Introduction to Engineering Optimization (ME6806)

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Module 4

Multi-variable Optimization Algorithms

Outlines

- **Optimality Criteria**
- **Direct Search Methods**
    - Nelder and Mead (Simplex Search)
    - Hook and Jeeves (Pattern Search)
    - Powell's Method (The Conjugated Direction Search)
- **Gradient Based Methods**
    - Cauchy's Method
    - Newton's Method
    - Modified Newton's Method
    - Marquardt's Method
    - Conjugate Gradient Method
    - Quasi-Newton Method
    - Trust Regions
    - Gradient-Based Algorithm
    - Numerical Gradient Approximations

The Optimality Criteria

- Given a function (objective function) *f*(**x**), where $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$ and let,

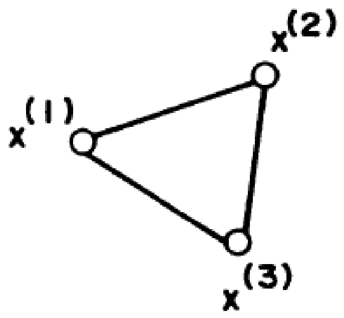
$$f(\mathbf{x}) = f(\mathbf{x}^*) + \nabla f(\mathbf{x}^*)^T(\mathbf{x}-\mathbf{x}^*) + \frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^T \nabla^2 f(\mathbf{x}^*)(\mathbf{x}-\mathbf{x}^*) + O_3(\Delta\mathbf{x})$$

- Stationary Condition: $\nabla f(\mathbf{x}^*) = 0$
- Sufficient minimum criteria $\nabla^2 f(\mathbf{x}^*)$ positive definite
- Sufficient maximum criteria $\nabla^2 f(\mathbf{x}^*)$ negative definite

Nelder and Mead (Simplex Search)

Rule 1   Minimum "Straddled"

If the selected "worse" vertex was generated in the previous iteration, then choose instead the vertex with the next highest function value.



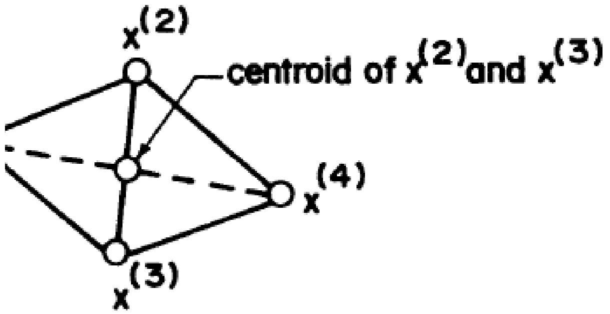
(a) Old Simplex ;

$x^{(1)}, x^{(2)}, x^{(3)}$

Rule 2   Cycling

If a given vertex remains unchanged for more than M iterations, reduce the size of the simplex by some factor. Set up a new simplex with the currently lowest point as the base point. Spendley et al. suggest that M be predicted via

$$M = 1.65N + 0.05N^2$$



) New Simplex ;

$x^{(2)}, x^{(3)}, x^{(4)}$

where N is the problem dimension and M is rounded to the nearest integer. This rule requires the specification of a reduction factor.

Nelder and Mead (Simplex Search)

Rule 3 Termination Criterion

The search is terminated when the simplex gets small enough or else if the standard deviation of the function values at the vertices gets small enough. This rule requires the specification of a termination parameter.

The implementation of this algorithm requires only two types of calculations: (1) generation of a regular simplex given a base point and appropriate scale factor and (2) calculation of the reflected point. The first of these calculations is readily carried out, since it can be shown from elementary geometry that given an N-dimensional starting or base point $x^{(0)}$ and a scale factor α, the other N vertices of the simplex in N dimensions are given by

$$x_j^{(i)} = \begin{cases} x_j^{(0)} + \delta_1 & \text{if } j = i \\ x_j^{(0)} + \delta_2 & \text{if } j \neq i \end{cases}$$

for i and $j = 1, 2, 3, \ldots, N$.

Nelder and Mead (Simplex Search)

The increments δ_1 and δ_2, which depend only on N and the selected scale factor α, are calculated from

$$\delta_1 = \left[\frac{(N+1)^{1/2} + N - 1}{N\sqrt{2}}\right]\alpha$$

$$\delta_2 = \left[\frac{(N+1)^{1/2} - 1}{N\sqrt{2}}\right]\alpha$$

Note that the scale factor α is chosen by the user to suit the problem at hand. The choice $\alpha = 1$ leads to a regular simplex with sides of unit length.

The second calculation, reflection through the centroid, is equally straightforward. Suppose $x^{(j)}$ is the point to be reflected. Then the centroid of the remaining N points is

$$x_c = \frac{1}{N}\sum_{\substack{i=0 \\ i\neq j}}^{N} x^{(i)}$$

Nelder and Mead (Simplex Search)

All points on the line from $x^{(j)}$ through x_c are given by

$$x = x^{(j)} + \lambda(x_c - x^{(j)})$$

The choice $\lambda = 0$ yields the original point $x^{(j)}$, while the choice $\lambda = 1$ corresponds to the centroid x_c. To retain the regularity of the simplex, the reflection should be symmetric. Hence, $\lambda = 2$ will yield the desired new vertex point. Thus,

$$x_{\text{new}}^{(j)} = 2x_c - x_{\text{old}}^{(j)}$$

Nelder and Mead (Simplex Search)

$$\text{Minimize } f(x) = (1 - x_1)^2 + (2 - x_2)^2$$

The construction of the initial simplex requires the specification of an initial point and a scale factor. Suppose $x^{(0)} = [0, 0]^T$ and $\alpha = 2$ are selected.

$$\delta_1 = \left[\frac{\sqrt{3} + 1}{2\sqrt{2}}\right]\alpha = 1.9318 \qquad \delta_2 = \left[\frac{\sqrt{3} - 1}{2\sqrt{2}}\right]\alpha = 0.5176$$

With these two parameters, the other two vertices are calculated as

$$x^{(2)} = [0 + 0.5176, 0 + 1.9318]^T = [0.5176, 1.9318]^T$$

$$x^{(1)} = [0 + 1.9318, 0 + 0.5176]^T = [1.9318, 0.5176]^T$$

with function values $f(x^{(1)}) = 3.0658$ and $f(x^{(2)}) = 0.2374$. Since $f(x^{(0)}) = 5$, $x^{(0)}$ is the point to be reflected to form the new simplex. The replacement $x^{(3)}$ is calculated as follows:

$$x_c = \frac{1}{2}\sum_{i=1}^{2} x^{(i)} = \frac{1}{2}(x^{(1)} + x^{(2)})$$

Nelder and Mead (Simplex Search)

$$x^{(3)} = x^{(1)} + x^{(2)} - x^{(0)}$$

$$x^{(3)} = [2.4494, 2.4494]^T$$

At the new point $f(x^{(3)}) = 2.3027$, an improvement. The new simplex is composed of points $x^{(1)}$, $x^{(2)}$, and $x^{(3)}$. The algorithm would now continue by reflecting out the point with the highest function value, $x^{(1)}$. The iteration proceeds as before except when situations are encountered that require rules 1, 2, or 3 given before.