Optimasi Tanpa Kendala: Multivariat

Pertemuan ke-5

STA1373- Optimisasi Statistika

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METODE

Table 6.1 Unconstrained Minimization Methods

Direct search methods[a]	Descent methods[b]
Random search method	Steepest descent (Cauchy) method
Grid search method	Fletcher–Reeves method
Univariate method	Newton's method
Pattern search methods	Marquardt method
Powell's method	Quasi-Newton methods
	Davidon–Fletcher–Powell method
	Broyden–Fletcher–Goldfarb–Shanno method
Simplex method	

[a]Do not require the derivatives of the function.
[b]Require the derivatives of the function.

SIMPLEX METHOD

- This method was originally given by Spendley, Hext, and Himsworth; and was developed later by Nelder and Mead.
- **Definisi Simplex:** The geometric figure formed by a set of n + 1 points in an n-dimensional space is called a simplex. When the points are equidistant, the simplex is said to be regular. Thus in two dimensions, the simplex is a triangle, and in three dimensions, it is a tetrahedron.
- **Basic idea simplex method:** compare the values of the objective function at the n + 1 vertices of a general simplex and move the simplex gradu ally toward the optimum point during the iterative process.
- The movement of the simplex is achieved by using three operations, known as **reflection, contraction, and expansion**.

REFLECTION

- If $\boldsymbol{X}_h$ is the vertex corresponding to the highest value of the objective function among the vertices of a simplex, we can expect the point $\boldsymbol{X}_r$ obtained by reflecting the point $\boldsymbol{X}_h$ in the opposite face to have the smallest value. If this is the case, we can construct a new simplex by rejecting the point $\boldsymbol{X}_h$ from the simplex and including the new point $\boldsymbol{X}_h$.

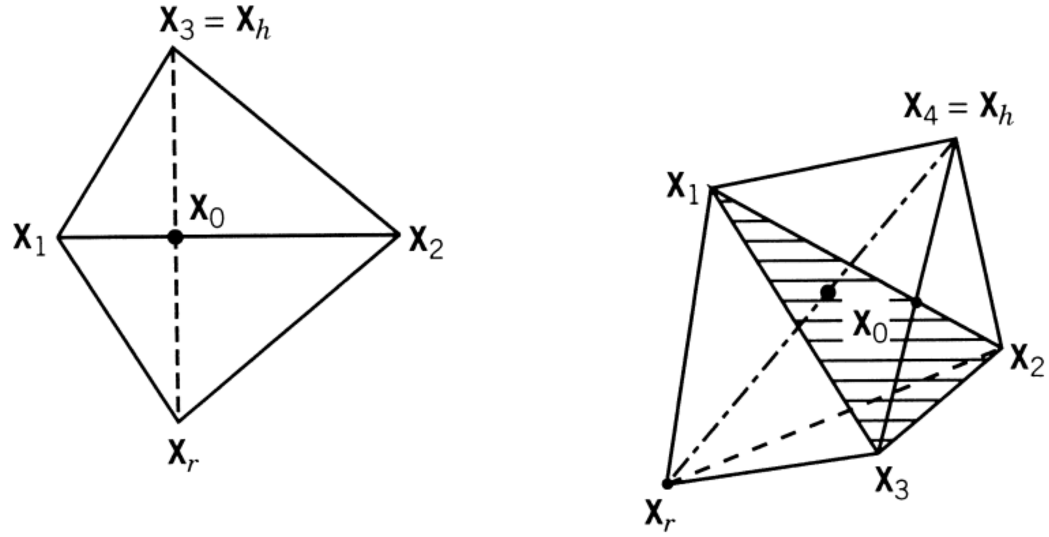

Figure 6.10 Reflection.

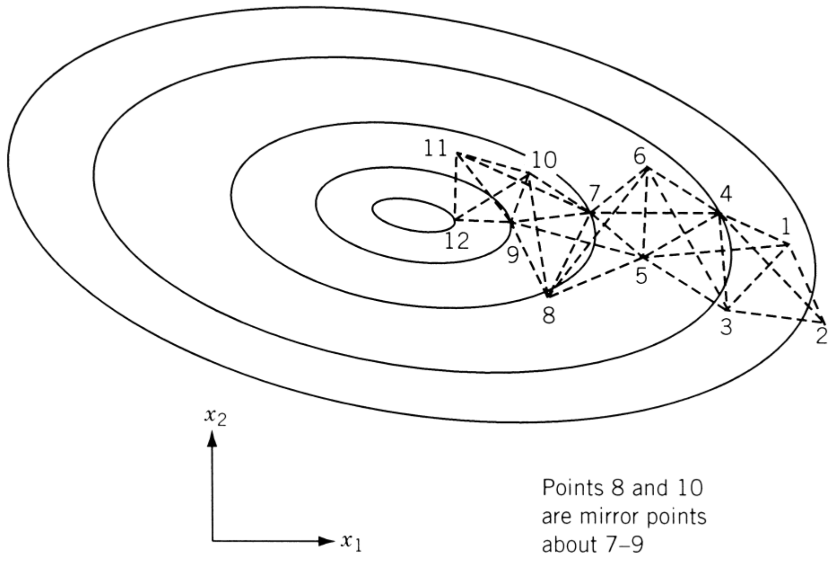

Figure 6.11 Progress of the reflection process.

