Lecture 11 - The Karush-Kuhn-Tucker Conditions

- The Karush-Kuhn-Tucker conditions are optimality conditions for inequality constrained problems discovered in 1951 (originating from Karush's thesis from 1939).
- Modern nonlinear optimization essentially begins with the discovery of these conditions.

The basic notion that we will require is the one of feasible descent directions.

Definition. Consider the problem

$$\begin{array}{ll} \min & h(\mathbf{x}) \\ \text{s.t.} & \mathbf{x} \in C, \end{array}$$

need not be convex

where h is continuously differentiable over the set $C \subseteq \mathbb{R}^n$. Then a vector $\mathbf{d} \neq 0$ is called a feasible descent direction at $\mathbf{x} \in C$ if $\nabla f(\mathbf{x})^T \mathbf{d} < 0$ and there exists $\varepsilon > 0$ such that $\mathbf{x} + t\mathbf{d} \in C$ for all $t \in [0, \varepsilon]$.

E.g.: n = 3, x is in the interior/boundary of a 2-D disk/3-D ball. Try to picture what the condition means in each of the 4 cases.

The Basic Necessary Condition - No Feasible Descent Directions

Lemma. Consider the problem

$$(\mathrm{G}) \quad \begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & \mathbf{x} \in C, \end{array}$$

where h is continuously differentiable over C. If $\mathbf{x}^*$ is a local optimal solution of (G), then there are no feasible descent directions at $\mathbf{x}^*$.

Proof.

- By contradiction, assume that there exists a vector $\mathbf{d}$ and $\varepsilon_1 > 0$ such that $\mathbf{x} + t\mathbf{d} \in C$ for all $t \in [0, \varepsilon_1]$ and $\nabla f(\mathbf{x}^*)^T \mathbf{d} < 0$.
- By definition of the directional derivative there exists $\varepsilon_2 < \varepsilon_1$ such that $f(\mathbf{x}^* + t\mathbf{d}) < f(\mathbf{x}^*)$ for all $t \in [0, \varepsilon_2] \Rightarrow$ contradiction to the local optimality of $\mathbf{x}^*$.

Consequence

Lemma. Let $\mathbf{x}^*$ be a local minimum of the problem

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m, \end{array}$$

where $f, g_1, \ldots, g_m$ are continuously differentiable functions over $\mathbb{R}^n$. Let $I(\mathbf{x}^*)$ be the set of active constraints at $\mathbf{x}^*$:

$$I(\mathbf{x}^*) = \{i : g_i(\mathbf{x}^*) = 0\}.$$

Then there does not exist a vector $\mathbf{d} \in \mathbb{R}^n$ such that

$$\begin{array}{ll} \nabla f(\mathbf{x}^*)^T \mathbf{d} & < 0, \\ \nabla g_i(\mathbf{x}^*)^T \mathbf{d} & < 0, i \in I(\mathbf{x}^*) \end{array}$$

This means if x* moves in the direction d a little, the active constraints will continue to be satisfied, but become inactive. The inactive ones will stay inactive (and satisfied).

Proof

- Suppose that $\mathbf{d}$ satisfies the system of inequalities.
- Then $\exists \varepsilon_1 > 0$ such that $f(\mathbf{x}^* + t\mathbf{d}) < f(\mathbf{x}^*)$ and $g_i(\mathbf{x}^* + t\mathbf{d}) < g_i(\mathbf{x}^*) = 0$ for any $t \in (0, \varepsilon_1)$ and $i \in I(\mathbf{x}^*)$.
- For any $i \notin I(\mathbf{x}^*)$ we have that $g_i(\mathbf{x}^*) < 0$, and hence, by the continuity of g_i, there exists $\varepsilon_2 > 0$ such that $g_i(\mathbf{x}^* + t\mathbf{d}) < 0$ for any $t \in (0, \varepsilon_2)$ and $i \notin I(\mathbf{x}^*)$.
- Consequently,

$$\begin{aligned} f(\mathbf{x}^* + t\mathbf{d}) &< f(\mathbf{x}^*), \\ g_i(\mathbf{x}^* + t\mathbf{d}) &< 0, \quad i = 1, 2, \ldots, m, \end{aligned}$$

  for all $t \in (0, \min\{\varepsilon_1, \varepsilon_2\})$.
- A contradiction to the local optimality of $\mathbf{x}^*$.

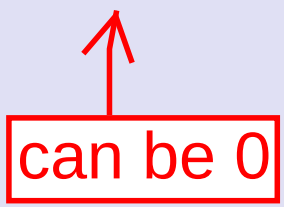
The Fritz-John Necessary Condition

Theorem. Let $\mathbf{x}^*$ be a local minimum of the problem

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m, \end{array}$$

where $f, g_1, \ldots, g_m$ are continuously differentiable functions over $\mathbb{R}^n$. Then there exist multipliers $\lambda_0, \lambda_1, \ldots, \lambda_m \geq 0$, which are not all zeros, such that

$$\begin{aligned} \lambda_0 \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) &= \mathbf{0}, \\ \lambda_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m. \end{aligned}$$



Proof of Fritz-John Conditions

- The following system is infeasible

$$(\mathrm{S}) \quad \nabla f(\mathbf{x}^*)^T \mathbf{d} < 0, \nabla g_i(\mathbf{x}^*)^T \mathbf{d} < 0, i \in I(\mathbf{x}^*)$$

