Self grades are due at 11 PM on March 23, 2023.

1. **Convergence of Gradient Descent for Ridge Regression**

   Let $A \in \mathbb{R}^{m \times n}, \vec{y} \in \mathbb{R}^m$, and $\lambda > 0$. Consider a slight variation of the ridge regression problem where the least squares loss is normalized by the number of data points:

   $$\min_{\vec{x} \in \mathbb{R}^n} f_\lambda(\vec{x}) \qquad \text{where} \qquad f_\lambda(\vec{x}) \doteq \frac{1}{2} \left\{ \frac{1}{m} \|A\vec{x} - \vec{y}\|_2^2 + \lambda \|\vec{x}\|_2^2 \right\}. \tag{1}$$

   In this problem, we will examine the behavior of gradient descent (GD) on this problem, and in particular the interplay between the learning rate $\eta > 0$ and regularization parameter $\lambda > 0$ in determining convergence.

   (a) Show that the unique solution to the problem in Equation (1) is

   $$\vec{x}_\lambda^\star = \left(A^\top A + \lambda m I\right)^{-1} A^\top \vec{y}. \tag{2}$$

   Solution: The function $\lambda \|\vec{x}\|_2^2$ in Equation (1) is strictly convex, so f_λ is strictly convex. Thus the problem in Equation (1) has strictly convex objective and convex feasible set $\mathbb{R}^n$, so it has at most one solution. And we can find a solution by setting the gradient to $\vec{0}$:

   $$\nabla f_\lambda(\vec{x}_\lambda^\star) = \frac{1}{m} A^\top (A\vec{x}_\lambda^\star - \vec{y}) + \lambda \vec{x}_\lambda^\star \tag{3}$$

   $$= \left(\frac{A^\top A}{m} + \lambda I\right) \vec{x}_\lambda^\star - \frac{1}{m} A^\top \vec{y} \tag{4}$$

   $$\implies \left(\frac{A^\top A}{m} + \lambda I\right) \vec{x}_\lambda^\star = \frac{1}{m} A^\top \vec{y} \tag{5}$$

   $$\implies \left(A^\top A + \lambda m I\right) \vec{x}_\lambda^\star = A^\top \vec{y} \tag{6}$$

   $$\implies \vec{x}_\lambda^\star = \left(A^\top A + \lambda m I\right)^{-1} A^\top \vec{y}. \tag{7}$$

   (b) Show that the GD update

   $$\vec{x}_{t+1} = \vec{x}_t - \eta \left(\frac{1}{m} A^\top (A\vec{x}_t - \vec{y}) + \lambda \vec{x}_t\right) \tag{8}$$

   can be rearranged into the form

   $$\vec{x}_{t+1} - \vec{x}_\lambda^\star = \left(I - \eta \left(\frac{A^\top A}{m} + \lambda I\right)\right) (\vec{x}_t - \vec{x}_\lambda^\star). \tag{9}$$

   Use this to show that

   $$\vec{x}_t - \vec{x}_\lambda^\star = \left(I - \eta \left(\frac{A^\top A}{m} + \lambda I\right)\right)^t (\vec{x}_0 - \vec{x}_\lambda^\star). \tag{10}$$

   for every positive integer t.

   Solution: We have

   $$\vec{x}_{t+1} = \vec{x}_t - \eta \left(\frac{1}{m} A^\top (A\vec{x}_t - \vec{y}) + \lambda \vec{x}_t\right) \tag{11}$$

$$= \vec{x}_t - \eta \cdot \frac{A^\top A}{m} \vec{x}_t + \eta \cdot \frac{1}{m} A^\top \vec{y} + \eta \lambda \vec{x}_t \tag{12}$$

$$= \left(I - \eta \left(\frac{A^\top A}{m} + \lambda I \right) \right) \vec{x}_t + \eta \cdot \frac{1}{m} A^\top \vec{y} \tag{13}$$

$$\implies \vec{x}_{t+1} - \vec{x}_\lambda^\star = \left(I - \eta \left(\frac{A^\top A}{m} + \lambda I \right) \right) \vec{x}_t + \eta \cdot \left(\frac{A^\top A}{m} + \lambda I \right) \vec{x}_\lambda^\star - \vec{x}_\lambda^\star \tag{14}$$

$$= \left(I - \eta \left(\frac{A^\top A}{m} + \lambda I \right) \right) (\vec{x}_t - \vec{x}_\lambda^\star). \tag{15}$$

Iterating this relation obtains the second equality.

