ORF522 – Linear and Nonlinear Optimization

13. Optimality conditions for nonlinear optimization

Bartolomeo Stellato — Fall 2022

Upcoming Lectures

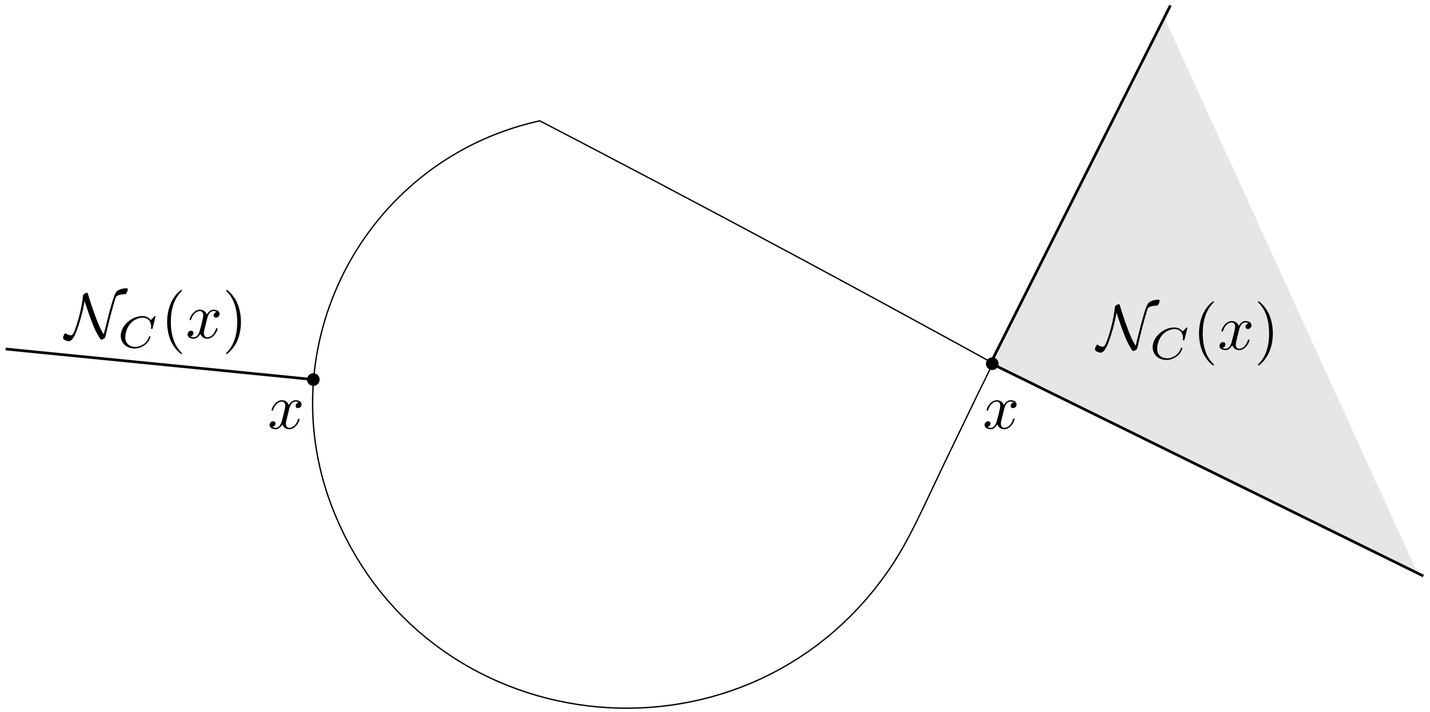
13	10/27	Optimality conditions		[Ch 2 and 12, NO] [Ch 4 and 5, CO]
14	11/01	Gradient descent		[Ch 1 and 2, ICLO] [Ch 9, CO] [Ch 5, FMO]
15	11/03	Subgradient methods	3 Out	[Ch 3 and 8, FMO] [ee364b] [Ch 3, ILCO]
16	11/08	Proximal algorithms		[Ch 3 and 6, FMO] [PA] [PMO]
17	11/10	Operator theory I	3 Due	[Ch 4, FMO] [PA] [PMO] [LSMO]
18	11/15	Operator theory II		[Ch 4, FMO] [PA] [PMO] [LSMO]
19	11/17	Operator splitting algorithms	4 Out	[PMO] [PA] [LSMO] [ADMM]
20	11/29	Acceleration schemes	4 Due	[Ch 1, FMO] [Ch 2, ILCO] [Ch 3, COAC]

Recap

Normal cone

For any set C and point $x \in C$, we define

$$\mathcal{N}_C(x) = \left\{ g \mid g^T(y - x) \leq 0, \quad \text{for all } y \in C \right\}$$



Gradient

Derivative

If $f(x) : \mathbf{R}^n \to \mathbf{R}^m$ continuously differentiable, we define

$$Df(x)_{ij} = \frac{\partial f_i(x)}{\partial x_j}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n$$

Gradient

If $f : \mathbf{R}^n \to \mathbf{R}$, we define

$$\nabla f(x) = Df(x)^T$$

Example

$$f(x) = (1/2)x^T P x + q^T x$$

$$\nabla f(x) = Px + q$$

First-order approximation

$$f(y) \approx f(x) + \nabla f(x)^T (y - x)$$

(affine function of y)

Hessian

Hessian matrix (second derivative)

If $f(x) : \mathbf{R}^n \to \mathbf{R}$ second-order differentiable, we define

$$\nabla^2 f(x)_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n$$

Example

$$f(x) = (1/2)x^T P x + q^T x$$
$$\nabla^2 f(x) = P$$

Second-order approximation

$$f(y) \approx f(x) + \nabla f(x)^T (y - x) + (1/2)(y - x)^T \nabla^2 f(x)(y - x)$$

(quadratic function of y)

Today's lecture

[Chapter 2 and 12, N and W][Chapter 4 and 5, B and V]

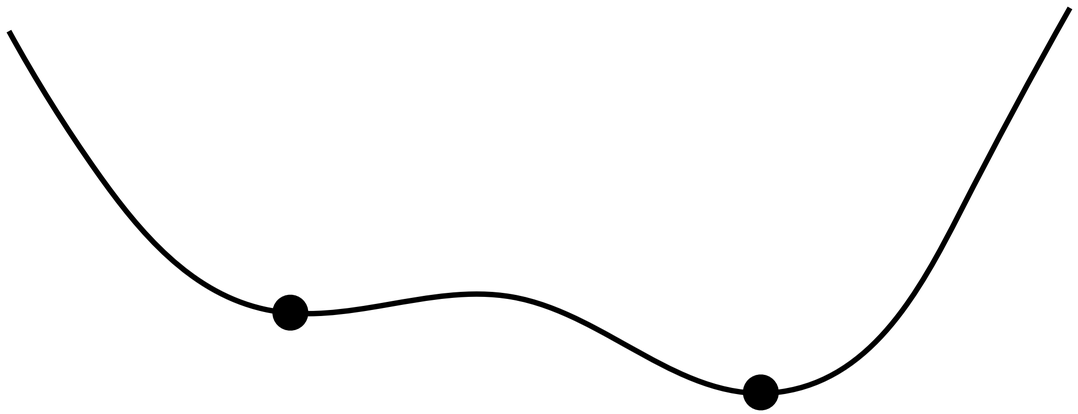
Optimality conditions for nonlinear optimization

