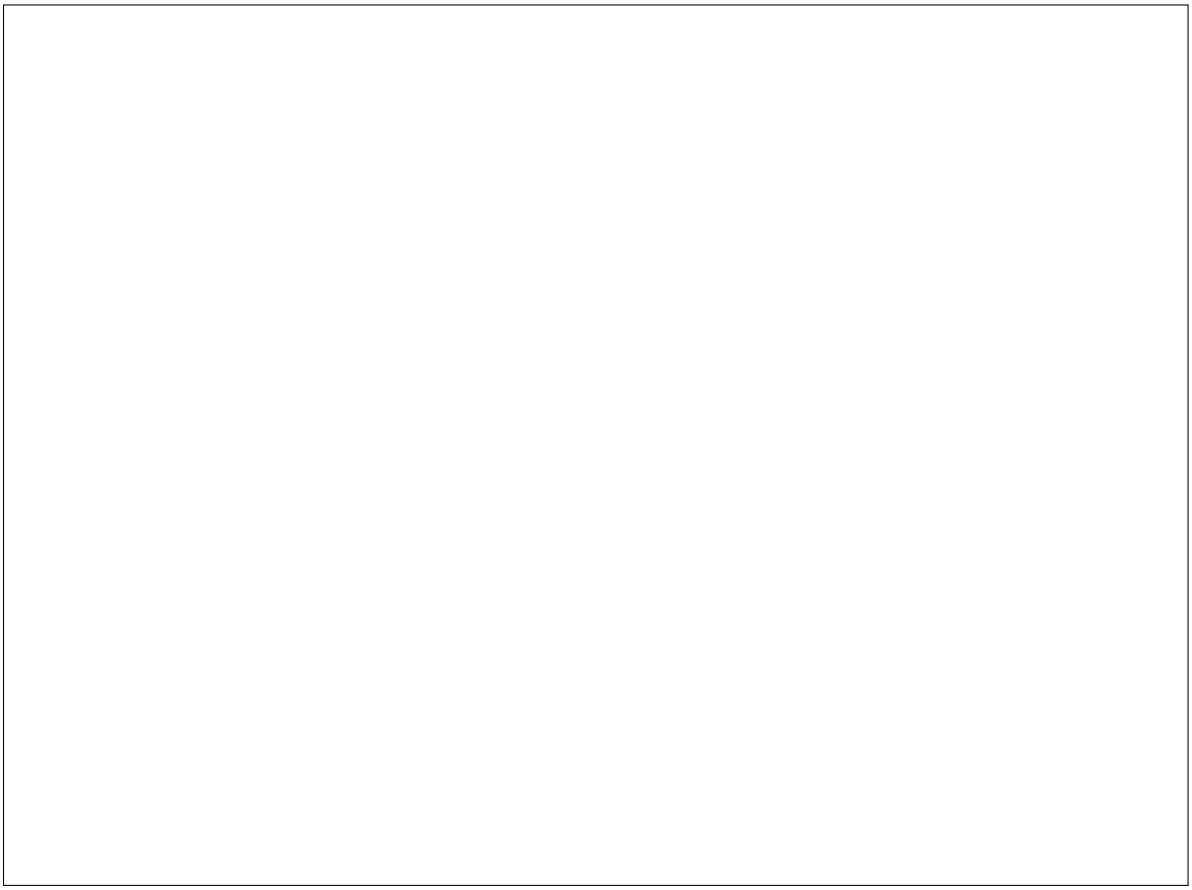
We argue that SGD with Dropout on the empirical objective above amounts to minimizing the following objective:

$$\widehat{L}_{\text{Dropout}}(\mathrm{w}) := \mathbb{E}_{\epsilon_1,\ldots,\epsilon_d}\left[\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \sum_{j=1}^{d}\epsilon_j w_j x_{ij}\right)^2\right]. \tag{5}$$

Problem 3 [15 **points**] Show that doing least squares regression using Dropout, as described above, amounts to doing ridge regression. Formally, show that

$$\widehat{L}_{\text{Dropout}}(\mathrm{w}) = \widehat{L}_{\text{ERM}}(\mathrm{w}) + \lambda\|\mathrm{w}\|^2.$$

What is the value of λ? How does the regularization parameter change with the Dropout rate, p. How does the regularizer change if we do not assume that the data is normalized to have zero mean and unit variance?



