1. Spectrahedron

This question explores the structure of the feasibility set associated to a linear matrix inequality. The feasibility set of any semidefinite program is the feasibility set of a linear matrix inequality, so this question aimed at developing a better understanding of the feasibility sets of semidefinite programs. Given symmetric matrices $F_0, F_1, \ldots, F_m \in \mathbb{S}^n$, the set of symmetric matrices

$$\{F_0 + x_1 F_1 + \ldots + x_m F_m : \vec{x} \in \mathbb{R}^m\},\$$

where \vec{x} denotes $\begin{bmatrix} x_1 & \dots & x_m \end{bmatrix}^\top$, is called a *linear matrix pencil*. It is an affine subspace of the vector space \mathbb{S}^n . We write $F(\vec{x})$ for $F_0 + \sum_{i=1}^m x_i F_i$. The intersection of a linear matrix pencil with the cone of symmetric positive semidefinite matrices is called a *spectrahedron*. The condition that needs to be satisfied for this, namely

$$F(\vec{x}) \succ 0$$
,

is called a *linear matrix inequality*. The term "spectrahedron" is also used to refer to

$$\{\vec{x} \in \mathbb{R}^m : F(\vec{x}) \succeq 0\},\$$

in which case we think of it as a subset of \mathbb{R}^m . This set is also called the feasibility set of the LMI. In this question we will study the spectrahedron associated to the linear matrix pencil

$$F(x,y) = \begin{bmatrix} 1 & 1-x & -x \\ 1-x & 1 & -y \\ -x & -y & 2y \end{bmatrix}.$$

We will think of this spectrahedron as a subset of \mathbb{R}^2 , with the vectors in \mathbb{R}^2 being written as $\begin{bmatrix} x & y \end{bmatrix}^\top$.

(a) Find all the principal minors of F(x,y). **Remark**: For a square $n \times n$ matrix A, for each $1 \le k \le n$ there are $\binom{n}{k}$ principal k-minors. These are found by picking a subset $J \subset \{1,\ldots,n\}$ of size k and considering the $k \times k$ matrix one gets from A by erasing all the rows with index not in J and all the columns with index not in J and then taking the determinant of this $k \times k$ matrix. Since F(x,y) is a 3×3 matrix, there will be three principal 1-minors (which are just the diagonal entries), three principal 2-minors, and one principal 3-minor (which is just the determinant). You are asked to find these.

Solution: The principal 1-minors are 1, 1 and 2y.

The principal 2-minors are $2x - x^2$, $2y - x^2$ and $2y - y^2$.

The principal 3-minor, i.e. the determinant, is $-x^2 - y^2 + 6xy - 4x^2y$.

(b) For a symmetric matrix $A \in \mathbb{S}^n$, it is known that A is symmetric positive semidefinite if and only if all its principal minors are nonnegative. Based on this, find a finite collection of polynomials in the variables (x, y), such that the spectrahedron can be defined as the set of (x, y) values where these polynomials are non-negative. A graph of the spectrahedron is shown in Figure 1.

Solution: F(x,y) is symmetric positive semidefinite if and only if the following conditions all hold:

$$2y > 0$$
,

$$2x - x^2 \ge 0,$$

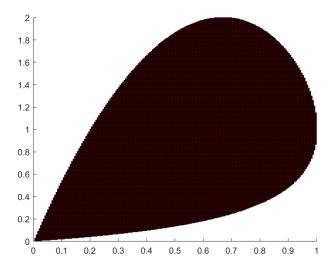


Figure 1: Spectrahedron. This is a convex set.

$$2y - x^{2} \ge 0,$$

$$2y - y^{2} \ge 0,$$

$$-x^{2} - y^{2} + 6xy - 4x^{2}y \ge 0.$$

(c) Show that if F(x, y) is symmetric positive semidefinite then $0 \le x \le 2$.

