LECTURE 3: OPTIMALITY CONDITIONS

- 1. First order and second order information
- 2. Necessary and sufficient conditions of optimality
- 3. Convex functions
- 4. Elementary solution methods

General setting

General form nonlinear programming problem

Min f(x)s. t. $x \in S \subset E^n$

where S can be a "simple" set

or
$$S \triangleq \{x \in E^n \mid g_i(x) \le 0, i = 1, ..., m;$$

 $h_j(x) = 0, j = 1, ..., n;$
 $x \in X\}$

Local minimum

Definition A point $x^* \in S$ is said to be a relative minimum point or a local minimum point of f over Sif there is an $\epsilon > 0$ such that $f(x) \ge f(x^*)$ for all $x \in$ $S \cap N(x^*, \epsilon)$, where $N(x^*, \epsilon)$ is the neighborhood of x^* of radius ϵ . If $f(x) > f(x^*)$ for all $x \in S \cap N(x^*, \epsilon)$ and $x \ne x^*$, then x^* is said to be a strictly relative minimum point of f over S.

Global minimum

Definition A point $x^* \in S$ is said to be a global minimum point of f over S if $f(x) \ge f(x^*)$ for all $x \in$ S. If $f(x) > f(x^*)$ for all $x \in S, x \neq x^*$, then x^* is said to be a strictly global minimum point of f over S.

Comments

- We always intend to seek a global minimum when formulating an optimization problem.
- In most situations, optimization theory and methodologies only enable us to locate local minimums.
- Global optimality can be achieved when certain convexity conditions are imposed.

A general iterative scheme

• A general scheme of an iterative solution procedure:

Step 1: Start from a feasible solution *x* in S.

Step 2: Check if the current solution is optimal.If the answer is Yes, stop.If the answer is No, continue.

Step 3: Move to a better feasible solution and return to Step 2.

What are the feasible moves that lead to a better solution?

Feasible direction

- Along any given direction, the objective function can be regarded as a function of a single variable.
- Given x ∈ S ⊂ Eⁿ, a vector d ∈ Eⁿ is a feasible direction at x if there is an ᾱ > 0 such that x + αd ∈ S for all α, 0 ≤ α ≤ ᾱ.
- A feasible direction is a good direction, if the objective function is reduced along the direction.

How do we know we have attained a minimum solution?

- First order necessary condition
 - Proposition. Let S be a subset of Eⁿ and let f
 ∈ C¹ be a function on S. If x* is a relative
 minimum point of f over S, then for any d ∈ Eⁿ
 that is a feasible direction at x*, we have
 ∇f(x*)d ≥ 0.
 - Corollary (Unconstrained case). Let S be a subset of Eⁿ and let f ∈ C¹ be a function on S. If x^{*} is a relative minimum point of f over S and if x^{*} is an interior point of S, then ∇f(x^{*}) = 0.

Example 1

Example: Constrained problem:

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

Check if $x^* = [1/2, 0]$ satisfies the first-order necessary condition or not.

$$abla f(x) \mid_{x^{\star}} = [2x_1 - 1 + x_2, 1 + x_1] \mid_{x_1 = 1/2, x_2 = 0}$$

= [0, 3/2]

 $\Rightarrow \nabla f(x^*)d \ge 0$ for all d with $d_2 \ge 0$ (feasible direction at x^*).

Example 2

Example: Unconstrained problem:

$$\min f(x_1, x_2) = x_1^2 - x_1 x_2 + x_2^2 - 3x_2$$

Global minimum is known at $x_1 = 1, x_2 = 2$. At this point, $\nabla f(x) = [2x_1 - x_2, -x_1 + 2x_2 - 3]$ = [0, 0]

Comments

- The necessary conditions in the pure unconstrained case lead to a system of *n* equations in *n* unknowns.
- Is the condition a sufficient condition? Why?
- How about the condition of

 $\nabla f(x^*)d > 0?$

Proof of the proposition

If \exists a feasible direction $d \in E^n$ at x^* with $\nabla f(x^*)d < 0$, then $\exists \bar{\alpha} > 0$ s.t. $x(\alpha) = x^* + \alpha d \in S$ with $0 < \alpha < \bar{\alpha}$ and

$$\begin{aligned} f(x(\alpha)) &= f(x^*) + \nabla f(x^*)(x(\alpha) - x^*) + O(\alpha^2) \\ &= f(x^*) + \alpha \nabla f(x^*)d + O(\alpha^2) \\ &< f(x^*) , \text{ if } \alpha \text{ is sufficiently small.} \end{aligned}$$

This contradicts to the fact that x^* is a local minimum point of f over S.

