UIUC IE510 Applied Nonlinear Programming

Lecture 11: Lagrangian Multipliers Part a: Equality Constraints

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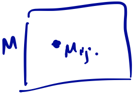
Review Question for Lecture 10

- **Question 1**: If x^* is a local-min of $\min_x f(x)$, s.t. $x \in X$ (convex), what condition does it satisfy?



$$\langle \nabla f(x^*), x - x^* \rangle \geq 0, \ \forall x \in X.$$

- **Question 2**: You work on recommendation systems in Netflix, which uses $x_i^T y_j$ to estimate rating M_{ij}, where x_i, y_j are vectors.
  - ◇ You noticed an implicit requirement: rating is often positive.
  - ◇ But your team is using SGD.
  - ◇ What can you say to your team leader?

$$\min_{x_i, y_j's} \sum_{1 \le i,j \le n} (M_{ij} - x_i^T y_j)^2.$$

$$\text{s.t.} \quad x_i^T y_j \geq 0, \ \forall i,j.$$

Here $x_i, y_j \in \mathbb{R}^{r \times 1}$, $i,j = 1, \ldots, n$.

Wrong method → right answer.

First check: at optimum, $x_i^{*T} y_j^* \geq 0$, $\forall i,j$.

If so, then not an issue. Otherwise, an issue.

Second, how to resolve the issue?

- SGD with projection; or CD with projection; or ADMM (to be learned).

Not easy answer.

Summary of Last Lecture

- Optimality condition for

$$\min_x f(x), \text{ s.t. } x \in X.$$

Suppose X convex, f cts-diffentiable. If x^* is a local-min, then

$$\langle \nabla f(x^*), x - x^* \rangle \geq 0, \quad \forall x \in X.$$

When X convex, necessary; when f convex, sufficient.

- Gradient projection method

$$\text{GP1}: x^{r+1} = \text{proj}_X(x^r - s_r \nabla f(x^r)).$$

x^r $\quad x^{r+1}$ $\quad \bar{x}^{r+1}$

GP2: pick new iterate along the direction given by GP1.

- Projection simple for: bounds, ball, simplex; sometimes linear
- Stepsize rules: constant; line search for s_r or α_r

This Lecture

set X: implicit description.
e.g. $X = \{\lambda \mid \lambda$ is an eigenvalue of a matrix A^3+2A^2+A for some matrix $A\}$.

- From today: **constrained optimization** with explicit equality/inequality constraints
- After the lecture, you should be able to
  - Write down the 1st and 2nd order conditions for equality constrained problems
  - Define Lagrangian multipliers and Lagrangian functions
  - Compute/verify optimal solutions for simple equality constrained problems
- Advanced goal: explain the two proof ideas and why they are useful

Outline

Optimization Over Convex-set: Criticism

- What is the drawback of the optimality condition

$$\langle \nabla f(x^*), x - x^* \rangle \geq 0, \forall\, x \in X? \tag{1}$$

- Back to the origin: what should be an "optimality condition"?
  - Of course, $f(x) \geq f(x^*)$, $\forall x \in X$ is also optimality condition
  - Issue: hard to check
  - Is the condition (1) really better? Sort of; unclear
- There can be multiple optimality conditions. How to judge?
  - Easily checkable
  - Leading to algorithm design

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Equality Constrained Problem

Let us first consider the following equality constrained problem

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

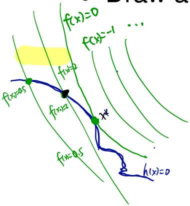
e.g. $\|x\|^2 = 1$, $Ax = b$, $XY^T = A$, etc.

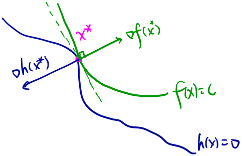
where $f : R^n \mapsto R$, $h_i : R^n \mapsto R, i = 1, ..., m$, are continuously differentiable functions.