(c) We now discuss the insight that the SVD can give us regarding the convergence of GD. Let $A = U\Sigma V^\top$ be a full SVD of A. Let $\vec{z}_t = V^\top \vec{x}_t$ and $\vec{z}_\lambda^\star = V^\top \vec{x}_\lambda^\star$. Show that

$$\vec{z}_t - \vec{z}_\lambda^\star = \left(I - \eta \left(\frac{\Sigma^\top \Sigma}{m} + \lambda I \right) \right)^t (\vec{z}_0 - \vec{z}_\lambda^\star), \tag{16}$$

and, moreover, show that for each $i \in \{1, \ldots, n\}$, we have

$$(\vec{z}_t)_i - (\vec{z}_\lambda^\star)_i = \left(1 - \eta \left(\frac{\sigma_i\{A\}^2}{m} + \lambda \right) \right)^t ((\vec{z}_0)_i - (\vec{z}_\lambda^\star)_i) \tag{17}$$

where $\sigma_i\{A\}$ is the ith largest singular value of A. This shows that the *rate of convergence* of $\vec{z}_t$ to $\vec{z}_\lambda^\star$ along the ith component is influenced by the interaction between $\sigma_i\{A\}$, λ, and η, but critically no other singular values. Thus, one considers the V basis to be the "natural" basis for thinking about GD for ridge regression.

Solution: If $A = U\Sigma V^\top$ then

$$A^\top A = V\Sigma^\top U^\top U\Sigma V^\top = V\Sigma^\top \Sigma V^\top. \tag{18}$$

Thus we have

$$\vec{x}_t - \vec{x}_\lambda^\star = \left(I - \eta \left(\frac{A^\top A}{m} + \lambda I \right) \right)^t (\vec{x}_0 - \vec{x}_\lambda^\star) \tag{19}$$

$$= \left(I - \eta \left(\frac{V\Sigma^\top \Sigma V^\top}{m} + \lambda I \right) \right)^t (\vec{x}_0 - \vec{x}_\lambda^\star) \tag{20}$$

$$= \left(I - \eta \left(V \left(\frac{\Sigma^\top \Sigma}{m} + \lambda I \right) V^\top \right) \right)^t (\vec{x}_0 - \vec{x}_\lambda^\star) \tag{21}$$

$$= \left(I - \eta V \left(\frac{\Sigma^\top \Sigma}{m} + \lambda I \right) V^\top \right)^t (\vec{x}_0 - \vec{x}_\lambda^\star) \tag{22}$$

$$= \left(V \left(I - \eta \left(\frac{\Sigma^\top \Sigma}{m} + \lambda I \right) \right) V^\top \right)^t (\vec{x}_0 - \vec{x}_\lambda^\star) \tag{23}$$

$$= V \left(I - \eta \left(\frac{\Sigma^\top \Sigma}{m} + \lambda I \right) \right)^t V^\top (\vec{x}_0 - \vec{x}_\lambda^\star) \tag{24}$$

$$\implies V^\top (\vec{x}_t - \vec{x}_\lambda^\star) = \left(I - \eta \left(\frac{\Sigma^\top \Sigma}{m} + \lambda I \right) \right)^t V^\top (\vec{x}_0 - \vec{x}_\lambda^\star) \tag{25}$$

$$\implies \vec{z}_t - \vec{z}_\lambda^\star = \left(I - \eta \left(\frac{\Sigma^\top \Sigma}{m} + \lambda I \right) \right)^t (\vec{z}_0 - \vec{z}_\lambda^\star). \tag{26}$$