Solution: If F(x,y) is symmetric positive semidefinite, its leading 2×2 block is also symmetric positive semidefinite, so the determinant of this block must be nonnegative. This gives $2x - x^2 \ge 0$, i.e. $0 \le x \le 2$.

(d) Suppose x = 0. Show that the only value of y for which F(0, y) is symmetric positive semidefinite is y = 0. What is the rank of F(0, 0)?

Solution: We have

$$F(0,y) = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & -y \\ 0 & -y & 2y \end{bmatrix}.$$

Since the (3,3) entry of this matrix must be nonnegative if the matrix is symmetric positive semidefinite, we must have $y \ge 0$. Since the determinant of the matrix must be nonnegative, we get $-y^2 \ge 0$. The only solution to these two inequalities is y = 0. The rank of the resulting matrix F(0,0) is 1.

(e) Suppose x = 2. Show that there is no value of y for which F(2, y) is symmetric positive semidefinite.

Solution: We have

$$F(2,y) = \begin{bmatrix} 1 & -1 & -2 \\ -1 & 1 & -y \\ -2 & -y & 2y \end{bmatrix}.$$

Since the (3,3) entry of this matrix must be nonnegative if the matrix is symmetric positive semidefinite, we must have $y \ge 0$. Since the determinant of the matrix must be nonnegative, we get $-4 - 4y - y^2 \ge 0$. There is no value of y that satisfies both these inequalities.

(f) What condition must the pair (x, y) satisfy for the rank of F(x, y) to be strictly less than 3?

Solution: The rank of F(x, y) is strictly less than 3 precisely when its determinant is zero. The condition that (x, y) must satisfy is therefore

$$-x^2 - y^2 + 6xy - 4x^2y = 0.$$

(g) Assume 0 < x < 2. Verify that this makes the leading 2×2 block of F(x,y) symmetric positive definite. Fixing x, apply the Schur complement criterion to show that F(x,y) is symmetric positive semidefinite if and only if the determinant of F(x,y) is nonnegative and symmetric positive definite if and only if the determinant of F(x,y) is strictly positive.

Remark: From this part of the question we learn that the boundary of the spectrahedron in Figure 1 consists of pairs (x, y) where the rank of F(x, y) is strictly less than 3.

Solution: When 0 < x < 2 the determinant of the leading 2×2 block of F(x, y), which is $2x - x^2$, is strictly positive. Its trace, i.e. 2, is also strictly positive, so it is symmetric positive definite.

The Schur complement criterion now tells us that F(x,y) is symmetric positive semidefinite if and only if we have

$$2y - \begin{bmatrix} -x & -y \end{bmatrix} \begin{bmatrix} 1 & 1-x \\ 1-x & 1 \end{bmatrix}^{-1} \begin{bmatrix} -x \\ -y \end{bmatrix} \ge 0,$$

and symmetric positive definite if and only if this expression is strictly positive. Multiplying through by $2x - x^2$ (which is strictly positive), this reads

$$2y(2x-x^2) - \begin{bmatrix} -x & -y \end{bmatrix} \begin{bmatrix} 1 & -1+x \\ -1+x & 1 \end{bmatrix} \begin{bmatrix} -x \\ -y \end{bmatrix} \ge 0,$$

which can be simplified to read

$$-x^2 - y^2 + 6xy - 4x^2y \ge 0,$$

i.e. that the determinant of F(x,y) is nonnegative. We therefore conclude that, under the condition 0 < x < 2, we have F(x,y) symmetric positive semidefinite if and only if the determinant of F(x,y) is nonnegative and symmetric positive definite if and only if the determinant of F(x,y) is strictly positive.

(h) Show that for (x, y) in the spectrahedron, the rank of F(x, y) is 1 precisely when (x, y) = (0, 0).

Remark: From this part and the preceding part of the question we learn that the rank of F(x, y) is 3 on the interior of the spectrahedron, is 2 at all points on the boundary of the spectrahedron except the point (x, y) = (0, 0). where the rank of F(0, 0) is 1.