Is this "optimization over convex set"? No, unless $h_i(x^*)$'s are affine.

Intuition: One Constraint

- Consider one constraint $\min_x f(x),$ s.t. $h(x) = 0$.
- Draw a plot of level set of f and the set $h(x) = 0$





- Observation: at an optimal solution, $\nabla f(x^*) \,//\, \nabla h(x^*)$,

  or $\nabla f(x^*) = \lambda^* \nabla h(x^*)$, for some λ^*.

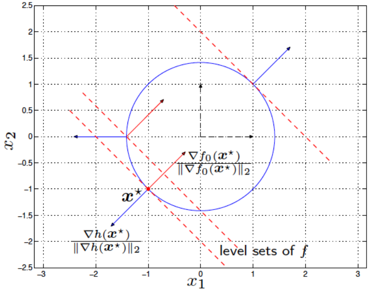
Example 1

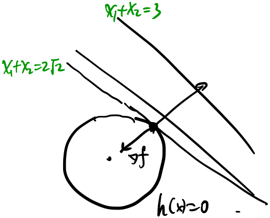
$$\nabla f = \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

$$\nabla h = \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix} = 2\begin{pmatrix} x_1^* \\ x_1^* \end{pmatrix}.$$

They touch at point

$$(x_1^*, x_2^*) = (x_1^*, x_1^*) = (\sqrt{2}, \sqrt{2}).$$





Consider the problem

$$\begin{aligned} \underset{x\in\mathbb{R}^2}{\text{minimize}} \quad & f_0(x) = x_1 + x_2 \\ \text{subject to} \quad & h(x) = x_1^2 + x_2^2 - 2 = 0. \end{aligned}$$

This is a problem with a linear objective function $f(x)$ and one nonlinear equality constraint $h(x) = 0$. At the solution $x^\star$, the gradient of the constraint $\nabla h(x^\star)$ is orthogonal to the level set of the function at x^*, and hence $\nabla h(x^\star)$ and $\nabla f_0(x^\star)$ are parallel *i.e.*, there is a scalar $\nu^\star$ such that

$$\nabla f_0(x^\star) + \nu^\star \nabla h(x^\star) = \mathbf{0}.$$

Clearly, in this example $x^\star$ is regular (because $\nabla h(x^\star) \neq \mathbf{0}$).

Degenerate Case

- Still one-constraint problem $\min_x f(x)$, s.t. $h(x) = 0$.
- Is $\nabla f(x^*) = \lambda \nabla h(x^*)$ always true? Assuming f and h are smooth.

- **Example 2**: $\min_{x \in \mathbb{R}} x^2$, s.t. $(x-1)^2 = 0$.

  Feasible set $\{1\}$. So optimal solution $x^* = 1$.

  Exercise: Check whether $\nabla f(x^*) = \lambda \nabla h(x^*)$.

  $\nabla f(x^*) = 2x^* = 2$,

  $\nabla h(x^*) = 2(x^*-1) = 0$.

  $2 \neq \lambda \cdot 0, \forall \mathbb{R}$.

- Modified problem: $\min_{x \in \mathbb{R}} x^2$, s.t. $x - 1 = 0$.
  Check: $\nabla f(x^*) = 2$, $\nabla h(x^*) = 1$, so $\nabla f(x^*) = 2 \cdot \nabla h(x^*)$.

Equality Constrained Problem: Optimality Conditions

Lagrange Multiplier Theorem

- Let x^* be a local min and a regular point ($\nabla h_i(x^*)$: linearly independent). Then there exist unique scalars $\lambda_1^*, ..., \lambda_m^*$ such that

  $$\text{1st order: } \nabla f(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla h_i(x^*) = 0.$$

  If in addition f and h are twice continuously differentiable,

  $$\text{2nd order: } y'\left(\nabla^2 f(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla^2 h_i(x^*)\right) y \geq 0, \quad \forall \underset{y \in \mathbb{R}^n.}{y} \text{ s.t. } \nabla h_i(x^*)' y = 0, \ \forall i.$$

Characterizes a set of necessary conditions for local min.