Corollary – Variational Inequalities

 Proposition: Let S ⊂ Eⁿ be convex and f: Eⁿ → R be C¹(S). If x* is a relative minimum point of f over S, then x* is a solution of the following variational inequality problem:

Find $x \in S$ (VI) s. t. $\langle x' - x, \nabla f(x) \rangle \ge 0$, $\forall x' \in S$.

Second order conditions

Proposition (Second-order necessary conditions). Let S be a subset of E^n and let $f \in C^2$ be a function on S. If x^* is a relative minimum point of f over S, then for any $d \in E^n$ that is a feasible direction at x^* , we have

(i) ∇ f(x*)d ≥ 0.
(ii) if ∇ f(x*)d = 0, then d^T∇²f(x*)d ≥ 0.

Proof:

$$\begin{aligned} f(x(\alpha)) &= f(x^*) + \frac{1}{2}(x(\alpha) - x^*)^T \nabla^2 f(x^*)(x(\alpha) - x^*) + O(\alpha^3) \\ &= f(x^*) + \frac{1}{2}\alpha^2 d^T \nabla^2 f(x^*) d + O(\alpha^3) \end{aligned}$$

Example 3

Example: Constrained problem:

min
$$f(x_1, x_2) = x_1^2 - x_1 + x_2 + x_1 x_2$$

s. t. $x_1, x_2 \ge 0$

Check if $x^* = [1/2, 0]$ satisfies the second-order necessary condition or not.

 $\nabla f(x) \mid_{x^*} = [0, 3/2]$, since $\nabla f(x^*)d = 3/2d_2 = 0$ $\Rightarrow d_2 = 0$ $\Rightarrow d^T \nabla^2 f(x^*)d = 2d_1^2 \ge 0$

Second order necessary condition

Proposition (Second-order necessary conditions – unconstrained case). Let x* be an interior point of the set S, and suppose x* is a relative minimum point of f ∈ C². Then
(i) ∇f(x*) = 0.
(ii) F(x*) is positive semidefinite.

Example 4

Example: Unconstrained problem:

$$\min f(x_1, x_2) = x_1^2 - x_1 x_2 + x_2^2 - 3x_2$$

Global minimum is known at $x_1 = 1, x_2 = 2$. At this point, $\nabla f(x) = [2x_1 - x_2, -x_1 + 2x_2 - 3]$ = [0, 0]

and F(x) is positive definite.

Example 5

Example: Constrained problem:

min
$$f(x_1, x_2) = x_1^3 - x_1^2 x_2 + 2x_2^2$$

s. t. $x_1, x_2 \ge 0$

 $x^* = [6, 9]$ is a solution to the first-order necessary condition:

$$\nabla f(x) |_{x} = [3x_{1}^{2} - 2x_{1}x_{2}, -x_{1}^{2} + 4x_{2}] = 0$$

But, x^* does not satisfy the second-order necessary condition,

$$F = \begin{bmatrix} 6x_1 - 2x_2 & -2x_1 \\ -2x_1 & 4 \end{bmatrix} \Big|_{x^*} = \begin{bmatrix} 18 & -12 \\ -12 & 4 \end{bmatrix}$$

Second order sufficient condition

Proposition (Second-order sufficient conditions

 unconstrained case). Let f ∈ C² be a function
 on a region in which the point x* is an interior point.

 Suppose in addition that

(i)
$$\nabla f(x^*) = 0$$
.

(ii) F(x^{*}) is positive definite.

Then x^* is a strictly relative minimum point of f.

Example 6

Min
$$f(x) = \frac{1}{4}x^4 - 2x^3 + \frac{11}{2}x^2 - 6x + 1$$

s. t. $0 \le x \le 4$.