- System (S) is the same as $\mathbf{Ad} < \mathbf{0}$ where $\mathbf{A} = \begin{pmatrix} \nabla f(\mathbf{x}^*)^T \\ \nabla g_{i_1}(\mathbf{x}^*)^T \\ \vdots \\ \nabla g_{i_k}(\mathbf{x}^*)^T \end{pmatrix}$
- By Gordan's theorem of alternative, system (S) is infeasible if and only if there exists a vector $\boldsymbol{\eta} = (\lambda_0, \lambda_{i_1}, \ldots, \lambda_{i_k})^T \neq \mathbf{0}$ such that

$$\mathbf{A}^T \boldsymbol{\eta} = \mathbf{0}, \boldsymbol{\eta} \geq \mathbf{0},$$

- which is the same as $\lambda_0 \nabla f(\mathbf{x}^*) + \sum_{i \in I(\mathbf{x}^*)} \lambda_i \nabla g_i(\mathbf{x}^*) = \mathbf{0}$.
- Define $\lambda_i = 0$ for any $i \notin I(\mathbf{x}^*)$, and we obtain that

$$\lambda_0 \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) = \mathbf{0}, \lambda_i g_i(\mathbf{x}^*) = 0, i = 1, 2, \ldots, m$$

The KKT Conditions for Inequality Constrained Problems

A major drawback of the Fritz-John conditions is that they allow λ_0 to be zero. Under an additional regularity condition, we can assume that $\lambda_0 = 1$.

Theorem. Let $\mathbf{x}^*$ be a local minimum of the problem

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m, \end{array}$$

where $f, g_1, \ldots, g_m$ are continuously differentiable functions over $\mathbb{R}^n$. Suppose that the gradients of the active constraints $\{\nabla g_i(\mathbf{x}^*)\}_{i \in I(\mathbf{x}^*)}$ are linearly independent. Then there exist multipliers $\lambda_1, \lambda_2 \ldots, \lambda_m \geq 0$ such that

$$\begin{aligned} \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) &= \mathbf{0}, \\ \lambda_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m. \end{aligned}$$

Proof of the KKT Conditions for Inequality Constrained Problems

- By the Fritz-John conditions it follows that there exists $\tilde{\lambda}_0, \tilde{\lambda}_1, \ldots, \tilde{\lambda}_m$, not all zeros, such that

$$\begin{aligned} \tilde{\lambda}_0 \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \tilde{\lambda}_i \nabla g_i(\mathbf{x}^*) &= \mathbf{0}, \\ \tilde{\lambda}_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m. \end{aligned}$$

- $\tilde{\lambda}_0 \neq 0$ since otherwise, if $\tilde{\lambda}_0 = 0$

$$\sum_{i \in I(\mathbf{x}^*)} \tilde{\lambda}_i \nabla g_i(\mathbf{x}^*) = \mathbf{0},$$

  where not all the scalars $\tilde{\lambda}_i, i \in I(\mathbf{x}^*)$ are zeros, which is a contradiction to the regularity condition.
- $\tilde{\lambda}_0 > 0$. Defining $\lambda_i = \frac{\tilde{\lambda}_i}{\tilde{\lambda}_0}$, the result follows.

KKT Conditions for Inequality/Equality Constrained Problems

Theorem. Let $\mathbf{x}^*$ be a local minimum of the problem

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m, \\ & h_j(\mathbf{x}) = 0, j = 1, 2, \ldots, p. \end{array} \tag{1}$$

where $f, g_1, \ldots, g_m, h_1, h_2, \ldots, h_p$ are continuously differentiable functions over $\mathbb{R}^n$. Suppose that the gradients of the active constraints and the equality constraints: $\{\nabla g_i(\mathbf{x}^*), \nabla h_j(\mathbf{x}^*), i \in I(\mathbf{x}^*), j = 1, 2, \ldots, p\}$ are linearly independent. Then there exist multipliers $\lambda_1, \lambda_2 \ldots, \lambda_m \geq 0, \mu_1, \mu_2, \ldots, \mu_p \in \mathbb{R}$ such that

$$\begin{aligned} \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) + \sum_{j=1}^{p} \mu_j \nabla h_j(\mathbf{x}^*) &= \mathbf{0}, \\ \lambda_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m. \end{aligned}$$

Terminology

Definition (KKT point) Consider problem (1) where $f, g_1, \ldots, g_m, h_1, h_2, \ldots, h_p$ are continuously differentiable functions over $\mathbb{R}^n$. A feasible point $\mathbf{x}^*$ is called a KKT point if there exist $\lambda_1, \lambda_2 \ldots, \lambda_m \geq 0, \mu_1, \mu_2, \ldots, \mu_p \in \mathbb{R}$ such that

$$\begin{aligned} \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) + \sum_{j=1}^{p} \mu_j \nabla h_j(\mathbf{x}^*) &= \mathbf{0}, \\ \lambda_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m. \end{aligned}$$

Definition (regularity) A feasible point $\mathbf{x}^*$ is called regular if the set $\{\nabla g_i(\mathbf{x}^*), \nabla h_j(\mathbf{x}^*), i \in I(\mathbf{x}^*), j = 1, 2, \ldots, p\}$ is linearly independent.

