Process Optimization

Jinhoon Choi

Department of Chemical Engineering
Sogang University

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Part I

Preliminaries

Chapter 1

Introduction

Optimization is associated with decision.

- When there are some alternatives (degree of freedom) to choose, the goal of optimization is to find the one that we like most.

In this lecture, we will focus on the mathematical programming among various optimization problems.

Ingredients of Mathematical Program

- Decision variables ($x \in \mathbf{R}^n$): undetermined parameters (degree of freedom)
- Cost function ($f : \mathbf{R}^n \to \mathbf{R}$): the measure of preference
- Constraints ($h(x) = 0$, $g(x) \leq 0$): equalities and inequalities that the decision variables must satisfy

$$\min_{x \in \mathbf{R}^n} f(x)$$
$$h(x) = 0, \quad g(x) \leq 0$$

Types of Mathematical Program

- Linear Program

$$\min_{x \in \mathbf{R}^n} c^T x$$
$$Ax + b = 0, \quad Dx + e \leq 0$$

- Unconstrained Nonlinear Program

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

- Constrained Nonlinear Program

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

$$h(x) = 0, \quad g(x) \leq 0$$

<u>Terminologies</u>

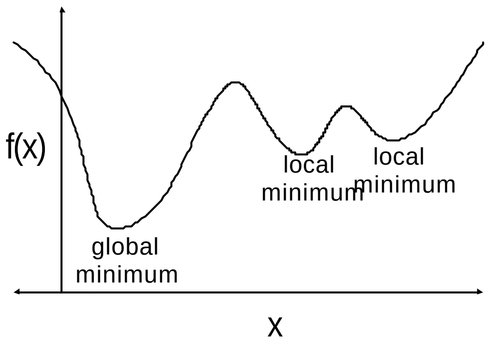
Feasible set:

$$\Omega = \{x \in \mathbf{R}^n : h(x) = 0, \; g(x) \leq 0\}$$

Feasible point: any $x \in \Omega$

Local minimum: $x^* \in \Omega$ such that $\exists \epsilon > 0$ for which $f(x^*) \leq f(x)$ for all $x \in \Omega \cap \{x \in \mathbf{R}^n : ||x - x^*|| < \epsilon\}$.

Global minimum: $x^* \in \Omega$ such that $f(x^*) \leq f(x)$ for all $x \in \Omega$.



Example (Optimal Design of an Oxygen Supply System):

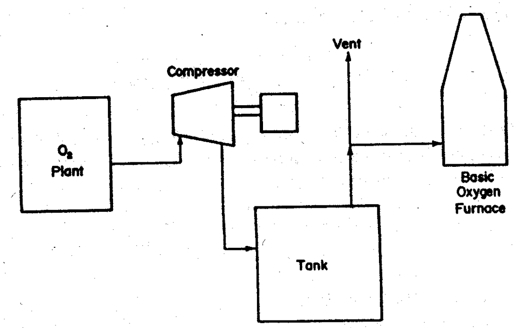


Figure 1.3. Design of oxygen production system, Example 1.1.

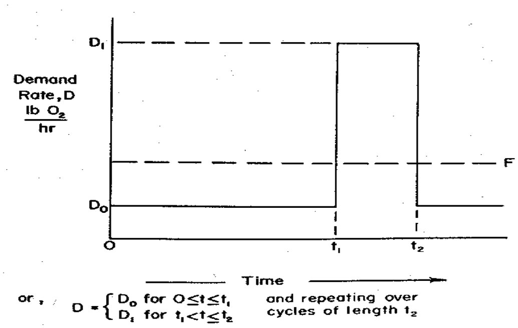


Figure 1.2. Oxygen demand cycle, Example 1.1.

- Decision variables:
  - the oxygen plant production rate (F ($lb\ O_2/hr$))
  - the compressor capacity (H (hp))
  - storage tank capacity (V (ft^3))

- maximum tank pressure (p (psi))

- Cost function: total annual cost that consists of
  - capital and operating cost of oxygen plant

$$C_1(\$/yr) = a_1 + a_2 F$$

    where a_1, a_2 are empirical constants for plants of this general type and include fuel, water and labor cost.
  - capital cost of storage vessel

$$C_2(\$) = b_1 V^{b_2}$$

    where b_1, b_2 are empirical constants appropriate for vessels of a specific construction.
  - capital cost of compressor

$$C_3(\$) = b_3 H^{b_4}$$

  - compressor operating cost per cycle (power consumption)

$$C_4(\$) = b_5 t_1 H$$

    where b_5 is the cost of power.
  - Total annual cost

$$C = a_1 + a_2 F + d(b_1 V^{b_2} + b_3 H^{b_4}) + N b_5 t_1 H$$

    where N is the number of cycles per year and d is an appropriate annual cost factor.

- Constraints:
  - The maximum amount of oxygen that must be stored

$$I_{max} = (D_1 - F)(t_2 - t_1)$$

    Then by the corrected gas law

$$V = \frac{I_{max}}{M}\frac{RT}{p}z = \frac{(D_1 - F)(t_2 - t_1)}{M}\frac{RT}{p}z$$

    where R: gas constant, T: gas temperature, z: compressibility factor and M: molecular weight of O_2.

- The compressor must be designed to handle gas at the flow rate $\frac{I_{max}}{t_1}$ and to compress the gas to the maximum pressure p. Under isothermal ideal gas compression assumption,

$$H = \frac{(D_1 - F)(t_2 - t_1)}{t_1} \frac{RT}{k_1 k_2} \ln\left(\frac{p}{p_0}\right)$$

where k_1: unit conversion factor, k_2: the compressor efficiency and p_0: the O_2 delivery pressure.

- O_2 production rate F must be adequate to supply total oxygen demand

$$F \geq \frac{D_0 t_1 + D_1(t_2 - t_1)}{t_2}$$

- maximum tank pressure must be greater than the O_2 delivery pressure

$$p \geq p_0$$

To this end,

$$\min_{F,H,V,p} a_1 + a_2 F + d(b_1 V^{b_2} + b_3 H^{b_4}) + N b_5 t_1 H$$

subject to

$$V = \frac{(D_1 - F)(t_2 - t_1)}{M} \frac{RT}{p} z$$

$$H = \frac{(D_1 - F)(t_2 - t_1)}{t_1} \frac{RT}{k_1 k_2} \ln\left(\frac{p}{p_0}\right)$$

$$F \geq \frac{D_0 t_1 + D_1(t_2 - t_1)}{t_2}$$

$$p \geq p_0$$

Chapter 2

Mathematical Preliminaries

2.1 Multivariable Calculus

$f : \mathbf{R} \to \mathbf{R}$ is differentiable at $x \in \mathbf{R}$ if

$$\lim_{\alpha \to 0} \frac{f(x+\alpha) - f(x)}{\alpha} \quad \text{exists.}$$

$$\Updownarrow$$

$\exists \eta(x) \in \mathbf{R}$ such that

$$\lim_{\alpha \to 0} \frac{f(x+\alpha) - f(x) - \alpha\eta(x)}{\alpha} = 0.$$

$\eta(x)$ is called the derivative of f, denoted $\frac{df(x)}{dx}$ or $f'(x)$.

<u>Gradients</u>

When $f : \mathbf{R}^n \to \mathbf{R}$, what do we mean by differentiability at $x \in \mathbf{R}^n$?

Definition: $f : \mathbf{R}^n \to \mathbf{R}$ is differentiable at $x \in \mathbf{R}^n$ if $\exists \eta(x) \in \mathbf{R}^n$ such that

$$\lim_{h \to 0} \frac{f(x+h) - f(x) - \eta^T(x)h}{||h||} = 0$$

where h is an n-D vector. $\eta(x)$ is called the gradient of f, denoted as $\nabla f(x)$.

Fact: If $f : \mathbf{R}^n \to \mathbf{R}$ is differentiable at x, then $\eta(x)$ is unique.

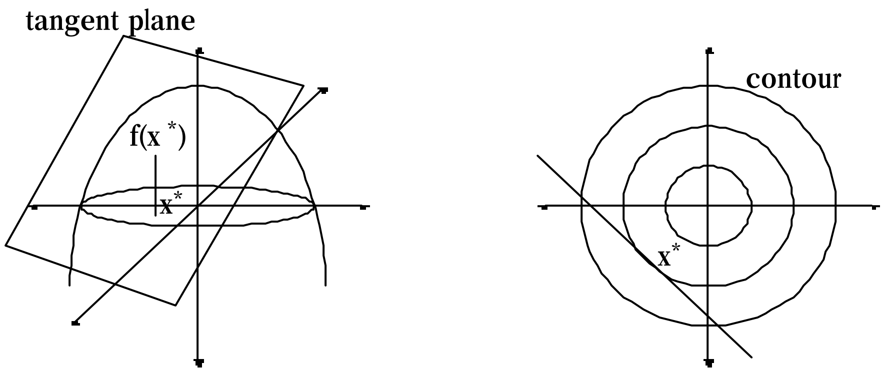
Proof: Suppose $\nu(x)$ is another gradient of f at x. Let $h = \alpha e_i$. Then

$$\nu_i(x) = \lim_{\alpha \searrow 0} \frac{f(x+\alpha e_i) - f(x)}{\alpha} = \eta_i(x).$$

Hence, the fact follows.

Geometric Interpretation of Gradient

Consider the tangent plane of f at $\bar{x}$. The the direction of the gradient is the steepest ascent direction.



Equation for tangent plane:

$$f(x) = f(\bar{x}) + \nabla f(\bar{x})^T (x - \bar{x}) \quad \Rightarrow \quad \triangle f = \nabla f^T \triangle x.$$

Note that $\frac{\triangle f}{|\triangle x|}$ is the slope in the direction of $\triangle x$. To find the steepest ascent direction, consider

$$\max_{|\triangle x|=1} \frac{\triangle f}{|\triangle x|} = \max_{|\triangle x|=1} \triangle f = \max_{|\triangle x|=1} \nabla f^T \triangle x$$

$$= \max_{|\triangle x|=1} |\nabla f||\triangle x| \cos(\angle(\nabla f, \triangle x)) = \max_{|\triangle x|=1} |\nabla f| |\cos(\angle(\nabla f, \triangle x)).$$

Notice that the maximum is achieved when $\angle(\nabla f, \triangle x) = 0$.

Moreover, consider $\triangle x$ in the tangent line of the contour. Then

$$0 = \triangle f = \nabla f^T \triangle x.$$

Hence, ∇f and $\triangle x$ are orthogonal.

Partial Derivatives

Definition: $f : \mathbf{R}^n \to \mathbf{R}$ is said to have a partial derivative at x with respect to x_i if

$$\lim_{\alpha \searrow 0} \frac{f(x + \alpha e_i) - f(x)}{\alpha} \quad \text{exists.}$$

$$\Updownarrow$$

$\exists\, \nu_i(x) \in \mathbf{R}$ such that

$$\lim_{\alpha \searrow 0} \frac{f(x + \alpha e_i) - f(x) - \alpha \nu_i(x)}{\alpha} = 0.$$

$\nu_i(x)$ is called the partial derivative of f w.r.t. x_i, denoted $\frac{\partial f(x)}{\partial x_i}$. Let

$$f_i(x_i) = f(x_1, \cdots, x_{i-1}, x_i, x_{i+1}, \cdots, x_n).$$

Then

$$\frac{\partial f}{\partial x_i}(x) = \lim_{\alpha \to 0} \frac{f(x + \alpha e_i) - f(x)}{\alpha} = \lim_{\alpha \to 0} \frac{f_i(x_i + \alpha) - f_i(x_i)}{\alpha} = \frac{df_i}{dx_i}(x_i).$$

Fact: If $f : \mathbf{R}^n \to \mathbf{R}$ is differentiable at x, then f has partial derivatives at x.

Proof: Since f is differentiable at x, there is a vector $\eta(x)$ so that

$$\lim_{h \to 0} \frac{f(x + h) - f(x) - \eta^T(x) h}{||h||} = 0.$$

This is true no matter how the vector h approaches to 0. Therefore, let $h(\alpha) = \alpha e_i$ and then $h(\alpha) \to 0$ as $\alpha \to 0$. Then

$$\lim_{\alpha \searrow 0} \frac{f(x + \alpha e_i) - f(x) - \alpha \eta^T(x) e_i}{\alpha} = 0.$$

This implies, by uniqueness, that $\nu_i(x) = \eta^T(x) e_i = \eta_i(x)$. Hence $\eta_i(x) = \frac{\partial f(x)}{\partial x_i}$.

From the proof of this theorem,

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}.$$

Directional Derivatives

Definition: $f : \mathbf{R}^n \to \mathbf{R}$ is said to be differentiable at x in the direction of d if

$$\lim_{\alpha \searrow 0} \frac{f(x+\alpha d) - f(x)}{\alpha ||d||} \quad \text{exists.}$$

When this limit exists, we will write it as $\boldsymbol{D}_d f(x)$.

Notice that

$$\lim_{\alpha \searrow 0} \frac{f(x+\alpha d) - f(x) - \alpha \boldsymbol{D}_d f(x) ||d||}{\alpha ||d||} = 0.$$

Note: When $d = e_i$, we have $\boldsymbol{D}_d f(x) = \frac{\partial f(x)}{\partial x_i}$.