Solution: Note that the rank of F(x,y) cannot be zero, because it can never be the zero matrix. For the rank of F(x,y) to equal 1, all three columns must be proportional. By looking at the first two columns, this gives the condition $(1-x)^2=1$, i.e. either x=0 or x=2. Since there is no value of y for which (2,y) is in the spectrahedron, as established in part (e) of this question, we must have x=0. From part (d) of this question this then means we must have y=0, and since the rank of F(0,0) is indeed 1, this proves what was required.

2. Soft-Margin SVM

Consider the soft-margin SVM problem,

$$p^{\star}(C) = \min_{\vec{w} \in \mathbb{R}^m, b \in \mathbb{R}, \vec{\xi} \in \mathbb{R}^n} \quad \frac{1}{2} \|\vec{w}\|_2^2 + C \sum_{i=1}^n \xi_i$$
 (1)

s.t.
$$1 - \xi_i - y_i(\vec{x}_i^\top \vec{w} - b) \le 0, \quad i = 1, 2, \dots, n$$
 (2)

$$-\xi_i \le 0, \quad i = 1, 2, \dots, n,$$
 (3)

where $\vec{x}_i \in \mathbb{R}^m$ refers to the i^{th} training data point, $y_i \in \{-1,1\}$ is its label, and $C \in \mathbb{R}_+$ (i.e. C>0) is a hyperparameter. Let α_i denote the dual variable corresponding to the inequality $1-\xi_i-y_i(\vec{x}_i^\top\vec{w}-b)\leq 0$ and let β_i denote the dual variable corresponding to the inequality $-\xi_i\leq 0$. The Lagrangian is then given by

$$\mathcal{L}(\vec{w}, b, \vec{\xi}, \vec{\alpha}, \beta) = \frac{1}{2} \|\vec{w}\|_{2}^{2} + C \sum_{i=1}^{n} \xi_{i} + \sum_{i=1}^{n} \alpha_{i} (1 - \xi_{i} - y_{i} (\vec{x}_{i}^{\top} \vec{w} - b)) - \sum_{i=1}^{n} \beta_{i} \xi_{i}.$$

$$\tag{4}$$

Suppose $\vec{w}^*, b^*, \vec{\xi}^*, \vec{\alpha}^*, \beta^*$ satisfy the KKT conditions. Classify the following statements as true or false and justify your answers mathematically.

(a) Suppose the optimal solution \vec{w}^* , b^* changes when the training point \vec{x}_i is removed. Then originally, we necessarily have $y_i(\vec{x}_i^\top \vec{w}^* - b^*) = 1 - \xi_i^*$.

Solution: True. Since optimal \vec{w}^* changes if we remove point \vec{x}_i we have $\alpha_i^* \neq 0$. By complementary slackness we have,

$$\alpha_i^{\star}(1 - \xi_i^{\star} - y_i(\vec{x}_i^{\mathsf{T}}\vec{w}^{\star} - b^{\star})) = 0, \tag{5}$$

which gives,

$$1 - \xi_i^* - y_i(\vec{x}_i^\top \vec{w}^* - b^*) = 0 \tag{6}$$

$$\implies y_i(\vec{x}_i^\top \vec{w}^* - b^*) = 1 - \xi_i^*. \tag{7}$$

(b) Suppose the optimal solution \vec{w}^* , b^* changes when the training point \vec{x}_i is removed. Then originally, we necessarily have $\alpha_i^* > 0$.

Solution: True. Since optimal \vec{w}^* changes if we remove point \vec{x}_i we have $\alpha_i^* \neq 0$. Further by dual feasibility we have $\alpha_i^* \geq 0$ which together gives $\alpha_i^* > 0$.

(c) Suppose the data points are strictly linearly separable, i.e. there exist $\vec{\tilde{w}}$ and \tilde{b} such that for all i,

$$y_i(\vec{x}_i^{\top}\vec{w} - \tilde{b}) > 0. \tag{8}$$

Then $p^*(C) \to \infty$ as $C \to \infty$.