- Unconstrained optimization
- Constrained optimization
- KKT optimality conditions
- Convex constrained nonconvex optimization

Unconstrained optimization

First-order necessary conditions

Fermat's Theorem



Theorem

If $x^\star$ is a local optimizer for the continuously differentiable function f, then

$$\nabla f(x^\star) = 0$$

First-order necessary condition

Proof (contraposition)

Assume that $\nabla f(x^\star) \neq 0$. Define $d = -\nabla f(x^\star)$. Then,

$$\nabla f(x^\star)^T d = -\|\nabla f(x^\star)\|^2 < 0$$

Then, by Taylor approximation

$$f(x^\star + td) = f(x^\star) + t\nabla f(x^\star)^T d + o(t)$$

With small enough t, we can find $y = x^\star + td$ in the neighborhood of $x^\star$ such that

$$f(y) < f(x^\star)$$

$\blacksquare$

Example: least-squares

$$\text{minimize} \quad \|Ax - b\|_2^2$$

$$f(x) = \|Ax - b\|_2^2 = (Ax - b)^T(Ax - b) = x^T A^T Ax - 2x^T A^T b + b^T b$$

First-order optimality condition

$$\nabla f(x) = 2A^T(Ax - b) = 0$$

$\longrightarrow$

Normal-equations

$$A^T Ax = A^T b$$

(they always have a solution)

Explicit solution

$$x^\star = (A^T A)^{-1} A^T b = A^\dagger b$$

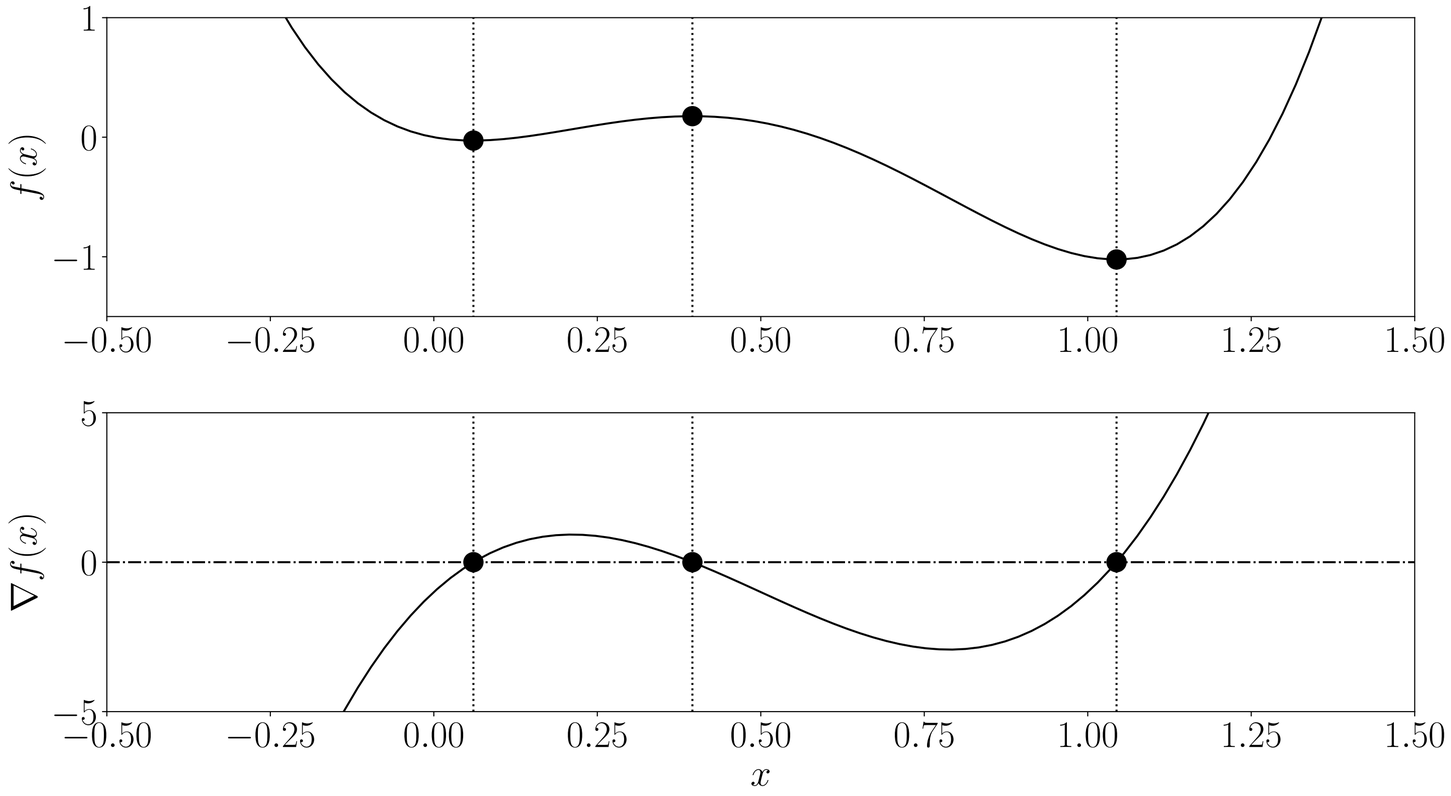
(pseudoinverse)

[Matrix Cookbook, https://www2.imm.dtu.dk/pubdb/edoc/imm3274.pdf]

First-order necessary condition is not sufficient

$$f(x) = 10x^2(1-x)^2 - x$$

$$\nabla f(x) = 40x^3 - 60x^2 + 20x - 1$$



Each local minimum/maximum satisfies

$$\nabla f(x) = 0$$

Second-order necessary condition

Theorem

If $x^\star$ is a local optimizer for the continuously differentiable function f, then

$$\nabla f(x^\star) = 0 \quad \text{and} \quad \nabla^2 f(x^\star) \succeq 0 \ \text{(positive semidefinite)}$$

Proof

If $\nabla f(x^\star) = 0$, then the second-order approximation is

$$\begin{aligned} f(x^\star + td) &= f(x^\star) + \cancel{t\nabla f(x^\star)^T d} + t^2(1/2)d^T\nabla^2 f(x^\star)d + o(t^2) \\ &= f(x^\star) + t^2(1/2)d^T\nabla^2 f(x^\star)d + o(t^2) \end{aligned}$$