Let

$$f_d(z) = f\left(x_1 + z\frac{d_1}{||d||}, x_2 + z\frac{d_2}{||d||}, \cdots, x_n + z\frac{d_n}{||d||}\right).$$

Then

$$\boldsymbol{D}_d f(x) = \lim_{\alpha \searrow 0} \frac{f(x+\alpha d) - f(x)}{\alpha ||d||} = \lim_{\alpha \searrow 0} \frac{f_d(\alpha ||d||) - f_d(0)}{\alpha ||d||} = \frac{df_d}{dz}(0).$$

Fact: Let $f : \mathbf{R}^n \to \mathbf{R}$ be differentiable at x. Let $d \neq 0$ be any direction. Then

$$\boldsymbol{D}_d f(x) = \frac{\nabla f^T(x) d}{||d||}.$$

Proof: Since f is differentiable at x, we know that

$$\lim_{h \to 0} \frac{f(x+h) - f(x) - \nabla f^T(x) h}{||h||} = 0$$

no matter how h approach 0. Now let $h(\alpha) = \alpha d$; then $h(\alpha) \to 0$ as $\alpha \to 0$. Therefore,

$$\lim_{\alpha \searrow 0} \frac{f(x+\alpha d) - f(x) - \alpha \nabla f^T(x) d}{\alpha ||d||} = 0.$$

However,

$$\lim_{\alpha \searrow 0} \frac{f(x+\alpha d) - f(x) - \alpha \boldsymbol{D}_d f(x) ||d||}{\alpha ||d||} = 0.$$

Therefore, by uniqueness, we must have

$$\nabla f^T(x) d = \boldsymbol{D}_d f(x) ||d||.$$

Corollary: the norm of the gradient is the slope of the steepest ascent direction.

Proof:

$$D_{\nabla f(x)} f(x) = \frac{\nabla f^T(x) \nabla f(x)}{||\nabla f(x)||} = \frac{||\nabla f(x)||^2}{||\nabla f(x)||} = ||\nabla f(x)||.$$

<u>Taylor's Theorem</u>

Taylor's Theorem for $f : \mathbf{R} \to \mathbf{R}$: Let f have an nth derivative and assume the $(n-1)$st derivative is continuous. Let $x \neq x^*$. Then $\exists\ \bar{\lambda} \in [0,1]$ so that $\bar{x} = x^* + \bar{\lambda}(x - x^*)$ and

$$f(x) = f(x^*) + \sum_{k=1}^{n-1} f^{(k)}(x^*) \frac{(x - x^*)^k}{k!} + f^{(n)}(\bar{x}) \frac{(x - x^*)^n}{n!}.$$

Note: For two vectors x, x^* the line through these two points is

$$\{y : y = \lambda x + (1 - \lambda) x^*,\ \lambda \in \mathbf{R}\}.$$

The line segment joining these two points is

$$\{y : y = \lambda x + (1 - \lambda) x^*,\ \lambda \in [0,1]\}.$$

Taylor's 1st and 2nd order results for $f : \mathbf{R}^n \to \mathbf{R}$: Let f have continuous 1st partial derivatives. Then, for any two points x, x^* so that $x \neq x^*$, $\exists$ $\bar{\lambda} \in [0,1]$ so that

$$(i) \quad f(x) = f(x^*) + \nabla f^T(\bar{\lambda} x + (1 - \bar{\lambda}) x^*)(x - x^*)$$

and if in addition f has continuous 2nd partials, $\exists\ \mathring{\lambda} \in [0,1]$ so that

$$(ii) \quad f(x) = f(x^*) + \nabla f(x^*)^T (x - x^*) + \frac{1}{2}(x - x^*) \boldsymbol{H}(\mathring{\lambda} x + (1 - \mathring{\lambda}) x^*)(x - x^*)$$

where $\boldsymbol{H}(z)$ is the $n \times n$ Hessian matrix for f, evaluated at z. That is,

$$\boldsymbol{H}(z) = \begin{bmatrix} \frac{\partial^2 f(z)}{\partial z_1^2} & \frac{\partial^2 f(z)}{\partial z_1 \partial z_2} & \cdots & \frac{\partial^2 f(z)}{\partial z_1 \partial z_n} \\ \frac{\partial^2 f(z)}{\partial z_2 \partial z_1} & \frac{\partial^2 f(z)}{\partial z_2^2} & \cdots & \frac{\partial^2 f(z)}{\partial z_2 \partial z_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(z)}{\partial z_n \partial z_1} & \frac{\partial^2 f(z)}{\partial z_n \partial z_2} & \cdots & \frac{\partial^2 f(z)}{\partial z_n^2} \end{bmatrix}.$$

Proof:

(i) Let $g(\lambda) = f(\lambda x + (1-\lambda)x^*)$. Then $g(1) = f(x)$ and $g(0) = f(x^*)$. Using Taylor's Theorem on $\mathbf{R}$, we get

$$g(1) = g(0) + g'(\bar{\lambda})$$

for some $\bar{\lambda} \in [0,1]$. Then, by the chain rule,

$$f(x) = f(x^*) + \nabla f^T(\bar{\lambda}x + (1-\bar{\lambda})x^*)(x - x^*).$$

(ii) Recall we have

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = \frac{\partial^2 f(x)}{\partial x_j \partial x_i}$$

i.e., $\boldsymbol{H}(x)$ is a symmetric matrix. Using Taylor's Theorem on $\mathbf{R}$, we have

$$g(1) = g(0) + g'(0) + \frac{1}{2}g''(\mathring{\lambda})$$

for some $\mathring{\lambda} \in [0,1]$. Then by the chain rule,

$$f(x) = f(x^*) + \nabla f^T(x^*)(x - x^*) + \frac{1}{2}(x - x^*)^T \boldsymbol{H}(\mathring{\lambda}x + (1-\mathring{\lambda})x^*)(x - x^*).$$

Definition: For a differentiable function $f : \mathbf{R}^n \to \mathbf{R}$, the first order approximation at x^* is defined to be

$$f(x^*) + \nabla f^T(x^*)(x - x^*).$$

Definition: For $f : \mathbf{R}^n \to \mathbf{R}$ with continuous 2nd partials, the second order approximation at x^* is defined to be

$$f(x^*) + \nabla f^T(x^*)(x - x^*) + \frac{1}{2}(x - x^*)\boldsymbol{H}(x^*)(x - x^*).$$

2.2 Quadratic Form

Let $\boldsymbol{A}$ be an $n \times n$ matrix and define the quadratic function $Q : \mathbf{R}^n \to \mathbf{R}$ by

$$Q(x) = x^T \boldsymbol{A} x.$$

$Q(x)$ is called a quadratic form.

Note that, in $Q(x) = x^T A x$, we can assume WLOG that A is symmetric. Indeed, if A is not symmetric, we may replace A with the symmetric matrix $\bar{A} = \frac{1}{2}(A + A^T)$ since

$$x^T A x = (x^T A x)^T = x^T A^T x = x^T \left[\frac{1}{2}(A + A^T)\right] x = x^T \bar{A} x.$$

Hence, whenever we consider a quadratic form, we will assume A is symmetric unless stated otherwise.

Def.: An $n \times n$ matrix A is said to be positive semi-definite (PSD) if

$$Q(x) = x^T A x \geq 0, \quad \forall x \in \mathbf{R}^n.$$

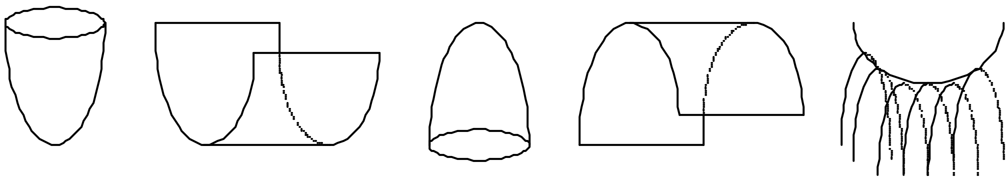
It is said to be positive definite (PD) if

$$Q(x) = x^T A x > 0 \quad \forall x \in \mathbf{R}^n, x \neq 0.$$

It is said to be negative semi-definite (NSD) if $-A$ is PSD.

It is said to be negative definite (ND) if $-A$ is PD.

If A is neither PSD nor NSD, it is called indefinite.



PD PSD ND NSD Indefinite

Fact:

1. If A is PD, $a_{ii} > 0$, $i = 1, \cdots, n$.

2. If A is PSD, $a_{ii} \geq 0$, $i = 1, \cdots, n$.

Proof: Set $x = e_i$. Then the fact follows.

Fact: Let A be PD. Then

1. $\boldsymbol{A}$ is a nonsingular matrix

2. $\boldsymbol{A}^{-1}$ is PD

Proof: 1. If $\boldsymbol{A}$ is singular, $\exists$ nonsero v such that $\boldsymbol{A}v = 0$ and thus $v^T av = 0$ (contradiction).

2. Since $\boldsymbol{A}$ is nonsingular, $\boldsymbol{A}^{-1}x \neq 0$ for all $x \neq 0$. Moreover $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I}$ implies $(\boldsymbol{A}^{-1})^T \boldsymbol{A}^T = \boldsymbol{I}$. Hence,

$$x^T \boldsymbol{A}^{-1} x = x^T (\boldsymbol{A}^{-1})^T \boldsymbol{A}^T \boldsymbol{A}^{-1} x = x^T (\boldsymbol{A}^{-1})^T \boldsymbol{A} \boldsymbol{A}^{-1} x > 0 \quad \forall x \neq 0.$$

Consider a 2×2 symmetric matrix:

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix}.$$

Then $x^T \boldsymbol{A} x = a_{11}x_1^2 + 2a_{12}x_1x_2 + a_{22}x_2^2$. Now assume $a_{11} \neq 0$. Then

$$x^T \boldsymbol{A} x = a_{11}\left[x_1^2 + 2\frac{a_{12}}{a_{11}}x_1x_2 + \frac{a_{22}}{a_{11}}x_2^2\right]$$

$$\begin{aligned} x^T \boldsymbol{A} x &= a_{11}\left[x_1^2 + 2\frac{a_{12}}{a_{11}}x_1x_2 + \frac{a_{12}^2}{a_{11}^2}x_2^2 - \frac{a_{12}^2}{a_{11}^2}x_2^2 + \frac{a_{22}}{a_{11}}x_2^2\right] \\ &= a_{11}\left[\left(x_1 + \frac{a_{12}}{a_{11}}x_2\right)^2 + \frac{a_{11}a_{22} - a_{12}^2}{a_{11}^2}x_2^2\right]. \end{aligned}$$

Now, if $a_{11} > 0$ and $det(\boldsymbol{A}) = a_{11}a_{22} - a_{12}^2 > 0$, $x^T \boldsymbol{A} x > 0$ for all $x \neq 0$ and, thus, $\boldsymbol{A}$ is PD. We now show that this condition is also necessary. Since $a_{11} > 0$, we need only to show that $det(\boldsymbol{A}) > 0$. Now

$$x^T \boldsymbol{A} x = a_{11}\left(x_1 + \frac{a_{12}}{a_{11}}x_2\right)^2 + \frac{det(\boldsymbol{A})}{a_{11}}x_2^2.$$

If $\det(\boldsymbol{A}) \leq 0$, let $x = \left[-\frac{a_{12}}{a_{11}} \; 1\right]^T$. Then $x^T \boldsymbol{A} x \leq 0$ where $x \neq 0$ and, thus, $\boldsymbol{A}$ is not PD (contradiction).

The above motivates the next fact which we state without proof.

Fact: Let $\boldsymbol{A}$ be a symmetric $n \times n$ matrix. Then $\boldsymbol{A}$ is PD iff

$$a_{11} > 0, \quad det\begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix} > 0, \quad det\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{23} \end{bmatrix} > 0, \quad \cdots, \quad det(\boldsymbol{A}) > 0$$

and, thus (since $det(-\boldsymbol{A}) = (-1)^n det(\boldsymbol{A})$), $\boldsymbol{A}$ is ND iff

$$a_{11} < 0, \quad det\begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix} > 0, \quad det\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{23} \end{bmatrix} < 0, \quad \cdots, \quad (-1)^n det(\boldsymbol{A}) > 0.$$

Let $\boldsymbol{A}$ be an $n \times n$ PSD matrix. For $\epsilon > 0$, define $\boldsymbol{A}(\epsilon) = \boldsymbol{A} + \epsilon \boldsymbol{I}$. Then $\boldsymbol{A}(\epsilon)$ is PD.

As a result of this, we have the following corollary.

Corollary: If $\boldsymbol{A}$ is an $n \times n$ symmetric matrix which is also PSD, then

$$a_{11} \geq 0, \quad det\begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix} \geq 0, \quad det\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{23} \end{bmatrix} \geq 0, \quad \cdots, \quad det(\boldsymbol{A}) \geq 0.$$

Proof: Since $\boldsymbol{A}(\epsilon)$ is PD, we must have

$$a_{11} + \epsilon > 0, \quad det\begin{bmatrix} a_{11} + \epsilon & a_{12} \\ a_{12} & a_{22} + \epsilon \end{bmatrix} > 0, \quad \cdots, \quad det(\boldsymbol{A}(\epsilon)) > 0.$$

But the determinant is a continuous function of the elements of the matrix and, thus, by letting $\epsilon \searrow 0$ we have

$$a_{11} \geq 0, \quad det\begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix} \geq 0, \quad \cdots \quad det(\boldsymbol{A}) \geq 0.$$

The above corollary is only sufficient. To see this, consider

$$\boldsymbol{A} = det\begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}.$$

Then

$$a_{11} = 0 \geq 0, \quad det(\boldsymbol{A}) = 0 \geq 0.$$

However, for $x = [0\ 1]^T$, $x^T ax = -1$ and thus A is not PSD.