Solution: False. Since

$$y_i(\vec{x}_i^{\top} \vec{\tilde{w}} - \tilde{b}) > 0, \tag{9}$$

we have for sufficiently small $\epsilon > 0$,

$$y_i(\vec{x}_i^{\top}\vec{\widetilde{w}} - \widetilde{b}) \ge \epsilon \implies y_i\left(\vec{x}_i^{\top}\frac{\vec{\widetilde{w}}}{\epsilon} - \frac{\widetilde{b}}{\epsilon}\right) \ge 1.$$
 (10)

Thus, $\vec{\overline{w}} = \frac{\vec{\widetilde{w}}}{\epsilon}, \vec{b} = \frac{\widetilde{b}}{\epsilon}, \vec{\overline{\xi}} = 0$ is a feasible point with objective value $\frac{1}{2} \left\| \vec{\overline{w}} \right\|_2^2 < \infty$ irrespective of value of C.

3. Gradient Descent on a Graph

This question studies a gradient descent method to solve an optimization problem where the variables are thought of as being parametrized by the vertices of an undirected graph. We are given an undirected simple graph G = (V, E) where $V = \{1, \dots, n\}$ is the set of vertices and $E \subseteq V \times V$ is the set of edges. Note that the notation is such that if $(i, j) \in E$ then we will also have $(j, i) \in E$. In particular, E will be of even cardinality.

(a) Consider the problem of assigning weights x_i to each vertex $i \in V$ such that adjacent vertices get similar weights, and the sum of weights is close to 1. That is, we want the solution to the optimization problem

$$\vec{x}^* := \arg\min_{\vec{x} \in \mathbb{R}^n} \sum_{(i,j) \in E} (x_i - x_j)^2 + 2\lambda \left(\sum_{i \in V} x_i - 1 \right)^2$$

where $\lambda \geq 0$ is a constant. Show that this optimization problem is equivalent to

$$\vec{x}^{\star} = \arg\min_{\vec{x} \in \mathbb{R}^n} \frac{1}{2} \vec{x}^{\top} (L + \lambda \vec{\mathbf{1}} \vec{\mathbf{1}}^{\top}) \vec{x} - \lambda \vec{\mathbf{1}}^{\top} \vec{x}$$

where L is the Laplacian matrix for G and $\vec{\mathbf{1}}$ is the all-ones vector in \mathbb{R}^n .

Note: Let G=(V,E) be a graph with $V=\{1,\cdots,n\}$. For each vertex $i\in V$, the degree of i, denoted $\deg(i)$, is defined as the number of edges incident to the vertex i. The Laplacian matrix L of G is the $n\times n$ matrix with i-th diagonal entry $\deg(i)$ and with (i,j)-th entry (with $i\neq j$) equal to -1 if $(i,j)\in E$ and equal to zero otherwise, for each $i,j\in V$.

Hint: For all $\vec{x} \in \mathbb{R}^n$ we have $\vec{x}^\top L \vec{x} = \frac{1}{2} \sum_{i,j \in V: (i,j) \in E} (x_i - x_j)^2$.

Solution: The optimization problem is

$$\vec{x}^* = \arg\min_{\vec{x} \in \mathbb{R}^n} \sum_{(i,j) \in E} (x_i - x_j)^2 + 2\lambda \left(\sum_{i \in V} x_i - 1\right)^2$$

$$= \arg\min_{\vec{x} \in \mathbb{R}^n} \frac{1}{4} \sum_{(i,j) \in E} (x_i - x_j)^2 + \frac{\lambda}{2} \left(\sum_{i \in V} x_i - 1\right)^2$$

$$= \arg\min_{\vec{x} \in \mathbb{R}^n} \frac{1}{2} \vec{x}^\top L \vec{x} + \frac{\lambda}{2} (\vec{\mathbf{1}}^\top \vec{x} - 1)^2$$

