CSE 512: Homework 1 — Due Monday, Sept. 14

1. *Bayes' rule.*

   (a) I look out of my window and see 10 people in the street. 8 have umbrellas, 2 do not. None of these people know each other; they make decisions independently.

   In general, the area is very windy, so people do not always use an umbrella when it rains. But each day has a 50% chance of getting rain. In fact, even when it rains, people only use an umbrella 75% of the time. When it's not raining, people sometimes use an umbrella as a parasol, 5% of the time.

   i. What is the probability that anyone would have an umbrella, given that it's raining?

   ii. What is the probability that it is raining today, given my observation?

   (b) According to the CDC[1], the current percentage of positive COVID tests in the US is 9.1%. Let's use this as a marker for $\mathbf{Pr}(\text{COVID}|\text{took a test})$.

   There are many available tests, each with different performance metrics. For example, if I take a combined IgG/IgM seriology test, then for one company [2], the PPV (the chance of a positive test when COVID is present) is estimated at 82.5%, and the NPV (the chance of a negative test when COVID is not present) is estimated at 99.9%.

   i. If a person goes in for a test and gets a positive result, what are the chances that that person has COVID?

   ii. If a person goes in for a test and gets a negative result, what are the chances that that person does not have COVID?

2. *Logistic regression for Binary MNIST*

   (a) For a twice-differentiable function $f : \mathbb{R}^d \to \mathbb{R}$, the *gradient* and *Hessian* are defined as

$$\nabla f(\theta) = \begin{bmatrix} \frac{\partial f}{\partial \theta_1} \\ \frac{\partial f}{\partial \theta_2} \\ \vdots \\ \frac{\partial f}{\partial \theta_d} \end{bmatrix} \in \mathbb{R}^d, \qquad \nabla^2 f(\theta) = \begin{bmatrix} \frac{\partial^2 f}{\partial \theta_1^2} & \frac{\partial^2 f}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 f}{\partial \theta_1 \partial \theta_d} \\ \frac{\partial^2 f}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 f}{\partial \theta_2^2} & \cdots & \frac{\partial^2 f}{\partial \theta_2 \partial \theta_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial \theta_d \partial \theta_1} & \frac{\partial^2 f}{\partial \theta_d \partial \theta_2} & \cdots & \frac{\partial^2 f}{\partial \theta_d^2} \end{bmatrix} \in \mathbb{R}^{d \times d}.$$

   For example, for the function $f(\theta) = \theta_1^2 + 2\theta_1\theta_2 + \theta_3^3$, the gradient and Hessian are

$$\nabla f(\theta) = \begin{bmatrix} 2\theta_1 + 2\theta_2 \\ 2\theta_1 \\ 3\theta_3^2 \end{bmatrix}, \qquad \nabla^2 f(\theta) = \begin{bmatrix} 2 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 6\theta_3 \end{bmatrix}.$$

   What is the gradient and Hessian of the logistic loss function

$$\mathcal{L}(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \log(y_i \sigma(x_i^T \theta)), \quad \sigma(s) = \frac{1}{1 + e^{-s}}$$

   where $y_i \in \{-1, 1\}$?

   (b) **Coding.**

   - Download mnist.mat [**?**]. We will use logistic regression to diffrentiate 4's from 9's, a notoriously tricky problem. If you are using python, you can use `scipy.io.loadmat` to read the matrix. If you are using MATLAB, just `load mnist.mat` should suffice.

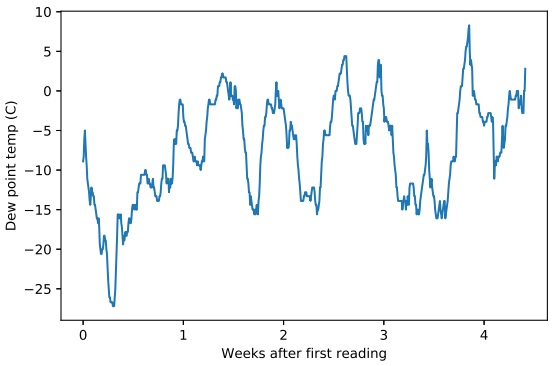
[1] `https://www.cdc.gov/coronavirus/2019-ncov/covid-data/covidview/index.html`

[2] `https://www.fda.gov/medical-devices/coronavirus-disease-2019-covid-19-emergency-use-authorizations-medical-devices/eua-authorized-serology-test-performance`

