Numerical Optimization

Lecture Notes #28
Constrained Optimization

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Outline

Introduction

We have spent a lots of effort on the Unconstrained Optimization problem, we now take a very quick look at the fundamentals of Constrained Optimization — we will quickly realize that things get quite "interesting!"

Problem 0: Constrained Optimization

$$\min_{\vec{x}\in\mathbb{R}^n} f(\vec{x}) \quad \text{subject to} \begin{cases} c_i(\vec{x}) = 0, & i \in \mathcal{E} \\ c_i(\vec{x}) \geq 0, & i \in \mathcal{I} \end{cases}$$

where $i \in \mathcal{E}$ are the equality constraints, and $i \in \mathcal{I}$ the inequality constraints.

The smoothness (or lack thereof) for the objective $f(\vec{x})$ and the constraint functions $c_i(\vec{x})$ will impact the difficulty of solving the problem.

The Feasible Set

With the following definition of all allowable points:

Definition (The Feasible Set)

Let

$$\Omega = \{\vec{x} \in \mathbb{R}^n \,:\, c_i(\vec{x}) = 0 \;\forall i \in \mathcal{E}, \text{ and } c_i(\vec{x}) \geq 0 \;\forall i \in \mathcal{I}\}$$

We can rewrite the problem more compactly as

Problem 1: Constrained Optimization

$$\min_{\vec{x}\in\Omega} f(\vec{x}).$$

Our goal is to state necessary and sufficient conditions for optimality.

Local Solution

Definition (Local Solution)

A point $\vec{x}^*$ is a local solution of Problem 1 if $\vec{x}^* \in \Omega$ and there is a neighborhood $\mathcal{N}$ of $\vec{x}^*$ such that $f(\vec{x}) \geq f(\vec{x}^*)$ $\forall \vec{x} \in \mathcal{N} \cap \Omega$.

Definition (Strict Local Solution)

A point $\vec{x}^*$ is a strict local solution of Problem 1 if $\vec{x}^* \in \Omega$ and there is a neighborhood $\mathcal{N}$ of $\vec{x}^*$ such that $f(\vec{x}) > f(\vec{x}^*)$ $\forall \vec{x} \in \mathcal{N} \cap \Omega$.

Definition (Isolated Local Solution)

A point $\vec{x}^*$ is an isolated local solution of Problem 1 if $\vec{x}^* \in \Omega$ and there is a neighborhood $\mathcal{N}$ of $\vec{x}^*$ such that $\vec{x}^*$ is the only local solution in $\mathcal{N} \cap \Omega$.

Smoothness

It is usually (always?) advantageous to express constraints and objectives in as smooth a way as possible; *e.g.* we can replace single non-smooth conditions, like

ns $\|\vec{x}\|_1 = |x_1| + |x_2| \leq 1$

with several smooth constraints

s#1 $x_1 + x_2 \leq 1$

s#2 $x_1 - x_2 \leq 1$

s#3 $-x_1 + x_2 \leq 1$

s#4 $-x_1 - x_2 \leq 1$

The Active Set

Definition (Active Set)

The active set $\mathcal{A}(\vec{x})$ at any feasible $\vec{x}$ consists of the equality constraint indices from $\mathcal{E}$ and the indices of the inequality constraint indices from $\mathcal{I}$ for which $c_i(\vec{x}) = 0$, *i.e.*

$$\mathcal{A}(\vec{x}) = \mathcal{E} \cup \{\, i \in \mathcal{I} \,:\, c_i(\vec{x}) = 0 \,\}.$$

At a feasible point $\vec{x}$, the inequality constraint $i \in \mathcal{I}$ is said to be active if $c_i(\vec{x}) = 0$ and inactive if $c_i(\vec{x}) > 0$.

Linear Independence Constraint Qualification

Definition (LICQ: Linear Independence Constraint Qualification)

Give a the point $\vec{x}$ and the active set $\mathcal{A}(\vec{x})$, we say that the linear independence constrain qualification (LICQ) holds if the set of active constraint gradients

$$\{\nabla c_i(\vec{x}),\ i \in \mathcal{A}(\vec{x})\}$$

is linearly independent.