So far we have developed a necessary and sufficient condition for A to be PD (ND). However, we have developed only a necessary condition for A to be PSD (NSD).

We now sketch a condition which is both necessary and sufficient for A to be PSD.

Fact: Let A be symmetric.

1. $x^* Ax$ is real.

2. eigenvalues of A are all real.

3. n real eigenvectors exist and are all orthogonal.

Proof: 1) $(x^* Ax)^* = x^* A^* x = x^* Ax$.

2) Let λ be an eigenvalue and v be the corresponding eigenvector. Then $v^* Av = \lambda v^* v$. Note that LHS is real, and $v^* v$ is real and > 0.

3) (Proof of orthogonality) For multiple eigenvalues, we can always choose mutually orthogonal eigenvectors. Suppose $Au = \lambda u$ and $Av = \mu v$ with $\lambda \neq \mu$. Note that $u^T A = \lambda u^T$. Hence

$$u^T Av = \lambda u^T v \quad \text{and} \quad u^T Av = \mu u^T v$$

$\Rightarrow \lambda u^T v = \mu u^T v \Rightarrow u^T v = 0$.

Theorem: TFAE

1. A is PSD (PD).

2. all its eigenvalues are nonnegative (positive).

Proof: $(1 \Rightarrow 2)$ Let λ_i be an eigenvalue and v_i be the corresponding unit eigenvector. Then

$$Av_i = \lambda_i v_i \quad \Rightarrow \quad 0 \leq (<) v_i^* Av_i = \lambda_i v_i^* v_i = \lambda_i.$$

$(2 \Rightarrow 1)$ $\{v_i\}$ orthonormal eigenvectors

$$Ax = A(a_1 v_1 + \cdots + a_n v_n) = a_1 Av_1 + \cdots + a_n Av_n = a_1 \lambda_1 v_1 + \cdots + a_n \lambda_n v_n$$

$$\Downarrow$$

$$x^t Ax = (a_1 v_1^t + \cdots + a_n v_n^t)(a_1 \lambda_1 v_1 + \cdots + a_n \lambda_n v_n) = a_1^2 \lambda_1 + \cdots + a_n^n \lambda_n \geq (>) 0.$$

Note: The above fact is not true for a nonsymmetric $n \times n$ matrix A. Consider

$$\begin{bmatrix} 1 & 0 \\ -3 & 1 \end{bmatrix}.$$

Clearly 1 is the double eigenvalue of A. However, for $x = [1\,1]^T$, $x^T Ax = -1$ and thus A is not PD.

2.3 Convexity

Convex Sets and Functions

Let $x, \bar{x} \in \mathbf{R}^n$. Define

$$[x, \bar{x}] = \{y | y = \lambda x + (1 - \lambda)\bar{x},\ \lambda \in [0, 1]\}$$

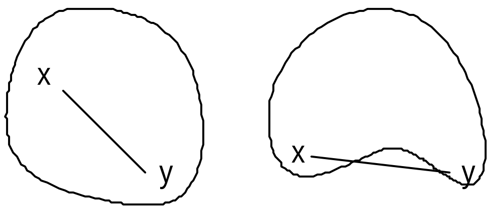
and

$$(x, \bar{x}) = \{y | y = \lambda x + (1 - \lambda)\bar{x},\ \lambda \in (0, 1)\}.$$

Notice that $[x, \bar{x}] = [\bar{x}, x]$ and $(x, \bar{x}) = (\bar{x}, x)$.

Definition: A set $C \subset \mathbf{R}^n$ is convex if

$$[x^1, x^2] \subset C \quad \forall x^1, x^2 \in C.$$

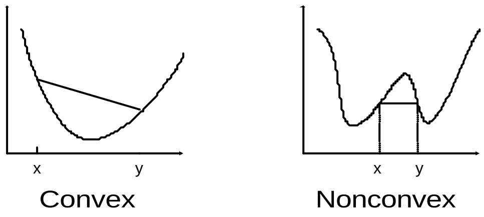


Convex Nonconvex

Definition: Let $C \subset \mathbf{R}^n$ be a nonempty convex set. A function $f : C \to \mathbf{R}$ is convex if

$$f(\lambda x^1 + (1 - \lambda)x^2) \leq \lambda f(x^1) + (1 - \lambda)f(x^2) \quad \forall x^1, x^2 \in C, \forall \lambda \in [0, 1].$$

$f : C \to \mathbf{R}$ is concave if $-f$ is convex.



Definition: Let C be a nonempty convex set of $\mathbf{R}^n$. $f : C \to \mathbf{R}$ is strictly convex if

$$f(\lambda x^1+(1-\lambda)x^2) < \lambda f(x^1)+(1-\lambda)f(x^2) \quad \forall x^1, x^2 \in C, x^1 \neq x^2, \quad \forall \lambda \in (0,1).$$

Simple Facts:

1. Let f_1 and f_2 be two convex functions on a convex set C. $\alpha_1 f_1 + \alpha_2 f_2$ is convex on C if $\alpha_1 \geq 0$, $\alpha_2 \geq 0$.

2. The intersection of any collection of convex sets in $\mathbf{R}^n$ is convex.

Proof: 1. Suppose $x^1, x^2 \in C$. Then for all $\lambda \in [0,1]$,

$$(\alpha_1 f_1+\alpha_2 f_2)(\lambda x^1+(1-\lambda)x^2) = \alpha_1 f_1(\lambda x^1+(1-\lambda)x^2)+\alpha_2 f_2(\lambda x^1+(1-\lambda)x^2)$$

$$\leq \alpha_1\lambda f_1(x^1) + \alpha_1(1-\lambda)f_1(x^2) + \alpha_2\lambda f_2(x^1) + \alpha_2(1-\lambda)f_2(x^2)$$
$$= \lambda(\alpha_1 f_1 + \alpha_2 f_2)(x^1) + (1-\lambda)(\alpha_1 f_1 + \alpha_2 f_2)(x^2).$$

2. Suppose $C = \cap_i C_i$ where C_i's are all convex. Then $x, x' \in C \Rightarrow x, x' \in C_i$ for all $i \Rightarrow [x, x'] \in C_i$ for all $i \Rightarrow [x, x'] \in C$.

Theorem: Let $C \subset \mathbf{R}^n$ be convex and let $f : C \to \mathbf{R}$ be convex. If x^* is a local minimum for

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

then x^* is a global minimum.

Proof: Suppose x^* is locally optimal but $\exists x \in C$ such that $f(x) < f(x^*)$. Consider $z = \lambda x + (1-\lambda)x^*$ with $\lambda \in [0,1]$. Then for all $\lambda \in (0,1]$, $z \in C$ and

$$f(z) = f(\lambda x + (1-\lambda)x^*) \leq \lambda f(x) + (1-\lambda)f(x^*) < f(x^*).$$

This is a contradiction and the fact follows.

The level sets of convex functions have an important property.

Fact: Let C be a nonempty convex set of $\mathbf{R}^n$. Let $f : C \to \mathbf{R}$ be convex. Then

$$\boldsymbol{L}_f(\alpha) = \{x \in C | f(x) \leq \alpha\}$$

is convex for all $\alpha \in \mathbf{R}$.

Proof: Let $x^1, x^2 \in \boldsymbol{L}_f(\alpha)$. Then $f(x^i) \leq \alpha$, $i = 1, 2$. Then by convexity of f, we have

$$f(\lambda x^1 + (1-\lambda)x^2) \leq \lambda f(x^1) + (1-\lambda) f(x^2) \leq \lambda\alpha + (1-\lambda)\alpha = \alpha \quad \forall \lambda \in [0,1].$$

$$\Downarrow$$

$$\lambda x^1 + (1-\lambda)x^2 \in \boldsymbol{L}_f(\alpha) \quad \forall \lambda \in [0,1].$$

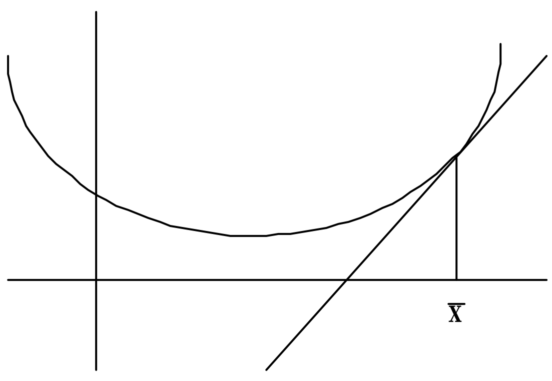
Note: The above shows that if f is concave on C then $\{x \in C | f(x) \geq \alpha\}$ is convex for all $\alpha \in \mathbf{R}$.

Corollary: Suppose $f_i(x)$'s are all convex. Then the feasible set satisfying the inequality constraints $f_i(x) \leq c_i$:

$$\Omega = \{x \in \mathbf{R}^n : f_i(x) \leq c_i, \ \forall i\} = \cap_i \{x \in \mathbf{R}^n : f_i(x) \leq c_i\}$$

is convex.

Differentiable Convex Functions



This picture motivates the following theorem:

Theorem: Let $f : \mathbf{R}^n \to \mathbf{R}$ be differentiable. Then f is convex on the the convex set $C \subset \mathbf{R}^n$ iff

$$f(x) \geq f(\bar{x}) + \nabla f(\bar{x})(x - \bar{x}) \quad \forall x, \bar{x} \in C.$$

Proof: ($\Rightarrow$) For $x, \bar{x} \in C$, we have

$$f(\lambda x + (1-\lambda)\bar{x}) \leq \lambda f(x) + (1-\lambda) f(\bar{x}) \quad \forall \lambda \in [0,1]$$

$$\Downarrow$$

$$f(\bar{x} + \lambda(x - \bar{x})) \leq f(\bar{x}) + \lambda(f(x) - f(\bar{x})) \quad \forall \lambda \in [0,1]$$

$$\Downarrow$$

$$\frac{f(\bar{x} + \lambda(x - \bar{x})) - f(\bar{x})}{\lambda} \leq f(x) - f(\bar{x}) \quad \forall \lambda \in (0,1]$$

$$\Downarrow$$

$$\frac{\nabla f^T(\bar{x})(x - \bar{x})}{|x - \bar{x}|} = D_{(x-\bar{x})} f(\bar{x}) = \lim_{\lambda \searrow 0} \frac{f(\bar{x} + \lambda(x - \bar{x})) - f(\bar{x})}{\lambda |x - \bar{x}|}$$

$$= \frac{1}{|x - \bar{x}|} \lim_{\lambda \searrow 0} \frac{f(\lambda x + (1-\lambda)\bar{x}) - f(\bar{x})}{\lambda} \leq \frac{1}{|x - \bar{x}|} \lim_{\lambda \searrow 0} [f(x) - f(\bar{x})]$$

$$= \frac{1}{|x - \bar{x}|}[f(x) - f(\bar{x})].$$

($\Leftarrow$) Let $x^1, x^2 \in C$ and let $\lambda \in [0,1]$. Define $x = \lambda x^1 + (1-\lambda)x^2$. Then

$$f(x^1) \geq f(x) + \nabla f(x)(x^1 - x)$$

$$f(x^2) \geq f(x) + \nabla f(x)(x^2 - x)$$

$$\Downarrow$$

$$\lambda f(x^1) + (1-\lambda) f(x^2) \geq f(x) + \nabla f(x)(\lambda x^1 + (1-\lambda)x^2 - x)$$
$$= f(x) = f(\lambda x^1 + (1-\lambda)x^2).$$

We now provide a necessary and sufficient condition for $f : C \to \mathbf{R}$ to be convex when, in addition, f has continuous second partials. For this, we need the following rather obvious geometric fact.

Lemma: Let $f : \mathbf{R} \to \mathbf{R}$ be convex on the open interval C and have a continuous 2nd derivative, f''. Then f'' is nonnegative on C.

Proof: Let $x \neq \bar{x}$ be points of C and let $x(\alpha) = \bar{x} + \alpha(x - \bar{x})$ for $\alpha \in [0,1]$. By Taylor's theorem, for $\alpha \in [0,1]$, there is $\lambda_\alpha \in [0,1]$ so that

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

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

By the convexity of f, we have

$$f(x(\alpha)) \geq f(\bar{x}) + f'(\bar{x})(x(\alpha) - \bar{x}) \quad \forall \alpha \in [0,1]$$

$$\Downarrow$$

$$f''(\bar{x} + \alpha\lambda_\alpha(x - \bar{x}))(x(\alpha) - \bar{x})^2 = 2[f(x(\alpha)) - f(\bar{x}) + f'(\bar{x})(x(\alpha) - \bar{x})] \geq 0 \quad \forall \alpha \in [0,1]$$

$$\Downarrow$$

$$f''(\bar{x} + \alpha\lambda_\alpha(x - \bar{x})) \geq 0 \quad \forall \alpha \in (0,1].$$

Then by the continuity of f'', we must then have $f''(\bar{x}) \geq 0$.

Theorem: Let $C \subset \mathbf{R}^n$ be open and convex and let $f : C \to \mathbf{R}$ have continuous 2nd partials on C. Then f is convex on C iff the Hessian matrix $\boldsymbol{H}(x)$ of f is PSD for all $x \in C$.