- The KKT theorem states that a necessary local optimality condition of a regular point is that it is a KKT point.
- The additional requirement of regularity is not required in linearly constrained problems in which no such assumption is needed. (The question is why... this subtlety is hidden in the use of Farkas' and Gordan's theorems)

Examples

1.

$$\begin{array}{ll} \min & x_1 + x_2 \\ \text{s.t.} & x_1^2 + x_2^2 = 1. \end{array}$$

not a convex constraint

Claim: Two KKT points: [1/sqrt(2), 1/sqrt(2)] & [-1/sqrt(2),-1/sqrt(2)]. The latter must be the minimizer.

2.

$$\begin{array}{ll} \min & x_1 + x_2 \\ \text{s.t.} & (x_1^2 + x_2^2 - 1)^2 = 0. \end{array}$$

In class Since 2. is equivalent to 1., the minimizer of 1. must be that of 2. also. However, 2. has no KKT point !

Sufficiency of KKT Conditions in the Convex Case

In the convex case the KKT conditions are always sufficient.

Note: if h(x) is convex, {x : h(x)<=0} is a convex set, but {x: h(x)=0} is NOT a convex set.

Theorem. Let $\mathbf{x}^*$ be a feasible solution of

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m, \\ & h_j(\mathbf{x}) = 0, \quad j = 1, 2, \ldots, p. \end{array} \tag{2}$$

where $f, g_1, \ldots, g_m, h_1, \ldots, h_p$ are continuously differentiable convex functions over $\mathbb{R}^n$ and $h_1, h_2, \ldots, h_p$ are affine functions. Suppose that there exist multipliers $\lambda_1, \ldots, \lambda_m \geq 0, \mu_1, \mu_2, \ldots, \mu_p \in \mathbb{R}$ such that

$$\begin{aligned} \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) + \sum_{j=1}^{p} \mu_j \nabla h_j(\mathbf{x}^*) &= \mathbf{0}, \\ \lambda_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m. \end{aligned}$$

Then $\mathbf{x}^*$ is the optimal solution of (2).

Proof

- Let $\mathbf{x}$ be a feasible solution of (2). We will show that $f(\mathbf{x}) \geq f(\mathbf{x}^*)$.
- The function $s(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{i=1}^{m} \mu_i h_i(\mathbf{x})$ is convex.
- Since $\nabla s(\mathbf{x}^*) = \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) + \sum_{j=1}^{p} \mu_j \nabla h_j(\mathbf{x}^*) = \mathbf{0}$, it follows that $\mathbf{x}^*$ is a minimizer of s over $\mathbb{R}^n$, and in particular $s(\mathbf{x}^*) \leq s(\mathbf{x})$.
- Thus,

$$\begin{aligned} f(\mathbf{x}^*) &= f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}^*) + \sum_{j=1}^{p} \mu_j h_j(\mathbf{x}^*) \\ &= s(\mathbf{x}^*) \\ &\leq s(\mathbf{x}) \\ &= f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{p} \mu_j h_j(\mathbf{x}) \\ &\leq f(\mathbf{x}) \end{aligned}$$

Convex Constraints - Necessity under Slater's Condition

If the constraints are convex, regularity can be replaced by Slater's condition.

Theorem (necessity of the KKT conditions under Slater's condition) Let $\mathbf{x}^*$ be a local optimal solution of the problem

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m. \end{array} \tag{3}$$

where $f, g_1, \ldots, g_m$ are continuously differentiable over $\mathbb{R}^n$. In addition, $g_1, g_2, \ldots, g_m$ are convex over $\mathbb{R}^n$. Suppose $\exists \hat{\mathbf{x}} \in \mathbb{R}^n$ such that

$$g_i(\hat{\mathbf{x}}) < 0, \quad i = 1, 2, \ldots, m.$$

Then there exist multipliers $\lambda_1, \lambda_2 \ldots, \lambda_m \geq 0$ such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) = \mathbf{0}, \tag{4}$$

$$\lambda_i g_i(\mathbf{x}^*) = 0, \quad i = 1, 2, \ldots, m. \tag{5}$$

Proof

- Since $\mathbf{x}^*$ is an optimal solution of (3), the Fritz-John conditions are satisfied: there exist $\tilde{\lambda}_0, \tilde{\lambda}_1, \ldots, \tilde{\lambda}_m \geq 0$ not all zeros, such that

$$\begin{aligned} \tilde{\lambda}_0 \nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \tilde{\lambda}_i \nabla g_i(\mathbf{x}^*) &= \mathbf{0}, \\ \tilde{\lambda}_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m. \end{aligned} \tag{6}$$

- We will prove that $\tilde{\lambda}_0 > 0$, and then conditions (4) and (5) will be satisfied with $\lambda_i = \frac{\tilde{\lambda}_i}{\tilde{\lambda}_0}, i = 1, 2, \ldots, m$.
- Assume in contradiction that $\tilde{\lambda}_0 = 0$. Then

$$\sum_{i=1}^{m} \tilde{\lambda}_i \nabla g_i(\mathbf{x}^*) = \mathbf{0}. \tag{7}$$

- By the gradient inequality,

$$0 > g_i(\hat{\mathbf{x}}) \geq g_i(\mathbf{x}^*) + \nabla g_i(\mathbf{x}^*)^T (\hat{\mathbf{x}} - \mathbf{x}^*), i = 1, 2, \ldots, m.$$

Proof Contd.

