Introduction and Math Preliminaries

Yinyu Ye
Department of Management Science and Engineering
Stanford University
Stanford, CA 94305, U.S.A.

http://www.stanford.edu/~yyye

What you lean in CME307/MS&E311?

- Present a core element, mathematical optimization theories and algorithms, for the ICME disciplines.
- Provide mathematical proofs and in-depth theoretical analyses of optimization models/algorithms discussed in MS&E211
- Introduce additional conic-linear and nonlinear/nonconvex optimization models/problems comparing to MS&E310.
- Describe new/recent effective optimization methods/algorithms in Data Science, Machine Learning and AI.

Mathematical Optimization

The field of optimization is concerned with the study of maximization and minimization of mathematical functions. Very often the arguments of (i.e., variables or unknowns in) these functions are subject to side conditions or constraints. By virtue of its great utility in such diverse areas as applied science, engineering, economics, finance, medicine, and statistics, optimization holds an important place in the practical world and the scientific world. Indeed, as far back as the Eighteenth Century, the famous Swiss mathematician and physicist Leonhard Euler (1707-1783) proclaimed[a] that ... nothing at all takes place in the Universe in which some rule of maximum or minimum does not appear.

[a]See Leonhardo Eulero, *Methodus Inviendi Lineas Curvas Maximi Minimive Proprietate Gaudentes*, Lausanne & Geneva, 1744, p. 245.

Mathematical Optimization/Programming (MP)

The class of mathematical optimization/programming problems considered in this course can all be expressed in the form

$$
\begin{array}{lll}
\text{(P)} & \text{minimize} & f(\mathbf{x}) \\
& \text{subject to} & \mathbf{x} \in \mathcal{X}
\end{array}
$$

where $\mathcal{X}$ usually specified by constraints:

$$
\begin{array}{rcll}
c_i(\mathbf{x}) & = & 0 & i \in \mathcal{E} \\
c_i(\mathbf{x}) & \leq & 0 & i \in \mathcal{I}.
\end{array}
$$

Global and Local Optimizers

A global minimizer for (P) is a vector $\mathbf{x}^*$ such that

$$\mathbf{x}^* \in \mathcal{X} \quad \text{and} \quad f(\mathbf{x}^*) \le f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X}.$$

Sometimes one has to settle for a local minimizer, that is, a vector $\bar{\mathbf{x}}$ such that

$$\bar{\mathbf{x}} \in \mathcal{X} \quad \text{and} \quad f(\bar{\mathbf{x}}) \le f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X} \cap N(\bar{x})$$

where $N(\bar{\mathbf{x}})$ is a neighborhood of $\bar{\mathbf{x}}$. Typically, $N(\bar{\mathbf{x}}) = B_\delta(\bar{\mathbf{x}})$, an open ball centered at $\bar{\mathbf{x}}$ having suitably small radius $\delta > 0$.

The value of the objective function f at a global minimizer or a local minimizer is also of interest. We call it the global minimum value or a local minimum value, respectively.

Important Terms

- decision variable/activity, data/parameter
- objective/goal/target
- constraint/limitation/requirement
- satisfied/violated
- feasible/allowable solutions
- optimal (feasible) solutions
- optimal value

Size and Complexity of Problems

- number of decision variables
- number of constraints
- bit size/number required to store the problem input data
- problem difficulty or complexity number
- algorithm complexity or convergence speed

Real n-Space; Euclidean Space

- $\mathcal{R}, \quad \mathcal{R}_+, \quad \text{int}\,\mathcal{R}_+$
- $\mathcal{R}^n, \quad \mathcal{R}^n_+, \quad \text{int}\,\mathcal{R}^n_+$
- $\mathbf{x} \geq \mathbf{y}$ means $x_j \geq y_j$ for $j = 1, 2, ..., n$
- $\mathbf{0}$: all zero vector; and $\mathbf{e}$: all one vector
- Column vector:

$$\mathbf{x} = (x_1; x_2; \ldots; x_n)$$

  and row vector:

$$\mathbf{x} = (x_1, x_2, \ldots, x_n)$$

- Inner-Product:

$$\mathbf{x} \bullet \mathbf{y} := \mathbf{x}^T\mathbf{y} = \sum_{j=1}^{n} x_j y_j$$