Proof: ($\Leftarrow$) Suppose $x, \bar{x} \in C$. Then by the Taylor's theorem, we have for a $\lambda \in [0,1]$

$$f(x) = f(\bar{x}) + \boldsymbol{\nabla} f^T(\bar{x})(x - \bar{x}) + \frac{1}{2}(x - \bar{x})^T \boldsymbol{H}(\lambda x + (1 - \lambda)\bar{x})(x - \bar{x}).$$

Since $\boldsymbol{H}$ is PSD on C,

$$(x - \bar{x})^T \boldsymbol{H}(\lambda x + (1 - \lambda)\bar{x})(x - \bar{x}) \geq 0$$

$$\Downarrow$$

$$f(x) \geq f(\bar{x}) + \boldsymbol{\nabla} f^T(\bar{x})(x - \bar{x}).$$

Therefore f is convex on C.

($\Rightarrow$) Let $x \in C$, let $d \in \mathbf{R}^n$, and define g by

$$g(\tau) = f(x + \tau d).$$

Since C is open and f is convex on C, it follows that g is convex in some neighborhood of $\tau = 0$. Therefore, from the previous lemma, $g''(0) \geq 0$. Now notice that

$$g'(\tau) = \nabla f^T(x + \tau d)d$$

and

$$g''(\tau) = (\boldsymbol{H}(x + \tau d)d)^T d = d^T \boldsymbol{H}(x + \tau d)d.$$

Hence,

$$0 \leq g''(0) = d^T \boldsymbol{H}(x)d$$

$$\Downarrow$$

$$\boldsymbol{H}(x) \text{ is PSD for all } x \in C.$$

Corollary: The Quadratic form $x^T Q x$ is convex iff Q is PSD.

Part II

Linear Programming

Chapter 3

Fundamentals of Linear Programming

3.1 Standard Form

Standard form of linear program:

$$\min c_1x_1 + c_2x_2 + \cdots + c_nx_n$$

subject to

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$
$$\vdots$$
$$a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n = b_m$$
$$x_1 \geq 0, \;\; x_2 \geq 0, \;\; \cdots, \;\; x_n \geq 0$$

or in vector form

$$\min_{x \geq 0} c^T x$$

subject to

$$Ax = b.$$

However, in general, a linear program is given in the form of

$$\min c^T x$$

subject to

$$\boldsymbol{A}_1 x = b_1$$
$$\boldsymbol{A}_2 x \leq b_2$$
$$\boldsymbol{A}_3 x \geq b_3.$$

Clearly the last inequality can be rewritten as

$$-\boldsymbol{A}_3 x \leq -b_3$$

and any inequality can be rewritten in the form of the first inequality. We now show how the above linear program can be transformed into the standard form.

Inequalities

Given an inequality, it can be transformed into an equality by introducing an additional variable. Consider an inequality

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n \leq b.$$

This inequality is equivalent to the equality

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n + s_1 = b$$

with $s_1 \geq 0$. s_1 is called "slack" variable.

Free Variable

Suppose we don't have the constraint $x_i \geq 0$ and thus x_i can be negative. Then x_i can be decomposed into two nonnegative variables.

$$x_i = x_i^+ - x_i^-$$

with $x_i^+, x_i^- \geq 0$.

To this end, any linear program can be transformed into the standard form.

Note: Given an equality, it can be transformed into two inequalities. Consider an equality

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = b.$$

This equality is equivalent to the inequalities

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n \leq b$$

$$-a_1x_1 - a_2x_2 - \cdots - a_nx_n \leq -b.$$

Hence, a linear program can be transformed into

$$\min c^T x$$

subject to

$$Ax \leq b.$$

This form is called the inequality form.

3.2 Basics of Linear Program

Consider

$$Ax = b$$

where A is an $m \times n$ matrix with $m \leq n$ (for degree of freedom). If the rank of A is m, there exists m linearly independent columns. WLOG, we assume first m columns are linearly independent. Now we rewrite the above equation as

$$[B\,N]\begin{bmatrix} x_B \\ x_N \end{bmatrix} = b$$

where B be $m \times m$ matrix composed of first m linearly independent columns. Then B is invertible and

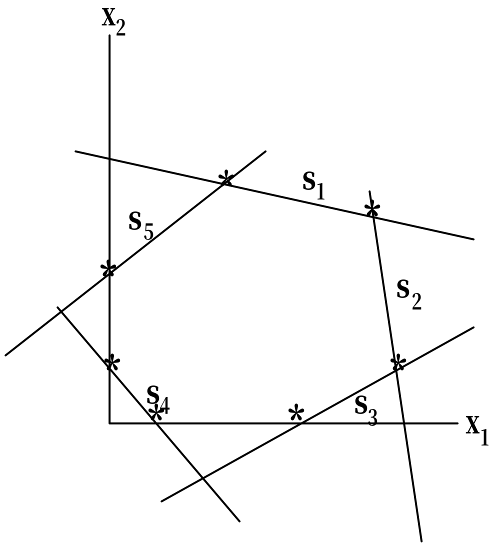
$$Bx_B = b$$

have unique solution and $(x_B, 0)$ is a solution of the full equation.

Definition: Among many solutions, $(x_B, 0)$ type solutions are called basic solutions. Moreover, x_B is called basic variables. If $(x_B, 0) \geq 0$ in addition, it is called the feasible basic solution.

In the inequality form, a basic solution is a corner point of the feasible set defined by

$$\Omega = \{x \in \mathbf{R}^n : x \geq 0,\ Ax \leq b\}.$$



Standard form:

variables x_1, x_2, s_1, $\cdots$, $s_5 \Rightarrow n = 7$

5 equalities $\Rightarrow m = 5$

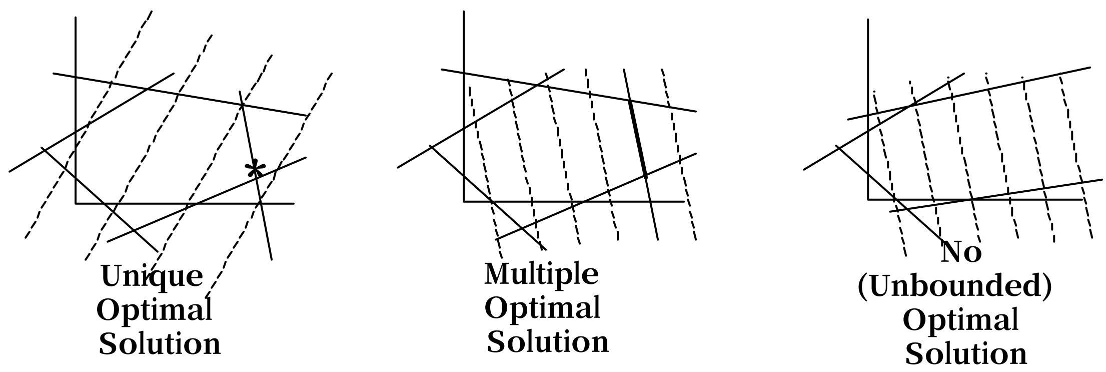
Definition: If one or more of the basic variables in a basic solution has value zero, that solution is said to be a degenerate basic solution.

Note that in a degenerate basic solution, the zero valued basic and non-basic variables are indistinguishable.

Fundamental theorem of linear programing: If there exists an optimal feasible solution, there is an optimal feasible basic solution.

Note: If there are no constraints, the optimal solution of a linear program doesn't exist.

- Unique optimal solution:
- Multiple optimal solution
- No (unbounded) optimal solution:



Thanks to the above theorem, the task of solving a linear program is reduced to searching over basic feasible solutions. Since at most

$$C_m^n = \begin{pmatrix} n \\ m \end{pmatrix} = \frac{n!}{m!(n-m)!}$$

basic solutions exist, there are only finite number of possibilities.

Chapter 4

Simplex Method

Main idea: proceed from one basic feasible solution to another in such a way to continually decrease the objective function value until a minimum is achieved.

4.1 Gauss-Jordan Elimination

Goal: Given $Ax = [B\,N]x = b$ or

$$
\begin{aligned}
a_{11}x_1 + \cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + \cdots + a_{2n}x_n &= b_2 \\
&\vdots \\
a_{m1}x_1 + \cdots + a_{mn}x_n &= b_m,
\end{aligned}
$$

transform it into canonical form: $[I\,B^{-1}N]x = B^{-1}b$ or

$$
\begin{aligned}
x_1 + y_{1,m+1}x_{m+1} + \cdots + y_{1n}x_n &= y_{10} \\
x_2 + y_{2,m+1}x_{m+1} + \cdots + y_{2n}x_n &= y_{20} \\
&\vdots \\
x_m + y_{m,m+1}x_{m+1} + \cdots + y_{mn}x_n &= y_{m0}
\end{aligned}
$$

from which we can easily find a basic solution.

Answer to the goal: Gauss-Jordan Elimination
Illustration of Gauss-Jordan Elimination Steps with Example:

$$\begin{bmatrix} 0 & -2 & 0 & 0 & 7 \\ 2 & -10 & 4 & 6 & 12 \\ 2 & -5 & 4 & 6 & -5 \end{bmatrix} x = \begin{bmatrix} 12 \\ 28 \\ -1 \end{bmatrix}$$

- Step 1: make the tableau $[\boldsymbol{A}\, b]$

$$\begin{bmatrix} 0 & -2 & 0 & 0 & 7 & 12 \\ 2 & -10 & 4 & 6 & 12 & 28 \\ 2 & -5 & 4 & 6 & -5 & -1 \end{bmatrix}$$

- Step 2: reshuffle the variables so that $\boldsymbol{B}$ is nonsingular

$$\begin{bmatrix} 0 & -2 & 7 & 0 & 0 & 12 \\ 2 & -10 & 12 & 6 & 4 & 28 \\ 2 & -5 & -5 & 6 & 4 & -1 \end{bmatrix}$$

- Step 3: reshuffle the equations so that $a_{ii} \neq 0$.

$$\begin{bmatrix} 2 & -10 & 12 & 6 & 4 & 28 \\ 0 & -2 & 7 & 0 & 0 & 12 \\ 2 & -5 & -5 & 6 & 4 & -1 \end{bmatrix}$$

- Step 4: divide the first equation by the first element

$$\begin{bmatrix} 1 & -5 & 6 & 3 & 2 & 14 \\ 0 & -2 & 7 & 0 & 0 & 12 \\ 2 & -5 & -5 & 6 & 4 & -1 \end{bmatrix}$$

- Step 5: make $a_{i1} = 0$, $i = 2, \cdots, m$ by subtracting an appropriate multiple of the first equation

$$\begin{bmatrix} 1 & -5 & 6 & 3 & 2 & 14 \\ 0 & -2 & 7 & 0 & 0 & 12 \\ 0 & 5 & -17 & 0 & 0 & -29 \end{bmatrix}$$

- Step 6: repeat Steps 4,5 with $(m-i)\times(n-i+1)$ right and down most tableau:

$$\begin{bmatrix} 1 & -5 & 6 & 3 & 2 & 14 \\ 0 & 1 & -\frac{7}{2} & 0 & 0 & -6 \\ 0 & 5 & -17 & 0 & 0 & -29 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -5 & 6 & 3 & 2 & 14 \\ 0 & 1 & -\frac{7}{2} & 0 & 0 & -6 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & -5 & 6 & 3 & 2 & 14 \\ 0 & 1 & -\frac{7}{2} & 0 & 0 & -6 \\ 0 & 0 & 1 & 0 & 0 & 2 \end{bmatrix}$$

- Step 7: Apply Steps 4,5,6 backward

$$\begin{bmatrix} 1 & -5 & 0 & 3 & 2 & 2 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 2 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 3 & 2 & 7 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 2 \end{bmatrix}$$

Hence, a basic solution is $x = [7\ 1\ 0\ 0\ 2]$.

4.2 Pivoting

Goal: Given a canonical form, find new canonical form by switching a basic variable with a nonbasic variable so as to find another basic solution.

Answer: pivoting

Switching basic variable x_p, $1 \le p \le m$ in the canonical form with a nonbasic variable x_q is possible iff $y_{pq} \ne 0$.

Pivoting:

- Step 1: divide pth row by the pivot y_{pq}

$$y'_{pj} = \frac{y_{pj}}{y_{pq}}$$

where y''s are the coefficients for the new canonical form.

- Step 2: subtract suitable multiples of p th row from each of the other rows in order to get a zero coefficient for x_q in all other equations.

$$y'_{ij} = y_{ij} - \frac{y_{pj}}{y_{pq}} y_{iq}, \quad i \neq p$$

Illustration of Pivoting Steps with Example:

$$\begin{bmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & \\ 1 & 0 & 0 & 1 & 1 & -1 & 5 \\ 0 & 1 & 0 & 2 & -3 & 1 & 3 \\ 0 & 0 & 1 & -1 & 2 & -1 & -1 \end{bmatrix}, \quad \text{basic solution: } \begin{bmatrix} 5 \\ 3 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Switch x_1 with x_4 by pivoting

$$\begin{bmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & \\ 1 & 0 & 0 & 1 & 1 & -1 & 5 \\ -2 & 1 & 0 & 0 & -5 & 3 & -7 \\ 1 & 0 & 1 & 0 & 3 & -2 & 4 \end{bmatrix}, \quad \text{basic solution: } \begin{bmatrix} 0 \\ -7 \\ 4 \\ 5 \\ 0 \\ 0 \end{bmatrix}$$

Switch x_2 with x_5 by pivoting

$$\begin{bmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & \\ \frac{3}{5} & \frac{1}{5} & 0 & 1 & 0 & -\frac{2}{5} & \frac{18}{5} \\ \frac{2}{5} & -\frac{1}{5} & 0 & 0 & 1 & -\frac{3}{5} & \frac{7}{5} \\ -\frac{1}{5} & \frac{3}{5} & 1 & 0 & 0 & -\frac{1}{5} & -\frac{1}{5} \end{bmatrix}, \quad \text{basic solution: } \begin{bmatrix} 0 \\ 0 \\ -\frac{1}{5} \\ \frac{18}{5} \\ \frac{7}{5} \\ 0 \end{bmatrix}$$

Switch x_3 with x_6 by pivoting

$$\begin{bmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & \\ 1 & -1 & -2 & 1 & 0 & 0 & 4 \\ 1 & -2 & -3 & 0 & 1 & 0 & 2 \\ 1 & -3 & -5 & 0 & 0 & 1 & 1 \end{bmatrix}, \quad \text{basic solution: } \begin{bmatrix} 0 \\ 0 \\ 0 \\ 4 \\ 2 \\ 1 \end{bmatrix}$$

4.3 Adjacent Basic Solutions

For linear program, we need to consider

$$Ax = b$$

$$x \geq 0.$$

However, pivoting may not yield nonnegative basic solution.

