Part 1: Optimality conditions and why they are important

Nick Gould (RAL)

$$c(x) \geq 0, \quad g(x) + A^T(x)y = 0, \quad y \geq 0$$

MSc course on nonlinear optimization

OPTIMIZATION PROBLEMS

Unconstrained minimization:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x)$$

where the **objective function** $f : \mathbb{R}^n \longrightarrow \mathbb{R}$

Equality constrained minimization:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x) \; \text{ subject to } \; c(x) = 0$$

where the **constraints** $c : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ $(m \leq n)$

Inequality constrained minimization:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x) \; \text{ subject to } \; c(x) \geq 0$$

where $c : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ (m may be larger than n)

NOTATION

Use the following throughout the course:

$g(x)$	$\stackrel{\text{def}}{=}$	$\nabla_x f(x)$	**gradient** of f
$H(x)$	$\stackrel{\text{def}}{=}$	$\nabla_{xx} f(x)$	**Hessian matrix** of f
$a_i(x)$	$\stackrel{\text{def}}{=}$	$\nabla_x c_i(x)$	**gradient** of ith constraint
$H_i(x)$	$\stackrel{\text{def}}{=}$	$\nabla_{xx} c_i(x)$	**Hessian** of ith constraint
$A(x)$	$\stackrel{\text{def}}{=}$	$\nabla_x c(x) \equiv \begin{pmatrix} a_1^T(x) \\ \cdots \\ a_m^T(x) \end{pmatrix}$	**Jacobian matrix** of c
$\ell(x,y)$	$\stackrel{\text{def}}{=}$	$f(x) - y^T c(x)$	**Lagrangian** function, where y are **Lagrange multipliers**
$H(x,y)$	$\stackrel{\text{def}}{=}$	$\nabla_{xx} \ell(x,y) \equiv H(x) - \sum_{i=1}^{m} y_i H_i(x)$	**Hessian** of the Lagrangian

LIPSCHITZ CONTINUITY

- $\mathcal{X}$ and $\mathcal{Y}$ open sets
- $F : \mathcal{X} \rightarrow \mathcal{Y}$
- $\|\cdot\|_{\mathcal{X}}$ and $\|\cdot\|_{\mathcal{Y}}$ are norms

Then

- F is **Lipschitz continuous at** $x \in \mathcal{X}$ if $\exists\ \gamma(x)$ such that

$$\|F(z) - F(x)\|_{\mathcal{Y}} \leq \gamma(x) \|z - x\|_{\mathcal{X}}$$

  for all $z \in \mathcal{X}$.

- F is **Lipschitz continuous throughout/in** $\mathcal{X}$ if $\exists\ \gamma$ such that

$$\|F(z) - F(x)\|_{\mathcal{Y}} \leq \gamma \|z - x\|_{\mathcal{X}}$$

  for all x and $z \in \mathcal{X}$.

USEFUL TAYLOR APPROXIMATIONS

Theorem 1.1. Let $\mathcal{S}$ be an open subset of IR^n, and suppose $f : \mathcal{S} \longrightarrow \mathrm{IR}$ is continuously differentiable throughout $\mathcal{S}$. Suppose further that $g(x)$ is Lipschitz continuous at x, with Lipschitz constant $\gamma^L(x)$ in some appropriate vector norm. Then, if the segment $x + \theta s \in \mathcal{S}$ for all $\theta \in [0, 1]$,

$$|f(x+s) - m^L(x+s)| \leq \tfrac{1}{2}\gamma^L(x)\|s\|^2, \quad \text{where}$$

$$m^L(x+s) = f(x) + g(x)^T s.$$

If f is twice continuously differentiable throughout $\mathcal{S}$ and $H(x)$ is Lipschitz continuous at x, with Lipschitz constant $\gamma^Q(x)$,

$$|f(x+s) - m^Q(x+s)| \leq \tfrac{1}{6}\gamma^Q(x)\|s\|^3, \quad \text{where}$$

$$m^Q(x+s) = f(x) + g(x)^T s + \tfrac{1}{2}s^T H(x)s.$$

MEAN VALUE THEOREM

Theorem 1.2. Let $\mathcal{S}$ be an open subset of IR^n, and suppose $f : \mathcal{S} \longrightarrow \mathrm{IR}$ is twice continuously differentiable throughout $\mathcal{S}$. Suppose further that $s \neq 0$, and that the interval $[x, x+s] \in \mathcal{S}$. Then

$$f(x+s) = f(x) + g(x)^T s + \tfrac{1}{2}s^T H(z)s$$

for some $z \in (x, x+s)$.