- The matrices X and y should contain the vectorized images and corresponding labels. To take a look at how the data is stored, run the following code:
  Python
  ```
  data = sio.loadmat('mnist.mat')
  for k in xrange(9):
      plt.subplot(3,3,k+1)
      plt.imshow(np.reshape(data['trainX'][k,:],(28,28)))
      plt.title(data['trainY'][0,k])
  plt.tight_layout()
  ```
  Matlab
  ```
  load mnist.mat
  for k = 1:9:
      subplot(3,3,k)
      imshow(reshape(trainX(k,:),28,28))
      title(trainY(k))
  end
  ```
- Select only the data rows corresponding to the labels 4 and 9, and set the remaining labels to be binary.
  Python
  ```
  idx = np.logical_or(np.equal(y,4) ,  np.equal(y,9))
  X = X[idx,:]
  y = y[idx]
  y[np.equal(y,4)] = -1
  y[np.equal(y,9)] = 1
  ```
  Matlab
  ```
  idx = (y == 4) || (y == 9)
  X = X(idx,:)
  y = y(idx)
  y(y==4) = -1
  y(y==9)= 1
  ```
  You should be left with 11791 train images and 1991 test images. Make sure they are stored separately, e.g. X = train images, X_t = test images.
- Normalize the data matrix so that all the values are between 0 and 1, and that the mean value per pixel is 0 (e.g. if I sum up all the images, I get a 0 image). [3]
- Use gradient descent to minimize the logistic loss for this classification problem. Use a step size of 0.001, and run for 5000 iterations. Plot the train / test loss, and train/test misclassification rate, and also report these final values.
- Comment a bit on what you see.

3. Using the properties of norms, verify that the following are norms, or prove that they are not norms
   (a) *Direct sum.* $f : \mathbb{R}^d \to \mathbb{R}$, $f(x) = \sum_i x_i$
   (b) *Sum of square roots.* $f : \mathbb{R}^d \to \mathbb{R}$, $f(x) = \sum_{i=1}^d \sqrt{x^p}$ for $p > 1$
   (c) *Weighted 2-norm.* $f : \mathbb{R}^d \to \mathbb{R}$, $f(x) = \sqrt{\sum_{i=1}^d \frac{|x_i|^2}{i}}$
4. *Polyfit via linear regression.*
   (a) Download weatherDewTmp.mat. Plot the data (`plot(weeks,dew)`). It should look like the following

[3] There are other ways to normalize, but this is a reasonable one I have found works in practice, and in the interest of "normalizing" the assignment, it's what we'll go with.



(b) We want to form a polynomial regression of this data. That is, given w = weeks and d = dew readings, we want to find $\theta_1, ..., \theta_p$ as the solution to

$$\underset{\theta \in \mathbb{R}^p}{\text{minimize}} \quad \frac{1}{2} \sum_{i=1}^{m} (\theta_1 + \theta_2 w_i + \theta_3 w_i^2 + \cdots + \theta_p w_i^{p-1} - d_i)^2. \tag{1}$$

Find X and y such that (**??**) is equivalent to the least squares problem

$$\underset{\theta \in \mathbb{R}^p}{\text{minimize}} \quad \frac{1}{2} \|X\theta - y\|_2^2. \tag{2}$$

(c) What are the normal equations for problem (**??**)? In particular, if θ^* is the minimizer of (**??**), then θ^* solves a linear system $A\theta^* = b$. What are A and b?

(d) *Ridge regression* Oftentimes, it is helpful to add a *regularization term* to (**??**), to improve stability. This also has an interpretation as Bayesian linear regression with a Gaussian 0-mean prior. In other words, we solve

$$\underset{\theta \in \mathbb{R}^p}{\text{minimize}} \quad \frac{1}{2} \|X\theta - y\|_2^2 + \frac{\alpha}{2} \|\theta\|_2^2. \tag{3}$$

for some $\alpha > 0$. The θ^* that minimizes (**??**) is the solution to a different linear system $A_{\text{reg}}\theta^* = b_{\text{reg}}$. What are A_{reg} and b_{reg}?

(e) If A is a positive semidefinite matrix with condition number 5 and largest eigenvalue 1, what is the condition number of $A + \alpha I$ for some $\alpha > 0$?

(f) In MATLAB or Python, write a function that takes as argument p and returns X and y so that (**??**) is equivalent to (**??**). Report the *condition numbers* for A and A_{reg} by filling out this table:

p	A ($\alpha = 0$)	A_{reg}, $\alpha = 0.1 \cdot m$	A_{reg}, $\alpha = m$	A_{reg}, $\alpha = 10 \cdot m$	A_{reg}, $\alpha = 100 \cdot m$
1					
2					
5					
10					

(g) Compute a polynomial fit by solving (**??**) for polynomials of order $1, 2, 10, 100, 150$, and 200. Plot all the fits on separate plots (use `subplot`). Comment on your observations.

