

This homework is due at 11 PM on April 20, 2023.

Submission Format: Your homework submission should consist of a single PDF file that contains all of your answers (any handwritten answers should be scanned).

1. Newton's Method, Coordinate Descent and Gradient Descent

In this question, we will compare three different optimization methods: Newton's method, coordinate descent and gradient descent. We will consider the simple set-up of unconstrained convex quadratic optimization; i.e we will consider the following problem:

$$\min_{\vec{x} \in \mathbb{R}^d} \vec{x}^\top A \vec{x} - 2\vec{b}^\top \vec{x} + c \quad (1)$$

where $A \succ 0$ and $\vec{b} \in \mathbb{R}^d$.

- (a) How many steps does Newton's method take to converge to the optimal solution? Recall that the update rule for Newton's method is given by the equation:

$$\vec{x}_{t+1} = \vec{x}_t - (\nabla^2 f(\vec{x}_t))^{-1} \nabla f(\vec{x}_t). \quad (2)$$

when optimizing a function f .

- (b) Now, consider the simple two variable quadratic optimization problem for $\sigma > 0$:

$$\min_{\vec{x} \in \mathbb{R}^2} f(\vec{x}) = \sigma x_1^2 + x_2^2. \quad (3)$$

How many steps does coordinate descent take to converge on this problem? Assume that we start by updating the variable x_1 in the first step, x_2 in step two and so on; therefore, we will update x_1 and x_2 in odd and even iterations respectively:

$$(x_{t+1})_1 = \begin{cases} \operatorname{argmin}_{x_1} f(x_1, (x_t)_2) & \text{for odd } t \\ (x_t)_1 & \text{otherwise} \end{cases} \quad \text{and} \quad (x_{t+1})_2 = \begin{cases} \operatorname{argmin}_{x_2} f((x_t)_1, x_2) & \text{for even } t \\ (x_t)_2 & \text{otherwise} \end{cases} \quad (4)$$

Here, $(x_t)_2$ represents x_2 at time t and so on.

- (c) We will now analyze the performance of coordinate descent on another quadratic optimization problem:

$$\min_{\vec{x} \in \mathbb{R}^2} f(\vec{x}) = \sigma(x_1 + x_2)^2 + (x_1 - x_2)^2. \quad (5)$$

where we have, as before, $\sigma > 0$. Note that $(0, 0)$ is the optimal solution to this problem. Now, starting from the point $\vec{x}_0 = (1, 1)$, write how each coordinate of $(\vec{x}_{t+1})_i$ relates to $(\vec{x}_t)_i$ for $i = 1, 2$. Use this to show how the algorithm converges from the initial point $(1, 1)$ to $(0, 0)$. What happens when σ grows large? *HINT: First find the update rule for $(\vec{x}_t)_1$, i.e. keep $(\vec{x}_t)_2$ fixed and figure out how $(\vec{x}_t)_1$ changes when t is odd. Then do the same for $(\vec{x}_t)_2$ when $(\vec{x}_t)_1$ is fixed for even t .*

- (d) Now, let $f(\vec{x}) = \frac{1}{2} \vec{x}^\top A \vec{x} + \vec{x}^\top \vec{b} + c$ where A is PD. When we run gradient descent on $f(\vec{x})$, the convergence along each of the unit eigenvectors \vec{v}_i of A is

$$|1 - \eta(\lambda_i\{A\})| \quad (6)$$

This can be derived similar to HW 8 Question 1e, which you may reference. Formally, in the current setting, we have

$$(\vec{x}_k - \vec{x}^*) = (I - \eta A)^k (\vec{x}_0 - \vec{x}^*)$$

One way we can derive an “optimal” learning rate η^* is to minimize the largest rate of convergence:

$$\eta^* \in \operatorname{argmin}_{\eta \in \mathbb{R}} \max_{i \in \{1, \dots, n\}} |1 - \eta(\lambda_i\{A\})|. \quad (7)$$

One important property of η^* is that it makes the rates of convergence $|1 - \eta(\lambda_i\{A\})|$ associated with the largest and smallest singular values of A equal, i.e.,

$$|1 - \eta(\lambda_{\max}\{A\})| = |1 - \eta(\lambda_{\min}\{A\})|$$

Use this property to show that

$$\eta^* = \frac{2}{\lambda_{\max}\{A\} + \lambda_{\min}\{A\}} \quad (8)$$

where $\lambda_{\min}\{A\} = \lambda_n\{A\}$ is the n^{th} largest singular value of A and similar for the maximum.