Question: Given a new basic variable, how can we guarantee the new basic solution obtained from the pivoting satisfies $x \geq 0$?

Temporary nondegeneracy assumption for easier illustration of simplex method: Every basic feasible solution is nondegenerate.

<u>Determination of Vector to Leave Basis to Obtain the New Basic Solution with $x > 0$</u>

Consider the basic feasible solution $x = (x_1, \cdots, x_m, 0, \cdots, 0)$. Then

$$\boldsymbol{B}^{-1}b = [\boldsymbol{I}\ \boldsymbol{B}^{-1}\boldsymbol{N}]x = x_1 e_1 + x_2 e_2 + \cdots + x_m e_m.$$

Assumption $\Rightarrow$ $x_i > 0$, $i = 1, \cdots, m$

Let a_i be the $(i - m)$th column of $\boldsymbol{B}^{-1}\boldsymbol{N}$. Then

$$a_q = y_{1q} e_1 + y_{2q} e_2 + \cdots + y_{mq} e_m \quad q > m.$$

Then for $\epsilon \geq 0$,

$$\boldsymbol{B}^{-1}b = [\boldsymbol{I}\ \boldsymbol{B}^{-1}\boldsymbol{N}]x - \epsilon a_q + \epsilon a_q$$

$$= (x_1 - \epsilon y_{1q}) e_1 + (x_2 - \epsilon y_{2q}) e_2 + \cdots + (x_m - \epsilon y_{mq}) e_m + \epsilon a_q.$$

Hence, $[x_1 - \epsilon y_{1q}\ x_2 - \epsilon y_{2q}\ \cdots\ x_m - \epsilon y_{mq}\ 0\ \cdots\ 0\ \epsilon\ 0\ \cdots\ 0]$ is a solution of $\boldsymbol{A}x = b$.

For $\epsilon = 0$, this solution reduces to old basic solution.

For small enough ϵ, this solution is a feasible but nonbasic solution.

If $y_{iq} > 0$, $x_i - \epsilon y_{iq} \searrow$ as $\epsilon \nearrow$.

If $y_{iq} < 0$, $x_i - \epsilon y_{iq} \nearrow$ as $\epsilon \nearrow$.

Case 1: $\exists y_{iq} > 0$

Note that $x_i - \epsilon y_{iq} = 0 \Rightarrow \epsilon = \frac{x_i}{y_{iq}}$

Hence, if

$$\epsilon = \min_i \left\{ \frac{x_i}{y_{iq}} : y_{iq} > 0 \right\},$$

then $[x_1-\epsilon y_{1q} \ \cdots \ x_{p-1}-\epsilon y_{(p-1)q} \ 0 \ x_{p+1}-\epsilon y_{(p+1)q} \ \cdots \ x_m-\epsilon y_{mq} \ 0 \ \cdots \ 0 \ \epsilon \ 0 \ \cdots \ 0]$ is a new basic feasible solution with $x \geq 0$ that is obtained switching x_q and x_p where p is the minimising index.

Case 2: $y_{iq} \leq 0$ for all i

ϵ can be arbitrarily big and thus the new basic solution cannot be obtained switching x_q and any basic variable. Notice that there exist unbounded feasible solutions in this case.

Example:

$$\begin{bmatrix} a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & b \\ 1 & 0 & 0 & 2 & 4 & 6 & 4 \\ 0 & 1 & 0 & 1 & 2 & 3 & 3 \\ 0 & 0 & 1 & -1 & 2 & 1 & 1 \end{bmatrix}.$$

Basic feasible solution: $x = [4, 3, 1, 0, 0, 0]^T \geq 0$.

Want to bring a_4 into the basis. Then $\frac{x_i}{y_{iq}}$'s are

$$\frac{x_1}{y_{14}} = \frac{4}{2} = 2, \quad \frac{x_2}{y_{24}} = \frac{3}{1} = 3, \quad \frac{x_3}{y_{34}} = \frac{1}{-1} = -1$$

Hence, $y_{14} = 2$ is the pivot and

$$\begin{bmatrix} a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & b \\ \frac{1}{2} & 0 & 0 & 1 & 2 & 3 & 2 \\ -\frac{1}{2} & 1 & 0 & 0 & 0 & 0 & 1 \\ \frac{1}{2} & 0 & 1 & 0 & 4 & 4 & 3 \end{bmatrix}.$$

New basic feasible solution: $x = [0, 1, 3, 2, 0, 0]^T \geq 0$.

4.4 Minimality Condition

We want to change basis in such a way to decrease the objective function.

From the canonical form, the basic feasible solution is

$$(x_B, 0) = (y_{10}, y_{20}, \cdots, y_{m0}, 0, \cdots, 0).$$

Now the objective function for any x is

$$z = c_1 x_1 + c_2 x_2 + \cdots + c_n x_n.$$

Hence for the above basic solution,

$$z_0 = c_B^T x_B, \quad \text{where } \; c_B^T = [c_1 \; \cdots \; c_m].$$

Instead of $x_N = 0$, pick some $x_N \neq 0$. Then $x_B = \boldsymbol{B}^{-1} b - \boldsymbol{B}^{-1} \boldsymbol{N} x_N$ and thus

$$x_1 = y_{10} - \sum_{j=m+1}^{n} y_{1j} x_j$$

$$x_2 = y_{20} - \sum_{j=m+1}^{n} y_{2j} x_j$$

$$\vdots$$

$$x_m = y_{m0} - \sum_{j=m+1}^{n} y_{mj} x_j.$$

Then

$$z = c^T x$$

$$= c_1 \left(y_{10} - \sum_{j=m+1}^{n} y_{1j} x_j \right) + \cdots + c_m \left(y_{m0} - \sum_{j=m+1}^{n} y_{mj} x_j \right) + c_{m+1} x_{m+1} + \cdots + c_n x_n$$

$$= z_0 - \sum_{j=m+1}^{n} c_1 y_{1j} x_j - \cdots - \sum_{j=m+1}^{n} c_m y_{mj} x_j + c_{m+1} x_{m+1} + \cdots + c_n x_n$$

$$= z_0 + (c_{m+1} - z_{m+1}) x_{m+1} + (c_{m+2} - z_{m+2}) x_{m+2} + \cdots + (c_n - z_n) x_n$$

where

$$z_j = c_B^T a_j = c_1 y_{1j} + c_2 y_{2j} + \cdots + c_m y_{mj}, \quad m+1 \leq j \leq n.$$

z for all feasible solution is now parametrized in terms of x_N.

If $c_j - z_j < 0$, $z \searrow$ as $x_j \nearrow$.

Theorem (improvement of basic feasible solution):

- If $c_j - z_j < 0$, there exists a feasible solution such that $z < z_0$.
- If a_j can be switched with one of the basis, the new basic feasible solution yields $z < z_0$.

- If a_j cannot be switched with one of the basis, the optimum is unbounded.

Proof: WLOG suppose $c_{m+1} - z_{m+1} < 0$. Then the new feasible solution is of the form $(x'_1, \cdots, x'_{m+1}, 0, \cdots, 0)$ with $x'_{m+1} > 0$. Then

$$z - z_0 = (c_{m+1} - z_{m+1})x'_{m+1} < 0.$$

Hence, we want to make x'_{m+1} as large as possible. x'_{m+1} can be increased until one component of x_B becomes zero and pivoting is complete. If no elements of x_B decrease, the optimum is unbounded.

Optimality Condition Theorem: If for some basic feasible solution $c_j - z_j \geq 0$ for all j, the solution is optimal.

Proof: Any other feasible solution must have $x_i \geq 0$ for all i. Hence, the value z of the objective will satisfy $z - z_0 \geq 0$.

Definition: relative (reduced) cost coefficient

$$r_j = c_j - z_j.$$

For basic variable x_j, $z_j = c_B^T e_j = c_j$ and thus $r_j = 0$.

4.5 Simplex Method

Assumption: At the initial stage we can find a canonical form that gives a basic solution with $x \geq 0$.

A way to find such initial canonical form will be given in the next section.

Simplex Method

- Step 0: Find canonical form that gives a basic solution with $x \geq 0$. Compute relative cost coefficients.
- Step 1: If each $r_j \geq 0$, stop; current basic feasible solution is optimal.
- Step 2: Select q such that $r_q < 0$ to determine which nonbasic variable is to become basic.
- Step 3: Calculate $\frac{y_{i0}}{y_{iq}}$ for $y_{iq} > 0$, $i = 1, \cdots, m$. If no $y_{iq} > 0$, stop; problem is unbounded. Otherwise select p as the index i corresponding to the minimum ratio.

- Step 4: Pivot the pqth element, updating all rows including the last. Return to Step 1.

Ex:

$$\min_{x \geq 0} -3x_1 - x_2 - 3x_3$$

subject to

$$2x_1 + x_2 + x_3 \leq 2$$
$$x_1 + 2x_2 + 3x_3 \leq 5$$
$$2x_1 + 2x_2 + x_3 \leq 6.$$

Then

$$\left[\begin{array}{cccccccc} & a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & b \\ & 2 & 1 & 1 & 1 & 0 & 0 & 2 \\ & 1 & 2 & 3 & 0 & 1 & 0 & 5 \\ & 2 & 2 & 1 & 0 & 0 & 1 & 6 \\ (r^T, -z_0) & -3 & -1 & -3 & 0 & 0 & 0 & 0 \end{array}\right], \quad \text{basic solution:} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \\ 5 \\ 6 \end{bmatrix}.$$

Suppose the 2nd column is the candidate for new basis. Then 1 is the pivot.

$$\begin{bmatrix} 2 & 1 & 1 & 1 & 0 & 0 & 2 \\ -3 & 0 & 1 & -2 & 1 & 0 & 1 \\ -2 & 0 & -1 & -2 & 0 & 1 & 2 \\ -1 & 0 & -2 & 1 & 0 & 0 & 2 \end{bmatrix}, \quad \text{basic solution:} \begin{bmatrix} 0 \\ 2 \\ 0 \\ 0 \\ 1 \\ 2 \end{bmatrix}$$

$z_0 = -2$.

Pick the 3rd column as the candidate for new basis. Then 1 in the second row is the pivot.

$$\begin{bmatrix} 5 & 1 & 0 & 3 & -1 & 0 & 1 \\ -3 & 0 & 1 & -2 & 1 & 0 & 1 \\ -5 & 0 & 0 & -4 & 1 & 1 & 3 \\ -7 & 0 & 0 & -3 & 2 & 0 & 4 \end{bmatrix}, \quad \text{basic solution:} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 3 \end{bmatrix}$$

$z_0 = -4$.

Pick the 1st column as the candidate for new basis. Then 5 is the pivot.

$$\begin{bmatrix} 1 & \frac{1}{5} & 0 & \frac{3}{5} & -\frac{1}{5} & 0 & \frac{1}{5} \\ 0 & \frac{3}{5} & 1 & -\frac{1}{5} & \frac{2}{5} & 0 & \frac{8}{5} \\ 0 & 1 & 0 & -1 & 0 & 1 & 4 \\ 0 & \frac{7}{5} & 0 & \frac{6}{5} & \frac{3}{5} & 0 & \frac{27}{5} \end{bmatrix}, \quad \text{basic solution: } \begin{bmatrix} \frac{1}{5} \\ 0 \\ \frac{8}{5} \\ 0 \\ 0 \\ 4 \end{bmatrix}$$

$z_0 = -\frac{27}{5}$. The last row elements are all nonnegative. Hence, the optimal solution is found. The optimal solution is $x = \left[\frac{1}{5}\ 0\ \frac{8}{5}\ 0\ 0\ 4\right]^T$.

Degeneracy

Even if there exist some degenerate basic solutions, the simplex method works fine in most cases. One possible, but rare, problematic situation is the cycle among degenerate basic solutions. Suppose the degenerate variable needs to leave basis. Then the objective doesn't decrease and another degenerate basic solution is attained. This may lead to an indefinite cycle among degenerate basic solutions. The cycle problem can be avoided if the degenerate variable is slightly perturbed.

4.6 Initial Tableau

Consider

$$Ax \leq b, \quad b \geq 0$$
$$x \geq 0.$$

Then the corresponding standard form is

$$Ax + Is = b$$

and thus $[s, x] = [b, 0] \geq 0$ is a feasible basic solution.