Continue

First-order information:

$$f'(x) = x^3 - 6x^2 + 11x - 6 = (x - 1)(x - 2)(x - 3).$$

 $f'(0) = -6, \ f'(1) = f'(2) = f'(3) = 0, \ f'(4) = 6.$

Second-order information:

$$f''(x) = 3x^2 - 12x + 11$$

$$\Rightarrow f''(1) > 0, f''(2) < 0, f''(3) > 0.$$

By checking the 1st-order necessary conditions, only x = 1, x = 2 and x = 3 are satisfied.

By checking the 2nd-order necessary conditions, only x = 1 and x = 3 are satisfied.

By checking the 2nd-order sufficient conditions, we know $x^* = 1$ or 3 with $f(x^*) = -1.25$.

Convex functions - definition

• Let $\Omega \subset E^n$ be a convex set and

 $f:\Omega\to R$ be a real-valued function. Then f is convex on $\Omega,$ if

 $\begin{aligned} f(\alpha x^1 + (1 - \alpha)x^2) &\leq \alpha f(x^1) + (1 - \alpha)f(x^2) \\ \forall \ x^1, x^2 \in \Omega \quad \text{and} \quad \alpha \in [0, 1]. \\ \text{Moreover, } f \text{ is strictly convex on } \Omega, \text{ if} \\ f(\alpha x^1 + (1 - \alpha)x^2) &< \alpha f(x^1) + (1 - \alpha)f(x^2) \\ \forall \ x^1 \neq x^2, \ \ x^1, x^2 \in \Omega \quad \text{and} \quad \alpha \in (0, 1). \end{aligned}$

Concave functions

• $g: \Omega \to R$ is (strictly) concave on Ω , if f = -g is (strictly) convex on Ω .

Graph and epigraph of a function

• Let $\Omega \subset E^n$ and $f : \Omega \to R$.

The graph of f is

 $gra(f) \triangleq \{(x, z) \in E^{n+1} \mid x \in \Omega \text{ and}$ $f(x) = z\}$

The epigraph of f is

 $epi(f) \triangleq \{(x, z) \in E^{n+1} \mid x \in \Omega \text{ and} f(x) \leq z\}$



Set based definition of convex functions

- Definition
 - A function f : Ω ⊂ Eⁿ → R is convex if epi(f) is a convex subset of Eⁿ⁺¹.
 - <u>Theorem</u>:

For a convex function f, if each point in gra(f) is an extreme point of epi(f), then the function f is strictly convex.

Question

Let $f: \Omega \subset E^n \to R$ be convex and $f \in C^1(\Omega)$. For $x^0 \in \Omega$, what's the supporting hyperplane of epi(f) at $(x^0, f(x^0))$



Overestimate by two-point information



• <u>Theorem</u>:

Let f be a convex function on a convex set $\Omega \subset E^n$.

Then

$$f(\sum_{i=1}^{m} \alpha_{i} x^{i}) \leq \sum_{i=1}^{m} \alpha_{i} f(x^{i})$$

$$f(x^{i} \in \Omega, \quad \alpha_{i} \in [0, 1] \quad and \quad \sum_{i=1}^{m} \alpha_{i} = 1$$

(Jensen's inequality)

• <u>Theorem</u>:

Let $f \in C^1$. Then f is convex on a convex set $\Omega \subset E^n$ if, and only if,

 $f(y) \geq f(x) + \nabla f(x)(y-x), \quad \forall x, y \in \Omega$ f(x)y x X r (underestimate by one-point information)

Proof

$\begin{array}{l} (\Rightarrow) \mbox{ If } f \mbox{ is convex, then for } x,y \in \Omega, \\ f(\alpha y + (1 - \alpha)x) \ \leq \ \alpha f(y) + (1 - \alpha)f(x), \ \forall \alpha \in [0, 1] \\ \mbox{ For } \alpha \neq 0, \\ \\ \frac{f(x + \alpha(y - x)) - f(x)}{\alpha} \ \leq \ f(y) - f(x) \end{array}$