The Lagrangian Function

Our final building block before stating the first order conditions for optimality is the:

Definition (The Lagrangian Function, $\mathcal{L}(\vec{x}, \vec{\lambda})$)

$$\mathcal{L}(\vec{x}, \vec{\lambda}) = f(\vec{x}) - \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i c_i(\vec{x})$$

The Lagrange multipliers, λ_i, are used to "pull" the solution back to the feasible set.

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KKT First Order Necessary Conditions

Theorem (KKT:FONC — First Order Necessary Conditions)

Suppose that $\vec{x}^*$ is a local solution to Problem 1, that the functions f and c_i are continuously differentiable, and that the LICQ holds at $\vec{x}^*$. Then there is a Lagrange multiplier vector $\vec{\lambda}^*$, with components $\lambda_i(\vec{x}^*)$, $i \in \mathcal{E} \cup \mathcal{I}$, such that the following conditions are satisfied at $(\vec{x}^*, \vec{\lambda}^*)$:

$$\begin{aligned}
\nabla_{\vec{x}} \mathcal{L}(\vec{x}, \vec{\lambda}) &= 0, \\
c_i(\vec{x}^*) &= 0, \quad \forall i \in \mathcal{E} \\
c_i(\vec{x}^*) &\geq 0, \quad \forall i \in \mathcal{I} \\
\lambda_i^* &\geq 0, \quad \forall i \in \mathcal{I} \\
\lambda_i^* c_i(\vec{x}^*) &= 0, \quad i \in \mathcal{I} \cup \mathcal{E}.
\end{aligned}$$

The Karush–Kuhn–Tucker conditions.

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KKT First Order Necessary Conditions (compact form)

Theorem (KKT:FONC — Compact Form)

Suppose that $\vec{x}^*$ is a local solution to Problem 1, that the functions f and c_i are continuously differentiable, and that the LICQ holds at $\vec{x}^*$. Then there is a Lagrange multiplier vector $\vec{\lambda}^*$, with components $\lambda_i(\vec{x}^*)$, $i \in \mathcal{E} \cup \mathcal{I}$, such that the following conditions are satisfied at $(\vec{x}^*, \vec{\lambda}^*)$:

$$0 = \nabla_{\vec{x}} \mathcal{L}(\vec{x}, \vec{\lambda}) = \nabla f(\vec{x}^*) - \sum_{i \in \mathcal{A}(\vec{x}^*)} \lambda_i^* \nabla c_i(\vec{x}^*).$$

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Strict Complementarity

Definition (Strict Complementarity)

Given a local solution $\vec{x}^*$ of Problem 1, and a vector $\vec{\lambda}^*$ satisfying the KKT:FONC, we say that the strict complementarity condition holds if exactly one of λ_i^* or $c_i(\vec{x}^*)$ is zero for each index $i \in \mathcal{I}$. In other words, we have $\lambda_i^* > 0 \ \forall i \in \mathcal{I} \cap \mathcal{A}(\vec{x}^*)$.

We sweep the proof of KKT:FONC under our infinitely stretchable rug. Not because it is not important (it is!), but we are somewhat short on time.

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Linearized Feasible Directions

Definition (Set of Linearized Feasible Directions)

Given a feasible point $\vec{x}$ and the active constrain set $\mathcal{A}(\vec{x})$, the set of linearized feasible directions is

$$\mathcal{F}(\vec{x}) = \left\{ \vec{d} \text{ such that } \begin{array}{ll} \vec{d}^T \nabla c_i(\vec{x}) = 0, & \forall i \in \mathcal{E} \\ \vec{d}^T \nabla c_i(\vec{x}) \geq 0, & \forall i \in \mathcal{A}(\vec{x}) \cap \mathcal{I} \end{array} \right\}$$

Second Order Conditions

Second order conditions will help determine the impact of directions $\vec{w} \in \mathcal{F}(\vec{x}^*)$ for which $\vec{w}^T \nabla f(\vec{x}^*) = 0$, *i.e.* directions which are "locally flat."

From this point on we need the functions f and c_i to be twice continuously differentiable.