Now note that the quantity $I - \eta(\frac{\Sigma^\top \Sigma}{m} + \lambda I)$ is a diagonal matrix. Thus we have

$$\vec{z}_t - \vec{z}_\lambda^\star = \left(I - \eta\left(\frac{\Sigma^\top \Sigma}{m} + \lambda I\right)\right)^t (\vec{z}_0 - \vec{z}_\lambda^\star) \tag{27}$$

$$\implies (\vec{z}_t - \vec{z}_\lambda^\star)_i = \left(I - \eta\left(\frac{\Sigma^\top \Sigma}{m} + \lambda I\right)\right)^t_i (\vec{z}_0 - \vec{z}_\lambda^\star)_i \tag{28}$$

$$\implies (\vec{z}_t)_i - (\vec{z}_\lambda^\star)_i = \left(1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right)^t ((\vec{z}_0)_i - (\vec{z}_\lambda^\star)_i) \tag{29}$$

(d) Show that $\lim_{t\to\infty} \vec{z}_t = \vec{z}_\lambda^\star$ for all initializations $\vec{x}_0 = V\vec{z}_0$ if and only if

$$\max_{i\in\{1,\dots,n\}} \left|1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right| < 1. \tag{30}$$

Use this to show that GD converges for all initializations $\vec{x}_0$ if and only if

$$\eta \in \left(0, \frac{2m}{\sigma_{\max}\{A\}^2 + \lambda m}\right) \tag{31}$$

where $\sigma_{\max}\{A\} = \sigma_1\{A\}$ is the largest singular value of A.

Solution: We have

$$\lim_{t\to\infty} \vec{z}_t = \vec{z}_\lambda^\star, \qquad \forall \vec{x}_0 \tag{32}$$

$$\iff \lim_{t\to\infty} (\vec{z}_t)_i = (\vec{z}_\lambda^\star)_i, \qquad \forall i \quad \forall \vec{x}_0 \tag{33}$$

$$\iff \lim_{t\to\infty} \left(1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right)^t = 0, \qquad \forall i \tag{34}$$

$$\iff \left|1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right| < 1, \qquad \forall i \tag{35}$$

$$\iff \max_{i\in\{1,\dots,n\}} \left|1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right| < 1. \tag{36}$$

This proves the first part of the question. The second part of the question follows by noting that

$$\max_{i\in\{1,\dots,n\}} \left|1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right| < 1 \tag{37}$$

$$\iff \max_{i\in\{1,\dots,n\}} \left(1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right) < 1 \tag{38}$$

$$\text{and} \quad \min_{i\in\{1,\dots,n\}} \left(1 - \eta\left(\frac{\sigma_i\{A\}^2}{m} + \lambda\right)\right) > -1 \tag{39}$$

$$\iff 1 - \eta\left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda\right) < 1 \tag{40}$$

$$\text{and} \quad 1 - \eta\left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda\right) > -1. \tag{41}$$

Now the first equation is always satisfied for $\eta > 0$ and $\lambda > 0$ because $\frac{\sigma_{\min}\{A\}^2}{m} + \lambda > 0$ so $1 - \eta(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda) < 1$. The second equation is satisfied when $\eta < \frac{2m}{\sigma_{\max}\{A\}^2 + \lambda m}$. Since $\lim_{t\to\infty} \vec{x}_t = \vec{x}_\lambda^\star$ if and only if $\lim_{t\to\infty} \vec{z}_t = \vec{z}_\lambda^\star$, we have that gradient descent converges for all initializations $\vec{x}_0$ if and only if $0 < \eta < \frac{2m}{\sigma_{\max}\{A\}^2 + \lambda m}$.

(e) **(OPTIONAL)** One way we can derive an "optimal" learning rate $\eta^\star$ is to minimize the largest rate of convergence:

$$\eta^\star \in \underset{\eta \in \mathbb{R}}{\operatorname{argmin}} \; \max_{i \in \{1,\dots,n\}} \left| 1 - \eta \left(\frac{\sigma_i\{A\}^2}{m} + \lambda \right) \right|. \tag{42}$$

One important property of $\eta^\star$ is that it makes the rates of convergence $\left| 1 - \eta \left(\frac{\sigma_i\{A\}^2}{m} + \lambda \right) \right|$ associated with the largest and smallest singular values of A equal. Use this property to show that

$$\eta^\star = \frac{2m}{\sigma_{\max}\{A\}^2 + \sigma_{\min}\{A\}^2 + 2\lambda m} \tag{43}$$

where $\sigma_{\min}\{A\} = \sigma_n\{A\}$ is the nth largest singular value of A.