- (e) Finally, for the objective function (5), write an equation relating \vec{x}_t to \vec{x}_0 if $\vec{x}_0 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$. Assume for this part that $\sigma > 1$ and reason about how quickly gradient descent converges when σ grows large. *HINT: What is the optimal step size for gradient descent, using the previous part? HINT: Also note that f is given by:*

$$f(\vec{x}) = \vec{x}^\top A \vec{x} \text{ where } A = 2 \left(\sigma \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} + \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \right). \quad (9)$$

2. Gradient Descent vs Newton Method

Run the Jupyter notebook `gradient_vs_newton.ipynb` which demonstrates differences between gradient descent and Newton's method.

3. LASSO vs. Ridge

Say that we have the data set $\{(\vec{x}^{(i)}, y^{(i)})\}_{i=1,\dots,n}$ of samples $\vec{x}^{(i)} \in \mathbb{R}^d$ and values $y^{(i)} \in \mathbb{R}$.

Define $X = \begin{bmatrix} \vec{x}^{(1)} & \dots & \vec{x}^{(n)} \end{bmatrix}^\top$ and $y = \begin{bmatrix} y^{(1)} & \dots & y^{(n)} \end{bmatrix}^\top$.

For the sake of simplicity, assume that the data has been centered and whitened so that each feature has mean 0 and variance 1 and the features are uncorrelated, i.e. $X^\top X = nI$. Consider the linear least squares regression with regularization in the ℓ_1 -norm, also known as LASSO:

$$\vec{w}^* = \operatorname{argmin}_{\vec{w} \in \mathbb{R}^d} \|X\vec{w} - \vec{y}\|_2^2 + \lambda \|\vec{w}\|_1. \quad (10)$$

This problem will compare ℓ_1 -regularization with ℓ_2 -regularization (ridge regression) to understand their similarities and differences. We will do this by looking at the elements of \vec{w}^* in the solution to each problem.

- First, we decompose this optimization problem into d univariate optimization problems over each element of \vec{w} . Let $X = \begin{bmatrix} \vec{x}_1 & \dots & \vec{x}_d \end{bmatrix}$ and recall that $X^\top X = nI$.
- If $w_i^* > 0$, then what is the value of w_i^* ? What is the condition on $\vec{y}^\top \vec{x}_i$ for this to be possible?
- If $w_i^* < 0$, then what is the value of w_i^* ? What is the condition on $\vec{y}^\top \vec{x}_i$ for this to be possible?
- What can we conclude about w_i^* if $|\vec{y}^\top \vec{x}_i| \leq \frac{\lambda}{2}$? How does the value of λ impact the individual entries w_i^* ?
- Now consider the case of ridge regression, which uses the ℓ_2 regularization $\lambda \|\vec{w}\|_2^2$.

$$\vec{w}^* = \operatorname{argmin}_{\vec{w} \in \mathbb{R}^d} \|X\vec{w} - \vec{y}\|_2^2 + \lambda \|\vec{w}\|_2^2. \quad (11)$$

Write down the new condition for w_i^* to be 0. How does this differ from the condition obtained in part (4) and what does this suggest about LASSO?

4. More Fun with Lasso and Ridge

Complete the Jupyter notebook `ridge_vs_lasso.ipynb` which demonstrates differences between ridge regression and LASSO.

5. Connecting Ridge Regression, LASSO, and Constrained Least Squares

This question aims to help you develop an understanding of how a constraint in an optimization problem has the same effect as a penalty term in the objective.