- Vector norm: $\|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^T\mathbf{x}}$, $\|\mathbf{x}\|_\infty = \max\{|x_1|, |x_2|, ..., |x_n|\}$, in general, for $p \geq 1$

$$\|\mathbf{x}\|_p = \left(\sum_{j=1}^{n} |x_j|^p\right)^{1/p}$$

- A set of vectors $\mathbf{a}_1, ..., \mathbf{a}_m$ is said to be linearly dependent if there are multipliers $\lambda_1, ..., \lambda_m$, not all zero, the linear combination

$$\sum_{i=1}^{m} \lambda_i \mathbf{a}_i = \mathbf{0}$$

- A linearly independent set of vectors that span R^n is a basis.

Matrices

- $A \in \mathcal{R}^{m \times n}$; $\mathbf{a}_{i.}$, the ith row vector; $\mathbf{a}_{.j}$, the jth column vector; a_{ij}, the i,jth entry
- $\mathbf{0}$: all zero matrix, and I: the identity matrix
- The null space $\mathcal{N}(A)$, the row space $\mathcal{R}(A^T)$, and they are orthogonal.
- $\det(A)$, $\text{tr}(A)$: the sum of the diagonal entries of A
- Inner Product:

$$A \bullet B = \text{tr} A^T B = \sum_{i,j} a_{ij} b_{ij}$$

- The operator norm of matrix A:

$$\|A\|^2 := \max_{\mathbf{0} \neq \mathbf{x} \in \mathcal{R}^n} \frac{\|A\mathbf{x}\|^2}{\|\mathbf{x}\|^2}$$

  The Frobenius norm of matrix A:

$$\|A\|_f^2 := A \bullet A = \sum_{i,j} a_{ij}^2$$

- Sometimes we use $X = \text{diag}(\mathbf{x})$
- Eigenvalues and eigenvectors

$$A\mathbf{v} = \lambda \cdot \mathbf{v}$$

Symmetric Matrices

- $\mathcal{S}^n$
- The Frobenius norm:

$$\|X\|_f = \sqrt{\text{tr} X^T X} = \sqrt{X \bullet X}$$

- Positive Definite (PD): $Q \succ \mathbf{0}$ iff $\mathbf{x}^T Q \mathbf{x} > 0, \quad \text{for all} \quad \mathbf{x} \neq \mathbf{0}$. The sum of PD matrices is PD.
- Positive Semidefinite (PSD): $Q \succeq \mathbf{0}$ iff $\mathbf{x}^T Q \mathbf{x} \geq 0, \quad \text{for all} \quad \mathbf{x}$. The sum of PSD matrices is PSD.
- PSD matrices: $\mathcal{S}^n_+, \quad \text{int}\, \mathcal{S}^n_+$ is the set of all positive definite matrices.

Affine Set

$S \subset R^n$ is affine if

$$[\,\mathbf{x}, \mathbf{y} \in S \text{ and } \alpha \in R\,] \Longrightarrow \alpha\mathbf{x} + (1-\alpha)\mathbf{y} \in S.$$

When x and y are two distinct points in R^n and α runs over R ,

$$\{\mathbf{z} : \mathbf{z} = \alpha\mathbf{x} + (1-\alpha)\mathbf{y}\}$$

is the affine combination of $\mathbf{x}$ and $\mathbf{y}$.

When $0 \le \alpha \le 1$, it is called the convex combination of $\mathbf{x}$ and $\mathbf{y}$.

For $\alpha \ge 0$ and for $\beta \ge 0$

$$\{\mathbf{z} : \mathbf{z} = \alpha\mathbf{x} + \beta\mathbf{y}\},$$

is called the conic combination of $\mathbf{x}$ and $\mathbf{y}$.