To have a local minimum $d^T\nabla^2 f(x^\star)d \geq 0$ for any d ■

Least-squares continued

$$\text{minimize} \quad \|Ax - b\|_2^2$$

$$f(x) = x^T A^T A x - 2x^T A^T b + b^T b$$

First-order optimality condition

$$\nabla f(x) = 2A^T(Ax - b) = 0$$

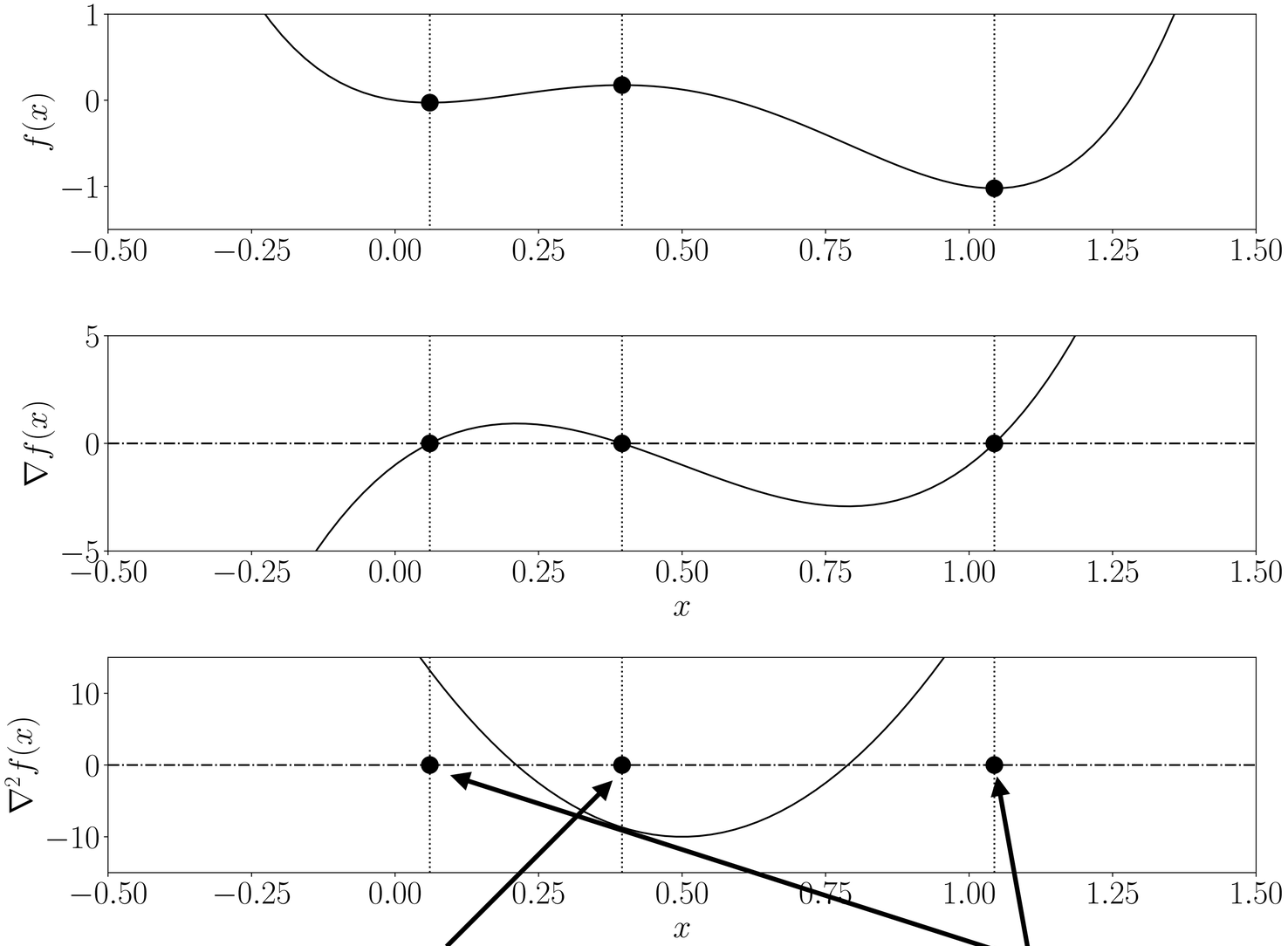
Explicit solution

$$x^\star = (A^T A)^{-1} A^T b = A^\dagger b$$

Second-order optimality condition

$$\nabla^2 f(x) = 2A^T A \succeq 0 \quad (\text{for any } A)$$

Example fixed



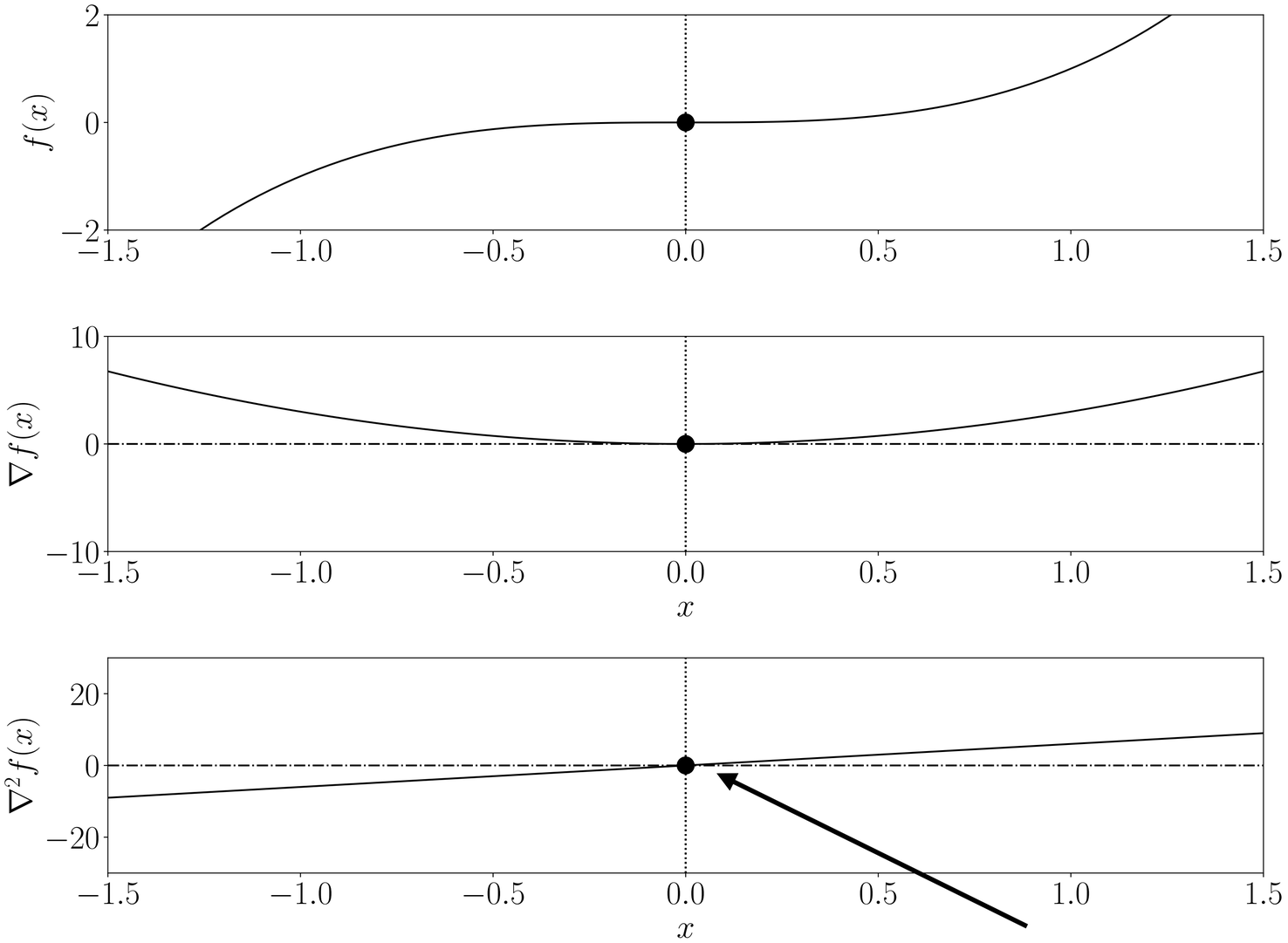
$$f(x) = 10x^2(1-x)^2 - x$$

$$\nabla f(x) = 40x^3 - 60x^2 + 20x - 1$$

$$\nabla^2 f(x) = 120x^2 - 120x + 20$$

Converse counterexample?

Second-order necessary condition is not sufficient



Cubic function

$$f(x) = x^3$$

$$\nabla f(x) = 3x^2$$

$$\nabla^2 f(x) = 6x$$

not local minimum

Conditions satisfied

$$\nabla f(0) = 0$$

$$\nabla^2 f(0) = 0 \succeq 0$$

Second-order sufficient condition

Theorem

Let f be a continuously differentiable function. If $x^\star$ satisfies

$$\nabla f(x^\star) = 0 \quad \text{and} \quad \nabla^2 f(x^\star) \succ 0$$

then $x^\star$ is a local minimum of f

Proof

If $\nabla^2 f(x^\star) \succ 0$, then $\exists \lambda > 0$ such that $d^T \nabla^2 f(x^\star) d > \lambda \|d\|_2^2$

