MATH3016: OPTIMIZATION

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1 Introduction

What is optimization?

Optimization is essentially about finding the best solution to a given problem from a set of feasible solutions. It consists of three components:

- the objective or objectives, that is, what do we want to optimize?
- a solution (decision) vector, that is, how can we achieve the optimal objective?
- the set of all feasible solutions, that is, among which possible options may we choose to optimize?

Examples

- Airline companies schedule crews and aircraft to minimize their costs
- Investors create portfolios to avoid the risks and achieve the maximum profits
- Manufacturers minimize the production costs and maximize the efficiency
- Bidders optimize their bidding strategies to achieve best results
- Physical system tends to a state of minimum energy

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Mathematical models

A familiar optimization model is *Linear programming* model which can be expressed as:

$$\begin{aligned} \min \quad & c^T \mathbf{x} \\ \text{subject to} \quad & A\mathbf{x} \leq b \\ & \mathbf{x} \geq 0 \end{aligned}$$

where c and b are n-dimensional vector, and A is an $m \times n$ matrix. Linear programming models have been proved as a useful tool in operational research.

In practical applications, however, a lot of optimization problems are nonlinear, that is, either the objective function or the constraints cannot be described by an affine function. Here we give one example.

Example 1.1 (Portfolio Optimization, see J. Nocedal and S.J. Wright (1999), *Numerical Optimisation*, Springer-Verlag.) Suppose that an investor has n investments with returns r_i, $i = 1, \cdots, n$. The returns are unknown in advance and are often assumed to be random variables with normal distribution. We characterize these variables by expected return $\mu_i = E[r_i]$ and their variance $\sigma_i = E[(r_i - \mu_i)^2]$.

The investor constructs a portfolio by putting a fraction x_i of his funds into investment i, for $i = 1, \cdots, n$. Assume all funds are invested and short-selling is not permitted. Then the constraints are $x_i \geq 0$, $i = 1, \cdots, n$ and $\sum_{i=1}^{n} x_i = 1$.

The return of the portfolio is given by

$$R = \sum_{i=1}^{n} x_i r_i.$$

To measure the desirability of the portfolio, we need to obtain measures of its expected return which is

$$E(R) = E\left[\sum_{i=1}^{n} x_i r_i\right] = \mathbf{x}^T \mu.$$

The variance can be calculated from elementary laws of statistics. It depends on the covariance between each pair of investments, which are defined by

$$\rho_{ij} = \frac{E[(r_i - \mu_i)(r_j - \mu_j)]}{\sigma_i \sigma_j} \text{ for } i, j = 1, \cdots, n.$$

The correlation measures the tendency of the return on investments i and j to move in the same direction. Two investments whose returns tend to rise and fall together have a positive covariance; the nearer ρ_{ij} is to 1, the more closely the two investments track each other. Investments whose returns tend to move in opposite directions have negative covariance.

The variance of the total portfolio R is

$$E[(R - E[R])^2] = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j \sigma_i \sigma_j \rho_{ij} = \mathbf{x}^T G \mathbf{x}$$

where $G_{ij} = \sigma_i \sigma_j \rho_{ij}$.

We are interested in a portfolio that the expected return is large while the variance is small. Marrkowitz combined these two aims into a single objective function using a "risk tolerance" parameter η and formulated the following (QP)

$$\begin{aligned} \max \quad & \mathbf{x}^T \mu - \eta \mathbf{x}^T G \mathbf{x} \\ \text{s.t.} \quad & \sum_{i=1}^{n} x_i = 1, \\ & \mathbf{x} \geq 0. \end{aligned}$$

We will get back to this example later on (in Chapter 6 Quadratic Programming).

In general, an optimization problem can be formulated as

$$(\max) \min_{\mathbf{x}\in\mathcal{F}} f(\mathbf{x}), \tag{1}$$

where f is called the *objective function* and $\mathcal{F}$ is called *feasible set*, x is called *decision vector*.

We only consider minimization problem since a maximization problem can be easily converted into a minimization problem. Also, we restrict x to be a vector of n variables.

The focus of this course is NOT on linear programming. It will be on nonlinear programming, particularly the following programs:

Unconstrained minimization:

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

Quadratic programming:

$$\begin{aligned} \min \quad & \frac{1}{2}\mathbf{x}^T G\mathbf{x} + g^T\mathbf{x} \\ \text{s.t.} \quad & A\mathbf{x} \le b \\ & \mathbf{x} \ge 0 \end{aligned}$$

where G is a symmetric matric and g is an n-dimensional vector.

Equality and inequality constrained minimization problem:

$$\begin{aligned} \min \quad & f(\mathbf{x}) \\ \text{s.t.} \quad & g_i(\mathbf{x}) \le 0, i = 1, \cdots, m, \\ & h_i(\mathbf{x}) = 0, i = 1, \cdots, r. \end{aligned}$$

Note also that **this course is NOT about modeling of practical problems**, instead, it is about theory and methods of the optimization models described above.

2 Direct search methods

In this chapter, we will discuss direct methods for solving unconstrained minimization problems.