ANOTHER USEFUL TAYLOR APPROXIMATION

Theorem 1.3. Let $\mathcal{S}$ be an open subset of IR^n, and suppose $F : \mathcal{S} \rightarrow \mathrm{IR}^m$ is continuously differentiable throughout $\mathcal{S}$. Suppose further that $\nabla_x F(x)$ is Lipschitz continuous at x, with Lipschitz constant $\gamma^L(x)$ in some appropriate vector norm and its induced matrix norm. Then, if the segment $x + \theta s \in \mathcal{S}$ for all $\theta \in [0,1]$,

$$\|F(x+s) - M^L(x+s)\| \leq \tfrac{1}{2}\gamma^L(x)\|s\|^2,$$

where

$$M^L(x+s) = F(x) + \nabla_x F(x) s$$

OPTIMALITY CONDITIONS

Optimality conditions are useful because:

- ⊙ they provide a means of guaranteeing that a candidate solution is indeed optimal (**sufficient conditions**), and
- ⊙ they indicate when a point is not optimal (**necessary conditions**)

Furthermore they

- ⊙ guide in the design of algorithms, since lack of optimality $\Longleftrightarrow$ indication of improvement

UNCONSTRAINED MINIMIZATION

First-order necessary optimality:

Theorem 1.4. Suppose that $f \in C^1$, and that x_* is a local minimizer of $f(x)$. Then

$$g(x_*) = 0.$$

Second-order necessary optimality:

Theorem 1.5. Suppose that $f \in C^2$, and that x_* is a local minimizer of $f(x)$. Then $g(x_*) = 0$ and $H(x_*)$ is positive semi-definite, that is

$$s^T H(x_*) s \geq 0 \text{ for all } s \in \mathbb{R}^n.$$

UNCONSTRAINED MINIMIZATION (cont.)

Second-order sufficient optimality:

Theorem 1.6. Suppose that $f \in C^2$, that x_* satisfies the condition $g(x_*) = 0$, and that additionally $H(x_*)$ is positive definite, that is

$$s^T H(x_*) s > 0 \text{ for all } s \neq 0 \in \mathbb{R}^n.$$

Then x_* is an isolated local minimizer of f.

EQUALITY CONSTRAINED MINIMIZATION

First-order necessary optimality:

Theorem 1.7. Suppose that $f,\ c \in C^1$, and that x_* is a local minimizer of $f(x)$ subject to $c(x) = 0$. Then, so long as a first-order constraint qualification holds, there exist a vector of Lagrange multipliers y_* such that

$$c(x_*) = 0 \ \ (\textbf{primal feasibility}) \text{ and}$$
$$g(x_*) - A^T(x_*) y_* = 0 \ \ (\textbf{dual feasibility}).$$

PROOF OF THEOREM 1.7

Constraint qualification $\Longrightarrow$ $\exists$ vector valued C^2 (C^3 for Theorem 1.8) function $x(\alpha)$ of the scalar α for which

$$x(0) = x_* \ \text{ and } \ c(x(\alpha)) = 0$$

and

$$x(\alpha) = x_* + \alpha s + \tfrac{1}{2}\alpha^2 p + O(\alpha^3)$$

+ Taylor's theorem $\Longrightarrow$

$$\begin{aligned} 0 &= c_i(x(\alpha)) = c(x_* + \alpha s + \tfrac{1}{2}\alpha^2 p + O(\alpha^3)) \\ &= c_i(x_*) + a_i^T(x_*)\left(\alpha s + \tfrac{1}{2}\alpha^2 p\right) + \tfrac{1}{2}\alpha^2 s^T H_i(x_*) s + O(\alpha^3) \\ &= \alpha a_i^T(x_*) s + \tfrac{1}{2}\alpha^2\left(a_i^T(x_*) p + s^T H_i(x_*) s\right) + O(\alpha^3) \end{aligned}$$