Then, if $\nabla f(x^\star) = 0$, in a neighborhood of $x^\star$ we have

$$f(x^\star + td) = f(x^\star) + t^2 (1/2) d^T \nabla^2 f(x^\star) d + o(t^2) > f(x^\star)$$

for any d

$\blacksquare$

Examples

Cubic function

$$f(x) = x^3 \longrightarrow \nabla^2 f(x) = 6x \longrightarrow \nabla^2 f(0) = 0$$

(does not satisfy sufficient condition)

Least-squares

$$f(x) = x^T A^T A x - 2x^T A^T b + b^T b \longrightarrow \nabla^2 f(x) = 2A^T A$$

$2A^T A \succ 0$ if A is full rank
(linear independent columns in A)

Constrained optimization

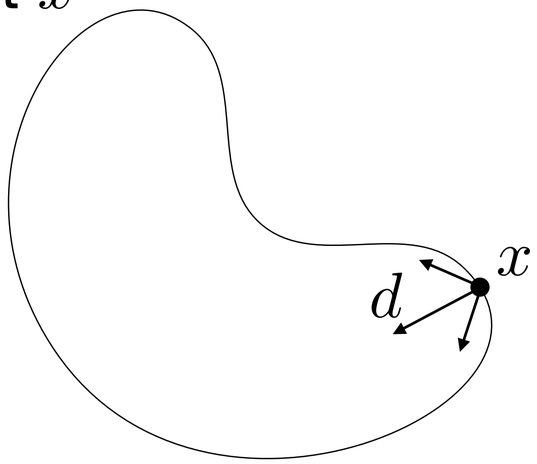
Feasible direction

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in C \end{array}$$

Given $x \in C$, we call d a **feasible direction** at x if there exists $\bar{t} > 0$ such that

$$x + td \in C, \quad \forall t \in [0, \bar{t}]$$

$F(x)$ is the **set of all feasible directions** at x



Examples

$C = \{Ax = b\} \quad \Longrightarrow F(x) = \{d \mid Ad = 0\}$

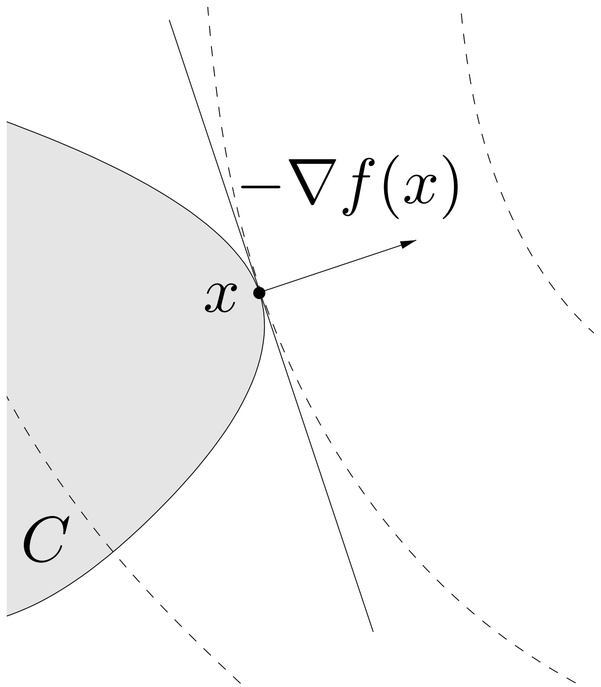
$C = \{Ax \leq b\} \quad \Longrightarrow F(x) = \{d \mid a_i^T d \leq 0 \quad \text{if } a_i^T x = b_i\}$

$C = \{g_i(x) \leq 0, \text{ (nonlinear)}\} \quad \Longrightarrow F(x) = \{d \mid \nabla g_i(x)^T d < 0 \quad \text{if } g_i(x) = 0\}$