As $\alpha \rightarrow 0$, we have

$$\nabla f(x)(y-x) \leq f(y) - f(x)$$

Proof

(⇐) Assume that

 $\begin{array}{ll} f(y) \ \ge \ f(x) + \nabla f(x)(y-x), & \forall x, y \in \Omega \\ \text{Given } x^1, x^2 \in \Omega \ , \ \text{and any } \bar{\alpha} \in [0,1]. \\ \text{Consider} & \bar{x} = \bar{\alpha}x^1 + (1-\bar{\alpha})x^2, \ \text{then} \\ & f(x^1) \ \ge \ f(\bar{x}) + \nabla f(\bar{x})(x^1 - \bar{x}) \\ & f(x^2) \ \ge \ f(\bar{x}) + \nabla f(\bar{x})(x^2 - \bar{x}) \end{array}$

Multiplying the first by $\bar{\alpha}$ and the second by $1 - \bar{\alpha}$ and adding up, we have

$$\bar{\alpha}f(x^{1}) + (1-\bar{\alpha})f(x^{2}) \ge f(\bar{x}) + \nabla f(\bar{x})(\bar{\alpha}x^{1} + (1-\bar{\alpha})x^{2} - \bar{x})$$

$$= f(\bar{\alpha}x^{1} + (1-\bar{\alpha})x^{2}) + \nabla f(\bar{x})(0)$$

$$= f(\bar{\alpha}x^{1} + (1-\bar{\alpha})x^{2})$$

Basic properties - 4 and 5

• <u>Theorem</u>:

Let $\Omega \subset E^n$ be a convex set, $f_1, f_2 : \Omega \to R$ be convex functions.

Then (i) $f_1 + f_2$ is convex on Ω (ii) βf_1 is convex on Ω , $\forall \beta \ge 0$

• <u>Theorem</u>:

Let f be a convex function on a convex set $\Omega \subset E^n$. Then the set

 $I_c \triangleq \{x \in \Omega \mid f(x) \le c\}$ is convex, $\forall c \in R$.

• <u>Theorem</u>:

Let $f \in C^2$ and $\Omega \subset E^n$ is convex with $int(\Omega) \neq \phi$. Then f is convex on Ω , if and only if, the Hessian matrix F is positive semidefinite over Ω .

Proof

By Taylor's Theorem, $\begin{aligned} f(y) &= f(x) + \nabla f(x)(y-x) \\ &+ \frac{1}{2}(y-x)^T F(x+\alpha(y-x))(y-x) \end{aligned}$ for some $\alpha \in [0,1].$

• <u>Theorem</u>:

Let $S \subset E^n$ be convex and $f : S \to R$. Then f is (strictly) convex if, and only if, $g(s) \triangleq f(x^0 + sd)$ is (strictly) convex on $I \triangleq \{s \in R \mid x^0 + sd \in S\}$ for any given $x^0 \in S$ and $d \in E^n$.

• <u>Theorem</u>:

Let f be (strictly) convex on $S \subset E^n$ and x = My + b is an affine transformation from E^m to E^n . Then $g(y) \triangleq f(My + b)$ is (strictly) convex on $\{y \in E^m \mid My + b \in S\}$, if M has full rank.

• <u>Theorem</u>:

Let f_j , j = 1, ..., p, be convex on $S \subset E^n$ and $\alpha_j \ge 0$. Then $f \triangleq \sum_{j=1}^p \alpha_j f_j$ is convex on S. In addition, if $\exists i$ such that f_i is strictly convex on S and $\alpha_i > 0$, then $f \triangleq \sum_{j=1}^p \alpha_j f_j$ is strictly convex on S.

• <u>Theorem</u>:

Let f_j , j = 1, 2, ..., be convex on $S \subset E^n$. If $\lim_{j \to \infty} f_j(x)$ exists for each $x \in S$, then $f(x) \triangleq \lim_{j \to \infty} f_j(x)$ is convex on S.

• <u>Theorem</u>:

Let Ω be an index set and $\{f_w \mid w \in \Omega\}$ be a family of convex functions on $S \subset E^n$.

Then,
$$f(x) \triangleq \sup_{w \in \Omega} f_w(x)$$
 is convex on

 $\{x \in S \mid \sup_{w \in \Omega} f_w(x) < +\infty\}$. In addition, if Ω

is finite and f_w is strictly convex for each

 $w \in \Omega$, then f is strictly convex on S.

