Solutions for Discussion 8

1 Least squares with equality constraints

Consider the least squares problem with equality constraints

$$\min_x \|Ax - b\|_2^2 \;:\; Gx = h, \tag{1}$$

where $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$, $G \in \mathbb{R}^{p\times n}$ and $h \in \mathbb{R}^p$. For simplicity, we will assume that $\text{rank}(A) = n$ and $\text{rank}(G) = p$.

Using the KKT conditions, determine the optimal solution of this optimization problem.

Solution:

This is a convex optimization problem with equality constraints. Let $\nu \in \mathbb{R}^p$ denote the dual variables, which are unconstrained. If we can find a primal point $x^* \in \mathbb{R}^n$ and a dual point $\nu^* \in \mathbb{R}^p$ that together satisfy the KKT conditions then, because this is a convex optimization problem, we will learn that x^* is a primal optimal point, ν^* is a dual optimal point, and strong duality holds. We will therefore write the KKT equations and attempt to solve them in order to find a primal optimal point.

The Lagrangian is

$$\begin{aligned}\mathcal{L}(x,\nu) &= (Ax-b)^T(Ax-b) + \nu^T(Gx-h) && (2)\\ &= x^TA^TAx + (G^T\nu - 2A^Tb)^Tx - \nu^Th + b^Tb. && (3)\end{aligned}$$

The KKT conditions are

$$\begin{aligned}Gx^* &= h, && (4)\\ 2A^TAx^* + G^T\nu^* - 2A^Tb &= 0, && (5)\end{aligned}$$

which are the primal feasibility and the Lagrangian stationarity conditions respectively. Since the dual variables are unconstrained there is no dual feasiblity condition on ν^*, and since there are no inequality constraints there are no complementary slackness conditions. As for the Lagrangian stationarity conditions, they come from computing

$$\nabla_x \mathcal{L}(x,\nu^*) = 2A^TAx + G^T\nu^* - 2A^Tb.$$

Since $\text{rank}(A) = n$, we can invert A^TA, and from the Lagrangian stationary conditions in (5) we get

$$x^* = (A^TA)^{-1}\left(A^Tb - \frac{1}{2}G^T\nu^*\right). \tag{6}$$

Substituting this in the primal feasibility condition in (4), we get

$$G(A^TA)^{-1}A^Tb - \frac{1}{2}G(A^TA)^{-1}G^T\nu^* = h,$$

which gives

$$\nu^* = -2\left(G(A^TA)^{-1}G^T\right)^{-1}\left(h - G(A^TA)^{-1}A^Tb\right), \tag{7}$$

where we have used the assumption that $\text{rank}(G) = p$ to conclude that $G(A^TA)^{-1}G^T$ is invertible.

At this point we have found a primal point x^* and a dual point ν^* that satisfy the KKT conditions, so we can claim that this x^* is primal optimal, this ν^* is dual optimal, and strong duality holds. We can get an explicit formula for x^* by substituting (7) in (6), which gives

$$x^* = (A^TA)^{-1}\left(A^Tb + G^T\left(G(A^TA)^{-1}G^T\right)^{-1}\left(h - G(A^TA)^{-1}A^Tb\right)\right).$$

In Lecture 7, we discussed a way to reduced the least squares problem with equality constraints, assuming it was feasible, to an unconstrained least squares problem. It is instructive to examine the solution found here in the context of the procedure suggested there.

First of all, since we have assumed that $\operatorname{rank}(G) = p$, the problem in (1) is feasible. Now note that that

$$G(A^TA)^{-1}G^T\left(G(A^TA)^{-1}G^T\right)^{-1}h = h,$$

so $\tilde{x} := (A^TA)^{-1}G^T\left(G(A^TA)^{-1}G^T\right)^{-1}h$ is a primal feasible point. Further, we have

$$x^* = \tilde{x} + \left(I_n - (A^TA)^{-1}G^T\left(G(A^TA)^{-1}G^T\right)^{-1}G\right)(A^TA)^{-1}A^Tb,$$

which is the sum of a specific point in the primal feasible set, namely $\tilde{x}$, and a point in the null space of G, as we can see from

$$G\left(I_n - (A^TA)^{-1}G^T\left(G(A^TA)^{-1}G^T\right)^{-1}G\right)(A^TA)^{-1}A^Tb = 0.$$