In general, multiplying -1 to some equations, the standard form can be written as

$$Ax = b \geq 0$$
$$x \geq 0.$$

Consider an artificial problem

$$\min \sum_{i=1}^{m} y_i$$

subject to

$$\boldsymbol{A}x + y = b$$

$$x \geq 0, \quad y \geq 0.$$

If the original problem is feasible, the artificial problem has a minimum value of zero with $y = 0$. Since all y_i's are nonbasic at the optimum with possible exchange with nonbasic ones in the degenerate case, the optimal solution provides a feasible basic solution of the original problem.

The artificial problem is already in canonical form with basic feasible solution $y = b$ and thus the simplex method can be directly applicable to yield the initial tableau for the original problem.

Part III

Unconstrained Nonlinear Programming

Chapter 5

Necessary Conditions and Sufficient Conditions of Optimality

Consider the optimization problem

$$\min f(x)$$

where $f : \mathbf{R}^n \to \mathbf{R}$.

Fact (1st order necessary condition for local minimum): Let $f : \mathbf{R}^n \to \mathbf{R}$ be differentiable. If x^* is a local minimum then, we must have

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

or, equivalently,

$$D_d f(x^*) = \nabla f(x^*) d = 0, \quad \forall d \in \mathbf{R}^n.$$

Proof: Suppose there exists $d^* \in \mathbf{R}^n$ such that $\nabla f(x^*) d^* \neq 0$. WLOG assume $\nabla f(x^*) d^* < 0$ by possibly considering $-d^*$. Then

$$\lim_{\alpha \searrow 0} \frac{f(x^* + \alpha d^*) - f(x^*)}{\alpha ||d^*||} < 0.$$

$\Rightarrow \exists \alpha^* > 0$ so that $f(x^* + \alpha d^*) < f(x^*)$ for all $\alpha \in (0, \alpha^*]$.

$\Rightarrow$ x^* not a local minimum.

Consider $f = -x^2$. Clearly $f'(0) = 0$. However, x^* is not a local minimum but a local maximum. Hence, the above theorem is only necessary.

Fact (2nd order necessary conditions of local minimality): Let $f : \mathbf{R}^n \to \mathbf{R}$ have continuous 2nd partials and let x^* be a local minimum. Then, for any $d \in \mathbf{R}^n$, we have

1. $\nabla f(x^*) = 0$, and
2. $d^T \boldsymbol{H}(x^*) d \geq 0$ for all $d \in \mathbf{R}^n$ ($\boldsymbol{H}(x^*)$ PSD).

Proof: 1) is just a restatement of 1st order necessary condition. Let $x(\alpha) = x^* + \alpha d$ for $\alpha \geq 0$. By Taylor's theorem, for some $\lambda_\alpha \in [0, 1]$,

$$f(x(\alpha)) = f(x^*) + \alpha \nabla f(x^*) d + \frac{1}{2} \alpha^2 d^T \boldsymbol{H}(x^* + \alpha \lambda_\alpha d) d.$$

Suppose $d\boldsymbol{H}(x^*)d < 0$. Then, by the continuity of the second partials, there exists $\alpha' > 0$ such that

$$d^T \boldsymbol{H}(x^* + \alpha \lambda_\alpha d) d < 0, \quad \forall \alpha \in [0, \alpha'].$$

Then for all $\alpha \in [0, \alpha']$, $f(x(\alpha)) < f(x^*)$. Hence x^* cannot be a local minimum.

Consider $f = x^3$. Clearly $f'(0) = 0$ and $f''(0) = 0$ (PSD). However, $x^* = 0$ is not a local minimum. Hence, the above theorem is only necessary.

Fact (2nd order sufficient condition for a strict local minimum): Let $f : \mathbf{R}^n \to \mathbf{R}$ have continuous 2nd partials . If

1. $\nabla f(x^*) = 0$, and
2. $\boldsymbol{H}(x^*)$ is PD,

then x^* is a strict local minimum.

Proof: Suppose x^* is not a strict local minimum. Then for all $\epsilon > 0$, there exists $x_\epsilon \in \boldsymbol{B}(x^*, \epsilon)$ and $x_\epsilon \neq x^*$ such that $f(x^*) \geq f(x_\epsilon)$. Let $\epsilon_k = \frac{1}{k}$ for an integer $k \geq 1$. Then $f(x_{\epsilon_k}) \leq f(x^*)$ for all k. By Taylor's theorem, for each k,

$$f(x_{\epsilon_k}) = f(x^*) + \frac{1}{2}(x_{\epsilon_k} - x^*)^T \boldsymbol{H}(\lambda_k x_{\epsilon_k} + (1 - \lambda_k) x^*)(x_{\epsilon_k} - x^*)$$

for some $\lambda_k \in [0,1]$. Therefore, for each k,

$$\frac{1}{2}(x_{\epsilon_k} - x^*)^T \boldsymbol{H}(\lambda_k x_{\epsilon_k} + (1-\lambda_k)x^*)(x_{\epsilon_k} - x^*) = f(x_{\epsilon_k}) - f(x^*) \leq 0.$$

This is a contradiction since $\boldsymbol{H}(\cdot)$ is continuous and thus $\boldsymbol{H}$ is PD in a neighborhood of x^*.

Consider $f = x^4$. Clearly $x^* = 0$ is the strict global minimum. However, $f'(0) = 0$ and $f''(0) = 0$ (PSD). Hence, the above theorem is only sufficient.

Chapter 6

Numerical Methods

6.1 One Dimensional Search Techniques

Consider

$$\min_{x \in [c_1, c_2]} f(x).$$

6.1.1 Brute Force Search

Find N evenly spaced points $\{x_k\}$ in $[c_1, c_2]$. Then pick x_i such that $f(x_i)$ is the smallest among $f(x_k)$'s.

6.1.2 Unimodal Functions

Throughout the rest of this section, we only consider unimodal functions. Hence, we present the preliminaries on the unimodal functions.

Def: A function f on $[c_1, c_2]$ is said to be (strictly) unimodal if it is (strictly) monotonic on either side of single optimal point x^* in the interval.

Fact: Suppose f is strictly unimodal on $[c_1, c_2]$ with a minimum at x^*. Let x_1 and x_2 be two points in the interval such that $c_1 < x_1 < x_2 < c_2$. Then

1. If $f(x_1) > f(x_2)$, then $x^* \in (x_1, c_2)$.
2. If $f(x_1) < f(x_2)$, then $x^* \in (c_1, x_2)$.

Proof: 1) Suppose $x^* \in (c_1, x_1)$. Since x^* is minimum,

$$f(x^*) \leq f(x_1) > f(x_2) \quad \text{with} \quad x^* < x_1 < x_2.$$

f is not unimodal (contradiction).

6.1.3 Fibonacci and Golden Section Search

Throughout this subsection, $f(x)$ is unimodal.

Main idea: eliminate the region where the minimum doesn't exist.

Fibonacci Search

Fibonacci Sequence $\{F_i\}$: generated by the Fibonacci difference equation

$$F_N = F_{N-1} + F_{N-2}, \quad F_0 = F_1 = 1$$

$$\Downarrow$$

$$\{F_i\} = \{1, 1, 2, 3, 5, 8, 13, \cdots\}.$$

Goal: Find N points:

$$c_1 = x_0 \leq x_1 < \cdots < x_N \leq x_{N+1} = c_2$$

such that the interval $[x_{i-1}, x_{i+1}]$ where $f(x_i)$ is the minimum among $f(x_k)$'s has length $\frac{2}{F_N}(c_2 - c_1)$.

Notice that this search is much more efficient than the brute force search for large N although it requires the function be unimodal.

Let $d_1 = c_2 - c_1$ and $I_1 = [c_1, c_2]$.

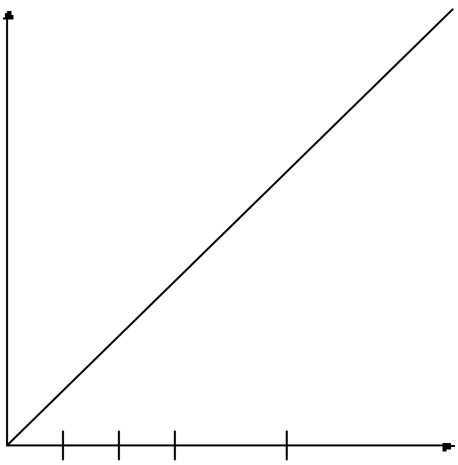
The Fibonacci search consists of $N-1$ steps. At the ith step, we perform the following:

- Let $I_i = [a_1^i, a_2^i]$. Find $f\left(a_1^i + \frac{F_{N-i}}{F_N} d_1\right)$ and $f\left(a_2^i - \frac{F_{N-i}}{F_N} d_1\right)$
- If $f\left(a_1^i + \frac{F_{N-i}}{F_N} d_1\right) \leq f\left(a_2^i - \frac{F_{N-i}}{F_N} d_1\right)$, set $I_{i+1} = \left[a_2^i - \frac{F_{N-i}}{F_N} d_1, a_2^i\right]$. Otherwise, set $I_{i+1} = \left[a_1^i, a_1^i + \frac{F_{N-i}}{F_N} d_1\right]$.

Example: $f = x$, $c_1 = 0, c_2 = 1$, $N = 5$

$I_1 = [0, 1]$

Step 1: $f\left(\frac{5}{8}\right) = \frac{5}{8}$, $f\left(\frac{3}{8}\right) = \frac{3}{8} \Rightarrow I_2 = \left[0, \frac{5}{8}\right]$.



Step 2: $f\left(\frac{3}{8}\right)=\frac{3}{8}$, $f\left(\frac{2}{8}\right)=\frac{2}{8} \Rightarrow I_3=\left[0,\frac{3}{8}\right]$.
Step 3: $f\left(\frac{2}{8}\right)=\frac{2}{8}$, $f\left(\frac{1}{8}\right)=\frac{1}{8} \Rightarrow I_4=\left[0,\frac{2}{8}\right]$.
Step 4: $f\left(\frac{1}{8}\right)=\frac{1}{8}$.

Golden Section Search

Fibonacci search with $N=\infty$

The solution to Fibonacci difference equation is

$$F_N = A\tau_1^N + B\tau_2^N$$

where τ_1, τ_2 are roots of the characteristic equation

$$\tau^2 = \tau + 1$$

or equivalently,

$$\tau_1 = \frac{1+\sqrt{5}}{2}, \quad \tau_2 = \frac{1-\sqrt{5}}{2}.$$

Since $|\tau_2| < 1$,

$$\lim_{N\to\infty} \frac{F_{N-1}}{F_N} = \frac{1}{\tau_1} \approx 0.618.$$

Hence,

$$d_k = \left(\frac{1}{\tau_1}\right)^{k-1} d_1$$
$$\Downarrow$$
$$\frac{d_{k+1}}{d_k} = \frac{1}{\tau_1} = 0.618.$$

Hence, the golden section search converges linearly.

6.1.4 Line Search by Curve Fitting

Throughout this subsection, $f(x)$ is unimodal.

Main idea: approximate f with polynomials successively and find the optimum of the approximate polynomials.

Quadratic Fit

1. Choose $x_1, x_2, x_3 \in [c_1, c_2]$.
2. Set
$$\boldsymbol{F_{min}} = \min\{f(x_1), f(x_2), f(x_3)\}$$
$$\boldsymbol{X_{min}} = x_i \text{ such that } f(x_i) = \boldsymbol{F_{min}}$$
3. Using $f(x_1)$, $f(x_2)$, $f(x_3)$, fit the quadratic function:
$$f(x) = a_0 + a_1(x - x_1) + a_2(x - x_1)(x - x_2)$$
4. Find the optimum x^* of the quadratic funtion on $[c_1, c_2]$.
5. If $\boldsymbol{F_{min}} > f(x^*)$, pick x^* and its two neighbor points as new $x_1, x_2, x_3 \in [c_1, c_2]$, and go to Step 2.

   Otherwise, pick $\boldsymbol{X_{min}}$ and its two neighbor points as new $x_1, x_2, x_3 \in [c_1, c_2]$, and go to Step 2.

This search converges faster than the Golden section search.

6.1.5 Miscellanious techniques

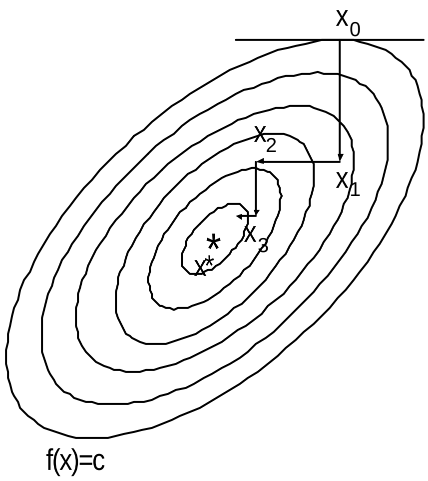
There are other one dimensional techniques. However, most of them require the derivative of f and thus are not recommended.