III. Multilayer neural networks

In this section we will return to the problem of handwritten digit recognition and attack it with a two-layer neural network. The general architecture of the network is as follows: let $\mathbf{x}$ be the input (pixels of the $d \times d$ digit image). Then, the first layer (with k hidden units) computes

$$\mathbf{f}_1(\mathbf{x}) \;=\; h\left(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1\right), \tag{6}$$

where $\mathbf{W}_1$ is a $k \times d^2$ matrix of weights, $\mathbf{b}_1$ is the k-dimensional vector of bias terms, and h is a nonlinearity (activation function for the hidden units); the syntax in (6) means that h is computed on each element of its k-dimensional argument vector (the output of $\mathbf{W}_1\mathbf{x}+\mathbf{b}_1$), yielding k-dimensional activation vector, called in neural network literature the feature map of the layer.

The second layer computes the network activation:

$$\mathbf{f}_2(\mathbf{x}) \;=\; \mathbf{W}_2\mathbf{f}_1(\mathbf{x}) + \mathbf{b}_2, \tag{7}$$

where $\mathbf{W}_2$ is a $10 \times k$ matrix and $\mathbf{b}_2$ a 10-dimensional vector. The values of the 10-dimensional vector $\mathbf{f}_2$ are interpreted as the scores (unnormalized log-probabilities) for the 10 classes. So, the posterior for class c computed by the network is

$$p(c|\mathbf{x}) \;=\; \frac{\exp(f_{2,c}(\mathbf{x}))}{\sum_j \exp(f_{2,j}(\mathbf{x}))}, \tag{8}$$

and the loss used to train the network is

$$-\frac{1}{n}\sum_{i=1}^{n} \log p(y_i|\mathbf{x}_i) \tag{9}$$

where the summation is over the indices of training examples. You can of course add regularization (e.g., squared norm penalty over elements of $\mathbf{W}_1$, $\mathbf{W}_2$) to the loss.

Again, we will revisit and improve our results on a familiar data set, this time MNIST.

Problem 4 [60 points] Implement a two-layer neural network for MNIST. We have set up a Kaggle competition for the clean version:

- https://www.kaggle.com/t/3be87d0815194c0998adfde42f0c10a0

We have provided skeleton code `PS5_neuralnet.ipynb` that features a complete forward and backward pass. However, you will have to work out what the gradients are.

We provide several different update algorithms in `utils.py`: SGD, SGD with momentum and SGD with Nestorov momentum. Try these methods, and report the differences in their performances.

You should also decide what the activation function h is. The options are ReLU, Logistic and Tanh. For all activations you try, you need to implement their forward and backward functions.

This task will require you to understand the code that we have provided, so read the inline documentation carefully. We encourage you to re-use parts of your code and hyperparameters from

Problem Set 2, e.g. `softmaxloss`, stopping criteria, stepsize reduction, batch_size, etc.

If you used loops in your solution in Problem Set 2, you will quickly find that it is not fast enough. Learn to write things in terms of matrix multiplications.

Optional:

More layers You can try more than two-layers, and it should be trivial given the code we provide.

Dropout Dropout is a popular technique in neural network. Instead of using (7), the feed-forward operation during training becomes:

$$r_j \sim Bernoulli(p) \tag{10}$$

$$\mathbf{f}_2(\mathbf{x}) = \mathbf{W}_2(\frac{1}{p}\mathbf{r} * \mathbf{f}_1(\mathbf{x})) + \mathbf{b}_2, \tag{11}$$

$\mathbf{r}$ is a vector of independent Bernoulli random variables each of which has probability p of being 1. This vector is multiplied element-wisely to the output of previous layer. Some of the outputs of previous layer are dropped out, and the remained are scaled by $\frac{1}{p}$ to make sure the"scale" of the input to remain the same. During evaluation, we do the same thing as (7).