Optimality Conditions in Words

To learn math, you should be able to translate “math language” to “human language”.

Lagrangian multiplier theorem (in words): for (smooth) equality constrained problems, at a “regular” local-min (gradients of constraints are linearly independent), we have

- The gradient of the objective can be linearly spanned by the gradients of constraints.
- The Hessian of the objective function plus the same span of Hessian of constraints is positive semidefinite in the space orthogonal to all gradients of constraints.

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Short version: linear combination of Hessians is PSD in some space (orthogonal complement space).

Outline

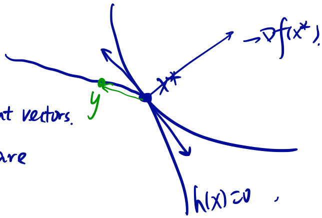
Proof Method 1: Feasible Direction

- Two ways to develop the theory of Lagrangian multipliers
  - **Feasible direction** viewpoint
  - **Penalty** approach

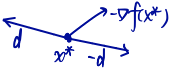
- For illustration, consider $\min_{x \in \mathbb{R}^n} f(x)$, s.t. $h(x) = 0$.

- Feasible variation $y - x^*, y \in X$ cannot be a descent variation. Draw a plot.

feasible variation: $y - x^*$, where $h(y)=0$.
As $y \to x^*$, becomes tangent vectors.
$\therefore$ Feasible variations are tangent vectors



Tangent vectors are not descent
$\Rightarrow$ tangent vectors $\perp \nabla f(x^*)$
(Since d is tangent
$\Rightarrow -d$ is tangent;
If $d \not\perp \nabla f(x^*)$, then either d or $-d$ is descent direction.)



Proof Method 1: Feasible Direction (cont'd)

- A bit more formally, use Taylor expansion:

$$f(x^* + d) = f(x^*) + \langle \nabla f(x^*), d\rangle + o(\|d\|^2) \geq f(x^*),$$

where $d = y - x^*$ in which $y \in X$ is any feasible variation.

$$\langle \nabla f(x^*), d\rangle + o(\|d\|^2) \geq 0 \qquad (2)$$

for any feasible variation d.

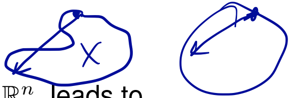
- Idea: Represent feasible variation d by Taylor expansion of h:

$$h(x^* + d) \approx h(x^*) + \langle \nabla h(x^*), d\rangle, \text{ i.e. } \quad 0 \approx \langle \nabla h(x^*), \underbrace{d}_{\text{tangent}}\rangle.$$

- If $\nabla h(x^*) \neq 0$ and $\nabla f(x^*) \nparallel \nabla h(x^*)$, then there is some d
  - orthogonal to $\nabla h(x^*)$
  - and positively related to $\nabla f(x^*)$,

violating (2).

Proof Method 1: More Formal Proof (Reading)



Remark 1: One issue of last-page proof.

- Unconstrained case: d can be anything in $\mathbb{R}^n$, leads to $\nabla f(x^*) = 0$.
    - Pick $d = -\alpha \nabla f(x^*)$ or positively related direction, let $\alpha \to 0$.
- **Issue**: for constrained case, d is restricted: cannot even scale.
    - thus finding one d is not enough
- **Correction**: there is such a sequence of d^k (norm going to zero)

Remark 2: A cleaner proof is by "elimination" [Sec. 3.1.2.]:

– represent some variables by others

– and transform to unconstrained problem.

It is essentially a "feasible direction" proof.

$h(x_1, x_2, x_3) = 0$

$\sim \ x_1 = \varphi(x_2, x_3)$

$\Rightarrow \min_{x_2, x_3} f(\varphi(x_2, x_3), x_2, x_3)$.