First-order necessary optimality condition

All feasible directions do not decrease the cost

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in C \end{array}$$



Theorem

If $x^\star$ is a local minimum, then

$$\nabla f(x^\star)^T d \geq 0, \quad \forall d \in F(x^\star)$$

Unconstrained case

$F(x^\star) = \mathbf{R}^n$, therefore $\nabla f(x^\star) = 0$

Descent direction

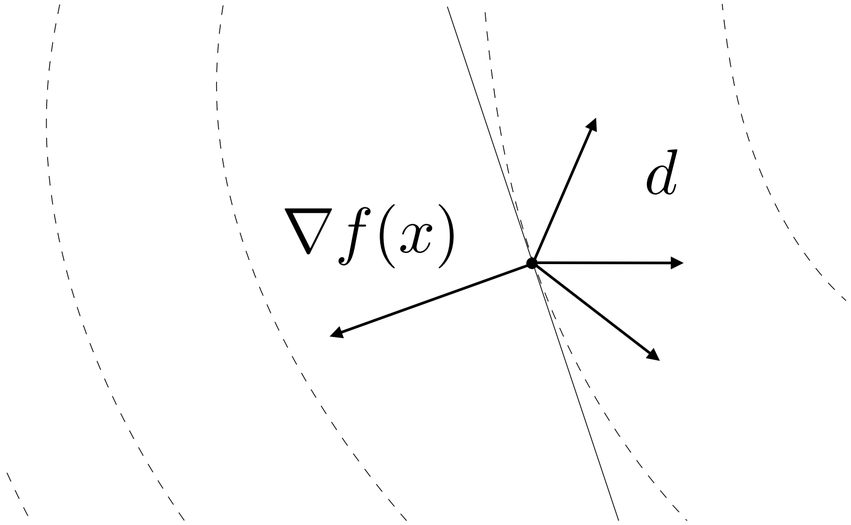
Given continuously differentiable f, we call d a **descent direction** at x if there exists $\bar{t}$ such that

$$f(x + td) < f(x), \quad \forall t \in [0, \bar{t}]$$

$D(x)$ is the **set of all descent directions**

Remark

For all descent directions d at x we have $\nabla f(x)^T d < 0$



Necessary optimality condition idea

All feasible directions are not descent directions

$$\downarrow$$

There is no feasible descent direction

If $x^\star$ is a local optimum, then

$$F(x^\star) \cap D(x^\star) = \emptyset$$

Nonlinear optimization with equality constraints

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & Ax = b \end{array}$$

Theorem

If $x^\star$ is a local optimum, then $\exists y$ such that $\nabla f(x^\star) + A^T y = 0$

Proof

Feasible directions

$F(x) = \{d \mid Ad = 0\}$

Descent directions

$D(x) = \{d \mid \nabla f(x)^T d < 0\}$

$F(x^\star) \cap D(x^\star) = \emptyset$ if and only if $\exists \nu$ such that $A^T \nu = \nabla f(x^\star)$ (thm. of alternatives)

Let $y = -\nu$

$\blacksquare$

Interpretation

$\nabla f(x^\star) \in \mathbf{range}(A^T) = \mathbf{null}(A)^\perp \longrightarrow \nabla f(x^\star) \perp \mathbf{null}(A)$

(perpendicular to hyperplane)

Example: constrained least squares

$$\begin{array}{ll} \text{minimize} & \|Ax - b\|_2^2 \\ \text{subject to} & Cx = d \end{array}$$

$$f(x) = x^T A^T A x - 2x^T A^T b + b^T b$$
$$\nabla f(x) = 2A^T(Ax - b)$$

Optimality conditions

Feasibility $\quad Cx = d$

Optimality $\quad 2A^T(Ax - b) + C^T y = 0$

$\longrightarrow$

Linear system solution

$$\begin{bmatrix} 2A^T A & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 2A^T b \\ d \end{bmatrix}$$

Necessary conditions for smooth nonlinear optimization

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \end{array} \qquad (g_i(x) \text{ nonlinear})$$

Linearly independence constraint qualification (LICQ)

Given x and the set of active constraints $\mathcal{A}(x) = \{i \mid g_i(x) = 0\}$, we say that LICQ holds if and only if

$$\{\nabla g_i(x), \quad i \in \mathcal{A}(x)\} \text{ is } \textbf{linearly independent}$$

Theorem

If $x^\star$ is a local minimum and LICQ holds, then there exists $y \geq 0$ such that

$$\nabla f(x^\star) + \sum_{i=1}^{m} y_i \nabla g_i(x^\star) = 0$$

$$y_i g_i(x^\star) = 0, \quad i = 1, \ldots, m$$

Useful Lemma

Farkas lemma variation

Given A, exactly one of the following statements is true

1. There exists an d with $Ad < 0$
2. There exists a u with $A^T u = 0$, $\mathbf{1}^T u = 1$, and $u \geq 0$

Proof

They cannot be both true (easy to show)

Let's show they they are alternatives:

We can write 1. as $B\tilde{d} \leq 0, \quad c^T \tilde{d} > 0$

where $B = \begin{bmatrix} A & \mathbf{1} \end{bmatrix}, c = (0, \ldots, 0, 1)$ and $\tilde{d} = (d, \epsilon)$

By Farkas lemma, we have the alternative $B^T u = c, \; u \geq 0$, equivalent to 2. ■

Necessary conditions for smooth nonlinear optimization

Proof

Feasible directions

$$F(x) = \{d \mid \nabla g_i(x)^T d < 0, \quad i \in \mathcal{A}(x)\}$$

Descent directions

$$D(x) = \{d \mid \nabla f(x)^T d < 0\}$$

Optimality condition

$$F(x) \cap D(x) = \emptyset \longrightarrow$$

Infeasible system

$$Ad < 0, \quad A = \begin{bmatrix} \nabla f(x) & \nabla g_{\mathcal{A}(x)_1}(x) & \dots & \nabla g_{\mathcal{A}(x)_n}(x) \end{bmatrix}^T$$

Farkas lemma variation $\longrightarrow$ $\exists u \geq 0$ such that $A^T u = 0$ and $\mathbf{1}^T u = 1$

Therefore,

$$u_0 \nabla f(x^\star) + \sum_{i \in \mathcal{A}(x^\star)} u_i \nabla g_i(x^\star) = 0$$

$$u \geq 0, \quad \mathbf{1}^T u = 1$$

Necessary conditions for smooth nonlinear optimization

Proof (continued)

$$u_0 \nabla f(x^\star) + \sum_{i \in \mathcal{A}(x^\star)} u_i \nabla g_i(x^\star) = 0$$

$$u \geq 0, \quad \mathbf{1}^T u = 1$$

If $u_0 = 0$, then $\sum_{i \in \mathcal{A}(x^\star)} u_i \nabla g_i(x^\star) = 0$ (LICQ violated).

Hence, $u_0 > 0$. Let's define $y = u/u_0$, obtaining $\nabla f(x^\star) + \sum_{i \in \mathcal{A}(x)} y_i \nabla g_i(x^\star) = 0$

Which can be rewritten as $\nabla f(x^\star) + \sum_{i=1}^{m} y_i \nabla g_i(x^\star) = 0$

$$y_i g_i(x^\star) = 0, \quad i = 1, \ldots, m \qquad \blacksquare$$

What happens if LICQ fails?