(h) Now compute a *regularized* polynomial fit by solving (**??**) for polynomials of order $1, 2, 10, 100, 150$, and 200, for $\alpha = 0.0001$. Plot all the fits on separate plots (use `subplot`). Comment on your observations. How does this compare to the unregularized polynomial fit?

(i) Picking your favorite set of hyperparameters (p, α), forecast the next week's dew point temperature. Plot the forecasted data over the current observations. Do you believe your forecast? Why?

Challenge!

In this problem we will investigate a *sparse* regularizer, in which we replace the 2-norm regularizer with a 1-norm regularizer. In other words, given $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$, and $\lambda \in \mathbb{R}$, we will solve

$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \quad \tfrac{1}{2m}\|Ax-b\|_2^2 + \lambda\|x\|_1 \tag{4}$$

1. This objective function is composed of a smooth (everywhere differentiable) and nonsmooth (not everywhere differentiable) term. Show that $\|x\|_1$ is nonsmooth by describing all the points x where $g(x) = \|x\|_1$ is not differentiable.

2. Because the objective has a nonsmooth point, gradient descent will not converge to the global minimum. To see that this is true, consider the case of $m = n = 1$, with $A = b = \lambda = 1$. In other words, we consider

$$\underset{x}{\text{minimize}} \quad \frac{1}{2}(x-1)^2 + |x|. \tag{5}$$

   Start with $x^{(0)} = 2$, and with a step size $t = 1/2$, write out the iterates $x^{(k)}$ for $k = 1, 2, 3$. What is the limit point $\lim_{k\to+\infty} x^{(k)}$? Is this limit point the problem's global minima?

3. We therefore will introduce a new method called the *proximal gradient descent* method. This method is similar to gradient descent, except we break away the nonsmooth term and deal with it separately. Explicitly, for solving

$$\underset{x}{\text{minimize}} \quad f(x) + g(x)$$

   where $f(x)$ is smooth and $g(x)$ is nonsmooth, the proximal gradient descent method picks a random point $x^{(0)}$ and iterates

$$x^{(k+1)} = \mathbf{Pro}x_{tg}(x^{(k)} - t\nabla f(x^{(t)}))$$

   where the mapping $\mathbf{Pro}x_{tg}$ is the *proximal operator*

$$\mathbf{Pro}x_{tg}(z) = \underset{x}{\text{argmin}}\ g(x) + \frac{1}{2t}\|x-z\|_2^2.$$

   We can interpret this as finding the variable x that trades off minimizing the nonsmooth term $g(x)$ and a proximity term (e.g. doesn't want to deviate too far from z).

   Show that the proximal operator of the 1-norm can be computed in closed form, as

$$\mathbf{Pro}x_{tg}(z) = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \qquad x_k = \begin{cases} (|z_k| - t)\mathbf{sign}(z_k) & \text{if } |z_k| > t \\ 0 & \text{else.} \end{cases}$$

   This operator is called the "shrinkage operator".

4. Again consider the scalar problem (**??**). Start with $x^{(0)} = 2$, and with a step size $t = 1/2$, write out the iterates $x^{(k)}$ for $k = 1, 2, 3$, but following the proximal gradient scheme. What is the limit point $\lim_{k\to+\infty} x^{(k)}$? Is this limit point the problem's global minima?

5. **Coding.** In MATLAB or Python, generate a sample problem with `A = randn(m,n)` and `b = randn(m,1)`. Pick $m = 100$, $n = 1000$. Solve (**??**). For $\lambda = 0, 0.001, 0.1$, show histograms of the elements of x^*. Comment on the sparsifying property of the 1-norm.

   Comparison with 2-norm regularization. We can also consider a 2-norm regularized version as well, where we solve

$$\underset{x}{\text{minimize}} \quad \frac{1}{2m}\|Ax-b\|_2^2 + \lambda\|x\|_2 \tag{6}$$

6. Show that this regularization term $\|x\|_2$ is also nonsmooth.

7. Derive the proximal operator $\mathbf{Pro}x_{tg}$ for $g(x) = \|x\|_2$.

8. Use proximal gradient descent to solve (**??**), using the same choices of A and b as in the previous section. Histogram the final solutions x^* for $\lambda = 0, 1, 2, 5, 10$. Comment on the sparsifying properties of the 2-norm vs the 1-norm.

References

[1] A. Beck, *Introduction to nonlinear optimization: theory, algorithms, and applications with MATLAB*, vol. 19, Siam, 2014.

[2] Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, "Gradient-based learning applied to document recognition." *Proceedings of the IEEE*, vol. 86, no. 11 (1998): 2278-2324.