Check unconstrained 1st order condition.

Will get desired 1st order condition

Proof Method 2: Penalty Approach

- For illustration, consider (P1): $\min_{x\in\mathbb{R}^n} f(x)$, s.t. $h(x) = 0$.
- Consider another problem (P2)
  $\min_{x\in\mathbb{R}^n} f(x) + k\|h(x)\|^2 + \|x - x^*\|^2. \overset{\Delta}{=} F(x).$
- Wish: If x^* is a local-min of (P1), then also a local-min of (P2).
  $\Downarrow$ $\nabla F(x^*) = 0$
  - This implies the desired 1st order condition, done.

$$\text{1oC:} \quad \nabla f(x^*) + \underbrace{2kh(x^*)}_{\lambda^*}\nabla h(x^*) = 0.$$

- Fact: it only holds for $k \to \infty$.

  Claim: As $k \to \infty$, there is a sequence of local-mins of (P2) $\{x^k\}$ that converge to x^*.

Question Is x^* global-min of (P2), provided that x^* is global-min of (P1)?
Answer: quite subtle .... Will discuss in later lectures.

Why are These Proofs Useful?

Geometrical understanding of Lagrangian multiplier condition.

- Viewpoint 1: $\nabla f(x^*)$ spanned by $\nabla h_k(x^*)$
- Viewpoint 2: $\nabla f(x^*)$ orthogonal to tangent space of constraint manifold
- Quick reason: feasible direction $\neq$ descent direction

Algorithm design.

- "Penalty" is critical for constrained-opt algorithm design
- Related constrained to unconstrained

Formal Proof of the Theorem (Sec. 3.1.1.) –Reading

- Suppose x^* is a local min satisfying $h(x^*) = 0$. Pick any $\alpha > 0$. Consider
$$f^k(x) = f(x) + k|h(x)|^2 + \frac{\alpha}{2} \|x - x^*\|^2 .$$
- Let x^k be a constrained minimizer of f^k over the region $\{x \mid f(x^*) \leq f(x), \|x - x^*\| \leq 1\}$. We will show that x^k is an unconstrained local min of f^k for all large k.
- Taking limit $k \to \infty$ of
$$f^k(x^k) = f(x^k) + k|h(x^k)|^2 + \frac{\alpha}{2} \left\|x^k - x^*\right\|^2 \leq f^k(x^*) = f(x^*)$$
along any convergent subsequence of $\{x^k\}$,we get $h(\bar{x}) = \lim_{k\to\infty} h(x^k) = 0$.
- Furthermore, taking limit of $f(x^k) + \frac{\alpha}{2} \|x - x^*\|^2 \leq f(x^*)$ shows
$$f(\bar{x}) + \frac{\alpha}{2} \|\bar{x} - x^*\|^2 \leq f(x^*)$$
- Since $h(\bar{x}) = 0$, it follows that $f(x^*) \leq f(\bar{x})$.Thus, we have $\bar{x} = x^*$ and $f(x^*) = f(\bar{x})$.

Formal Proof of the Theorem (Sec. 3.1.1.) –Reading

- Since $\bar{x}$ is any limit point, we have $x^k \to x^*$,so $\left\|x^k - x^*\right\| < 1$ for large k,$\Rightarrow$ x^k for k large enough, x^k is an unconstrained local min of f^k, satisfying

$$\nabla f^k(x^k) = 0, \quad \nabla^2 f^k(x^k) \succeq 0.$$

- Taking limit of the following optimality condition

$$0 \; = \; \nabla f(x^k) + 2kh(x^k)\nabla h(x^k) + \alpha(x^k - x^*) \tag{3}$$

Since $\nabla h(x^*)$ has rank m, $\nabla h(x^k)$ also has rank m for large k, so $\nabla h(x^k)'\nabla h(x^k)$: invertible.