REFLECTION

- Reflection point: $\mathbf{X}_r = (1+\alpha)\mathbf{X}_0 - \alpha\mathbf{X}_h$
- Vertex corresponding to the maximum function value ($\boldsymbol{X}_h$)

$$f(\mathbf{X}_h) = \max_{i=1 \text{ to } n+1} f(\mathbf{X}_i),$$

- Centroid of all the points $\boldsymbol{X}_i$ except $i = h$ ($\boldsymbol{X}_0$): $\mathbf{X}_0 = \frac{1}{n}\sum_{\substack{i=1 \\ i \neq h}}^{n+1} \mathbf{X}_i$
- Reflection coefficient (α):

$$\alpha = \frac{\text{distance between } \mathbf{X}_r \text{ and } \mathbf{X}_0}{\text{distance between } \mathbf{X}_h \text{ and } \mathbf{X}_0} \quad ; \alpha > 0$$

Thus $\mathbf{X}_r$ will lie on the line joining $\mathbf{X}_h$ and $\mathbf{X}_0$, on the far side of $\mathbf{X}_0$ from $\mathbf{X}_h$ with $|\mathbf{X}_r - \mathbf{X}_0| = \alpha|\mathbf{X}_h - \mathbf{X}_0|$. If $f(\mathbf{X}_r)$ lies between $f(\mathbf{X}_h)$ and $f(\mathbf{X}_l)$, where $\mathbf{X}_l$ is the vertex corresponding to the minimum function value,

$$f(\mathbf{X}_l) = \min_{i=1 \text{ to } n+1} f(\mathbf{X}_i)$$

$\boldsymbol{X}_h$ is replaced by $\boldsymbol{X}_r$ and a new simplex is started.

REFLECTION

- Certain difficulties:

if one of the simplexes (triangles in two dimensions) straddles a valley and if the reflected point Xr happens to have an objective function value equal to that of the point Xh, we will enter into a closed cycle of operations.