Further, this point in the null space of G, namely

$$\left(I_n - (A^TA)^{-1}G^T\left(G(A^TA)^{-1}G^T\right)^{-1}G\right)(A^TA)^{-1}A^Tb,$$

solves the least squares problem for projecting

$$b - A\tilde{x} = b - A(A^TA)^{-1}G^T\left(G(A^TA)^{-1}G^T\right)^{-1}h$$

onto the image under A of the null space of G, which, it was argued in Lecture 7, can be posed as an unconstrained least squares problem.

2 Distance between polytopes

Let $p^{(1)}, \ldots, p^{(r)}$ and $q^{(1)}, \ldots, q^{(s)}$ be points in $\mathbb{R}^d$, where $r, s \geq 1$. Let $\mathcal{P}$ denote the polytope defined as the convex hull of $\{p^{(1)}, \ldots, p^{(r)}\}$, and $\mathcal{Q}$ the polytope defined as the convex hull of $\{q^{(1)}, \ldots, q^{(s)}\}$. Thus every point in $\mathcal{P}$ can be written as $\sum_{i=1}^{r} x_i p^{(i)}$ for som $x_i \geq 0$, $1 \leq i \leq r$ such that $\sum_{i=1}^{r} x_i = 1$, and every point in $\mathcal{Q}$ can be written as $\sum_{j=1}^{s} x_{r+i} q^{(j)}$ for some $x_i \geq 0$, $r+1 \leq i \leq n$ such that $\sum_{i=r+1}^{n} x_i = 1$, where $n := r + s$.

Define the matrix $C \in \mathbb{R}^{d \times n}$ whose i-th column is $p^{(i)}$, $1 \leq i \leq r$ and whose $r+j$-th column is $-q^{(j)}$, $1 \leq j \leq s$.

(a) Pose the problem of finding the minimum squared ℓ_2 distance between points in $\mathcal{P}$ and points in $\mathcal{Q}$ as a quadratic program with objective function $\|Cx\|_2^2$, viewed as a function on $\mathbb{R}^n$.

Solution:
The problem can be posed as

$$\begin{aligned} \min_{x} \quad & x^T C^T C x \\ \text{subject to:} \quad & \sum_{i=1}^{r} x_i = 1, \\ & \sum_{j=1}^{s} x_{r+j} = 1, \\ & x_i \geq 0, \ i = 1, \ldots, n, \end{aligned}$$

where we recall that $n := r + s$. To see this, note that the objective is

$$\| \sum_{i=1}^{r} x_i p^{(i)} - \sum_{j=1}^{s} x_{r+j} q^{(j)} \|_2^2,$$

which is the squared ℓ_2 distance between the points $\sum_{i=1}^{r} x_i p^{(i)}$ and $\sum_{j=1}^{s} x_{r+j} q^{(j)}$, which lie in $\mathcal{P}$ and $\mathcal{Q}$ respectively, because of the constraints on x. Further, as x ranges over the feasible set, the pair $(\sum_{i=1}^{r} x_i p^{(i)}, \sum_{j=1}^{s} x_{r+j} q^{(j)})$ ranges over all possible pairs of point in $\mathcal{P} \times \mathcal{Q}$ (possibly with redundancy).

(b) Define $y := Cx$. Show that QP found in the preceding part of this question can be expressed as a QP with the objective function $\|y\|_2^2$, viewed as a function of $(x, y) \in \mathbb{R}^n \times \mathbb{R}^d$.