Matching similar asymptotic terms $\Longrightarrow$

$$A(x_*) s = 0 \tag{1}$$

and

$$a_i^T(x_*) p + s^T H_i(x_*) s = 0 \ \ \forall i = 1, \ldots, m \tag{2}$$

Now consider objective function

$$\begin{aligned} f(x(\alpha)) &= f(x_* + \alpha s + \tfrac{1}{2}\alpha^2 p + O(\alpha^3)) \\ &= f(x_*) + g(x_*)^T \left(\alpha s + \tfrac{1}{2}\alpha^2 p\right) + \tfrac{1}{2}\alpha^2 s^T H(x_*) s + O(\alpha^3) \\ &= f(x_*) + \alpha g(x_*)^T s + \tfrac{1}{2}\alpha^2 \left(g(x_*)^T p + s^T H(x_*) s\right) + O(\alpha^3) \end{aligned} \tag{3}$$

$f(x)$ unconstrained along $x(\alpha) \Longrightarrow$

$$g(x_*)^T s = 0 \;\text{ for all }\; s \;\text{ such that }\; A(x_*) s = 0. \tag{4}$$

Let S be a basis for null space of $A(x_*) \Longrightarrow$

$$g(x_*) = A^T(x_*) y_* + S z_* \tag{5}$$

for some y_* and z_*. (4) $\Longrightarrow$ $g^T(x_*) S = 0$ + $A(x_*) S = 0 \Longrightarrow$

$$0 = S^T g(x_*) = S^T A^T(x_*) y_* + S^T S z_* = S^T S z_*.$$

$\Longrightarrow$ $S^T S z_* = 0$ + S full rank $\Longrightarrow$ $z_* = 0$ + (5) $\Longrightarrow$

$$g(x_*) - A^T(x_*) y_* = 0.$$

EQUALITY CONSTRAINED MINIMIZATION (cont.)

Second-order necessary optimality:

Theorem 1.8. Suppose that $f,\; c \in C^2$, and that x_* is a local minimizer of $f(x)$ subject to $c(x) = 0$. Then, provided that first- and second-order constraint qualifications hold, there exist a vector of Lagrange multipliers y_* such that

$$s^T H(x_*, y_*) s \geq 0 \;\text{ for all }\; s \in \mathcal{N}$$

where

$$\mathcal{N} = \{ s \in \mathrm{IR}^n \mid A(x_*) s = 0 \}$$

PROOF OF THEOREM 1.8

$$g(x_*) - A^T(x_*)y_* = 0. \tag{6}$$

while (3) $\Longrightarrow$

$$f(x(\alpha)) = f(x_*) + \tfrac{1}{2}\alpha^2 \left(p^T g(x_*) + s^T H(x_*)s\right) + O(\alpha^3) \tag{7}$$

for all s and p satisfying $A(x_*)s = 0$ and

$$a_i^T(x_*)p + s^T H_i(x_*)s = 0 \;\; \forall i = 1, \ldots, m. \tag{8}$$

Hence, necessarily,
$$p^T g(x_*) + s^T H(x_*)s \geq 0 \tag{9}$$

But (6) + (8) $\Longrightarrow$
$$p^T g(x_*) = \sum_{i=1}^{m} (y_*)_i p^T a_i(x_*) = -\sum_{i=1}^{m} (y_*)_i s^T H_i(x_*)s$$

$\Longrightarrow$ (9) is equivalent to

$$s^T \left(H(x_*) - \sum_{i=1}^{m} (y_*)_i H_i(x_*) \right) s \equiv s^T H(x_*, y_*)s \geq 0$$

for all s satisfying $A(x_*)s = 0$.

INEQUALITY CONSTRAINED MINIMIZATION

First-order necessary optimality:

Theorem 1.9. Suppose that $f,\ c \in C^1$, and that x_* is a local minimizer of $f(x)$ subject to $c(x) \geq 0$. Then, provided that a first-order constraint qualification holds, there exist a vector of Lagrange multipliers y_* such that

$$c(x_*) \geq 0 \quad \text{(\textbf{primal feasibility})},$$

$$\left.\begin{array}{r} g(x_*) - A^T(x_*)y_* = 0 \\ \text{and} \;\; y_* \geq 0 \end{array}\right. \quad \text{(\textbf{dual feasibility}) and}$$