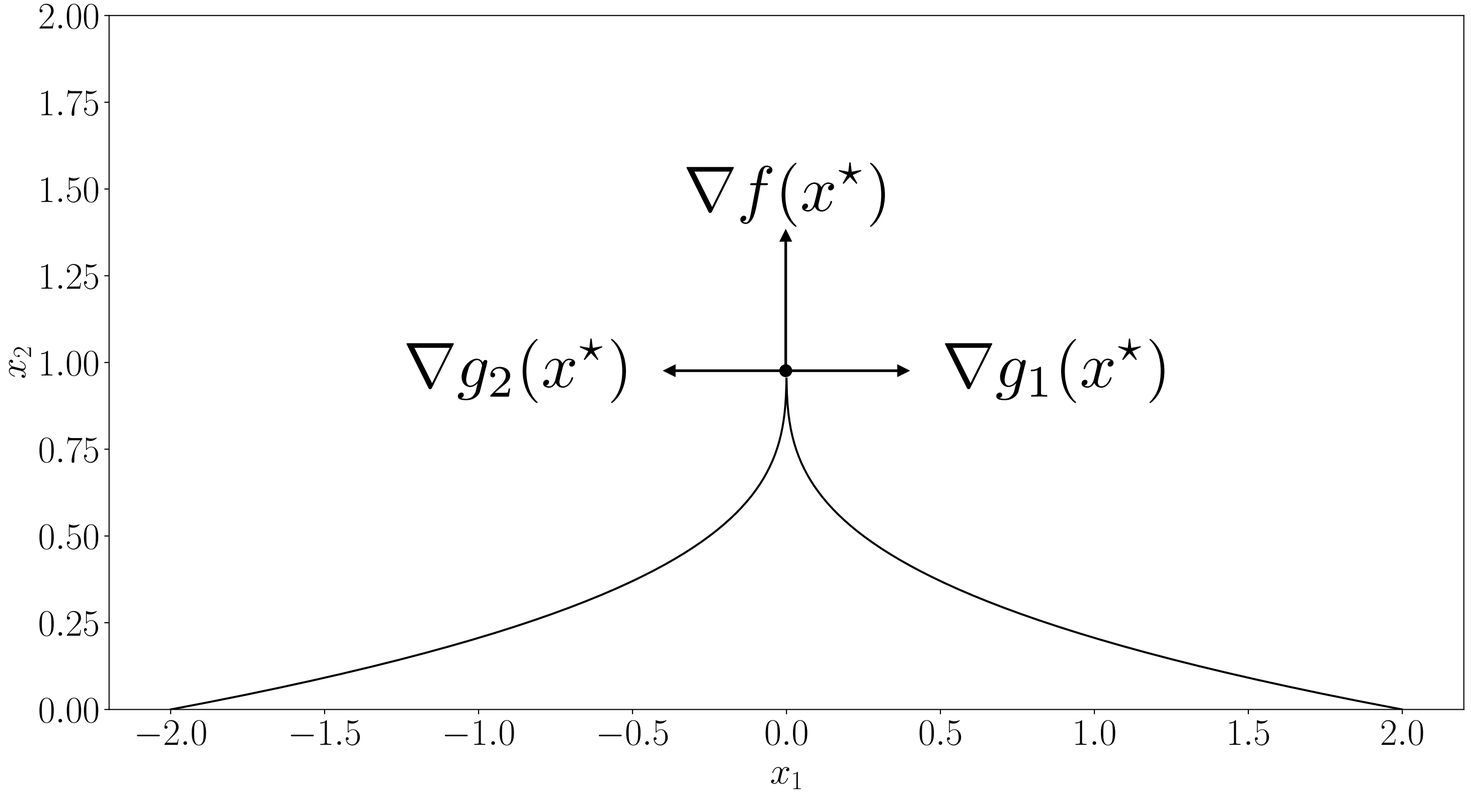
minimize $\quad -x_2$

subject to $\quad x_1 - 2(1-x_2)^3 \leq 0$

$\quad -x_1 - 2(1-x_2)^3 \leq 0$

$\quad x \geq 0$

$$x^\star = (0, 1)$$



Lagrangian function and duality

Lagrangian

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{array}$$

Optimal cost

$$f(x^\star) = p^\star$$

Lagrange multipliers

$$g_i(x) \leq 0 \quad \Longrightarrow \quad y_i \geq 0$$

$$h_i(x) = 0 \quad \Longrightarrow \quad v_i$$

Lagrangian

$$L(x, y, v) = f(x) + \sum_{i=1}^{m} y_i g_i(x) + \sum_{i=1}^{p} v_i h_i(x)$$

Lagrangian

Interpretation

Lower bound $f(x) \geq L(x, y, v)$ for each feasible x

Proof

$$L(x, y, v) = f(x) + \sum_{i=1}^{m} y_i \underbrace{g_i(x)}_{\leq 0} + \sum_{i=1}^{p} v_i \underbrace{h_i(x)}_{= 0} \leq f(x) \qquad \blacksquare$$

Dual function

$$q(y, v) = \underset{x}{\text{minimize}}\ L(x, y, v)$$

$$\mathbf{dom}\ q = \{(y, v) \mid q(y, v) > -\infty\}$$

Lagrange dual problem

Finding the best lower bound

Always concave (-convex) problem

$$\begin{array}{ll} \text{maximize} & q(y, v) \\ \text{subject to} & y \geq 0 \end{array} \longrightarrow$$

Dual problem

$$d^\star = \max_{y \geq 0, v} \min_{x} L(x, y, v)$$

Lower bound condition always holds

Weak duality

$$d^\star \leq p^\star$$

Stationarity condition

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{array}$$

$$L(x, y, v) = f(x) + \sum_{i=1}^{m} y_i g_i(x) + \sum_{i=1}^{p} v_i h_i(x)$$

Min-max formulation

$$p^\star = \min_x \max_{y \geq 0, v} \; L(x, y, v)$$ (minimize unconstrained version)

Stationarity condition on the Lagrangian

$$\nabla_x L(x, y, v) = \nabla f(x) + \sum_{i=1}^{m} y_i \nabla g_i(x) + \sum_{i=1}^{p} v_i \nabla h_i(x) = 0$$

KKT necessary conditions for optimality

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{array}$$

Theorem

If $x^\star$ is a local minimizer and LICQ holds, then there exists $y^\star, v^\star$ such that

$$\nabla f(x^\star) + \sum_{i=1}^{m} y_i^\star \nabla g_i(x^\star) + \sum_{i=1}^{p} v_i^\star \nabla h_i(x^\star) = 0$$ **stationarity**

$$y^\star \geq 0$$ **dual feasibility**

$$g_i(x^\star) \leq 0, \quad i = 1, \ldots, m$$
$$h_i(x^\star) = 0, \quad i = 1, \ldots, p$$ **primal feasibility**

$$y_i^\star g_i(x^\star) = 0, \quad i = 1, \ldots, m$$ **complementary slackness**

Strong duality theorem

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{array}$$

Theorem

If the problem is convex and there exists at least a strictly feasible x, *i.e.*,

$$\begin{array}{ll} g_i(x) \leq 0, & \text{(for all affine } g_i\text{)} \\ g_i(x) < 0, & \text{(for all non-affine } g_i\text{)} \\ h_i(x) = 0, & i = 1, \ldots, p \end{array}$$