Solution:
An equivalent QP to the one written in the preceding part of this question is

$$\begin{aligned} \min_{x,y} \quad & y^T y \\ \text{subject to:} \quad & y = Cx, \\ & \sum_{i=1}^{r} x_i = 1, \\ & \sum_{j=1}^{s} x_{r+j} = 1, \\ & x_i \geq 0, \ i = 1, \ldots, n, \end{aligned}$$

(c) Show that the dual to the QP in the preceding part of this question takes the form of the unconstrained QP

$$\max_z \left(-\frac{1}{4} z^T z + \min_{1 \le i \le r} z^T p^{(i)} - \max_{1 \le j \le s} z^T q^{(j)} \right),$$

Solution:
We introduce dual variables $\gamma \in \mathbb{R}^d$, $\alpha, \beta \in \mathbb{R}$ and $\lambda \in \mathbb{R}^n$, and write the Lagrangian for the QP in the preceding part of the question as

$$\mathcal{L}((x,y),\gamma,\alpha,\beta,\lambda) \tag{8}$$

$$= y^T y + \gamma^T (y - Cx) + \alpha(\sum_{i=1}^r x_i - 1) + \beta(\sum_{j=1}^s x_{r+j} - 1) - \sum_{i=1}^n \lambda_i x_i \tag{9}$$

$$= \sum_{l=1}^d \left(y_l^2 + \gamma_l y_l\right) + \sum_{i=1}^r \left(\sum_{l=1}^d \gamma_l c_{li} + \alpha - \lambda_i \right) x_i + \sum_{i=r+1}^n \left(\sum_{l=1}^d \gamma_l c_{li} + \beta - \lambda_i \right) x_i - \alpha - \beta. \tag{10}$$

Here γ, α, β are unconstrained, and we are interested in $\lambda \ge 0$, the inequality being interpreted coordinate-wise.

We compute the dual objective function

$$g(\gamma,\alpha,\beta,\lambda) := \inf_{x,y} \mathcal{L}((x,y),\gamma,\alpha,\beta,\lambda),$$

where the infimum is over $(x,y) \in \mathbb{R}^n \times \mathbb{R}^d$, because that is the domain of the primal problem.

We can minimize over each y_l separately, and we observe that

$$\min_{y_l} y_l^2 + \gamma_l y_l = -\frac{1}{4}\gamma_l^2,$$

by straightforward calculus (since the derivative of $y_l^2 + \gamma_l y_l$ is $2y_l + \gamma_l$, which becomes 0 at $y_l = -\frac{1}{2}\gamma_l$, and when we substitute this value for y_l the expression $y_l^2 + \gamma_l y_l$ becomes $-\frac{1}{4}\gamma_l^2$).

Fix λ. For $1 \le i \le r$ we observe that, since α is unconstrained, as long as we have:

$$\sum_{l=1}^d \gamma_l c_{li} - \lambda_i \text{ is the same for all } 1 \le i \le r, \tag{11}$$

we can choose α to make

$$\sum_{l=1}^d \gamma_l c_{li} + \alpha - \lambda_i = 0 \text{ for all } 1 \le i \le r,$$

whereas, if this condition in (11) does not hold then, irrespective of the choice of α, we will get $g(\gamma,\alpha,\beta,\lambda) = -\infty$.

Similarly, For $r+1 \leq i \leq n$ we observe that, since β is unconstrained, as long as we have

$$\sum_{l=1}^{d} \gamma_l c_{li} - \lambda_i \text{ is the same for all } r+1 \leq i \leq n, \tag{12}$$

we can choose β to make

$$\sum_{l=1}^{d} \gamma_l c_{li} + \beta - \lambda_i = 0 \text{ for all } r+1 \leq i \leq n,$$

whereas, if the condition in (12) does not hold then, irrespective of the choice of β, we will get $g(\gamma, \alpha, \beta, \lambda) = -\infty$.