6.2 Steepest Descent Method

Main idea: from the given point, search the minimum in the steepest descent direction

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$$

$$\alpha_k = \arg\min_{\alpha \geq 0} f(x_k - \alpha \nabla f(x_k))$$



6.3 Newton Method

Main idea:

1. Approximate the object function by quadradic function
2. Solve the resulting quadratic problem

3. Search for the solution direction to find the minimum in the direction

Quadratic approximation:

$$f(x) \approx f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2}(x - x_k)^T \boldsymbol{H}(x_k)(x - x_k).$$

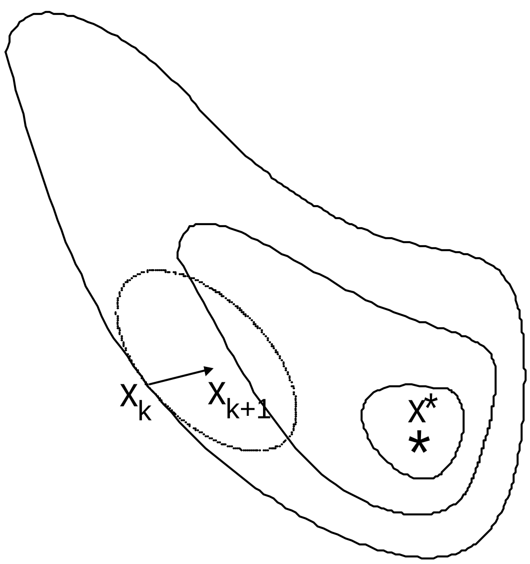
Exact solution of the quadratic program:

$$x = x_k - [\boldsymbol{H}(x_k)]^{-1} \nabla f(x_k).$$

Newton Method:

$$x_{k+1} = x_k - \alpha_k [\boldsymbol{H}(x_k)]^{-1} \nabla f(x_k),$$

$$\alpha_k = \arg\min_{\alpha \geq 0} f\left(x_k - \alpha [\boldsymbol{H}(x_k)]^{-1} \nabla f(x_k)\right).$$



Advantage: converges faster than the steepest descent method
Drawback: need to compute $[\boldsymbol{H}(x_k)]^{-1}$

Connections with the Newton Methods for Systems of Nonlinear Equations

Let $f : \mathbf{R}^n \to \mathbf{R}^n$ be differentiable. Then the Newton method for $f(x) = 0$ is to solve its linear approximation successively.

Linear Approximation:

$$0 = f(x) \approx f(x_k) + \nabla f(x_k)(x - x_k).$$

Newton Method:

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

In the unconstrained optimization above, $f : \mathbf{R}^n \to \mathbf{R}$. The necessary condition of local minimality is

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

where $\nabla f : \mathbf{R}^n \to \mathbf{R}^n$. Apply the Newton method to this equation. Then

$$x_{k+1} = x_k - [\boldsymbol{H}(x_k)]^{-1} \nabla f(x_k)$$

that is the Newton method for the unconstrained optimization.

6.3.1 Modified Newton Methods

In the Newton method, finding the exact inverse of Hessian matrix is often problematic (time consuming and sensitive). Hence, there are a couple of modified Newton methods depending on how to construct the approximation of Hessian inverse.

Notice that

$$\nabla f(x_{k+1}) - \nabla f(x_k) \approx \boldsymbol{H}(x_k)(x_{k+1} - x_k)$$

and thus

$$x_{k+1} - x_k = \boldsymbol{H}(x_k)^{-1}(\nabla f(x_{k+1}) - \nabla f(x_k)).$$

Indeed,

$$\boldsymbol{H}^{-1}(x_k)$$

$$\approx [x_{k+1}^1 - x_k, \cdots, x_{k+1}^n - x_k][\nabla f(x_{k+1}^1) - \nabla f(x_k), \cdots, \nabla f(x_{k+1}^n) - \nabla f(x_k)]^{-1}$$

provided that all the matrices are nonsingular.

Main idea: use the previous step data to update the approximation of Hessian inverse.

Rank One Method

$$H_{k+1}^{-1} = H_k^{-1} + \underbrace{a_k z_k z_k^T}_{\text{has rank 1}}$$

$$\Downarrow$$

$$p_k = H_{k+1}^{-1} q_k = H_k^{-1} q_k + a_k z_k z_k^T q_k$$

where

$$p_k = x_{k+1} - x_k, \quad q_k = \nabla f(x_{k+1}) - \nabla f(x_k)$$

$$\Downarrow$$

$$q_k^T p_k - q_k^T H_k^{-1} q_k = a_k (z_k^T q_k)^2$$

$$\Downarrow$$

$$H_{k+1}^{-1} = H_k^{-1} + a_k z_k z_k^T = H_k^{-1} + \frac{a_k z_k [a_k (q_k^T z_k)^2] z_k^T}{a_k (z_k^T q_k)^2}$$

$$= H_k^{-1} + \frac{a_k z_k z_k^T q_k q_k^T z_k z_k^T a_k}{a_k (z_k^T q_k)^2} = H_k^{-1} + \frac{(p_k - H_k^{-1} q_k)(p_k - H_k^{-1} q_k)^T}{q_k^T (p_k - H_k^{-1} q_k)}.$$

Fact: If $H(x)^{-1}$ is a constant, then

$$\nabla f(x_{i+1}) - \nabla f(x_i) = H_{k+1}(x_{i+1} - x_i) \quad \forall i \leq k.$$

Hence if $[\nabla f(x_1) - \nabla f(x_0), \cdots, \nabla f(x_n) - \nabla f(x_{n-1})]$ is nonsingular, the rank one correction converges to H^{-1} in n steps.

Davidon-Fletcher-Powell Method (Rank Two Method, Variable Metric Method)

1. Let H_0 be a symmetric positive definite matrix and x_0 any point.
2. Set $d_k = -H_k \nabla f(x_k)$.
3. Minimize $f(x_k + \alpha d_k)$ w.r.t. $\alpha \geq 0$ to obtain x_{k+1}.
4. Set
$$H_{k+1}^{-1} = H_k^{-1} + \frac{p_k p_k^T}{p_k^T q_k} - \frac{H_k^{-1} q_k q_k^T H_k^{-1}}{q_k^T H_k^{-1} q_k}$$
and go to step 2.

Fact: If H_k^{-1} is PD, then so is H_{k+1}^{-1}.
Fact: If $H(x)^{-1}$ is a constant, then

$$H_{k+1}^{-1} H p_i = p_i \quad \forall i \leq k.$$

Part IV

Constrained Nonlinear Programming

Chapter 7

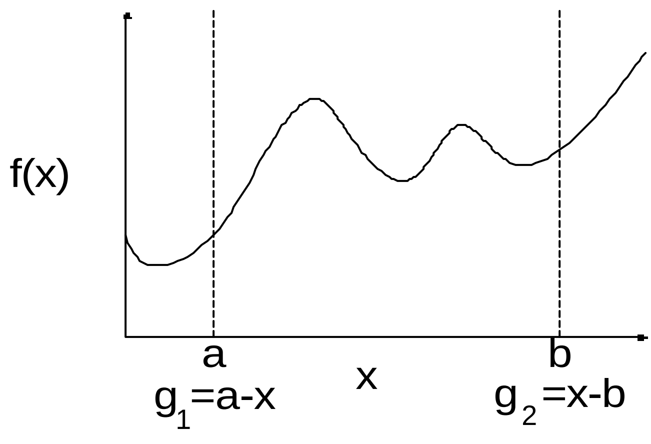
Necessary Conditions of Optimality

Consider

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

subject to

$$g_1(x) = a - x \leq 0$$
$$g_2(x) = x - b \leq 0.$$



$$\Downarrow$$

$\nabla f(x^*) = 0$ is not the necessary condition of optimality anymore.

Consider the optimization problem

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

where $f : \mathbf{R}^n \to \mathbf{R}$, $\Omega \subset \mathbf{R}^n$.

Definition (feasible directions): The vector $d \in \mathbf{R}^n$, is said to be a feasible direction at $x \in \Omega$ if there exists $\bar{\alpha} > 0$ such that

$$x + \alpha d \in \Omega, \quad \forall \alpha \in [0, \bar{\alpha}].$$

We let $D(x; \Omega)$ denote the set of all feasible directions at $x \in \Omega$.

Fact (1st order necessary condition for local minimum): Let $\Omega \subset \mathbf{R}^n$ and let $f : \mathbf{R}^n \to \mathbf{R}$ be differentiable. If $x^* \in \Omega$ is a local minimum then, for all $d \in D(x^*; \Omega)$ we must have

$$D_d f(x^*) = \nabla f(x^*) d \geq 0.$$

Proof: If there exists $d^* \in D(x^*; \Omega)$ such that $\nabla f(x^*) d^* < 0$,

$$\lim_{\alpha \searrow 0} \frac{f(x^* + \alpha d^*) - f(x^*)}{\alpha ||d^*||} < 0.$$

$\Rightarrow \exists \alpha^* > 0$ so that $f(x^* + \alpha d^*) < f(x^*)$ for all $\alpha \in [0, \alpha^*]$. But $d^* \in D(x^*; \Omega)$ $\Rightarrow \exists \alpha' > 0$ so that $x^* + \alpha d^* \in \Omega$ for all $\alpha \in [0, \alpha']$. Let $\bar{\alpha} = \min\{\alpha', \alpha^*\}$ and we then have $f(x^* + \alpha d) < f(x^*)$ and $x^* + \alpha d \in \Omega$ for all $\alpha \in [0, \bar{\alpha}] \Rightarrow x^*$ not a local minimum.

Corollary: If $x^* \in int\Omega$, Then $\nabla f(x^*) = 0$.

Proof: $x^* \in int\Omega \Rightarrow D(x^*; \Omega) = \mathbf{R}^n \setminus \{0\}$. Therefore, $\nabla f(x^*) d \geq 0$ for all $d \neq 0$, $\Rightarrow \nabla f(x^*) = 0$.

<u>Lagrange Multiplier</u>

Consider

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

subject to

$$h(x) = 0.$$

At the minimum, the m constraint equations must be satisfied

$$h(x^*) = 0.$$

Moreover, a feasible direction, $dx^\dagger$, from the minimum x^* must satisfy

$$dh(x^*) = \nabla h(x^*) dx^\dagger = [\nabla h_1(x^*) \; \cdots \; \nabla h_m(x^*)] dx^\dagger = 0.$$

This implies

$$y = \sum_{i=1}^{m} a_i \nabla h_i(x^*) \quad \Leftrightarrow \quad y^T dx^\dagger = 0, \; \forall dx^\dagger. \quad (*)$$

From the above theorem, at the minimum, it must hold that

$$df(x^*) = \nabla f(x^*)^T dx^\dagger \geq 0, \quad \forall dx^\dagger.$$

Since both $dx^\dagger$ and $-dx^\dagger$ are feasible directions, this is equivalent to

$$df(x^*) = \nabla f(x^*)^T dx^\dagger = 0, \quad \forall dx^\dagger.$$

From $(*)$, $\exists \; \{\lambda_i\}_{i=1}^m$ such that

$$\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(x^*) = \nabla f(x^*) + \nabla h(x^*) \lambda = 0$$

where $\lambda = [\lambda_1 \; \cdots \; \lambda_m]^T$.

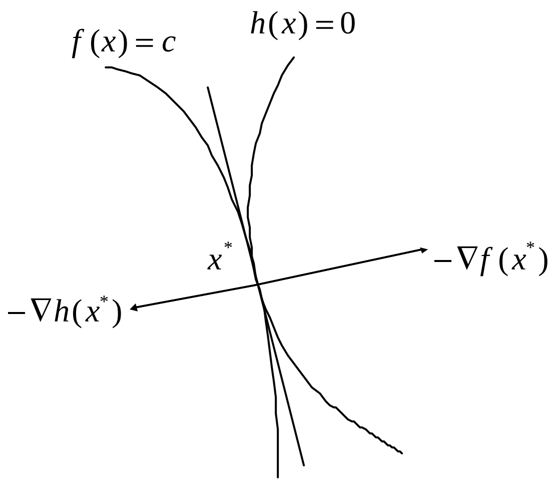
$$\Downarrow$$

Necessary Condition of Local Minimality:

$$h(x^*) = 0 \quad m \text{ equations}$$

$$\nabla f(x^*) + \nabla h(x^*) \lambda = 0 \quad n \text{ equations}$$

where λ_i's are called Lagrange Multipliers.
$(n + m$ equations and $n + m$ unknowns$)$



x* is a local minimum

Example: Consider

$$\min_{x \in \mathbf{R}^n} \frac{1}{2} x^T \boldsymbol{H} x + g^T x$$

subject to

$$\boldsymbol{A}x - b = 0$$

The necessary condition of local minimality for this problem is

$$\boldsymbol{\nabla} f(x^*) + \boldsymbol{\nabla} h(x^*)\lambda = \boldsymbol{H}x^* + g + \boldsymbol{A}^T\lambda = 0$$

$$h(x^*) = \boldsymbol{A}x^* - b = 0$$

$$\Downarrow$$

$$\boldsymbol{H}x^* + \boldsymbol{A}^T\lambda = -g$$

$$\boldsymbol{A}x^* = b$$

$$\Downarrow$$

$$\begin{bmatrix} \boldsymbol{H} & \boldsymbol{A}^T \\ \boldsymbol{A} & 0 \end{bmatrix} \begin{bmatrix} x^* \\ \lambda \end{bmatrix} = \begin{bmatrix} -g \\ b \end{bmatrix}.$$

If $\begin{bmatrix} \boldsymbol{H} & \boldsymbol{A}^T \\ \boldsymbol{A} & 0 \end{bmatrix}$ is invertible,

$$\begin{bmatrix} x^* \\ \lambda \end{bmatrix} = \begin{bmatrix} \boldsymbol{H} & \boldsymbol{A}^T \\ \boldsymbol{A} & 0 \end{bmatrix}^{-1} \begin{bmatrix} -g \\ b \end{bmatrix}.$$