- Multiplying the i-th equation by $\tilde{\lambda}_i$ and summing over $i = 1, 2, \ldots, m$ we obtain

$$0 > \sum_{i=1}^{m} \tilde{\lambda}_i g_i(\mathbf{x}^*) + \left[\sum_{i=1}^{m} \tilde{\lambda}_i \nabla g_i(\mathbf{x}^*) \right]^T (\hat{\mathbf{x}} - \mathbf{x}^*), \tag{8}$$

- Plugging the identities (7) and (6) into (8) we obtain the impossible statement that $0 > 0$, thus establishing the result.

Examples

1.

$$\begin{array}{ll} \min & x_1^2 - x_2 \\ \text{s.t.} & x_2 = 0. \end{array}$$

.

2.

$$\begin{array}{ll} \min & x_1^2 - x_2 \\ \text{s.t.} & x_2^2 \leq 0. \end{array}$$

The optimal solution is $(x_1, x_2) = (0, 0)$. Satisfies KKT conditions for problem 1, but not for problem 2. In class

The constraint in 2 does not satisfy the regularity condition at (0,0), nor does it satisfy Slater's condition. And indeed, the optimal solution cannot be solved based on solving the KKT condition (let's check it) !

The Convex Case - Generalized Slater's Condition

Definition (Generalized Slater's Condition) Consider the system

$$\begin{aligned} g_i(\mathbf{x}) &\leq 0, \quad i = 1, 2, \ldots, m, \\ h_j(\mathbf{x}) &\leq 0, \quad j = 1, 2, \ldots, p, \\ s_k(\mathbf{x}) &= 0, \quad k = 1, 2, \ldots, q, \end{aligned}$$

where $g_i, i = 1, 2, \ldots, m$ are convex functions over $\mathbb{R}^n$ and $h_j, s_k, j = 1, 2, \ldots, p, k = 1, 2, \ldots, q$ are affine functions over $\mathbb{R}^n$. Then we say that the generalized Slater's condition is satisfied if there exists $\hat{\mathbf{x}} \in \mathbb{R}^n$ for which

$$\begin{aligned} g_i(\hat{\mathbf{x}}) &< 0, \quad i = 1, 2, \ldots, m, \\ h_j(\hat{\mathbf{x}}) &\leq 0, \quad j = 1, 2, \ldots, p, \\ s_k(\hat{\mathbf{x}}) &= 0, \quad k = 1, 2, \ldots, q, \end{aligned}$$

In particular, when we only have the affine part of the constraints (i.e. back to the setting of Chapter 10), this demands only that the feasible set is non-empty.

Necessity of KKT under Generalized Slater

Theorem. Let $\mathbf{x}^*$ be an optimal solution of the problem

$$\begin{array}{lll} \min & f(\mathbf{x}) & \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, & i = 1,2,\ldots,m, \\ & h_j(\mathbf{x}) \leq 0, & j = 1,2,\ldots,p, \\ & s_k(\mathbf{x}) = 0, & k = 1,2,\ldots,q, \end{array} \tag{9}$$

where $f, g_1, \ldots, g_m$ are continuously differentiable convex functions and $h_j, s_k, j = 1,2,\ldots,p, k = 1,2,\ldots,q$ are affine. Suppose that the generalized Slater's condition is satisfied. Then there exist multipliers $\lambda_1, \lambda_2 \ldots, \lambda_m, \eta_1, \eta_2, \ldots, \eta_p \geq 0, \mu_1, \mu_2, \ldots, \mu_q \in \mathbb{R}$ such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\mathbf{x}^*) + \sum_{j=1}^{p} \eta_j \nabla h_j(\mathbf{x}^*) + \sum_{k=1}^{q} \mu_k \nabla s_k(\mathbf{x}^*) = \mathbf{0},$$

$$\lambda_i g_i(\mathbf{x}^*) = 0, \quad i = 1,2,\ldots,m,$$

$$\eta_j h_j(\mathbf{x}^*) = 0, \quad j = 1,2,\ldots,p.$$

Example

$$\begin{array}{ll} \min & 4x_1^2 + x_2^2 - x_1 - 2x_2 \\ \text{s.t.} & 2x_1 + x_2 \leq 1, \\ & x_1^2 \leq 1. \end{array}$$

In class

Slater's condition is clearly satisfied with (0,0). Together with convexity in both the objective and the constraints, the KKT conditions are both necc. and suff. for optimality.
So let's write and the KKT system and solve it:

Constrained Least Squares

$$\text{(CLS)} \quad \begin{array}{ll} \min & \|\mathbf{A}\mathbf{x}-\mathbf{b}\|^2, \\ \text{s.t.} & \|\mathbf{x}\|^2 \leq \alpha, \end{array}$$

where $\mathbf{A} \in \mathbb{R}^{m\times n}$ has full column rank, $\mathbf{b} \in \mathbb{R}^m, \alpha > 0$

- Problem (CLS) is a convex problem and satisfies Slater's condition.
- Lagrangian: $L(\mathbf{x},\lambda) = \|\mathbf{A}\mathbf{x}-\mathbf{b}\|^2 + \lambda(\|\mathbf{x}\|^2 - \alpha). \quad (\lambda \geq 0)$
- KKT conditions:

$$\begin{aligned} \nabla_{\mathbf{x}} L = 2\mathbf{A}^T(\mathbf{A}\mathbf{x}-\mathbf{b}) + 2\lambda\mathbf{x} &= 0, \\ \lambda(\|\mathbf{x}\|^2 - \alpha) &= 0, \\ \|\mathbf{x}\|^2 &\leq \alpha, \lambda \geq 0. \end{aligned}$$

- If $\lambda = 0$, then by the first equation

$$\mathbf{x} = \mathbf{x}_{\mathrm{LS}} \equiv (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}.$$

Optimal iff $\|\mathbf{x}_{\mathrm{LS}}\|^2 \leq \alpha$.