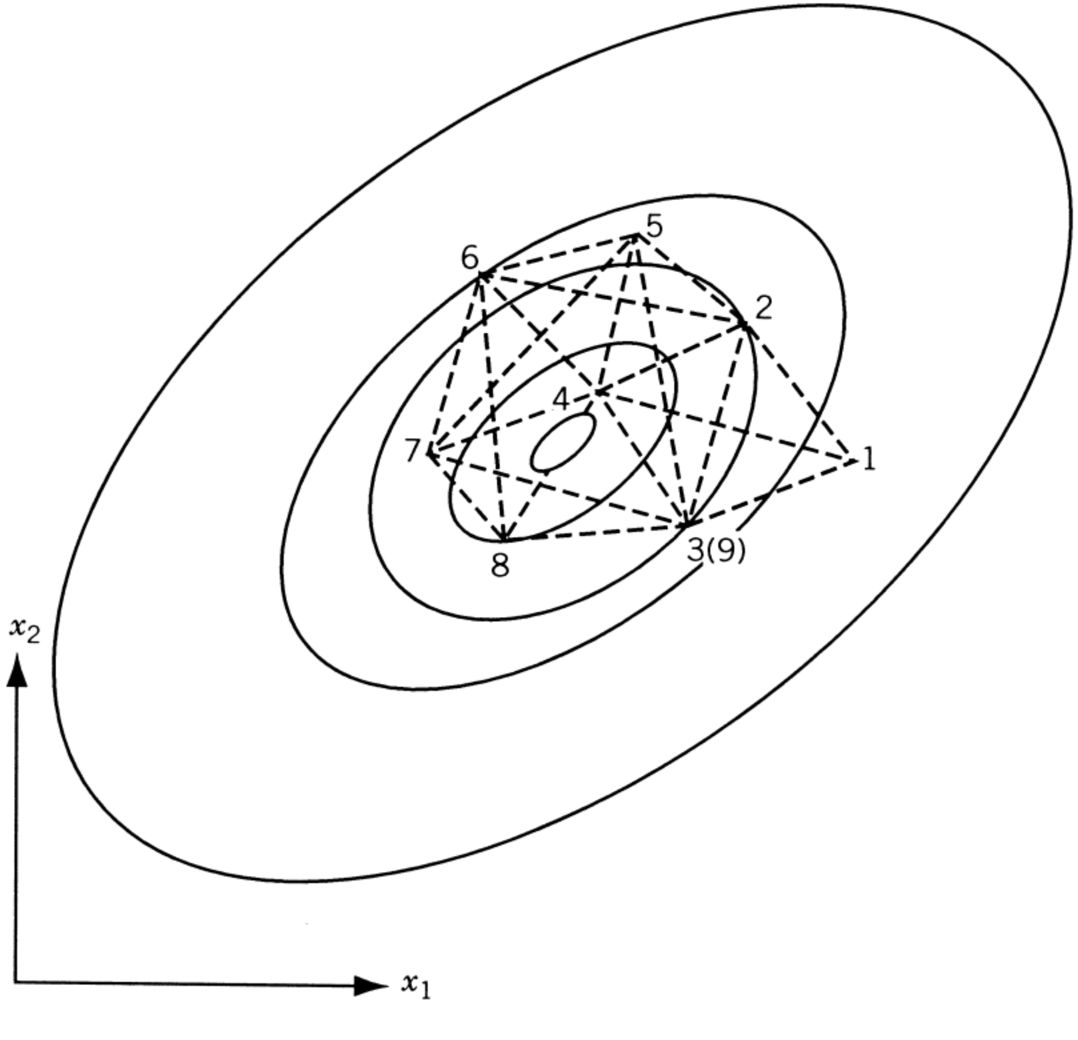

Figure 6.13 Reflection process leading to a cyclic process.

EXPANSION

- If a reflection process gives a point $\boldsymbol{X_r}$ for which $\mathrm{f}(\boldsymbol{X_r}) < \mathrm{f}(\boldsymbol{X_l})$, (i.e., if the reflection produces a new minimum), one can generally expect to decrease the function value further by moving along the direction pointing from $\boldsymbol{X_0}$ to $\boldsymbol{X_r}$. Hence we expand $\boldsymbol{X_r}$ to $\boldsymbol{X_e}$.

$$\mathbf{X}_e = \gamma \mathbf{X}_r + (1 - \gamma)\mathbf{X}_0$$

- γ is expansion coefficient: $\gamma = \dfrac{\text{distance between } \mathbf{X}_e \text{ and } \mathbf{X}_0}{\text{distance between } \mathbf{X}_r \text{ and } \mathbf{X}_0} > 1$

- If $\mathrm{f}(\boldsymbol{X_e}) < \mathrm{f}(\boldsymbol{X_l})$, we replace the point $\boldsymbol{X_h}$ by Xe and restart the process of reflection. On the other hand, if $\mathrm{f}(\boldsymbol{X_e}) > \mathrm{f}(\boldsymbol{X_l})$, it means that the expansion process is not successful and hence we replace point $\boldsymbol{X_h}$ by $\boldsymbol{X_r}$ and start the reflection process again.

CONSTRACTION

- If the reflection process gives a point $\boldsymbol{X_r}$ for which f$(\boldsymbol{X_r}) >$ f$(\boldsymbol{X_i})$ for all i except $i = h$, and f$(\boldsymbol{X_r}) <$ f$(\boldsymbol{X_h})$, we replace point $\boldsymbol{X_h}$ by $\boldsymbol{X_r}$. Thus the new $\boldsymbol{X_h}$ will be $\boldsymbol{X_r}$. In this case we contract the simplex as follows:

$$\mathbf{X}_c = \beta \mathbf{X}_h + (1 - \beta)\mathbf{X}_0$$

where β is called the contraction coefficient ($0 \le \beta \le 1$):

$$\beta = \frac{\text{distance between } \mathbf{X}_e \text{ and } \mathbf{X}_0}{\text{distance between } \mathbf{X}_h \text{ and } \mathbf{X}_0}$$

- If f$(\boldsymbol{X_r}) >$ f$(\boldsymbol{h})$, we still use Eq. to find $\boldsymbol{X_c}$ without changing the previous point $\boldsymbol{X_h}$. If the contraction process produces a point $\boldsymbol{X_c}$ for which $f(\boldsymbol{X_c}) < min[f(\boldsymbol{X}_h), f(\boldsymbol{X}_r)]$, we replace the point $\boldsymbol{X_h}$ in $\boldsymbol{X_1}, \boldsymbol{X_2}, \ldots, \boldsymbol{X_{n+1}}$ by $\boldsymbol{X_c}$ and proceed with the reflection process again. On the other hand, if $f(\boldsymbol{X_c}) \geq min[f(\boldsymbol{X}_h), f(\boldsymbol{X}_r)]$, the contraction process will be a failure, and in this case we replace all $\boldsymbol{X_i}$ by $(\boldsymbol{X_i} + \boldsymbol{X_l})/2$ and restart the reflection process.

CONVERGENCY

- The method is assumed to have converged whenever the standard deviation of the function at the $n + 1$ vertices of the current simplex is smaller than some prescribed small quantity ε.

$$Q = \left\{ \sum_{i=1}^{n+1} \frac{[f(\mathbf{X}_i) - f(\mathbf{X}_0)]^2}{n+1} \right\}^{1/2} \leq \varepsilon$$

Example

Example 6.7 Minimize $f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$. Take the points defining the initial simplex as

$$\mathbf{X}_1 = \begin{Bmatrix} 4.0 \\ 4.0 \end{Bmatrix}, \quad \mathbf{X}_2 = \begin{Bmatrix} 5.0 \\ 4.0 \end{Bmatrix}, \quad \text{and} \quad \mathbf{X}_3 = \begin{Bmatrix} 4.0 \\ 5.0 \end{Bmatrix}$$

and $\alpha = 1.0$, $\beta = 0.5$, and $\gamma = 2.0$. For convergence, take the value of ε as 0.2.