Homework 2

Deadline: Thursday, Feb. 18, at 11:59pm.

Submission: You need to submit three files through MarkUs[1]:

- Your answers to Questions 1, 2, and 3, as a PDF file titled `hw2_writeup.pdf`. You can produce the file however you like (e.g. LaTeX, Microsoft Word, scanner), as long as it is readable.
- Your completed code for Question 2, as the Python file `q2.py`.

If you wish to write the code in a Jupyter notebook instead, then please submit a PDF printout of the notebook, rather than the notebook itself.

Late Submission: 10% of the marks will be deducted for each day late, up to a maximum of 3 days. After that, no submissions will be accepted.

Computing: To install Python and required libraries, see the instructions on the course web page.

1. **[2pts] Robust Regression.** One problem with linear regression using squared error loss is that it can be sensitive to outliers. Another loss function we could use is the *Huber loss*, parameterized by a hyperparameter δ:

$$L_\delta(y,t) = H_\delta(y-t)$$
$$H_\delta(a) = \begin{cases} \frac{1}{2}a^2 & \text{if } |a| \leq \delta \\ \delta(|a| - \frac{1}{2}\delta) & \text{if } |a| > \delta \end{cases}$$

   (a) **[1pt]** Sketch the Huber loss $L_\delta(y,t)$ and squared error loss $L_{\mathrm{SE}}(y,t) = \frac{1}{2}(y-t)^2$ for $t = 0$, either by hand or using a plotting library. Based on your sketch, why would you expect the Huber loss to be more robust to outliers?

   (b) **[1pt]** Just as with linear regression, assume a linear model:

$$y = \mathbf{w}^\top \mathbf{x} + b.$$

   Give formulas for the partial derivatives $\partial L_\delta / \partial \mathbf{w}$ and $\partial L_\delta / \partial b$. (We recommend you find a formula for the derivative $H'_\delta(a)$, and then give your answers in terms of $H'_\delta(y-t)$.)

   (c) **[Optional]** Write Python code to perform (full batch mode) gradient descent on this model. Assume the training dataset is given as a design matrix `X` and target vector `y`. Initialize $\mathbf{w}$ and b to all zeros. Your code should be vectorized, i.e. you should not have a `for` loop over training examples or input dimensions. You may find the function `np.where` helpful.

[1] `https://markus.teach.cs.toronto.edu/csc2515-2021-01`

2. **[5pts] Locally Weighted Regression.**

   (a) **[2pts]** Given $\{(\mathbf{x}^{(1)}, y^{(1)}), .., (\mathbf{x}^{(N)}, y^{(N)})\}$ and positive weights $a^{(1)}, ..., a^{(N)}$ show that the solution to the *weighted* least squares problem

$$\mathbf{w}^* = \arg\min \frac{1}{2}\sum_{i=1}^{N} a^{(i)}(y^{(i)} - \mathbf{w}^T\mathbf{x}^{(i)})^2 + \frac{\lambda}{2}||\mathbf{w}||^2 \tag{1}$$

   is given by the formula

$$\mathbf{w}^* = \left(\mathbf{X}^T\mathbf{A}\mathbf{X} + \lambda\mathbf{I}\right)^{-1}\mathbf{X}^T\mathbf{A}\mathbf{y} \tag{2}$$

   where $\mathbf{X}$ is the design matrix (defined in class) and $\mathbf{A}$ is a diagonal matrix where $\mathbf{A}_{ii} = a^{(i)}$

   It may help you to review Section 3.1 of the csc321 notes[2].

   (b) **[2pts]** Locally reweighted least squares combines ideas from k-NN and linear regression. For each new test example $\mathbf{x}$ we compute distance-based weights for each training example $a^{(i)} = \frac{\exp(-||\mathbf{x}-\mathbf{x}^{(i)}||^2/2\tau^2)}{\sum_j \exp(-||\mathbf{x}-\mathbf{x}^{(j)}||^2/2\tau^2)}$, computes $\mathbf{w}^* = \arg\min \frac{1}{2}\sum_{i=1}^{N} a^{(i)}(y^{(i)} - \mathbf{w}^T\mathbf{x}^{(i)})^2 + \frac{\lambda}{2}||\mathbf{w}||^2$ and predicts $\hat{y} = \mathbf{x}^T\mathbf{w}^*$. Complete the implementation of locally reweighted least squares by providing the missing parts for `q2.py`.