Critical Cone

Given $\mathcal{F}(\vec{x}^*)$, and some Lagrange multiplier vector λ^* satisfying KKT:FONC, we define:

Definition (Critical Cone)

$$C(\vec{x}^*, \vec{\lambda}^*) = \{\, \vec{w} \in \mathcal{F}(\vec{x}^*) \,:\, \nabla c_i(\vec{x}^*)^T \vec{w} = 0, \forall i \in \mathcal{A}(\vec{x}^*) \cap \mathcal{I} \text{ with } \lambda_i^* = 0 \,\}.$$

Or equivalently

$$\vec{w} \in C(\vec{x}^*, \vec{\lambda}^*) \Leftrightarrow \left\{ \begin{array}{ll} \nabla c_i(\vec{x}^*)^T \vec{w} = 0, & \forall i \in \mathcal{E} \\ \nabla c_i(\vec{x}^*)^T \vec{w} = 0, & \forall i \in \mathcal{A}(\vec{x}^*) \cap \mathcal{I} \text{ with } \lambda_i^* > 0 \\ \nabla c_i(\vec{x}^*)^T \vec{w} \geq 0, & \forall i \in \mathcal{A}(\vec{x}^*) \cap \mathcal{I} \text{ with } \lambda_i^* = 0 \end{array} \right.$$

The critical cone $C(\vec{x}^*, \vec{\lambda}^*)$ contains the directions from $\mathcal{F}(\vec{x}^*)$ for which it is not clear from first derivative information whether f will increase or decrease.

Second Order Necessary Conditions

Theorem (Second Order Necessary Conditions)

Suppose that $\vec{x}^*$ is a local solution of Problem 1, and that the LICQ condition is satisfied. Let $\vec{\lambda}^*$ be the Lagrange multiplier vector for which the KKT:FONC are satisfied. Then

$$\vec{w}^T \nabla^2_{\vec{x}\vec{x}} \mathcal{L}(\vec{x}, \vec{\lambda}) \vec{w} \geq 0, \ \forall \vec{w} \in C(\vec{x}^*, \vec{\lambda}^*).$$

Interpretation: The Hessian of the Lagrangian has non-negative curvature along critical directions.

Second Order Sufficient Conditions

Theorem (Second Order Sufficient Conditions)

Suppose that for some feasible point $\vec{x}^* \in \mathbb{R}^n$ there is a Langrange multiplier vector $\vec{\lambda}^*$ such that KKT:FONC are satisfied. Suppose also that

$$\vec{w}^T \nabla^2_{\vec{x}\vec{x}} \mathcal{L}(\vec{x}, \vec{\lambda}) \vec{w} > 0,\ \forall \vec{w} \in C(\vec{x}^*, \vec{\lambda}^*),\ \ \vec{w} \neq \vec{0}.$$

Then $\vec{x}^*$ is a strict local solution for Problem 1.

Much remains to be said; however, everything grows out of these fundamental definitions and theorems; leveraging special cases, weakening and strengthening conditions, and looking for alternatives.

Some Approaches

- **Linear Programming — The Simplex Method**
  - f and c_i linear functions
  - Leonid Kantorovich, 1939 — Linear Programming.
  - George Datzig, 1947 — The Simplex Method.
  - John von Neumann, 1947 — Theory of Duality.
  - The *worst case complexity* for The Simplex Method is exponential, but it is remarkably efficient in practice.

Some Approaches

- **Interior Point Methods, Primal-Dual Methods**
  - c_i are *strict* inequalities.
  - Better theoretical behavior than The Simplex Method.
  - Leonid Khachiyan, 1979 — The Ellipsoid Method (polynomial runtime, $\mathcal{O}(n^6 L)$)
  - Narendra Karmarkar, 1984 — Projective Algorithm, $\mathcal{O}(n^{3.5} L^2 \cdot \log L \cdot \log\log L)$, where n is the number of variables and L is the number of bits of input to the algorithm.

Some Approaches

- **Quadratic Programming**
  - Special case: Exploit the structure of the problem:
  - Quadratic Objective, Linear Constraints
  - Active Set methods
  - Interior Point methods
  - Gradient Projection methods
  - Appears as sub-problems for: Sequential Quadratic Programming, Penalty/Augmented Lagrangian Methods, and Interior Point Methods.

Some Approaches

- **Penalty / Augmented Lagrangian Methods**
  - Constraints are represented by additions to the objective
  - *Quadratic Penalty Terms* — add the square of the constraint discrepancies: intuitive, fairly simple to implement
  - *Non-smooth Penalty Terms* — ℓ_1 and ℓ_0 penalty functions
  - *Method of Multipliers* — estimated for the Lagrange multipliers are used.

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