Convex Set

- Ω is said to be a convex set if for every $\mathbf{x}^1, \mathbf{x}^2 \in \Omega$ and every real number $\alpha \in [0, 1]$, the point $\alpha \mathbf{x}^1 + (1-\alpha)\mathbf{x}^2 \in \Omega$.
- Ball and Ellipsoid: for given $\mathbf{y} \in \mathcal{R}^n$ and positive definite matrix Q,
$$E(\mathbf{y}, Q) = \{\mathbf{x} : \ (\mathbf{x}-\mathbf{y})^T Q(\mathbf{x}-\mathbf{y}) \leq 1\}$$
- The Intersection of convex sets is convex
- The convex hull of a set Ω is the intersection of all convex sets containing Ω
- An extreme point in a convex set is a point that cannot be expressed as a convex combination of other two distinct points of the set.
- A set is polyhedral if it has finitely many extreme points; $\{\mathbf{x} : \ A\mathbf{x} = \mathbf{b}, \ \mathbf{x} \geq \mathbf{0}\}$ and $\{\mathbf{x} : \ A\mathbf{x} \leq \mathbf{b}\}$ are convex polyhedral.

Cone and Convex Cone

- A set C is a cone if $\mathbf{x} \in C$ implies $\alpha\mathbf{x} \in C$ for all $\alpha > 0$
- The intersection of cones is a cone
- A convex cone is a cone and also a convex set
- A pointed cone is a cone that does not contain a line
- Dual cone:

$$C^* := \{\mathbf{y} : \ \mathbf{x} \bullet \mathbf{y} \geq 0 \quad \text{for all} \quad \mathbf{x} \in C\}.$$

The dual cone is always a closed convex cone.

Cone Examples

- Example 1: The n-dimensional non-negative orthant, $\mathcal{R}^n_+ = \{\mathbf{x} \in \mathcal{R}^n : \ \mathbf{x} \ge \mathbf{0}\}$, is a convex cone. Its dual is itself.
- Example 2: The set of all PSD matrices in $\mathcal{S}^n$, $\mathcal{S}^n_+$, is a convex cone, called the PSD matrix cone. Its dual is itself.
- Example 3: The set $\{(t;\mathbf{x}) \in \mathcal{R}^{n+1} : \ t \ge \|\mathbf{x}\|_p\}$ for a $p \ge 1$ is a convex cone in $\mathcal{R}^{n+1}$, called the p-order cone. Its dual is the q-order cone with $\frac{1}{p} + \frac{1}{q} = 1$.
- The dual of the second-order cone ($p = 2$) is itself.

Polyhedral Convex Cones

- A cone C is (convex) polyhedral if C can be represented by

$$C = \{\mathbf{x} : A\mathbf{x} \leq \mathbf{0}\}$$

or

$$C = \{A\mathbf{x} : \mathbf{x} \geq \mathbf{0}\}$$

for some matrix A.