$$= \arg\min_{\vec{x} \in \mathbb{R}^n} \frac{1}{2} \vec{x}^\top L \vec{x} + \frac{\lambda}{2} (\vec{x}^\top \vec{\mathbf{1}} \vec{\mathbf{1}}^\top \vec{x} - 2 \vec{\mathbf{1}}^\top \vec{x} + 1)$$

$$= \arg\min_{\vec{x} \in \mathbb{R}^n} \frac{1}{2} \vec{x}^\top L \vec{x} + \frac{\lambda}{2} \vec{x}^\top \vec{\mathbf{1}} \vec{\mathbf{1}}^\top \vec{x} - \lambda \vec{\mathbf{1}}^\top \vec{x}$$

$$= \arg\min_{\vec{x} \in \mathbb{R}^n} \frac{1}{2} \vec{x}^\top (L + \lambda \vec{\mathbf{1}} \vec{\mathbf{1}})^\top \vec{x} - \lambda \vec{\mathbf{1}}^\top \vec{x}.$$

(b) What is the optimal \vec{x}^* ?

Solution: The objective $\sum_{(i,j)\in E}(x_i-x_j)^2+\frac{\lambda}{2}\left(\sum_{i\in V}x_i-1\right)^2$ is a sum of squares and thus is lower-bounded by zero. Setting $\vec{x}^*=\frac{1}{n}\vec{1}$ achieves this lower bound.

(c) Suppose we use gradient descent with step size $\eta > 0$ to find the optimal \vec{x}^* . Write the gradient descent step; i.e., express \vec{x}_{k+1} , the (k+1)th step of gradient descent, in terms of \vec{x}_k , L, η , and λ .

Solution: Let $A = L + \lambda \vec{1}\vec{1}^{\top}$ and $\vec{b} = -\lambda \vec{1}$, so the objective becomes $\vec{x}^{\top} A \vec{x} + \vec{b}^{\top} \vec{x}$. The gradient at each step is

$$\nabla_{\vec{x}} \left(\frac{1}{2} \vec{x}^\top A \vec{x} + \vec{b}^\top \vec{x} \right) = A \vec{x} + \vec{b}$$

since A is symmetric.

The gradient descent step is

$$\begin{aligned} \vec{x}_{k+1} &= -\eta \nabla_{\vec{x}} \left(\frac{1}{2} \vec{x}_k^\top A \vec{x}_k + \vec{b}^\top \vec{x}_k \right) + \vec{x}_k \\ &= -\eta (A \vec{x}_k + \vec{b}) + \vec{x}_k \\ &= -\eta ((L + \lambda \vec{\mathbf{1}} \vec{\mathbf{1}}^\top) \vec{x}_k - \lambda \vec{\mathbf{1}}) + \vec{x}_k \end{aligned}$$

(d) Show that $\vec{x}_{k+1} - \vec{x}^* = (I - \eta(L + \lambda \vec{\mathbf{1}}\vec{\mathbf{1}}^\top))(\vec{x}_k - \vec{x}^*).$

Solution: Again, let $A = L + \lambda \vec{\mathbf{1}} \vec{\mathbf{1}}^{\top}$ and $\vec{b} = -\lambda \vec{\mathbf{1}}$. Note that $\nabla_{\vec{x}}^2 \left(\frac{1}{2} \vec{x}^{\top} A \vec{x} + \vec{b}^{\top} \vec{x} \right) = A \succeq 0$ since A is the sum of PSD matrices, so we can set the gradient to zero to find the optimum:

$$\nabla_{\vec{x}} \left(\frac{1}{2} \vec{x}^\top A \vec{x} + \vec{b}^\top \vec{x} \right) = A \vec{x} + \vec{b} = 0,$$

so $A\vec{x}^* + \vec{b} = \vec{0}$. Thus, from the gradient descent step $\vec{x}_{k+1} = -\eta(A\vec{x}_k + \vec{b}) + \vec{x}_k$ we have