NOTE: There are several useful notions of optimal learning rate; this is just one of them.

Solution: We have

$$\left| 1 - \eta^\star \left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda \right) \right| = \left| 1 - \eta^\star \left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda \right) \right| \tag{44}$$

$$1 - \eta^\star \left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda \right) = - \left(1 - \eta^\star \left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda \right) \right) \tag{45}$$

$$1 - \eta^\star \left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda \right) = \eta^\star \left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda \right) - 1 \tag{46}$$

$$2 = \eta^\star \left(\frac{\sigma_{\max}\{A\}^2 + \sigma_{\min}\{A\}^2}{m} + 2\lambda \right) \tag{47}$$

$$\eta^\star = \frac{2m}{\sigma_{\max}\{A\}^2 + \sigma_{\min}\{A\}^2 + 2m\lambda}. \tag{48}$$

Here the second equality is the most challenging to derive. It follows from the first inequality by the following reasoning:

- If $1 - \eta^\star \left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda \right)$ and $1 - \eta^\star \left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda \right)$ have the same sign, then by the first equality, they must be equal. This means that $\sigma_{\max}\{A\} = \sigma_1\{A\} = \sigma_2\{A\} = \cdots = \sigma_n\{A\} = \sigma_{\min}\{A\}$ and the optimal learning rate $\eta^\star$ sets each rate $1 - \eta^\star \left(\frac{\sigma_i\{A\}^2}{m} + \lambda \right)$ to 0 simultaneously, ensuring convergence in one step. If both sides are 0 then the second equality holds (because $0 = -0$).

- Otherwise, $1 - \eta^\star \left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda \right)$ and $1 - \eta^\star \left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda \right)$ have opposite signs. Since $\sigma_{\max}\{A\} > \sigma_{\min}\{A\}$ (since if they were equal we would be in the first case), we have $1 - \eta^\star \left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda \right) > 1 - \eta^\star \left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda \right)$. Thus $1 - \eta^\star \left(\frac{\sigma_{\min}\{A\}^2}{m} + \lambda \right)$ must be positive and $1 - \eta^\star \left(\frac{\sigma_{\max}\{A\}^2}{m} + \lambda \right)$ must be negative. The absolute value of a negative number is its negative, so the second equality follows directly from the first equality.

(f) The attached notebook, `gd_convergence.ipynb`, will examine the computational aspects of GD on ridge regression. Implement the GD and stochastic gradient descent (SGD) functions at the top of the notebook, which are marked with `TODO`s.

(g) Click through the notebook and run the sections $n = 1$, $n = 2$, and $n \gg 2$. Change the values of λ and η and re-run the cells a few times. Write down your observations about how the convergence of GD works under different values of λ and η.

(h) In the sections $n = 1$, $n = 2$, and $n \gg 2$, change the calls to GD to instead call SGD. Write down your observations about how the convergence of SGD works under different values of λ and η. Compare the behavior of GD and SGD.

(i) You might have noticed that if we think of convergence in the "last iterate" sense, i.e., $\lim_{T \to \infty} \vec{x}_T = \vec{x}_\lambda^\star$, then *SGD rarely converges*. This is because even if we reach the global optimum, the gradient estimate used by SGD is in general nonzero, and so the iterates end up bouncing around near the optimum. Another different, weaker, notion of convergence under which one might show that SGD actually does converge is convergence "in time average", i.e., $\lim_{T \to \infty} \overline{\vec{x}}_T = \vec{x}_\lambda^\star$ where $\overline{\vec{x}}_T \doteq \frac{1}{T} \sum_{t=1}^{T} \vec{x}_t$. Visualize this by adding the argument `time_avg=True` to each plotting function; the plot will now visualize the sequence of $\overline{\vec{x}}_t$. Re-run the notebook. Write down your observations, especially regarding the stability of SGD and convergence in the last-iterate sense versus the time-average sense.

2. **Homework Process**

With whom did you work on this homework? List the names and SIDs of your group members.

NOTE: If you didn't work with anyone, you can put "none" as your answer.