- (a) Let $f: \mathbb{R}^n \rightarrow \mathbb{R}$ be strictly convex and such that $\lim_{\alpha \rightarrow \infty} f(\alpha \vec{v}) = \infty$ for any nonzero $\vec{v} \in \mathbb{R}^n$. Let $g: \mathbb{R}^n \rightarrow \mathbb{R}_+$ be convex and take non-negative values. Further, suppose that there exists $\vec{x}_0 \in \mathbb{R}^n$ such that $g(\vec{x}_0) = 0$.

For $\lambda \geq 0$ and $k \geq 0$, define the “penalty” and “constraint” programs

$$P(\lambda) \doteq \operatorname{argmin}_{\vec{x}} \{f(\vec{x}) + \lambda g(\vec{x})\} \quad (12)$$

$$C(k) \doteq \operatorname{argmin}_{\vec{x}: g(\vec{x}) \leq k} f(\vec{x}). \quad (13)$$

Show that:

- for every $\lambda \geq 0$ there exists $k \geq 0$ such that $P(\lambda) = C(k)$, and
- for every $k > 0$ there exists $\lambda \geq 0$ such that $P(\lambda) = C(k)$.

HINT: First show using strict convexity that, for $k \geq 0$ and $\lambda \geq 0$, both $P(\lambda)$ and $C(k)$ have exactly one element, i.e., each problem has exactly one optimal solution. You may use without proof that $P(\lambda)$ and $C(k)$ have at least one element each (this is true from assumptions but requires some analysis to show).

To show the first direction (i.e. for all λ there exists $k...$), let $\vec{x}^ \in P(\lambda)$ and show that $\vec{x}^* \in C(k)$ for $k = g(\vec{x}^*)$. You might need the fact that $P(\lambda)$ and $C(k)$ have exactly one element. To show the other direction (i.e. for all k there exists $\lambda...$), prove that strong duality holds for the constraint problem, let $\vec{x}^* \in C(k)$ and μ^* be optimal primal and dual variables for the constraint problem and show that $\vec{x}^* \in P(\lambda)$ for $\lambda = \mu^*$.*

Let $A \in \mathbb{R}^{m \times n}$ have full column rank, and let $\vec{y} \in \mathbb{R}^m$. In the course, we have looked at LASSO:

$$\text{LASSO}(\lambda) \doteq \operatorname{argmin}_{\vec{x}} \left\{ \|A\vec{x} - \vec{y}\|_2^2 + \lambda \|\vec{x}\|_1 \right\} \quad (14)$$

and ridge regression:

$$\text{Ridge}(\lambda) \doteq \operatorname{argmin}_{\vec{w}} \left\{ \|A\vec{w} - \vec{y}\|_2^2 + \lambda \|\vec{w}\|_2^2 \right\} \quad (15)$$

which add an ℓ^1 and ℓ^2 norm penalty to the least squares objective, respectively. The analogous constraint programs are the ℓ^1 - and ℓ^2 -constrained least squares problems:

$$\ell^1\text{CLS}(k) \doteq \operatorname{argmin}_{\vec{x}: \|\vec{x}\|_1 \leq k} \|A\vec{x} - \vec{y}\|_2^2 \quad (16)$$

$$\ell^2\text{CLS}(k) \doteq \operatorname{argmin}_{\vec{x}: \|\vec{x}\|_2 \leq k} \|A\vec{x} - \vec{y}\|_2^2. \quad (17)$$

- (b) Show that the result from part (a) can be used to show the equivalence of LASSO with $\ell^1\text{CLS}$ and the equivalence of ridge regression with $\ell^2\text{CLS}$. Namely, for each pair of equivalent formulations, find f and g , prove that f is strictly convex, prove that g is convex, and prove that there is an \vec{x}_0 such that $g(\vec{x}_0) = 0$.
- (c) Complete the Jupyter notebook, which will use this equivalence to show geometrically why LASSO solutions tend to be sparse (i.e. have many zeros) while ridge regression doesn't, and attach a PDF printout of your answers.

6. 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.