Constrained Least Squares Contd.

- On the other hand, if $\|\mathbf{x}_{\mathrm{LS}}\|^2 > \alpha$, then necessarily $\lambda > 0$. By the C-S condition we have that $\|\mathbf{x}\|^2 = \alpha$ and the first equation implies that

$$\mathbf{x} = \mathbf{x}_\lambda \equiv (\mathbf{A}^T\mathbf{A} + \lambda \mathbf{I})^{-1}\mathbf{A}^T\mathbf{b}.$$

  The multiplier $\lambda > 0$ should be chosen to satisfy $\|\mathbf{x}_\lambda\|^2 = \alpha$, that is, λ is the solution of

$$f(\lambda) = \|(\mathbf{A}^T\mathbf{A} + \lambda \mathbf{I})^{-1}\mathbf{A}^T\mathbf{b}\|^2 - \alpha = 0.$$

- $f(0) = \|(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}\|^2 - \alpha = \|\mathbf{x}_{\mathrm{LS}}\|^2 - \alpha > 0$, f strictly decreasing and $f(\lambda) \to -\alpha$ as $\lambda \to \infty$.
- Conclusion: the optimal solution of the CLS problem is given by

$$\mathbf{x} = \begin{cases} \mathbf{x}_{\mathrm{LS}} & \|\mathbf{x}_{\mathrm{LS}}\|^2 \leq \alpha, \\ (\mathbf{A}^T\mathbf{A} + \lambda \mathbf{I})^{-1}\mathbf{A}^T\mathbf{b} & \|\mathbf{x}_{\mathrm{LS}}\|^2 > \alpha \end{cases}$$

  where λ is the unique root of $f(\lambda)$ over $(0, \infty)$.

Second Order Necessary Optimality Conditions

Theorem. Consider the problem

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & f_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m, \end{array}$$

where $f_0, f_1, \ldots, f_m$ are continuously differentiable over $\mathbb{R}^n$. Let $\mathbf{x}^*$ be a local minimum, and suppose that $\mathbf{x}^*$ is regular meaning that $\{\nabla f_i(\mathbf{x}^*)\}_{i \in I(\mathbf{x}^*)}$ are linearly independent. Then $\exists \lambda_1, \lambda_2, \ldots, \lambda_m \geq 0$ such that

$$\begin{array}{rcl} \nabla_{\mathbf{x}} L(\mathbf{x}^*, \boldsymbol{\lambda}) & = & \mathbf{0}, \\ \lambda_i f_i(\mathbf{x}^*) & = & 0, \quad i = 1, 2, \ldots, m, \end{array}$$

and $\mathbf{y}^T \nabla^2_{\mathbf{xx}} L(\mathbf{x}^*, \boldsymbol{\lambda}) \mathbf{y} \geq 0$ for all $\mathbf{y} \in \Lambda(\mathbf{x}^*)$ where

$$\Lambda(\mathbf{x}^*) \equiv \{\mathbf{d} \in \mathbb{R}^n : \nabla f_i(\mathbf{x}^*)^T \mathbf{d} = 0, i \in I(\mathbf{x}^*)\}.$$

See proof of Theorem 11.18 in the book

Second Order Necessary Optimality Conditions for Inequality/Equality Constrained Problems

Theorem. Consider the problem

$$\begin{array}{ll} \min & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \ldots, m, \\ & h_j(\mathbf{x}) = 0, j = 1, 2, \ldots, p. \end{array}$$

where $f, g_1, \ldots, g_m, h_1, \ldots, h_p$ are continuously differentiable. Let $\mathbf{x}^*$ be a local minimum and suppose that $\mathbf{x}^*$ is regular meaning that the set $\{\nabla g_i(\mathbf{x}^*), \nabla h_j(\mathbf{x}^*), i \in I(\mathbf{x}^*), j = 1, 2, \ldots, p\}$ is linearly independent. Then $\exists \lambda_1, \lambda_2, \ldots, \lambda_m \geq 0$ and $\mu_1, \mu_2, \ldots, \mu_p \in \mathbb{R}$ such that

$$\begin{aligned} \nabla_{\mathbf{x}} L(\mathbf{x}^*, \boldsymbol{\lambda}, \boldsymbol{\mu}) &= \mathbf{0}, \\ \lambda_i g_i(\mathbf{x}^*) &= 0, \quad i = 1, 2, \ldots, m, \end{aligned}$$

and $\mathbf{d}^T \nabla^2_{\mathbf{xx}} L(\mathbf{x}^*, \boldsymbol{\lambda}, \boldsymbol{\mu}) \mathbf{d} \geq 0$ for all $\mathbf{d} \in \Lambda(\mathbf{x}^*) \equiv \{\mathbf{d} \in \mathbb{R}^n : \nabla g_i(\mathbf{x}^*)^T \mathbf{d} = 0, \nabla h_j(\mathbf{x}^*)^T \mathbf{d} = 0, i \in I(\mathbf{x}^*), j = 1, 2, \ldots, p\}$.