Slater's condition

then $p^\star = d^\star$ (**strong duality holds**)

Remarks

- For nonconvex optimization, we need harder conditions
- Generalizes LP conditions [Lecture 7]

KKT for convex problems

Always sufficient

For $x^\star, y^\star, v^\star$ that satisfy the KKT conditions

$$f(x^\star) = f(x^\star) + \sum_{i=1}^{m} y_i^\star g_i(x^\star) + \sum_{i=1}^{p} v_i^\star h_i(x^\star) = L(x^\star, y^\star v^\star)$$

$$\nabla f(x^\star) + \sum_{i=1}^{m} y_i^\star \nabla g_i(x^\star) + \sum_{i=1}^{p} v_i^\star \nabla h_i(x^\star) = 0 \quad \Rightarrow \quad q(y^\star, v^\star) = L(x^\star, y^\star, v^\star)$$

(L convex and differentiable $\Rightarrow \nabla_x L(x^\star, y^\star, v^\star) = 0$ implies $x^\star$ minimizes L)

Therefore, $f(x^\star) = q(y^\star, v^\star)$ and $x^\star, y^\star, v^\star$ are primal-dual optimal

Necessary when constraint qualifications (Slater's) condition holds

Slater condition $\Rightarrow$ strong duality $p^\star = d^\star$ and dual optimum attained.
Therefore, since $x^\star, y^\star, v^\star$ are optimal, they must satisfy the KKT conditions.

KKT remarks

History

- First appeared in publication by Kuhn and Tucker (1951)
- It already existed in Karush's unpublished master thesis (1939)

Unconstrained problems

They reduce to necessary first-order condition $\nabla f(x) = 0$

Strong duality

In general, we can replace LICQ assumption with strong duality

Convex problems

KKT conditions are always **sufficient**

If strong duality holds, KKT conditions are **necessary and sufficient**

Example: KKT conditions for convex QP

$$\begin{array}{ll} \text{minimize} & (1/2)x^T P x + q^T x \\ \text{subject to} & Ax = b \\ & Cx \leq d \end{array}$$

Lagrangian

$$L(x, y, v) = (1/2)x^T P x + q^T x + y^T(Cx - d) + v^T(Ax - b)$$

where $y \geq 0$

Stationarity condition

$$\nabla_x L(x, y, u) = Px + q + C^T y + A^T v = 0$$

Example: KKT conditions for convex QP

$$\begin{array}{ll} \text{minimize} & (1/2)x^T P x + q^T x \\ \text{subject to} & Ax = b \\ & Cx \leq d \end{array}$$

KKT Optimality conditions

$$Px^\star + q + C^T y^\star + A^T v^\star = 0$$ **stationarity condition**

$$y^\star \geq 0$$ **dual feasibility**

$$Ax - b = 0$$

$$Cx - d \leq 0$$ **primal feasibility**

$$y_i(c_i^T x^\star - d_i) = 0, \quad i = 1, \ldots, m$$ **complementary slackness**

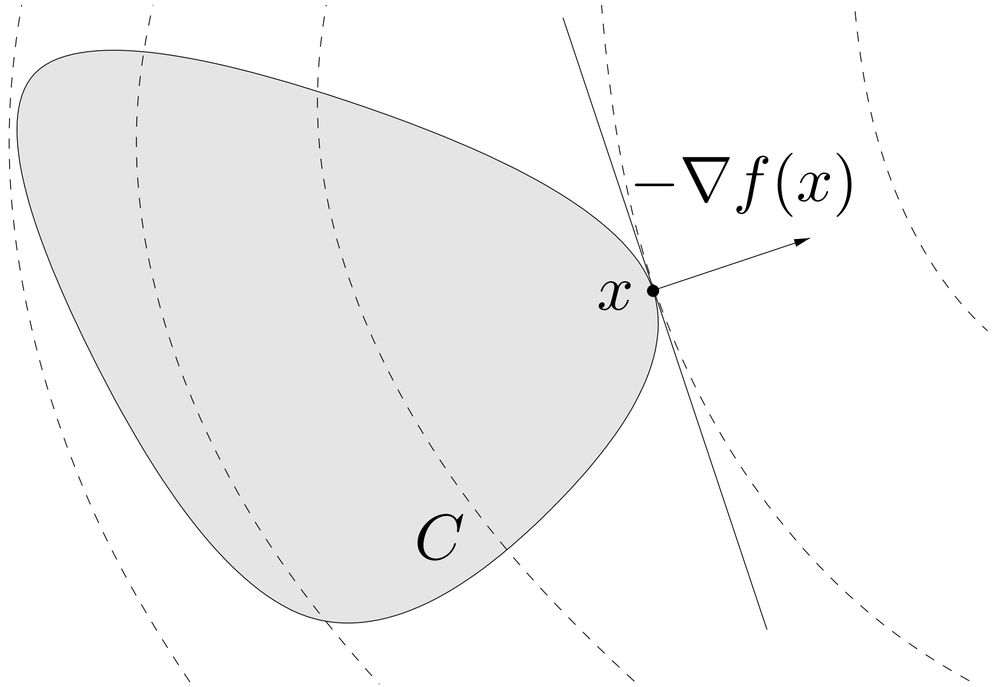
Convex constrained nonconvex optimization

Minimization over convex set

[Section 3.7.3 and Example 3.74, A. Beck]

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in C \end{array}$$

$\longleftarrow$ convex set



First-order optimality condition

If $x^\star$ is a local minimum, then

$$\nabla f(x^\star)^T (y - x^\star) \geq 0, \quad \forall y \in C$$

(f can be nonconvex)

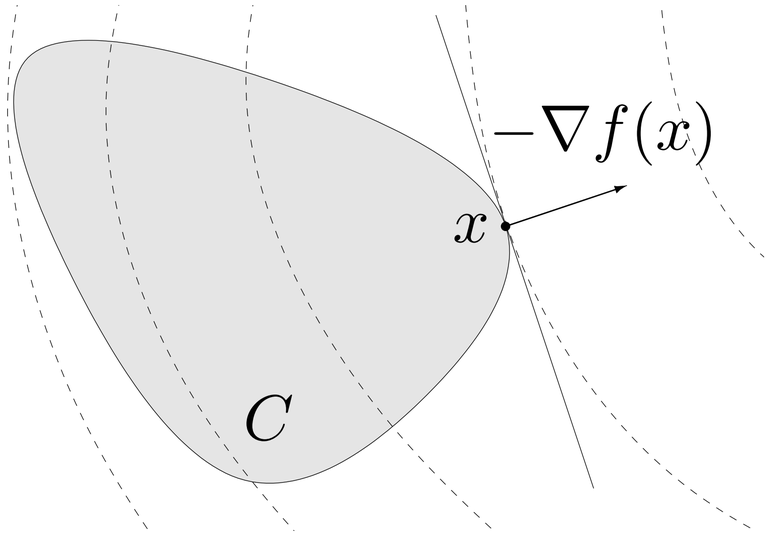
Why do you need a convex set?

