Downhill Simplex Algorithm

Definitions

Simplex

A simplex is an n-dimensional geometric figure formed by $n + 1$ non-collinear points (called **vertices**). It can be considered the most basic polytope in a high-dimensional space.

Measuring 'Best' and 'Worst'

Assume the objective function is $f(x)$. For all vertices of the current simplex $x_1, x_2, \ldots, x_{n+1}$:

- Best Point x_1 is the current 'best' point (i.e., the point with the smallest objective function value), satisfying:

$$f(x_1) = \min\left(f(x_1), f(x_2), \ldots, f(x_{n+1})\right) \tag{1}$$

- Worst Point x_{n+1} is the current 'worst' point (i.e., the point with the largest objective function value), satisfying:

$$f(x_{n+1}) = \max\left(f(x_1), f(x_2), \ldots, f(x_{n+1})\right) \tag{2}$$

Assumptions

Suppose:

- x_0 is the starting point.
- x_1 is the vertex with the smallest objective function value (the best point).
- x_{n+1} is the vertex with the largest objective function value (the worst point).

Algorithm

Initialization

In an n-dimensional space, choose $n + 1$ vertices to form the initial simplex. These vertices are typically generated by small displacements around the starting point x_0:

$$x_i = x_0 + \delta_i \mathbf{e}_i \quad \text{for } i = 1, 2, \ldots, n \tag{3}$$

where $\mathbf{e}_i$ are unit vectors, and δ_i are small displacement values.

Reflection

The reflection point can be computed using the formula:

$$x_r = x_c + \alpha(x_c - x_{n+1}) \tag{4}$$

where:

- x_c is the centroid of all vertices except the worst one:

$$x_c = \frac{1}{n}\sum_{i=1}^{n} x_i \tag{5}$$

- α is the **reflection coefficient**, typically set to 1.

Expansion

If the reflected point x_r shows an improvement in the objective function, an expansion along the reflection direction can be performed. The expansion point is calculated as:

$$x_e = x_c + \gamma(x_r - x_c) \tag{6}$$

where γ is the **expansion coefficient**, usually greater than 1.

Contraction

If reflection fails (i.e., the reflected point is worse than the original worst point), a contraction is performed. There are two types of contraction: outside and inside contraction.

Outside Contraction

If the reflected point is better than the worst point but not better than the second worst point, consider an outside contraction:

$$x_s = x_c + \beta(x_r - x_c) \tag{7}$$

where β is the **contraction coefficient**, typically between 0 and 1.

Inside Contraction

If the reflection point is even worse than the worst point, consider an inside contraction:

$$x_s = x_c + \beta(x_{n+1} - x_c) \tag{8}$$

Shrinking

If none of the above operations succeed, the entire simplex is shrunk towards the best point:

$$x_i = x_1 + \sigma(x_i - x_1) \quad \text{for all } i = 2, 3, \ldots, n+1 \tag{9}$$

where σ is the **shrinkage factor**, typically between 0 and 1.

Termination Conditions

Convergence of Function Values

The difference between the highest and lowest function values at the vertices of the simplex falls below a predefined threshold ϵ_f:

$$\max\left(f(x_1), f(x_2), \ldots, f(x_{n+1})\right) - \min\left(f(x_1), f(x_2), \ldots, f(x_{n+1})\right) < \epsilon_f \tag{10}$$

Convergence of Simplex Size

The simplex itself has become sufficiently small. This can be measured by checking the largest distance between any two vertices of the simplex:

$$\max\left(\|x_i - x_j\|\right) < \epsilon_x \quad \text{for all } i, j \tag{11}$$

Maximum Iterations

The algorithm has reached a predefined maximum number of iterations $N_{\max}$.

Lack of Progress

The algorithm has failed to make significant progress over a certain number of iterations.