Optimality Conditions for the Trust Region Subproblem

The Trust Region Subproblem (TRS) is the problem consisting of minimizing an indefinite quadratic function subject to an l_2-norm constraint:

$$\text{(TRS)}: \quad \min\{f(\mathbf{x}) \equiv \mathbf{x}^T\mathbf{A}\mathbf{x} + 2\mathbf{b}^T\mathbf{x} + c : \|\mathbf{x}\|^2 \leq \alpha\},$$

where $\mathbf{A} = \mathbf{A}^T \in \mathbb{R}^{n\times n}$, $\mathbf{b} \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Although the problem is nonconvex, it possesses necessary and sufficient optimality conditions.

Theorem A vector $\mathbf{x}^*$ is an optimal solution of problem (TRS) if and only if there exists $\lambda^* \geq 0$ such that

$$\begin{aligned}
(\mathbf{A} + \lambda^*\mathbf{I})\mathbf{x}^* &= -\mathbf{b} && (10)\\
\|\mathbf{x}^*\|^2 &\leq \alpha, && (11)\\
\lambda^*(\|\mathbf{x}^*\|^2 - \alpha) &= 0, && (12)\\
\mathbf{A} + \lambda^*\mathbf{I} &\succeq \mathbf{0}. && (13)
\end{aligned}$$

Proof

Sufficiency:

- Assume that $\mathbf{x}^*$ satisfies (10)-(13) for some $\lambda^* \geq 0$.
- Define the function

$$h(\mathbf{x}) = \mathbf{x}^T\mathbf{A}\mathbf{x}+2\mathbf{b}^T\mathbf{x}+c+\lambda^*(\|\mathbf{x}\|^2-\alpha) = \mathbf{x}^T(\mathbf{A}+\lambda^*\mathbf{I})\mathbf{x}+2\mathbf{b}^T\mathbf{x}+c-\alpha\lambda^*. \quad (14)$$

- Then by (13) we have that h is a convex quadratic function. By (10) it follows that $\nabla h(\mathbf{x}^*) = 0$, which implies that $\mathbf{x}^*$ is the unconstrained minimizer of h over $\mathbb{R}^n$.
- Let $\mathbf{x}$ be a feasible point, i.e., $\|\mathbf{x}\|^2 \leq \alpha$. Then

$$\begin{array}{lll} f(\mathbf{x}) & \geq f(\mathbf{x}) + \lambda^*(\|\mathbf{x}\|^2 - \alpha) & (\lambda^* \geq 0, \|\mathbf{x}\|^2 - \alpha \leq 0) \\ & = h(\mathbf{x}) & (\text{by (14)}) \\ & \geq h(\mathbf{x}^*) & (\mathbf{x}^* \text{ is the minimizer of } h) \\ & = f(\mathbf{x}^*) + \lambda^*(\|\mathbf{x}^*\|^2 - \alpha) & \\ & = f(\mathbf{x}^*) & (\text{by (12)}) \end{array}$$

Proof Contd.

Necessity:

- If $\mathbf{x}^*$ is a minimizer of (TRS), then by the second order necessary conditions there exists $\lambda^* \geq 0$ such that

$$\begin{aligned}
(\mathbf{A}+\lambda^*\mathbf{I})\mathbf{x}^* &= -\mathbf{b} && (15)\\
\|\mathbf{x}^*\|^2 &\leq \alpha, && (16)\\
\lambda^*(\|\mathbf{x}^*\|^2-\alpha) &= 0, && (17)\\
\mathbf{d}^T(\mathbf{A}+\lambda^*\mathbf{I})\mathbf{d} &\geq 0 \quad \text{for all } \mathbf{d} \text{ satisfying } \mathbf{d}^T\mathbf{x}^*=0. && (18)
\end{aligned}$$

- Need to show that (18) is true **for any d**.
- Suppose on the contrary that there exists a $\mathbf{d}$ such that $\mathbf{d}^T\mathbf{x}^* > 0$ and $\mathbf{d}^T(\mathbf{A}+\lambda^*\mathbf{I})\mathbf{d} < 0$.
- Consider the point $\bar{\mathbf{x}} = \mathbf{x}^* + t\mathbf{d}$, where $t = -2\frac{\mathbf{d}^T\mathbf{x}^*}{\|\mathbf{d}\|^2}$. The vector $\bar{\mathbf{x}}$ is a feasible point since

$$\begin{aligned}
\|\bar{\mathbf{x}}\|^2 &= \|\mathbf{x}^*+t\mathbf{d}\|^2 = \|\mathbf{x}^*\|^2 + 2t\mathbf{d}^T\mathbf{x}^* + t^2\|\mathbf{d}\|^2\\
&= \|\mathbf{x}^*\|^2 - 4\frac{(\mathbf{d}^T\mathbf{x}^*)^2}{\|\mathbf{d}\|^2} + 4\frac{(\mathbf{d}^T\mathbf{x}^*)^2}{\|\mathbf{d}\|^2} = \|\mathbf{x}^*\|^2 \leq \alpha.
\end{aligned}$$

Proof Contd.