• <u>Theorem</u>:

Let f_1 be convex on $S_1 \,\subset E^n$ and f_2 be convex and non-decreasing on a set $T \supset f_1(S_1)$. Then the composition function $f_2 \circ f_1(x) \triangleq f_2(f_1(x))$ is convex on S_1 . In addition, if f_1 is strictly convex on S_1 and f_2 is increasing, then $f_2 \circ f_1$ is strictly convex on S_1 .

Minimization of convex functions

• Theorem:

Let f be a convex function defined on the convex set S. Then any relative minimum of f is a global minimum and the set τ where f achieves its minimum is convex.

Proof

(i) If $x^* \in \Omega$ is a local minimum and $\exists y \in \Omega$ with $f(y) < f(x^*)$, then $f(\alpha y + (1 - \alpha)x^*) \le \alpha f(y) + (1 - \alpha)f(x^*) < f(x^*)$ for $\alpha \in (0, 1)$

This contradicts to the fact that x^* is a local minimum.

(*ii*) $\tau = \{x \mid f(x) \leq f(x^*), x \in \Omega\}$ is obviously convex.

Sufficient and necessary conditions

 For convex functions, the first order necessary condition is also a sufficient condition.

• Theorem:

Let $f \in C^1$ be convex on a convex set $\Omega \subset E^n$. If $\exists x^* \in \Omega$, s.t.

 $\nabla f(x^*)(y - x^*) \ge 0, \quad \forall y \in \Omega$

then x^* is a global minimum of f over Ω

Proof

Proof: Since

 $f(y) \ge f(x^*) + \nabla f(x^*)(y - x^*) \ge f(x^*), \ \forall y \in \Omega,$ and any $y \in \Omega$ can be reached from x^* along a feasible direction $y - x^*$.

Example

 Example: Check the convexity of the following optimization problem and find its (global) minimum.

$$\min f(x_1, x_2, x_3) = 4x_1^2 + 3x_2^2 + 5x_3^2 + 6x_1x_2 + x_1x_3 - 3x_1 - 2x_2$$

Maximization of convex functions

• Theorem:

Let f be a convex function defined on the bounded, closed convex set $\Omega \subset E^n$. If fachieves global maximum on Ω , then one maximizer falls in bdry (Ω).

Proof

Assume $x^* \in \Omega$ is a global maximizer of f. If x^* is not a boundary point of Ω , then $\exists x^1, x^2 \in bdry(\Omega)$ s.t. $x^* = \alpha x^1 + (1 - \alpha) x^2$ for some $\alpha \in (0, 1)$ By convexity of f, $f(x^*) \le \alpha f(x^1) + (1 - \alpha) f(x^2)$ $\leq \max \{f(x^1), f(x^2)\}$ Therefore either x^1 or x^2 is a global maximizer.

Non-differentiable convex functions

- Where is the first order information?
 - subgradient and subdifferential



Subgradient and subdifferential

Definition

A vector y is said to be a subgradient of a convex function f (over a set S) at a point x^0 if

$$f(x) \ge f(x^0) + \langle y, x - x^0 \rangle, \forall x \in S$$

Definition

The set of all subgradients of f at x^0 iis called the subdifferential of f at x^0 and is denoted by

$$\partial f(x^0) = \{ y \in E^n \mid f(x) \ge f(x^0) + \langle y, x - x^0 \rangle, \forall x \in S \}$$

Properties

1. The graph of the affine function

$$h(x) = f(x^0) + \langle y, x - x^0 \rangle_{t}$$

is a non-vertical supporting hyperplane to the convex set epi(f) at the point of $(x^0, f(x^0))$.

- 2. The subdifferential set $\partial f(x^0)$ is closed and convex.
- 3. $\partial f(x^0)$ can be empty, singleton, or a set with infinitely many elements. When it is not empty, *f* is said to be subdifferentiable at x^0 .
- 4. $\nabla f(x^0) \in \partial f(x^0)$ if f is differentiable at x^0 . $\{\nabla f(x^0)\} = \partial f(x^0)$ if f is convex and differentiable at $x^0 \in int(S)$.