$$\begin{split} \vec{x}_{k+1} - \vec{x}^* &= -\eta (A\vec{x}_k + \vec{b}) + \vec{x}_k - \vec{x}^* \\ &= (I - \eta A)\vec{x}_k - \eta \vec{b} - \vec{x}^* \\ &= (I - \eta A)(\vec{x}_k - \vec{x}^*) + (I - \eta A)\vec{x}^* - \eta \vec{b} - \vec{x}^* \\ &= (I - \eta A)(\vec{x}_k - \vec{x}^*) + \vec{x}^* + \eta \vec{b} - \eta \vec{b} - \vec{x}^* \\ &= (I - \eta A)(\vec{x}_k - \vec{x}^*) \\ &= (I - \eta (L + \lambda \vec{\mathbf{1}}\vec{\mathbf{1}}^\top))(\vec{x}_k - \vec{x}^*). \end{split}$$

(e) We saw that for all $\vec{x} \in \mathbb{R}^n$ we have $\vec{x}^\top L \vec{x} = \frac{1}{2} \sum_{i,j \in V: (i,j) \in E} (x_i - x_j)^2$. Hence L is symmetric positive semidefinite. Also $L\vec{1} = \vec{0}$, so the smallest eigenvalue of L is 0. Let $\lambda_1 \geq \cdots \geq \lambda_n = 0$ be the eigenvalues of L, and assume λ is given such that $\lambda_1 \geq n\lambda \geq \lambda_{n-1}$. Show that $\|\vec{x}_k - \vec{x}^\star\|_2 \leq \rho^k \|\vec{x}_0 - \vec{x}^\star\|_2$ for $\rho := \max\{|1 - \eta\lambda_{n-1}|, |1 - \eta\lambda_1|\}$, where \vec{x}_0 is the starting point of the gradient descent.

Solution: Since L is symmetric, by the spectral theorem we can diagonalize L as $L = V\Lambda V^{\top}$, where

$$\Lambda = egin{bmatrix} \lambda_1 & & & \ & \ddots & & \ & & \lambda_n \end{bmatrix}$$

and the columns of V are the corresponding eigenvectors.

Notice that $\vec{\mathbf{1}}$ is the eigenvector corresponding to the smallest eigenvalue of L, i.e., $\lambda_n=0$, and is normalized as $\vec{u}:=\frac{1}{\sqrt{n}}\vec{\mathbf{1}}$. Thus,

$$\vec{u}\vec{u}^{\top} = V \begin{bmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & \\ & & & 1 \end{bmatrix} V^{\top} = V e_n e_n^{\top} V^{\top}$$

so $\vec{\mathbf{1}}\vec{\mathbf{1}}^{\top} = nV\vec{e}_n\vec{e}_n^{\top}V$ and therefore

$$A = L + \lambda \vec{\mathbf{1}} \vec{\mathbf{1}}^{\top}$$

$$= V(\Lambda + n\lambda \vec{e}_n \vec{e}_n^{\top}) V^{\top}$$

$$= V \begin{bmatrix} \lambda_1 & & & \\ & \ddots & & \\ & & \lambda_{n-1} & \\ & & & \lambda_n + n\lambda \end{bmatrix} V^{\top}.$$

Note that since zero is an eigenvalue of L and $L \succeq 0$, the smallest eigenvalue is $\lambda_n = 0$. Thus, the eigenvalues of A are the eigenvalues $\lambda_1, \dots, \lambda_{n-1}$ of L, as well as $n\lambda$. In particular, since $\lambda_1 \geq n\lambda \geq \lambda_{n-1}$, the largest eigenvalue of A is λ_1 while the smallest is λ_{n-1} .