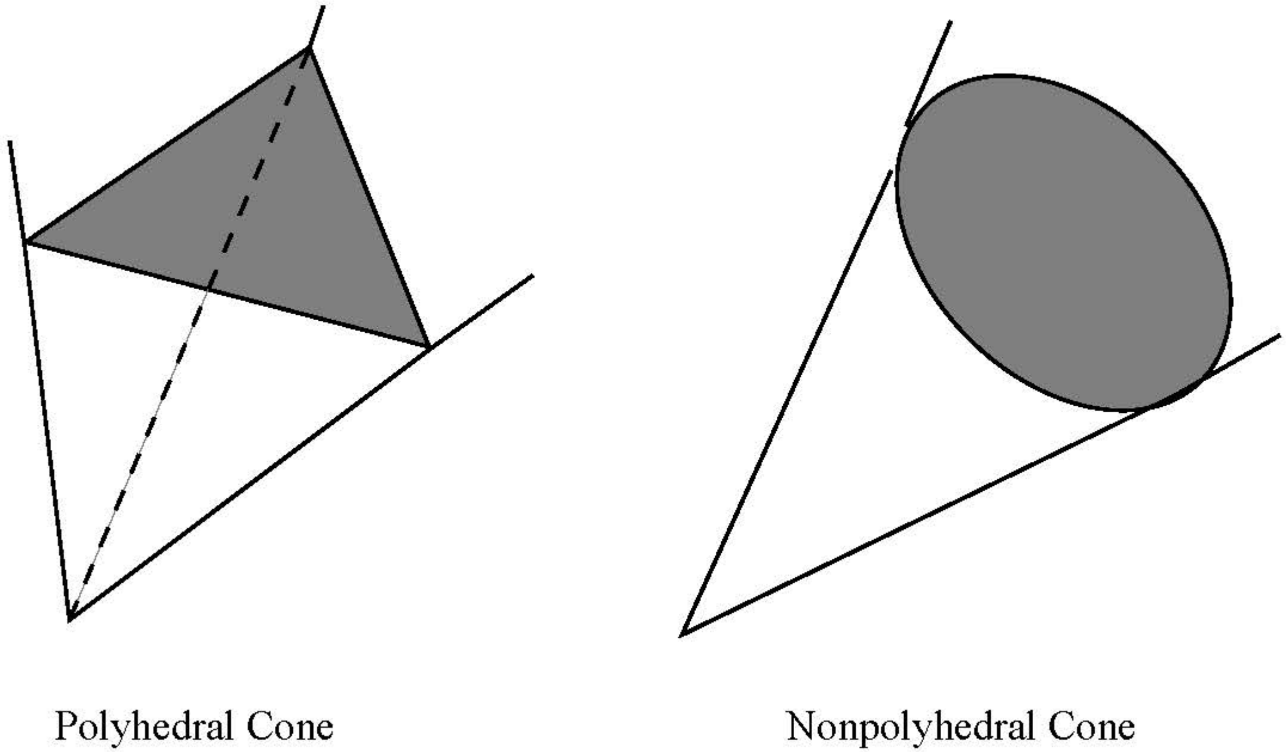

Figure 1: Polyhedral and nonpolyhedral cones.

- The non-negative orthant is a polyhedral cone, and neither the PSD matrix cone nor the second-order cone is polyhedral.

Real Functions

- Continuous functions

- Weierstrass theorem: a continuous function f defined on a compact set (bounded and closed) $\Omega \subset \mathcal{R}^n$ has a minimizer in Ω.

- A function $f(\mathbf{x})$ is called homogeneous of degree k if $f(\alpha\mathbf{x}) = \alpha^k f(\mathbf{x})$ for all $\alpha \geq 0$.

- Example: Let $\mathbf{c} \in \mathcal{R}^n$ be given and $\mathbf{x} \in \operatorname{int} \mathcal{R}^n_+$. Then $\mathbf{c}^T\mathbf{x}$ is homogeneous of degree 1 and

$$\mathcal{P}(\mathbf{x}) = n \log(\mathbf{c}^T\mathbf{x}) - \sum_{j=1}^{n} \log x_j$$

  is homogeneous of degree 0.

- Example: Let $C \in \mathcal{S}^n$ be given and $X \in \operatorname{int} \mathcal{S}^n_+$. Then $\mathbf{x}^T C\mathbf{x}$ is homogeneous of degree 2, $C \bullet X$ and $\det(X)$ are homogeneous of degree 1 and n, respectively; and

$$\mathcal{P}(X) = n \log(C \bullet X) - \log\det(X)$$

  is homogeneous of degree 0.

- The gradient vector: $\nabla f(\mathbf{x}) = \{\partial f / \partial x_i\}$, for $i = 1, ..., n.$
- The Hessian matrix: $\nabla^2 f(\mathbf{x}) = \left\{ \frac{\partial^2 f}{\partial x_i \partial x_j} \right\}$ for $i = 1, ..., n;\ j = 1, ..., n.$
- Vector function: $\mathbf{f} = (f_1; f_2; ...; f_m)$
- The Jacobian matrix of $\mathbf{f}$ is

$$\nabla \mathbf{f}(x) = \begin{pmatrix} \nabla f_1(\mathbf{x}) \\ \ldots \\ \nabla f_m(\mathbf{x}) \end{pmatrix}.$$

- The least upper bound or supremum of f over Ω

$$\sup\{f(\mathbf{x}) : \ x \in \Omega\}$$

and the greatest lower bound or infimum of f over Ω

$$\inf\{f(\mathbf{x}) : \ x \in \Omega\}$$

Convex Functions

- f is a convex function iff for $0 \le \alpha \le 1$,

$$f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y}) \le \alpha f(\mathbf{x}) + (1-\alpha)f(\mathbf{y}).$$

- The sum of convex functions is a convex function; the max of convex functions is a convex function;

- The (lower) level set of f is convex:

$$L(z) = \{\mathbf{x} : \quad f(\mathbf{x}) \le z\}.$$

- Convex set $\{(z;\mathbf{x}) : \ f(\mathbf{x}) \le z\}$ is called the epigraph of f.