$$c_i(x_*)[y_*]_i = 0 \quad \text{(\textbf{complementary slackness})}.$$

PROOF OF THEOREM 1.9

Consider feasible perturbations about x_*. $c_i(x_*) > 0 \Longrightarrow c_i(x) > 0$ for small perturbations $\Longrightarrow$ need only consider perturbations that are constrained by $c_i(x) \geq 0$ for $i \in \mathcal{A} \stackrel{\text{def}}{=} \{i : c_i(x_*) = 0\}$.
Consider $x(\alpha)$: $x(0) = x_*$, $c_i(x(\alpha)) \geq 0$ for $i \in \mathcal{A}$ and

$$x(\alpha) = x_* + \alpha s + \tfrac{1}{2}\alpha^2 p + O(\alpha^3)$$

$\Longrightarrow$

$$\begin{aligned} 0 &\leq c_i(x(\alpha)) = c(x_* + \alpha s + \tfrac{1}{2}\alpha^2 p + O(\alpha^3)) \\ &= c_i(x_*) + a_i(x_*)^T \alpha s + \tfrac{1}{2}\alpha^2 p + \tfrac{1}{2}\alpha^2 s^T H_i(x_*) s + O(\alpha^3) \\ &= \alpha a_i(x_*)^T s + \tfrac{1}{2}\alpha^2 \left(a_i(x_*)^T p + s^T H_i(x_*) s \right) + O(\alpha^3) \end{aligned}$$

$\forall i \in \mathcal{A} \Longrightarrow$

$$s^T a_i(x_*) \geq 0 \ \ \forall i \in \mathcal{A} \tag{10}$$

and

$$p^T a_i(x_*) + s^T H_i(x_*) s \geq 0 \ \ \text{when} \ \ s^T a_i(x_*) = 0 \ \ \forall i \in \mathcal{A} \tag{11}$$

Expansion (3) of $f(x(\alpha))$

$$f(x(\alpha)) = f(x_*) + \alpha g(x_*)^T s + \tfrac{1}{2}\alpha^2 \left(g(x_*)^T p + s^T H(x_*) s \right) + O(\alpha^3)$$

$\Longrightarrow$ x_* can only be a local minimizer if

$$\mathcal{S} = \{ s \mid s^T g(x_*) < 0 \ \ \text{and} \ \ s^T a_i(x_*) \geq 0 \ \ \text{for} \ \ i \in \mathcal{A} \} = \emptyset.$$

Result then follows directly from Farkas' lemma:

Farkas' lemma. Given any vectors g and a_i, $i \in \mathcal{A}$, the set

$$\mathcal{S} = \{ s \mid s^T g < 0 \ \ \text{and} \ \ s^T a_i \geq 0 \ \ \text{for} \ \ i \in \mathcal{A} \}$$

is empty if and only if

$$g = \sum_{i \in \mathcal{A}} y_i a_i$$

for some $y_i \geq 0$, $i \in \mathcal{A}$

Second-order necessary optimality:

Theorem 1.10. Suppose that $f,\ c \in C^2$, and that x_* is a local minimizer of $f(x)$ subject to $c(x) \geq 0$. Then, provided that first- and second-order constraint qualifications hold, there exist a vector of Lagrange multipliers y_* for which primal/dual feasibility and complementary slackness requirements hold as well as

$$s^T H(x_*, y_*) s \geq 0 \ \text{ for all } \ s \in \mathcal{N}_+$$

where

$$\mathcal{N}_+ = \left\{ s \in \mathbb{R}^n \ \middle| \ \begin{array}{l} s^T a_i(x_*) = 0 \text{ if } c_i(x_*) = 0 \ \& \ [y_*]_i > 0 \ \& \\ s^T a_i(x_*) \geq 0 \text{ if } c_i(x_*) = 0 \ \& \ [y_*]_i = 0 \end{array} \right\}.$$

PROOF OF THEOREM 1.10

Expansion

$$f(x(\alpha)) = f(x_*) + \alpha g(x_*)^T s + \tfrac{1}{2}\alpha^2 \left(g(x_*)^T p + s^T H(x_*) s \right) + O(\alpha^3)$$

for change in objective function dominated by $\alpha s^T g(x_*)$ for feasible perturbations unless $s^T g(x_*) = 0$, in which case the expansion

$$f(x(\alpha)) = f(x_*) + \tfrac{1}{2}\alpha^2 \left(p^T g(x_*) + s^T H(x_*) s \right) + O(\alpha^3)$$

is relevant $\Longrightarrow$

$$p^T g(x_*) + s^T H(x_*) s \geq 0 \tag{12}$$

holds for all feasible s for which $s^T g(x_*) = 0 \Longrightarrow$
$0 = s^T g(x_*) = \displaystyle\sum_{i \in \mathcal{A}} (y_*)_i s^T a_i(x_*) \Longrightarrow$ either $(y_*)_i = 0$ or $a_i(x_*)^T s = 0$.
$\Longrightarrow$ second-order feasible perturbations characterised by $s \in \mathcal{N}_+$.