We therefore have

$$g(\gamma, \alpha, \beta, \lambda) = -\frac{1}{4} \sum_{l=1}^{d} \gamma_l^2 - \alpha(\gamma, \lambda_1, \ldots, \lambda_r) - \beta(\gamma, \lambda_{r+1}, \ldots, \lambda_n),$$

if γ and λ are such that the conditions in (11) and (12) hold, where $\alpha(\gamma, \lambda_1, \ldots, \lambda_r)$ – which is uniquely determined by γ and $\lambda_1, \ldots, \lambda_r$ – and $\beta(\gamma, \lambda_{r+1}, \ldots, \lambda_n)$ – which is uniquely determined by γ and $\lambda_{r+1}, \ldots, \lambda_n$ – are defined so that

$$\sum_{l=1}^{d} \gamma_l c_{li} + \alpha - \lambda_i = 0 \text{ for all } 1 \leq i \leq r$$

and

$$\sum_{l=1}^{d} \gamma_l c_{li} + \beta - \lambda_i = 0 \text{ for all } r+1 \leq i \leq n.$$

Further, we have

$$g(\gamma, \alpha, \beta, \lambda) = -\infty$$

otherwise.

Let $\mathcal{F}$ denote the set of pairs (γ, λ) for which the conditions in (11) and (12) hold. Then the dual problem has the form

$$\max_{\gamma, \lambda} -\frac{1}{4} \sum_{l=1}^{d} \gamma_l^2 - \alpha(\gamma, \lambda_1, \ldots, \lambda_r) - \beta(\gamma, \lambda_{r+1}, \ldots, \lambda_n), \, : \, \lambda \geq 0, \ (\gamma, \lambda) \in \mathcal{F}.$$

For any given γ, we would therefore like to choose $\lambda \geq 0$ with $(\gamma, \lambda) \in \mathcal{F}$ to minimize $\alpha(\gamma, \lambda_1, \ldots, \lambda_r) + \beta(\gamma, \lambda_{r+1}, \ldots, \lambda_n)$.

Since we must have $\lambda_i \geq 0$ for all $1 \leq i \leq r$ and $\alpha(\gamma, \lambda_1, \ldots, \lambda_r)$ is being chosen so that $\sum_{l=1}^{d} \gamma_l c_{li} + \alpha - \lambda_i = 0$ for all $1 \leq i \leq r$, we see that we must have

$$\alpha(\gamma, \lambda_1, \ldots, \lambda_r) \geq -\sum_{l=1}^{d} \gamma_l c_{li}$$

for all $1 \leq i \leq r$ and all (γ, λ) such that $\lambda \geq 0$ and $(\gamma, \lambda) \in \mathcal{F}$. Further, for any γ, we see that there is $\lambda \geq 0$ with $(\gamma, \lambda) \in \mathcal{F}$ for which setting $\alpha = \max_{1 \leq i \leq r} - \sum_{l=1}^{d} \gamma_l c_{li}$ works to make $\sum_{l=1}^{d} \gamma_l c_{li} + \alpha - \lambda_i = 0$ for all $1 \leq i \leq r$.

A similar argument works in the range $r+1 \leq l \leq n$.

This allows us to fix λ based on γ and to replace $\alpha(\gamma, \lambda_1, \ldots, \lambda_r)$ by $\max_{1\leq i\leq r} -\sum_{l=1}^{d} \gamma_l c_{li}$ and $\beta(\gamma, \lambda_{r+1}, \ldots, \lambda_n)$ by $\max_{r+1\leq i\leq n} -\sum_{l=1}^{d} \gamma_l c_{li}$.

Since the columns of C for $1 \leq i \leq r$ are the $p^{(i)}$ and the columns of C for $r+1 \leq i \leq n$ are the $-q^{(r+1-i)}$, we now get the dual optimization problem in the form of the unconstrained QP that we were seeking, namely

$$\max_z -\frac{1}{4} z^T z + \min_{1\leq i\leq r} z^T p^{(i)} - \max_{1\leq j\leq s} z^T q^{(j)},$$

where we have used the notation z for γ.

(d) Provide a geometric interpretation of the dual problem formulated in the preceding part of this question.