Using part (d), we then have

$$\|\vec{x}_{k+1} - \vec{x}^*\|_2 \le \|I - \eta(L + \lambda \vec{\mathbf{1}}\vec{\mathbf{1}}^\top)\|_2 \|\vec{x}_k - \vec{x}^*\|_2.$$

Let $\rho = ||I - \eta(L + \lambda \vec{\mathbf{1}}\vec{\mathbf{1}}^{\top})||_2 = \max\{|1 - \eta\lambda_{n-1}|, |1 - \eta\lambda_1|\}$. Expanding the above equation,

$$\|\vec{x}_k - \vec{x}^*\|_2 \le \rho^k \|\vec{x}_0 - \vec{x}^*\|_2.$$

(f) Assuming that $\eta > 0$ is small enough that $0 < \rho < 1$, find the number of time steps needed to converge to some $\varepsilon > 0$ around x^* as a function of η , assuming $\|\vec{x}_0 - \vec{x}^*\|_2 > \varepsilon$. That is, find $t(\eta)$ such that $\|\vec{x}_k - \vec{x}^*\|_2 \le \varepsilon$ for $k \ge t(\eta)$.

Solution: We need t such that

$$\rho^t \|\vec{x}_0 - \vec{x}^{\star}\|_2 \le \varepsilon.$$

Taking the logarithm of both sides, we get

$$t {\rm log}\; \rho \leq {\rm log}\; \frac{\varepsilon}{\|\vec{x}_0 - \vec{x}^\star\|_2}$$

which is satisfied by

$$t \ge \log_{\rho} \frac{\varepsilon}{\|\vec{x}_0 - \vec{x}^{\star}\|_2},$$

so we can set $t(\eta) = \log_{\rho} \frac{\varepsilon}{\|\vec{x}_0 - \vec{x}^*\|_2}$.

(g) Find the optimal step size, i.e. the solution to

$$\eta^* = \arg\min_{\{\eta > 0: 0 < \rho < 1\}} t(\eta).$$

What is the corresponding $t(\eta^*)$?

Solution: Since we restrict attention to $\eta>0$ such that $0<\rho<1$ and since $0<\frac{\varepsilon}{\|\vec{x}_0-\vec{x}^\star\|_2}<1$, we see that $\log_\rho\frac{\varepsilon}{\|\vec{x}_0-\vec{x}^\star\|_2}$ increases monotonically with ρ . Thus, to minimize $t(\eta)=\log_\rho\frac{\varepsilon}{\|\vec{x}_0-\vec{x}^\star\|_2}$, it suffices to minimize ρ with respect to η . From part (e), we have $\rho=\max\{|1-\eta\lambda_{n-1},|1-\eta\lambda_1|\}$. By inspection, the minimum is attained when $1-\eta\lambda_{n-1}=-(1-\eta\lambda_1)$, so $\eta^\star=\frac{2}{\lambda_1+\lambda_{n-1}}$, with corresponding $\rho=1-\eta^\star\lambda_1=\frac{\lambda_1-\lambda_{n-1}}{\lambda_1+\lambda_{n-1}}$ and

$$t(\eta^{\star}) = \frac{\log \frac{\varepsilon}{\|\vec{x}_0 - \vec{x}^{\star}\|_2}}{\log \frac{\lambda_1 - \lambda_{n-1}}{\lambda_1 + \lambda_{n-1}}}.$$

4. 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:

$$\min_{\vec{x} \in \mathbb{R}^d} \vec{x}^\top A \vec{x} - 2 \vec{b}^\top \vec{x} + c \tag{11}$$

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:

$$\vec{x}_{t+1} = \vec{x}_t - (\nabla^2 f(\vec{x}_t))^{-1} \nabla f(\vec{x}_t). \tag{12}$$

when optimizing a function f.

Solution: Newton's method converges in a single step irrespective of the starting point. Let \vec{x}_0 be any starting point. We have:

$$\nabla^2 f(\vec{x}_0) = 2A \text{ and } \nabla f(\vec{x}_0) = 2(A\vec{x} - \vec{b}).$$
 (13)

Therefore, we have:

$$\vec{x}_1 = \vec{x}_0 - A^{-1}(A\vec{x}_0 - \vec{b}) = A^{-1}\vec{b}. \tag{14}$$