- $tf(\mathbf{x}/t)$ is a convex function of $(t;\mathbf{x})$ for $t > 0$; it's homogeneous with degree 1.

Convex Function Examples

- $\|\mathbf{x}\|_p$ for $p \geq 1$.

$$\|\alpha\mathbf{x} + (1-\alpha)\mathbf{y}\|_p \leq \|\alpha\mathbf{x}\|_p + \|(1-\alpha)\mathbf{y}\|_p \leq \alpha\|\mathbf{x}\|_p + (1-\alpha)\|\mathbf{y}\|_p,$$

  from the triangle inequality.

- $e^{x_1} + e^{x_2} + e^{x_3}$.

- $\log(e^{x_1} + e^{x_2} + e^{x_3})$: we will prove it later.

Example: Proof of convex function

Consider the minimal-objective function of $\mathbf{b}$ for fixed A and $\mathbf{c}$:

$$\begin{aligned} z(\mathbf{b}) := \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & A\mathbf{x} = \mathbf{b}, \\ & \mathbf{x} \geq \mathbf{0}, \end{aligned}$$

where $f(\mathbf{x})$ is a convex function.

Show that $z(\mathbf{b})$ is a convex function in $\mathbf{b}$.

Theorems on functions

Taylor's theorem or the mean-value theorem:

Theorem 1 *Let $f \in C^1$ be in a region containing the line segment $[\mathbf{x}, \mathbf{y}]$. Then there is a α, $0 \le \alpha \le 1$, such that*

$$f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y})(\mathbf{y} - \mathbf{x}).$$

Furthermore, if $f \in C^2$ then there is a α, $0 \le \alpha \le 1$, such that

$$f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{x})(\mathbf{y} - \mathbf{x}) + (1/2)(\mathbf{y} - \mathbf{x})^T \nabla^2 f(\alpha\mathbf{x} + (1-\alpha)\mathbf{y})(\mathbf{y} - \mathbf{x}).$$

Theorem 2 *Let $f \in C^1$. Then f is convex over a convex set Ω if and only if*

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})(\mathbf{y} - \mathbf{x})$$

for all $\mathbf{x},\ \mathbf{y} \in \Omega$.

Theorem 3 *Let $f \in C^2$. Then f is convex over a convex set Ω if and only if the Hessian matrix of f is positive semi-definite throughout Ω.*

Theorem 4 *Suppose we have a set of m equations in n variables*

$$h_i(\mathbf{x}) = 0, \ i = 1, ..., m$$

where $h_i \in C^p$ for some $p \geq 1$. Then, a set of m variables can be expressed as implicit functions of the other $n - m$ variables in the neighborhood of a feasible point when the Jacobian matrix of the m variables is nonsingular.

Known Inequalities

- Cauchy-Schwarz: given $\mathbf{x}, \mathbf{y} \in \mathcal{R}^n$, $|\mathbf{x}^T\mathbf{y}| \leq \|\mathbf{x}\|_p \|\mathbf{y}\|_q$, where $\frac{1}{p} + \frac{1}{q} = 1$ and $p \geq 1$.
- Triangle: given $\mathbf{x}, \mathbf{y} \in \mathcal{R}^n$, $\|\mathbf{x} + \mathbf{y}\|_p \leq \|\mathbf{x}\|_p + \|\mathbf{y}\|_p$ for $p \geq 1$.
- Arithmetic-geometric mean: given $\mathbf{x} \in \mathcal{R}^n_+$,