Focus on *subset* of all feasible arcs that ensure $c_i(x(\alpha)) = 0$ if $(y_*)_i > 0$ and $c_i(x(\alpha)) \geq 0$ if $(y_*)_i = 0$ for $i \in \mathcal{A} \Longrightarrow \; s \in \mathcal{N}_+$.
When $c_i(x(\alpha)) = 0 \Longrightarrow$

$$a_i^T(x_*)p + s^T H_i(x_*)s = 0$$

$\Longrightarrow$

$$\begin{aligned} p^T g(x_*) &= \sum_{i \in \mathcal{A}} (y_*)_i p^T a_i(x_*) = \sum_{\substack{i \in \mathcal{A} \\ (y_*)_i > 0}} (y_*)_i p^T a_i(x_*) \\ &= -\sum_{\substack{i \in \mathcal{A} \\ (y_*)_i > 0}} (y_*)_i s^T H_i(x_*)s = -\sum_{i \in \mathcal{A}} (y_*)_i s^T H_i(x_*)s \end{aligned}$$

$$+ \, (12) \Longrightarrow \quad s^T H(x_*, y_*)s \equiv s^T \left(H(x_*) - \sum_{i=1}^{m} (y_*)_i H_i(x_*) \right) s = p^T g(x_*) + s^T H(x_*)s \geq 0.$$

for all $s \in \mathcal{N}_+$

INEQUALITY CONSTRAINED MINIMIZATION (cont.)

Second-order sufficient optimality:

Theorem 1.11. Suppose that $f, \; c \in C^2$, that x_* and a vector of Lagrange multipliers y_* satisfy

$$c(x_*) \geq 0, g(x_*) - A^T(x_*)y_* = 0, y_* \geq 0, \quad \text{and} \quad c_i(x_*)[y_*]_i = 0$$

and that

$$s^T H(x_*, y_*)s > 0$$

for all s in the set

$$\mathcal{N}_+ = \left\{ s \in \mathrm{I\!R}^n \;\middle|\; \begin{array}{l} s^T a_i(x_*) = 0 \text{ if } c_i(x_*) = 0 \;\&\; [y_*]_i > 0 \;\& \\ s^T a_i(x_*) \geq 0 \text{ if } c_i(x_*) = 0 \;\&\; [y_*]_i = 0. \end{array} \right\}.$$

Then x_* is an isolated local minimizer of $f(x)$ subject to $c(x) \geq 0$.

PROOF OF THEOREM 1.11

Consider any feasible arc $x(\alpha)$. Already shown

$$s^T a_i(x_*) \geq 0 \;\; \forall i \in \mathcal{A} \tag{13}$$

and

$$p^T a_i(x_*) + s^T H_i(x_*) s \geq 0 \;\; \text{when} \;\; s^T a_i(x_*) = 0 \;\; \forall i \in \mathcal{A} \tag{14}$$

and that second-order feasible perturbations are characterized by $\mathcal{N}_+$.

$$(14) \implies p^T g(x_*) = \sum_{i \in \mathcal{A}} (y_*)_i p^T a_i(x_*) = \sum_{\substack{i \in \mathcal{A} \\ s^T a_i(x_*)=0}} (y_*)_i p^T a_i(x_*)$$

$$\geq -\sum_{\substack{i \in \mathcal{A} \\ s^T a_i(x_*)=0}} (y_*)_i s^T H_i(x_*) s = -\sum_{i \in \mathcal{A}} (y_*)_i s^T H_i(x_*) s,$$

and hence by assumption that

$$p^T g(x_*) + s^T H(x_*) s \geq s^T \left(H(x_*) - \sum_{i=1}^{m} (y_*)_i H_i(x_*) \right) s$$

$$\equiv s^T H(x_*, y_*) s > 0$$

$\forall s \in \mathcal{N}_+ + (3) + (13) \implies f(x(\alpha)) > f(x_*) \; \forall$ sufficiently small α.