Examples

- In *R*, f(x) = |x| is subdifferentiable at every point and $\partial f(0) = [-1, 1]$.
- In E^n , the Euclidean norm f(x) = ||x|| is subdifferentiable at every point and $\partial f(0)$ consists of all the vectors y such that

 $||x|| \ge \langle y, x \rangle$ for all x.

This means the Euclidean unit ball !

Elementary Solution Methods

 Two elementary solution methods for the unconstrained optimization problem

Minimize $f(\mathbf{x})$ for $\mathbf{x} \in \mathbf{E}^n$

1. First order information based Gradient descent method

(Steepest decent method)

2. Second order information based Newton's method (Newton-Raphson method)

Gradient Decent Method

- Motivation:
 - Negative gradient direction is the steepest decent direction to reduce the function value.
- Gradient Decent Method
 - 1. Start from a guess point $x_0 \in E^n$ (or *S*) and set k = 0.
 - 2. At iterate x_k , move along the negative gradient direction with an appropriate step size $\gamma_k > 0$ to generate the next iterate

 $\mathbf{x}_{k+1} = \mathbf{x}_{\mathbf{k}} - \gamma_k [\nabla f(\mathbf{x}_k)]^T$

and reset $k \leftarrow k + 1$

3. Return to 2 until $x_{k+1} \approx x_k$

Newton's Method

Motivation – one variable

$$f(x) : E^1 \to R \text{ and } f \in C^2$$

 $\min_{x \in R} f(x)$

• At a point $x_k \in E^1$, make the 2nd order Taylor expansion of f

$$f(x_k + t) \approx f(x_k) + f'(x_k)t + \frac{1}{2}f''(x_k)t^2$$

 If f''(x_k) ≥ 0, then the quadratic approximation is a convex function of variable t ∈ R, and its minimum can be found by setting the derivative to be 0.

Newton's Method

$$0 = \frac{d}{dt}(f(x_k) + f'(x_k) + \frac{1}{2}f''(x_k)t^2)$$

= $f'(x_k) + f''(x_k)t$

• The minimum is achieved at $t = -\frac{f'(x_k)}{f''(x_k)}$.

Hence, we take

$$x_k = x_k + t = x_k - \frac{f'(x_k)}{f''(x_k)}$$

Newton's Method

Extension to multi-variable

$$f(\mathbf{x}) : E^n \to R \text{ and } f \in C^2$$

$$\min_{\mathbf{x} \in E^n} f(\mathbf{x})$$

Newton step

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - F(\boldsymbol{x}_k)^{-1} \ [\nabla f(\boldsymbol{x}_k)]^T$$

- Newton's Method
 - 1. Start from a guess point $x_0 \in E^n$ (or *S*), and set k = 0.
 - 2. At iterate x_k , take a Newton step to generate the next iterate x_{k+1} , and reset $k \leftarrow k + 1$
 - 3. Return to 2 until $x_{k+1} \approx x_k$

Damped Newton's Method

Replace the Newton step

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - F(\boldsymbol{x}_k)^{-1} \ [\nabla f(\boldsymbol{x}_k)]^T$$

by a modified Newton step

$$x_{k+1} = x_k - \gamma F(x_k)^{-1} [\nabla f(x_k)]^T$$

for $\gamma \in (0,1]$

where γ is taken to satisfy the Wolfe conditions or Armijio's condition.

Performance

1. Newton's method is not necessarily convergent.

- 2. When it converges, it may converge to a local minimum, or a saddle point.
- 3. Depends on the existence and computations of the inverse of Hessian.
- 4. Convergence result:

When *f* is strongly convex with Lipschitz Hessian, provided that x_0 is close enough to the minimizer x^* , the Newton's method converges to the minimizer in a quadratic rate, i.e., $||x_{k+1} - x^*|| \le \frac{1}{2} ||x_k - x^*||^2, \forall k \ge 0$

Comments

- Newton step takes a "conditioned" negative gradient direction, when the second-order information is available.
- When it works, the Newton's method take "more computational efforts" to determine a "better direction" that may move in a "more straight-forward" path to reach the destination.
- See gradient decent method vs. Newton's method



https://en.wikipedia.org/wiki/File:Newton_optimization_vs_grad_descent.svg