   Report the training and test loss for $\tau = 10$.

   Important things to notice while implementing: First, do not invert any matrix, use a linear solver (numpy.linalg.solve is one example). Second, notice that $\frac{\exp(A_i)}{\sum_j \exp(A_j)} = \frac{\exp(A_i - B)}{\sum_j \exp(A_j - B)}$ but if we use $B = \max_j A_j$ it is much more numerically stable as $\frac{\exp(A_i)}{\sum_j \exp(A_j)}$ overflows/underflows easily. *This is handled automatically in the scipy package with the* `scipy.misc.logsumexp` *function*[3].

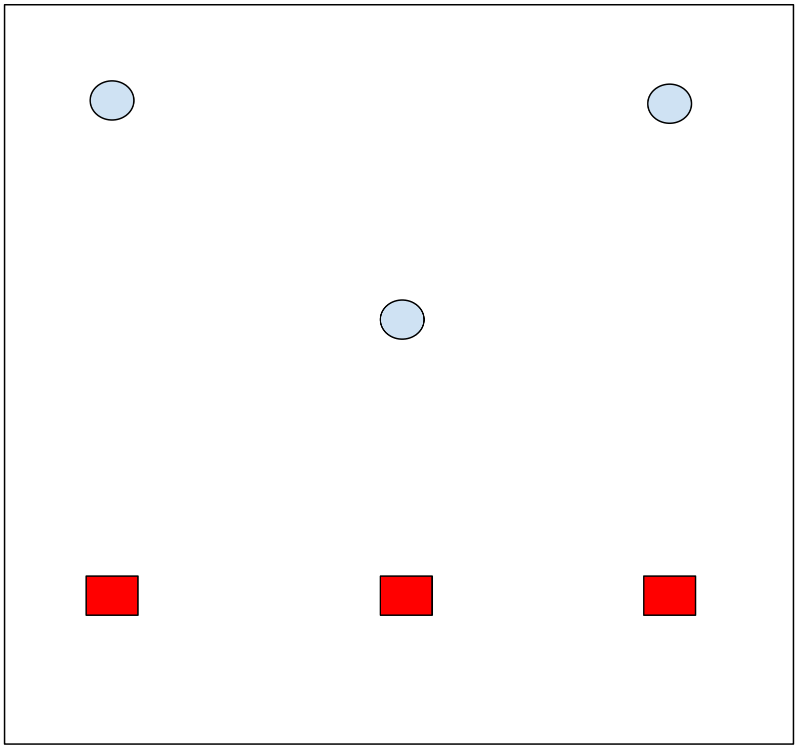
   (c) **[1pt]** Based on our understanding of overfitting and underfitting, how would you expect the training error and the validation error to vary as a function of τ? (I.e., what do you expect the curves to look like?)

   Now run the experiment. Randomly hold out 30% of the dataset as a validation set. Compute the average loss for different values of τ in the range [10,1000] on both the training set and the validation set. Plot the training and validation losses as a function of τ (using a log scale for τ). Was your guess correct?

3. **[3pts] Decision Boundaries**

   (a) **[1pt]** Draw a decision boundary for logistic regression and draw a decision boundary for 1-nearest-neighbors (1-NN) on the following 2-D binary classification dataset:

[2] `http://www.cs.toronto.edu/~rgrosse/courses/csc321_2018/readings/L02%20Linear%20Regression.pdf`
[3] `https://docs.scipy.org/doc/scipy-0.14.0/reference/generated/scipy.misc.logsumexp.html`



(b) **[1pt]** When we train models, we often want them to generalize to unseen data. We can use cross-validation to assess how our model might generalize. We discussed leave-p-out cross-validation in Tutorial 3 here, which is a cross-validation procedure that uses p observations as the validation set and the remaining observations as the training set.

Draw a 2-d binary classification dataset with at least 8 observations, where leave-1-out validation will have lower error with 1-NN than logistic regression for any choice of observation to leave out. A drawing by hand is sufficient.

(c) **[1pt]** Draw a 2-d binary classification dataset with at least 8 observations where leave-1-out validation will have lower error with logistic regression than 1-NN for any choice of observation to leave out. A drawing by hand is sufficient.