Note that since this is an unconstrained convex quadratic optimization problem with A being full rank, we can find the optimum point by setting the derivative of the function to 0. Therefore, we have:

$$\nabla f(\vec{x}^*) = 2(A\vec{x}^* - \vec{b}) = 0 \implies \vec{x}^* = A^{-1}\vec{b}.$$
 (15)

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

$$\min_{\vec{x} \in \mathbb{R}^2} f(\vec{x}) = \sigma x_1^2 + x_2^2. \tag{16}$$

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:

$$(x_{t+1})_1 = \begin{cases} \operatorname{argmin}_{x_1} f(x_1, (x_t)_2) & \text{for odd t} \\ (x_t)_1 & \text{otherwise} \end{cases} \text{ and } (x_{t+1})_2 = \begin{cases} \operatorname{argmin}_{x_2} f((x_t)_1, x_2) & \text{for even t} \\ (x_t)_2. & \text{otherwise} \end{cases}$$
(17)

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

Solution: On this problem, coordinate descent converges in 2 steps starting from any initialization point. Note that the optimal solution for each of the updates is 0, by setting the gradient to 0. Therefore, coordinate descent converges in two steps, one to update x_1 and the other to update x_2 .

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

$$\min_{\vec{x} \in \mathbb{R}^2} f(\vec{x}) = \sigma(x_1 + x_2)^2 + (x_1 - x_2)^2.$$
(18)

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.

Solution: We first find the update rule for x_1 . Note that we only update x_1 when t is odd. Now, by taking the gradient and setting it to 0, we get:

$$\sigma((x_{t+1})_1 + (x_t)_2) + ((x_{t+1})_1 - (x_t)_2) = 0 \implies (x_{(t+1)})_1 = \frac{(1-\sigma)}{(1+\sigma)}(x_t)_2.$$
(19)

Note that the function, f, is symmetric in the variables, x_1 and x_2 . Therefore, the update rule for x_2 (when t is even) is given by:

$$(x_{(t+1)})_2 = \frac{(1-\sigma)}{(1+\sigma)}(x_t)_1. \tag{20}$$

Therefore, we get for all $t \geq 2$:

$$(x_t)_1 = \left(\frac{1-\sigma}{1+\sigma}\right)^{2\left\lfloor\frac{t+1}{2}\right\rfloor - 1} \text{ and } (x_t)_2 = \left(\frac{1-\sigma}{1+\sigma}\right)^{2\left\lfloor\frac{t}{2}\right\rfloor}. \tag{21}$$

When σ grows large, the $\frac{1-\sigma}{1+\sigma}$ goes to -1 and this results in slow convergence as the algorithm converges quickly when $\left|\frac{1-\sigma}{1+\sigma}\right|$ is small.

(d) Finally, for the objective function (18), 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:*

$$f(\vec{x}) = \vec{x}^{\top} A \vec{x} \text{ where } A = 2 \left(\sigma \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} + \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \right). \tag{22}$$

Solution: We first note that f is given by:

$$f(\vec{x}) = \vec{x}^{\top} A \vec{x} \text{ where } A = 2 \left(\sigma \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} + \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \right). \tag{23}$$

Therefore, we have that λ_{\max} of A is 2σ and λ_{\min} is 2. Now, we have that:

$$\nabla f((1,-1)) = 2A \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 4 \\ -4 \end{bmatrix}. \tag{24}$$

Therefore, we have that:

$$\vec{x}_1 = \vec{x}_0 - \eta \nabla f((1, -1)) = \left(1 - \frac{2}{\sigma + 1}\right) \begin{bmatrix} 1\\ -1 \end{bmatrix}.$$
 (25)

By iterating the above procedure we see that:

$$\vec{x}_t = \left(1 - \frac{2}{\sigma + 1}\right)^t \begin{bmatrix} 1\\ -1 \end{bmatrix}. \tag{26}$$

Therefore, when σ is large, the convergence rate of gradient descent is really slow. However, Newton's method would find the optimum in one step.

5. Gradient Descent vs Newton Method

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

Solution: See Jupyter notebook.