First-order necessary optimality condition

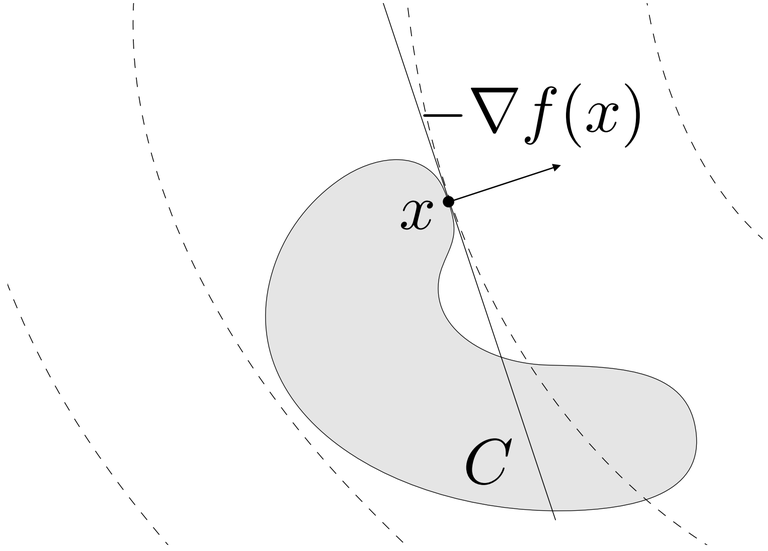
If $x^\star$ is a local minimum, then

$$\nabla f(x^\star)^T(y - x^\star) \geq 0, \quad \forall y \in C$$

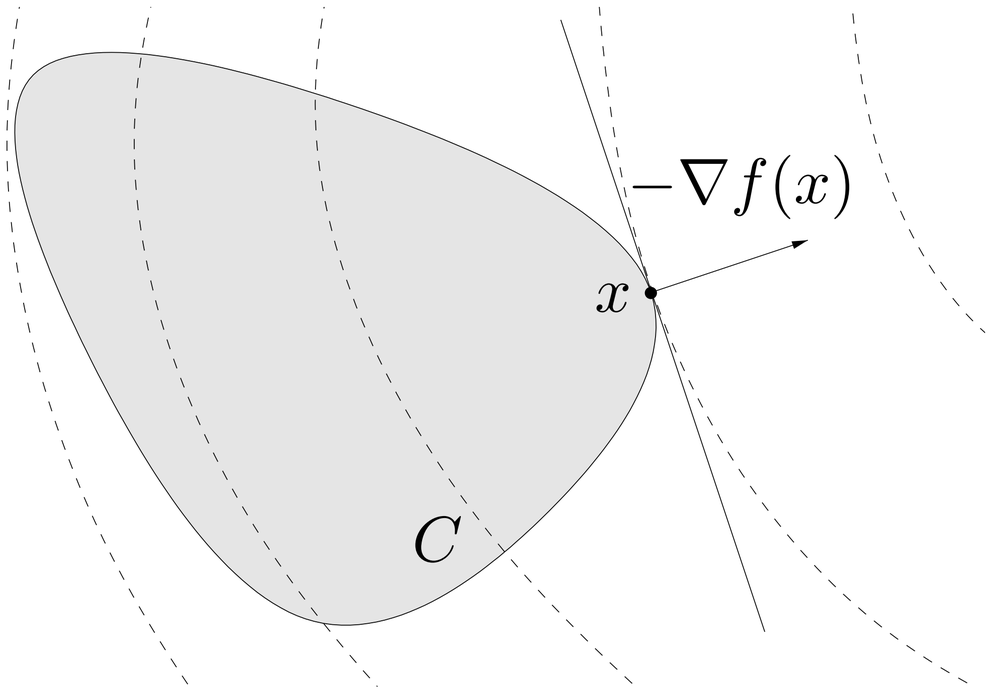
Convex set



Nonconvex set



Normal cone condition



First-order necessary optimality condition

If $x^\star$ is a local minimum, then

$$\nabla f(x^\star)^T(y - x^\star) \geq 0, \quad \forall y \in C$$

Normal cone

$$\mathcal{N}_C(x) = \{g \mid g^T(y - x) \leq 0, \quad \text{for all } y \in C\}$$

Reformulated condition

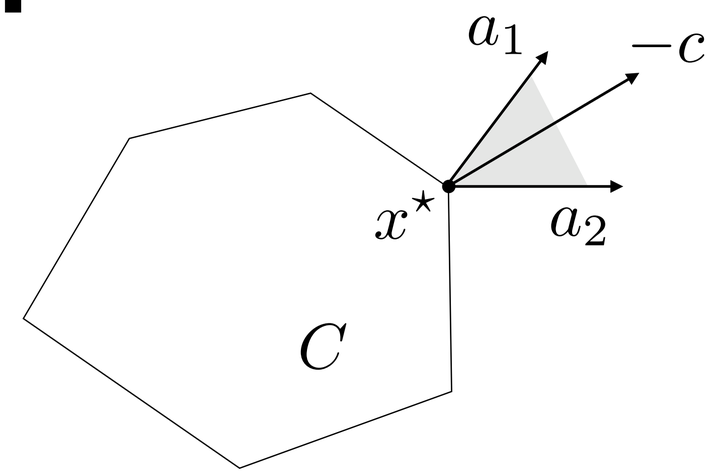
$$-\nabla f(x^\star) \in \mathcal{N}_C(x^\star)$$

Remark
If f and C are convex, then it is **necessary and sufficient**
[Section 4.2.3, B and V]

Normal cone condition

Linear program example

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Ax \leq b \end{array}$$



Recap from Lecture 8

Two active constraints at optimum: $a_1^T x^\star = b_1, \quad a_2^T x^\star = b_2$

Optimal dual solution y satisfies:

$$A^T y + c = 0, \quad y \geq 0, \quad y_i = 0 \text{ for } i \neq \{1, 2\}$$

In other words, $-c = a_1 y_1 + a_2 y_2$ with $y_1, y_2 \geq 0$

Normal cone to polyhedron

$$-c \in \mathcal{N}_{\{Ax \leq b\}}(x^\star) = \{A^T y \mid y \geq 0 \quad \text{and} \quad y_i(a_i^T x^\star - b_i) = 0\}$$

Optimality conditions in nonlinear optimization

Today, we learned to:

- **Prove** optimality conditions for unconstrained optimization
- **Compute** feasible and descent directions
- **Derive** optimality conditions for constrained optimization using Farkas lemma
- **Derive** optimality conditions for constrained optimization using Lagrangian
- **Apply** normal cone to derive necessary first-order conditions for nonconvex optimization over convex set

Next lecture

- Optimization algorithms: iteratively solve first-order optimality conditions