$$\frac{\sum x_j}{n} \geq \left(\prod x_j\right)^{1/n}.$$

System of linear equations

Given $A \in \mathcal{R}^{m \times n}$ and $\mathbf{b} \in \mathcal{R}^m$, the problem is to determine n unknowns from m linear equations:

$$A\mathbf{x} = \mathbf{b}$$

Theorem 5 *Let $A \in \mathcal{R}^{m \times n}$ and $\mathbf{b} \in \mathcal{R}^m$. The system $\{\mathbf{x} : \ A\mathbf{x} = \mathbf{b}\}$ has a solution if and only if that $A^T\mathbf{y} = \mathbf{0}$ and $\mathbf{b}^T\mathbf{y} \neq 0$ has no solution.*

A vector $\mathbf{y}$, with $A^T\mathbf{y} = 0$ and $\mathbf{b}^T\mathbf{y} \neq 0$, is called an infeasibility certificate for the system.

Alternative system pairs: $\{\mathbf{x} : \ A\mathbf{x} = \mathbf{b}\}$ and $\{\mathbf{y} : \ A^T\mathbf{y} = \mathbf{0}, \ \mathbf{b}^T\mathbf{y} \neq 0\}$.

Gaussian Elimination and LU Decomposition

$$\begin{pmatrix} a_{11} & A_{1.} \\ 0 & A' \end{pmatrix} \begin{pmatrix} x_1 \\ x' \end{pmatrix} = \begin{pmatrix} b_1 \\ b' \end{pmatrix}.$$

$$A = L \begin{pmatrix} U & C \\ 0 & 0 \end{pmatrix}$$

The method runs in $O(n^3)$ time for n equations with n unknowns.

Linear least-squares problem

Given $A \in \mathcal{R}^{m \times n}$ and $\mathbf{c} \in \mathcal{R}^n$,

$$\begin{array}{lll} (LS) & \text{minimize} & \|A^T\mathbf{y} - \mathbf{c}\|^2 \\ & \text{subject to} & \mathbf{y} \in \mathcal{R}^m, \quad \text{or} \end{array}$$

$$\begin{array}{lll} (LS) & \text{minimize} & \|\mathbf{s} - \mathbf{c}\|^2 \\ & \text{subject to} & \mathbf{s} \in \mathcal{R}(A^T). \end{array}$$

$$AA^T\mathbf{y} = A\mathbf{c}$$

Choleski Decomposition:

$$AA^T = L\Lambda L^T, \quad \text{and then solve} \quad L\Lambda L^T\mathbf{y} = A\mathbf{c}.$$

Projections Matrices: $A^T(AA^T)^{-1}A$ and $I - A^T(AA^T)^{-1}A$

Solving ball-constrained linear problem

$$
\begin{array}{lll}
(BP) & \text{minimize} & \mathbf{c}^T\mathbf{x} \\
 & \text{subject to} & A\mathbf{x} = \mathbf{0},\ \|\mathbf{x}\|^2 \le 1,
\end{array}
$$

$\mathbf{x}^*$ minimizes (BP) if and only if there always exists a $\mathbf{y}$ such that they satisfy

$$AA^T\mathbf{y} = A\mathbf{c},$$

and if $\mathbf{c} - A^T\mathbf{y} \neq \mathbf{0}$ then

$$\mathbf{x}^* = -(\mathbf{c} - A^T\mathbf{y})/\|\mathbf{c} - A^T\mathbf{y}\|;$$

otherwise any feasible $\mathbf{x}$ is a minimal solution.

Solving ball-constrained linear problem

$$
\begin{array}{lll}
(BD) & \text{minimize} & \mathbf{b}^T\mathbf{y} \\
 & \text{subject to} & \|A^T\mathbf{y}\|^2 \leq 1.
\end{array}
$$

The solution $\mathbf{y}^*$ for (BD) is given as follows: Solve

$$AA^T\bar{\mathbf{y}} = \mathbf{b}$$

and if $\bar{\mathbf{y}} \neq \mathbf{0}$ then set

$$\mathbf{y}^* = -\bar{\mathbf{y}}/\|A^T\bar{\mathbf{y}}\|;$$

otherwise any feasible $\mathbf{y}$ is a solution.