Solution:

The unconstrained dual QP found in the preceding part of this question can also be written as

$$-\min_z \left(\frac{1}{4} z^T z - \min_{1\leq i\leq r} z^T p^{(i)} + \max_{1\leq j\leq s} z^T q^{(j)} \right), \tag{13}$$

Suppose that $\mathcal{P} \cap \mathcal{Q} \neq \emptyset$. Then the optimal value of the primal problem is 0, because we can find $x_i \geq 0$, $1 \leq i \leq n$, with $\sum_{i=1}^{r} x_i = 1$ and $\sum_{i=r+1}^{n} x_i = 1$ such that $\sum_{i=1}^{r} x_i p^{(i)} = \sum_{j=1}^{s} x_{r+j} q^{(j)}$.

But then, for all $z \in \mathbb{R}^d$ we have

$$\sum_{i=1}^{r} x_i z^T p^{(i)} = \sum_{j=1}^{s} x_{r+j} z^T q^{(j)},$$

and so $\max_{1\leq j\leq s} z^T q^{(j)} \geq \min_{1\leq i\leq r} z^T p^{(i)}$. It follows that the optimal value of the dual problem is 0, achieved, at $z = 0$.

Now suppose that $\mathcal{P} \cap \mathcal{Q} = \emptyset$. Then, because $\mathcal{P}$ and $\mathcal{Q}$ are bounded closed sets, we can find $a \in \mathcal{P}$ and $b \in \mathcal{Q}$ such that the minimum ℓ_2 distance between $\mathcal{P}$ and $\mathcal{Q}$ equals $\|a-b\|_2$. There will be an affine hyperplane orthogonal to the vector $a-b$ which acts a separating hyperplane that strictly separates $\mathcal{P}$ from $\mathcal{Q}$.

An optimal point for the dual problem will then be given by $2(a-b)$. We will have $\min_{1\leq i\leq r}(a-b)^T p^{(i)} = 2(a-b)^T a$ and $\max_{1\leq j\leq s}(a-b)^T q^{(j)} = 2(a-b)^T b$. Also

$$\frac{1}{4}\left(4\|a-b\|_2^2\right) - 2(a-b)^T(a-b) = -\|a-b\|_2^2,$$

explaining why the optimal value of the dual problem equals that of the primal problem.

To see this, first consider dual feasible z of the form $\tau(a-b)$. The objective function for such z is

$$\frac{\tau^2}{4}(a-b)^T(a-b) - \tau \min_{1\leq i\leq r}(a-b)^T p^{(i)} + \tau \max_{1\leq j\leq s}(a-b)^T q^{(j)},$$

and since

$$\min_{1\leq i\leq r} (a-b)^T p^{(i)} = (a-b)^T a,$$

and

$$\max_{1\leq j\leq s} (a-b)^T q^{(j)} = (a-b)^T b,$$

this becomes

$$(\frac{\tau^2}{4} - \tau)(a-b)^T(a-b),$$

which is minimized over $\tau \in \mathbb{R}$ at $\tau = 2$, with value $-\|a-b\|_2^2$.

We now observe that the value of the optimization problem in (13) is the same as that of the optimization problem

$$-\min_z \left(\frac{1}{4}z^T z - \min_{1\leq i\leq r} z^T\left(p^{(i)} - \frac{1}{2}(a+b)\right) + \max_{1\leq j\leq s} z^T\left(q^{(j)} - \frac{1}{2}(a+b)\right)\right),$$

Consider z of the form $z = \tau(a-b) + w$ for some $\tau \in \mathbb{R}$ and $w \in \mathbb{R}^n$ such that $w^T(a-b) = 0$. For such z we can see geometrically that

$$\min_{1\leq i\leq r} (\tau(a-b)+w)^T\left(p^{(i)} - \frac{1}{2}(a+b)\right) \leq \min_{1\leq i\leq r} \tau(a-b)^T\left(p^{(i)} - \frac{1}{2}(a+b)\right),$$

and similarly that

$$\max_{1\leq j\leq s} (\tau(a-b)+w)^T\left(q^{(j)} - \frac{1}{2}(a+b)\right) \geq \max_{1\leq j\leq s} \tau(a-b)^T\left(q^{(j)} - \frac{1}{2}(a+b)\right)$$

so the best choice of w is $w = 0$.