- In addition,

$$\begin{aligned}
f(\bar{\mathbf{x}}) &= \bar{\mathbf{x}}^T\mathbf{A}\bar{\mathbf{x}} + 2\mathbf{b}^T\bar{\mathbf{x}} + c \\
&= (\mathbf{x}^* + t\mathbf{d})^T\mathbf{A}(\mathbf{x}^* + t\mathbf{d}) + 2\mathbf{b}^T(\mathbf{x}^* + t\mathbf{d}) + c \\
&= \underbrace{(\mathbf{x}^*)^T\mathbf{A}\mathbf{x}^* + 2\mathbf{b}^T\mathbf{x}^* + c}_{f(\mathbf{x}^*)} + t^2\mathbf{d}^T\mathbf{A}\mathbf{d} + 2t\mathbf{d}^T(\mathbf{A}\mathbf{x}^* + \mathbf{b}) \\
&= f(\mathbf{x}^*) + t^2\mathbf{d}^T(\mathbf{A} + \lambda^*\mathbf{I})\mathbf{d} + 2t\mathbf{d}^T(\underbrace{(\mathbf{A} + \lambda^*\mathbf{I})\mathbf{x}^* + \mathbf{b}}_{=\mathbf{0} \text{ by}(15)}) \\
&\quad -\lambda^* t\underbrace{\left[t\|\mathbf{d}\|^2 + 2\mathbf{d}^T\mathbf{x}^*\right]}_{=0} \\
&= f(\mathbf{x}^*) + t^2\mathbf{d}^T(\mathbf{A} + \lambda^*\mathbf{I})\mathbf{d} \\
&< f(\mathbf{x}^*),
\end{aligned}$$

which is a contradiction to the optimality of $\mathbf{x}^*$.

Total Least Squares

Consider the approximate set of linear equations:

$$\mathbf{A}\mathbf{x} \approx \mathbf{b}$$

- In the Least Squares (LS) approach we only assume that the RHS vector $\mathbf{b}$ is subjected to noise.

$$\begin{array}{ll} \min_{\mathbf{w},\mathbf{x}} & \|\mathbf{w}\|^2 \\ \text{s.t.} & \mathbf{A}\mathbf{x} = \mathbf{b} + \mathbf{w}, \\ & \mathbf{w} \in \mathbb{R}^m. \end{array}$$

- In the Total Least Squares (TLS) we assume that both the RHS vector $\mathbf{b}$ and the model matrix $\mathbf{A}$ are subjected to noise

$$\text{(TLS)} \quad \begin{array}{ll} \min_{\mathbf{E},\mathbf{w},\mathbf{x}} & \|\mathbf{E}\|_F^2 + \|\mathbf{w}\|^2 \\ \text{s.t.} & (\mathbf{A}+\mathbf{E})\mathbf{x} = \mathbf{b} + \mathbf{w}, \\ & \mathbf{E} \in \mathbb{R}^{m\times n}, \mathbf{w} \in \mathbb{R}^m. \end{array}$$

The TLS problem – as formulated – seems like a difficult nonconvex problem. We will see that it can be solved efficiently.

Eliminating the $\mathbf{E}$ and $\mathbf{w}$ variables

- Fixing $\mathbf{x}$, we will solve the problem

$$(P_{\mathbf{x}}) \quad \begin{array}{ll} \min_{\mathbf{E},\mathbf{w}} & \|\mathbf{E}\|_F^2 + \|\mathbf{w}\|^2 \\ \text{s.t.} & (\mathbf{A}+\mathbf{E})\mathbf{x} = \mathbf{b} + \mathbf{w}. \end{array}$$

- The KKT conditions are necessary and sufficient for problem $(P_{\mathbf{x}})$.
- Lagrangian: $L(\mathbf{E},\mathbf{w},\boldsymbol{\lambda}) = \|\mathbf{E}\|_F^2 + \|\mathbf{w}\|^2 + 2\boldsymbol{\lambda}^T[(\mathbf{A}+\mathbf{E})\mathbf{x} - \mathbf{b} - \mathbf{w}]$.
- By the KKT conditions, $(\mathbf{E},\mathbf{w})$ is an optimal solution of $(P_{\mathbf{x}})$ if and only if there exists $\boldsymbol{\lambda} \in \mathbb{R}^m$ such that

$$2\mathbf{E} + 2\boldsymbol{\lambda}\mathbf{x}^T = \mathbf{0} \qquad (\nabla_{\mathbf{E}} L = \mathbf{0}), \tag{19}$$

$$2\mathbf{w} - 2\boldsymbol{\lambda} = \mathbf{0} \qquad (\nabla_{\mathbf{w}} L = \mathbf{0}), \tag{20}$$

$$(\mathbf{A}+\mathbf{E})\mathbf{x} = \mathbf{b} + \mathbf{w} \quad \text{(feasibility)}. \tag{21}$$

- By (19), (20) and (21), $\mathbf{E} = -\boldsymbol{\lambda}\mathbf{x}^T, \mathbf{w} = \boldsymbol{\lambda}$ and $\boldsymbol{\lambda} = \frac{\mathbf{A}\mathbf{x}-\mathbf{b}}{\|\mathbf{x}\|^2+1}$. Plugging this into the objectve function, a reduced formulation in the variables $\mathbf{x}$ is obtained.