Kuhn-Tucker Condition

Let x^* be a local minimum of

$$\min f(x)$$

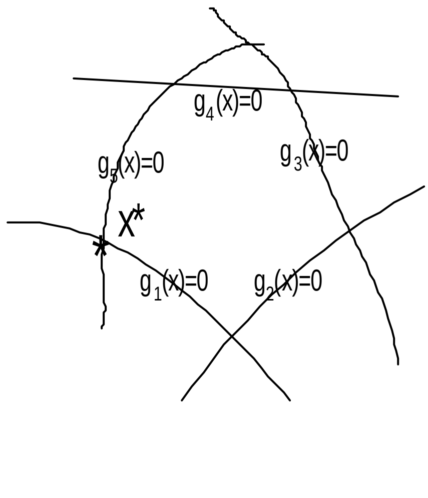
subject to

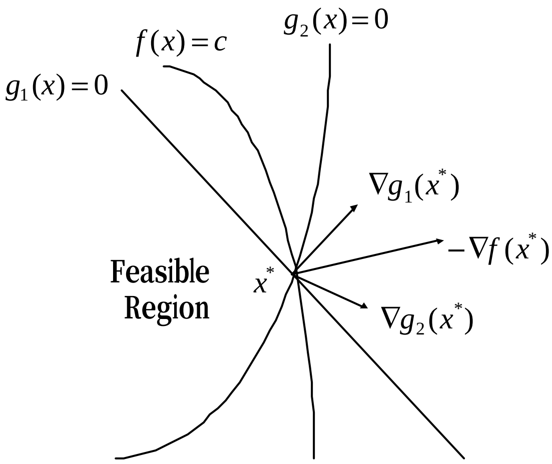
$$h(x) = 0$$
$$g(x) \leq 0$$

and suppose x^* is a regular point for the constraints. Then $\exists\ \lambda$ and μ such that

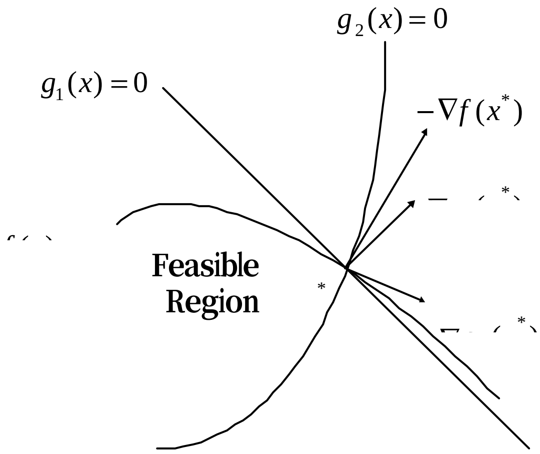
$$\nabla f(x^*) + \lambda^T \nabla h(x^*) + \mu^T \nabla g(x^*) = 0$$
$$\mu^T g(x^*) = 0$$
$$h(x^*) = 0$$
$$\mu \geq 0.$$

$g_i(x^*) < 0 \Rightarrow \mu_i = 0.$





x* is a local minimum



x* is not a local minimum

Chapter 8

Numerical Methods

8.1 Generalized Reduced Gradient Method for Constrained Nonlinear Programs

Main idea:

1. Linearize the equality constraints that are possibly obtained adding slack variables.
2. Solve the resulting linear equations for m variables.
3. Apply the steepest descent method with respect to $n - m$ variables.

Linearisation of Constraints:

$$dh = \nabla_y h(y,z)dy + \nabla_z h(y,z)dz = 0$$
$$\Downarrow$$
$$dy = -[\nabla_y h(y,z)]^{-1}\nabla_z h(y,z)dz.$$

Generalised Reduced Gradient of Objective Function:

$$df(y,z) = \nabla_y f(y,z)dy + \nabla_z f(y,z)dz$$
$$= [\nabla_z f(y,z) - \nabla_y f(y,z)[\nabla_y h(y,z)]^{-1}\nabla_z h(y,z)]dz$$
$$\Downarrow$$
$$r = \frac{df}{dz} = \nabla_z f(y,z) - \nabla_y f(y,z)[\nabla_y h(y,z)]^{-1}\nabla_z h(y,z).$$

8.2 Penalty Method for Constrained Nonlinear Programs

Consider

$$\min f(x)$$

subject to

$$g(x) \le 0.$$

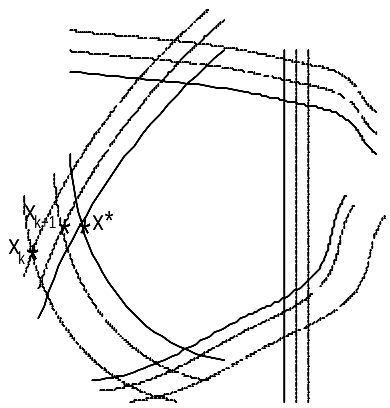
Main idea: Instead of forcing the constraints, penalise the violation of the constraints in the objective:

$$\min_x f(x) + c_k P(x) \qquad (P_k)$$

where $c_k > 0$ and

$$P(x) = \frac{1}{2} \sum_{i=1}^{m} (\max[0, g_i(x)])^2.$$

Theorem: Let x_k be the optimal solution of (P_k). Then as $c_k \to \infty$, $x_k \to x^*$.



8.3 Successive QP Method for Constrained Nonlinear Programs

Main idea:

1. Approximate the object function by quadradic function and constraints linear function.

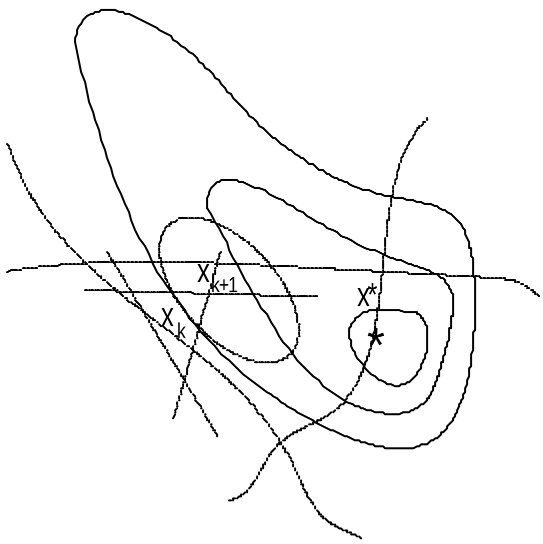
2. Solve the resulting quadratic problem.

Approximate Quadratic Program:

$$\min \nabla f dx + \frac{1}{2} dx^T \boldsymbol{H} dx$$

subject to

$$g(x) + \nabla g(x) dx \leq 0.$$



Consider the optimization problem

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

where $f : \mathbf{R}^n \to \mathbf{R}$, $\boldsymbol{F} \subset \mathbf{R}^n$.

Definition (feasible directions): The vector $d \in \mathbf{R}^n$, is said to be a feasible direction at $x \in \boldsymbol{F}$ if there is a number $\bar{\alpha} > 0$ so that the vector

$$x + \alpha d \in \boldsymbol{F}$$

for all $\alpha \in [0, \bar{\alpha}]$.

We let $\boldsymbol{D}(x; \boldsymbol{F})$ denote the set of feasible directions at $x \in \boldsymbol{F}$.

Fact (1st order necessary condition for local minimum): Let $\boldsymbol{F} \subset \mathbf{R}^n$ and let $f : \mathbf{R}^n \to \mathbf{R}$ be differentiable. If $x^* \in \boldsymbol{F}$ is a local minimum then, for all $d \in \boldsymbol{D}(x^*; \boldsymbol{F})$ we must have

$$D_d f(x^*) = \nabla f(x^*) d \geq 0.$$

Proof: If there is a $d^* \in \boldsymbol{D}(x^*; \boldsymbol{F})$ so that $\nabla f(x^*) d^* < 0$, we must then have

$$\lim_{\alpha \searrow 0} \frac{f(x^* + \alpha d^*) - f(x^*)}{\alpha ||d^*||} < 0$$

$\Rightarrow \exists \alpha^* > 0$ so that $f(x^* + \alpha d^*) < f(x^*)$ for all $\alpha \in [0, \alpha^*]$. But $d^* \in \boldsymbol{D}(x^*; \boldsymbol{F})$ $\Rightarrow \exists \alpha' > 0$ so that $x^* + \alpha d^* \in \boldsymbol{F}$ for all $\alpha \in [0, \alpha']$. Let $\bar{\alpha} = \min\{\alpha', \alpha^*\}$ and we then have $f(x^* + \alpha d) < f(x^*)$ and $x^* + \alpha d \in \boldsymbol{F}$ for all $\alpha \in [0, \bar{\alpha}] \Rightarrow x^*$ not a local minimum.

Corollary: If $x^* \in int\boldsymbol{F}$, Then $\nabla f(x^*) = 0$.

Proof: $x^* \in int\boldsymbol{F} \Rightarrow \boldsymbol{D}(x^*; \boldsymbol{F}) = \mathbf{R}^n \setminus \{0\}$. Therefore, $\nabla f(x^*) d \geq 0$ for all $d \neq 0$, $\Rightarrow \nabla f(x^*) = 0$.

Remark: For unconstrained problems, $\boldsymbol{F} = \mathbf{R}^n$ and thus $x^* \in int\boldsymbol{F}$ is always satisfied.

Consider $f = -x^2$ and $\boldsymbol{F} = \mathbf{R}$. Clearly $f'(0) = 0$. However, x^* is not a local minimum but a local maximum. Hence, the above theorem is only necessary.

Fact (2nd order necessary conditions of local minimality): Let $f : \mathbf{R}^n \to \mathbf{R}$ have continuous 2nd partials and let $x^* \in \boldsymbol{F}$ be a local minimum. Then for any $d \in \boldsymbol{D}(x^*, \boldsymbol{F})$ we have

1. $\nabla f(x^*)d \geq 0$, and

2. if $\nabla f(x^*)d = 0$, then $d^T H(x^*)d \geq 0$.

Proof: 1) is just a restatement of 1st order necessary condition. Therefore, assume $d^* \in D(x^*; F)$ is such that $\nabla f(x^*)d^* = 0$. Let $x(\alpha) = x^* + \alpha d^*$ for $\alpha \geq 0$. By Taylor's theorem,

$$f(x(\alpha)) = f(x^*) + \alpha \nabla f(x^*)d^* + \frac{1}{2}\alpha^2 d^{*T} H(x^* + \alpha\lambda_\alpha d^*)d^*$$

Now, if $d^* H(x^*)d^* < 0$ we see, by the continuity of the second partials, there exists an $\alpha' > 0$ so that $d^{*T} H(x^* + \alpha\lambda_\alpha d^*)d^* < 0$ for all $\alpha \in [0, \alpha']$, and then, for such α's, $f(x(\alpha)) < f(x^*)$. But, again $d^* \in D(x^*, F) \Rightarrow$ there is an $\bar{\alpha} > 0$ so that $x^* + \alpha d^* \in F$ for all $\alpha \in [0, \bar{\alpha}]$. By letting $\alpha^* = \min\{\alpha', \bar{\alpha}\}$ we see that x^* cannot be a local minimum.

Corollary: Let a local minimum, x^*, be an interior point of F. Then,

1. $\nabla f(x^*) = 0$, and

2. $d^T H(x^*)d \geq 0$ for all $d \in \mathbf{R}^n$

(i.e., $H(x^*)$ is a positive semi-definite matrix)

Proof: $D(x^*, F) = \mathbf{R}^n \setminus \{0\}$.

Remark: For unconstrained problems, $F = \mathbf{R}^n$ and thus $x^* \in intF$ is always satisfied.

Consider $f = x^3$ and $F = \mathbf{R}$. Clearly $f'(0) = 0$ and $f''(0) = 0$ (PSD). However, x^* is not a local minimum. Hence, the above theorem is only necessary.

Fact (2nd order sufficient condition for a strict local minimum): Let $f : \mathbf{R}^n \to \mathbf{R}$ have continuous 2nd partials and let $x^* \in F$. If

1. $\nabla f(x^*) = 0$, and

2. $H(x^*)$ is PD

then x^* is a strict local minimum.

Proof: Suppose x^* is not a strict local minimum. Then for all $\epsilon > 0$, there is an $x_\epsilon \in F \cap N(x^*, \epsilon)$ and $x_\epsilon \neq x^*$ so that $f(x^*) \geq f(x_\epsilon)$. Let $\epsilon_k = \frac{1}{k}$ for an integer $k \geq 1$. Then $f(x_{\epsilon_k}) \leq f(x^*)$ for all k. By Taylor's theorem, for each k,

$$f(x_{\epsilon_k}) = f(x^*) + \frac{1}{2}(x_{\epsilon_k} - x^*)^T \boldsymbol{H}(\lambda_k x_{\epsilon_k} + (1-\lambda_k)x^*)(x_{\epsilon_k} - x^*)$$

for some $\lambda_k \in [0,1]$. Therefore, for each k,

$$(x_{\epsilon_k} - x^*)^T \boldsymbol{H}(\lambda_k x_{\epsilon_k} + (1-\lambda_k)x^*)(x_{\epsilon_k} - x^*) = f(x_{\epsilon_k}) - f(x^*) \leq 0$$

This is a contradiction since $\boldsymbol{H}(\cdot)$ is continuous and thus $\boldsymbol{H}$ is PD in a neighborhood of x^*.

Consider $f = x^4$ and $\boldsymbol{F} = \mathbf{R}$. Clearly $x^* = 0$ is the strict local minimum. However, $f'(0) = 0$ and $f''(0) = 0$ (PSD). Hence, the above theorem is only sufficient.