Multiplying (1) with $\nabla h(x^k)'$ yields

$$kh(x^k) = -(\nabla h(x^k)'\nabla h(x^k))^{-1}\nabla h(x^k)'(\nabla f(x^k) + \alpha(x^k - x^*)).$$

- Taking limit as $k \to \infty$ and $x^k \to x^*$,

$$\{kh(x^k)\} \to (\nabla h(x^*)'\nabla h(x^*))^{-1}\nabla h(x^*)'\nabla f(x^*) \equiv \lambda.$$

Formal Proof of the Theorem (Sec. 3.1.1.) –Reading

Taking limit as $k \to \infty$ in Eq.(1), we obtain

$$\nabla f(x^*) + \nabla h(x^*)\lambda = 0.$$

- **Exercise**: 2nd order L-multiplier condition: Use 2nd order unconstrained condition for x^k, and algebra.

Outline

Optimality Conditions for Equally Constrained Problems

Two Proof Methods: Feasible Direction and Penalty

Lagrangian Function and Sufficient Conditions

Lagrangian Function

- Define the Lagrangian function (λ: Lagrangian multiplier)

$$L(x, \lambda) = f(x) + \sum_{i=1}^{m} \lambda_i h_i(x).$$

Different from $f(x) + \sum_i h_i(x)^2$.

Then, if x^* is a local minimum which is regular, $\nabla L = 0$.

1st order Condition (1oC): $\nabla_x L(x^*, \lambda^*) = 0, \quad \nabla_\lambda L(x^*, \lambda) = 0.$ $\longrightarrow$ $h_i(x^*) = 0, \forall i$.

$\nabla f(x^*) + \sum_i \lambda_i^* \nabla h_i(x^*) = 0$.

2nd Order Condition (2oC): $y' \nabla^2_{xx} L(x^*, \lambda^*) y \geq 0, \quad \forall y \ s.t. \ \nabla h(x^*)' y = 0.$

Note: $\nabla^2_{\lambda\lambda} L(x; \lambda) = 0$.

- **Remark**: $n + m$ variables, $n + m$ equations in 1oC
- **Example:**

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}(x_1^2 + x_2^2 + x_3^2) \\ \text{subject to} & x_1 + x_2 + x_3 = 3. \end{array}$$

Necessary conditions

$$x_1^* + \lambda^* = 0, \quad x_2^* + \lambda^* = 0, \quad x_3^* + \lambda^* = 0, \quad x_1^* + x_2^* + x_3^* = 3.$$

Original: 3 variables, 1 equation + $\min_x \square$.

1oC: 4 variables, 4 equations

Original: 5 var's 2 equations

1oC: 7 -- , 7. equations.

Optimality Conditions in Words

Lagrangian multiplier theorem (restated, in words): for (smooth) equality constrained problems, at a “regular” local-min (gradients of constraints are linearly independent), we have

- The gradient of the Lagrangian function is zero
- The Hessian of the Lagrangian function w.r.t. x is positive semidefinite in the space orthogonal to all gradients of constraints.
  - Another way: in the nullspace defined by all gradients of constraints

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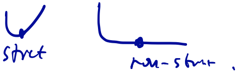
Suffciency Condition

- Second Order Suffciency Conditions: Let $x^* \in R^n$ and $\lambda \in R^m$ satisfy

$$\nabla_x L(x^*, \lambda^*) = 0, \;\; \nabla_\lambda L(x^*, \lambda^*) = 0,$$
$$y' \nabla^2_{xx} L(x^*, \lambda^*) y > 0, \forall y \neq 0 \text{ with } \nabla h_i(x^*)' y = 0. \; \forall i,$$

Then x^* is a strict local minimum.

Remark: No need to have regularity condition.