The New Formulation of (TLS)

$$\text{(TLS')} \quad \min_{\mathbf{x}\in\mathbb{R}^n} \frac{\|\mathbf{A}\mathbf{x}-\mathbf{b}\|^2}{\|\mathbf{x}\|^2+1}.$$

Theorem $\mathbf{x}$ is an optimal solution of (TLS') if and only if $(\mathbf{x},\mathbf{E},\mathbf{w})$ is an optimal solution of (TLS) where $\mathbf{E}=-\frac{(\mathbf{A}\mathbf{x}-\mathbf{b})\mathbf{x}^T}{\|\mathbf{x}\|^2+1}$ and $\mathbf{w}=\frac{\mathbf{A}\mathbf{x}-\mathbf{b}}{\|\mathbf{x}\|^2+1}$

- Still a nonconvex problem.
- Resembles the problem of minimizing the Rayleigh quotient.

Solving the Fractional Quadratic Formulation

Under a rather mild condition, the optimal solution of (TLS') can be derived via a homogenization argument.

- (TLS') is the same as

$$\min_{\mathbf{x}\in\mathbb{R}^n, t\in\mathbb{R}} \left\{ \frac{\|\mathbf{A}\mathbf{x} - t\mathbf{b}\|^2}{\|\mathbf{x}\|^2 + t^2} : t = 1 \right\}.$$

- the same as (denoting $\mathbf{y} = \begin{pmatrix} \mathbf{x} \\ t \end{pmatrix}$):

$$f^* = \min_{\mathbf{y}\in\mathbb{R}^{n+1}} \left\{ \frac{\mathbf{y}^T\mathbf{B}\mathbf{y}}{\|\mathbf{y}\|^2} : y_{n+1} = 1 \right\}, \tag{22}$$

where

$$\mathbf{B} = \begin{pmatrix} \mathbf{A}^T\mathbf{A} & -\mathbf{A}^T\mathbf{b} \\ -\mathbf{b}^T\mathbf{A} & \|\mathbf{b}\|^2 \end{pmatrix}.$$

Solving the Fractional Quadratic Formulation Contd.

We will consider the following relaxed version:

$$g^* = \min_{\mathbf{y} \in \mathbb{R}^{n+1}} \left\{ \frac{\mathbf{y}^T \mathbf{B} \mathbf{y}}{\|\mathbf{y}\|^2} : \mathbf{y} \neq \mathbf{0} \right\}, \tag{23}$$

Lemma. Let $\mathbf{y}^*$ be an optimal solution of (23) and assume that $y^*_{n+1} \neq 0$. Then $\tilde{\mathbf{y}} = \frac{1}{y^*_{n+1}} \mathbf{y}^*$ is an optimal solution of (22).

Proof.

- $f^* \geq g^*$.
- $\tilde{\mathbf{y}}$ is feasible for (22) and we have

$$f^* \leq \frac{\tilde{\mathbf{y}}^T \mathbf{B} \tilde{\mathbf{y}}}{\|\tilde{\mathbf{y}}\|^2} = \frac{\frac{1}{(y^*_{n+1})^2} (\mathbf{y}^*)^T \mathbf{B} \mathbf{y}^*}{\frac{1}{(y^*_{n+1})^2} \|\mathbf{y}^*\|^2} = \frac{(\mathbf{y}^*)^T \mathbf{B} \mathbf{y}^*}{\|\mathbf{y}^*\|^2} = g^*.$$

- Therefore, $\tilde{\mathbf{y}}$ is an optimal solution of both (22) and (23).

Main Result on TLS

Theorem. Assume that the following condition holds:

$$\lambda_{\min}(\mathbf{B}) < \lambda_{\min}(\mathbf{A}^T\mathbf{A}), \tag{24}$$

where

$$\mathbf{B} = \begin{pmatrix} \mathbf{A}^T\mathbf{A} & -\mathbf{A}^T\mathbf{b} \\ -\mathbf{b}^T\mathbf{A} & \|\mathbf{b}\|^2 \end{pmatrix}.$$

Then the optimal solution of problem (TLS') is given by $\frac{1}{y_{n+1}}\mathbf{v}$, where $\mathbf{y} = \begin{pmatrix} \mathbf{v} \\ y_{n+1} \end{pmatrix}$ is an eigenvector corresponding to the min. eigenvalue of $\mathbf{B}$.

Proof.

- All we need to prove is that under condition (24), an optimal solution $\mathbf{y}^*$ of (23) must satisfy $y^*_{n+1} \neq 0$.
- Assume on the contrary that $y^*_{n+1} = 0$. Then

$$\lambda_{\min}(\mathbf{B}) = \frac{(\mathbf{y}^*)^T\mathbf{B}\mathbf{y}^*}{\|\mathbf{y}^*\|^2} = \frac{\mathbf{v}^T\mathbf{A}^T\mathbf{A}\mathbf{v}}{\|\mathbf{v}\|^2} \geq \lambda_{\min}(\mathbf{A}^T\mathbf{A}),$$

which is a contradiction to (24).