- **Example:**

$$\begin{array}{ll} \text{minimize} & -(x_1x_2 + x_2x_3 + x_1x_3) \\ \text{subject to} & x_1 + x_2 + x_3 = 3. \end{array}$$

$\nabla L = 0.$

We have that $x_1^* = x_2^* = x_3^* = 1$ and $\lambda^* = 2$ satisfy the 1st order conditions. Also

$$\nabla^2_{xx} L(x^*, \lambda^*) = \begin{bmatrix} 0 & -1 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix}$$

We have for all $y \neq 0$ with $\nabla h(x^*)' y = 0$ or $y_1 + y_2 + y_3 = 0$,

$$y' \nabla^2_{xx} L(x^*, \lambda^*) y = -y_1(y_2 + y_3) - y_2(y_1 + y_3) - y_3(y_1 + y_2) = y_1^2 + y_2^2 + y_3^2 > 0$$

Hence, x^* is a strict local minimum.

Proof Preparation: A Useful Lemma (Reading)

- Let P and Q be two symmetric matrices. Assume that $Q \succ 0$ and $P \succ 0$ on the nullspace of Q,i.e.,$x'Px > 0$ for all $x \neq 0$ with $x'Qx = 0$. Then there exists a scalar c such that

$$P + cQ : \text{positive definite}, \forall c > \bar{c}.$$

- Proof: Assume the contrary. Then for every k, there exists a vector x^k with $x^k = 1$ such that

$$(x^k)'Px^k + k(x^k)'Qx^k < 0.$$

Consider a subsequence $\{x^k\}_{k \in \mathcal{K}}$ converging to some x with $x = 1$. Taking the limit superimum,

$$x'Px + \limsup_{k \to \infty \ k \in \mathcal{K}} (k(x^k)'Qx^k) \leq 0.$$

We have $(x^k)'Qx^k \geq 0$ (since $Q \succeq 0$), so

$$\{(x^k)'Qx^k\}_{k \in \mathcal{K}} \to 0.$$

Therefore, $x'Qx = 0$ and using the hypothesis, $x'Px > 0$, a contradiction.

Proof by Penalty Approach (Reading)

Consider the *augmented Lagrangian function*

$$L_c(x, \lambda) = f(x) + \lambda' h(x) + \frac{c}{2} \|h(x)\|^2 ,$$

where c is a scalar. We have

$$\nabla_x L_c(x, \lambda) = \nabla_x L(x, \tilde{\lambda}), \ \nabla^2_{xx} L_c(x, \lambda) = \nabla^2_{xx} L(x, \tilde{\lambda}) + c \nabla h(x) \nabla h(x)'$$

where $\tilde{\lambda} = \lambda + ch(x)$. If (x^*, λ^*) satisfy the suffciency conditions, we have using the lemma (why?),

$$\nabla_x L_c(x^*, \lambda^*) = 0, \ \nabla^2_{xx} L_c(x^*, \lambda^*) > 0,$$

for suffciently large c. Hence for some $\gamma > 0, \epsilon > 0$, (x^* unconstrained local min)

$$L_c(x, \lambda^*) \geq L_c(x^*, \lambda^*) + \frac{\gamma}{2} \|x - x^*\|^2 ,$$

if $\|x - x^*\| < \epsilon$. Since $L_c(x, \lambda^*) = f(x)$ when $h(x) = 0$,

$$f(x) \geq f(x^*) + \frac{\gamma}{2} \|x - x^*\|^2 , \ if \ h(x) = 0, \|x - x^*\| < \epsilon.$$

Summary

In this lecture, we learned the following: (think about what you have learned)

- Optimality conditions (1st and 2nd order) for equally constrained problems
- Two proofs: feasible direction and penalty
- Lagrangian multipliers λ and Lagrangian function $L(x, \lambda)$

  Express optimality conditions by derivatives of L

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In this lecture, we learned the following:

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- Two proofs: feasible direction and penalty

- Lagrangian multipliers λ and Lagrangian function $L(x, \lambda)$

  Express optimality conditions by derivatives of L