A *direct search method* is a method which relies only on evaluating $f(\mathbf{x})$ on a sequence $\mathbf{x}_1$, $\mathbf{x}_2$, $\cdots$ and comparing values in order to calculate a minimizer of f. Direct methods are usually applied in the following circumstance

- the function $f(\mathbf{x})$ is not differentiable;
- the derivatives of f are complicated to compute or even do not exist;
- the function has few variables;
- the location of an optimal solution is roughly known.

There are many direct search methods. Here we introduce the most popular five:

- Golden section method
- Fibonacci method
- Hooke and Jeeves' method
- Spendley, Hext and Himsworth's method
- Nelder and Mead's method

The first two methods deal with a function of a single variable, the rest four deal with a function of several variables.

2.1 Golden section method

2.1.1 Unimodal function

We consider the following minimization problem

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & x \in [a, b] \end{array} \tag{2}$$

where $f : \mathbb{R} \to \mathbb{R}$ is a univariate function and $[a, b]$ is an interval.

Let x^* denote a minimizer of $f(x)$ in $[a, b]$. f is said to be *unimodal* on $[a, b]$ if $f(x)$ is decreasing for $a \leq x \leq x^*$ and increasing for $x^* \leq x \leq b$.

Remark 2.1 1. In some textbooks, a function which is increasing for $a \leq x \leq x^*$ and decreasing for $x^* \leq x \leq b$ is also called a unimodal function. Of course in this case x^* is a maximizer.

2. A sufficient condition for f to be unimodal on $[a, b]$ is that $f(x)$ is convex (to be introduced in Chapter 3) over $[a, b]$. But a unimodal function is NOT necessarily a convex function.

2.1.2 Golden section

Throughout this subsection, we assume the objective function f in (2) is unimodal over $[a, b]$.

What is **the golden section**?

The golden section is a line segment divided into two parts. Point C is positioned such that the ratio of the short half to the long half is equal to the ratio of the long half to the whole. Symbolically:

A——C—B where $\frac{CB}{AC} = \frac{AC}{AB} = \tau$, or $AC^2 = BC \times AB$.

2.1.3 Golden section algorithm

Algorithm 2.1 *(Golden section algorithm)*

Step 1. Given initial interval $[a_1, b_1]$ *and precision* ϵ. *Set* $\tau = 0.618$. *Calculate*

$$x_1^1 = b_1 - \tau(b_1 - a_1)$$

and

$$x_2^1 = a_1 + \tau(b_1 - a_1)$$

set $i := 1$;

Step 2. If $f(x_2^i) > f(x_1^i)$,

$$\begin{aligned} a_{i+1} &= a_i \\ b_{i+1} &= x_2^i \\ x_2^{i+1} &= x_1^i \\ x_1^{i+1} &= b_{i+1} - \tau(b_{i+1} - a_{i+1}) \end{aligned}$$

If $f(x_2^i) \leq f(x_1^i)$,

$$\begin{aligned} a_{i+1} &= x_1^i \\ b_{i+1} &= b_i \\ x_1^{i+1} &= x_2^i \\ x_2^{i+1} &= a_{i+1} + \tau(b_{i+1} - a_{i+1}) \end{aligned}$$

Step 3. If $|b_{i+1} - a_{i+1}| \leq \epsilon$, *stop; otherwise, set* $i := i + 1$, *go to Step 2.*

2.1.4 Derivation of the golden section method

Consider minimization problem (2). Observe first that

- It is necessary to evaluate the function at two interior points of $[a, b]$ before the minimizer can be located in a sub-interval of $[a, b]$.

- By the repeated evaluation of f, the minimum can be located to any prescribed precision.
- The efficiency of this process depends on the choice of the points at which function is evaluated.
- Although two function evaluations are required initially, only one further function value is required in the subsequent process because the other lies in the interior of the reduced interval.

Motivation: *Is it possible to arrange that the size of the interval containing the minimum be decreased by a constant factor τ at each step?*

Let the current interval be (a_i, b_i) and let the points at which f is evaluated be x_1^i and x_2^i where $x_1^i < x_2^i$. For $i = 1$, $a_1 = a$, $b_1 = b$. Then

1. The reduced interval is either $[a_i, x_2^i]$ or $[x_1^i, b_i]$.
2. To make the length of the reduced interval to be a constant factor of $[a_i, b_i]$, it is necessary that x_1^i, x_2^i satisfy
$$\frac{x_2^i - a_i}{b_i - a_i} = \frac{b_i - x_1^i}{b_i - a_i} = \tau. \tag{3}$$
3. To update, if $f(x_2^i) > f(x_1^i)$, then the minimizer must be located in $[a_i, x_2^i]$, hence we set
$$a_{i+1} = a_i,\ b_{i+1} = x_2^i, \tag{4}$$
and
$$\begin{aligned} x_2^{i+1} &= x_1^i \\ x_1^{i+1} &= b^{i+1} - (x_2^{i+1} - a_{i+1}). \end{aligned} \tag{5}$$
If $f(x_2^i) \leq f(x_1^i)$, then the minimizer must be located in $[x_1^i, b_i]$, hence we set
$$a_{i+1} = x_1^i,\ b_{i+1} = b_i$$
and
$$\begin{aligned} x_1^{i+1} &= x_2^i \\ .x_2^{i+1} &= a_{i+1} + b_{i+1} - x_1^{i+1} \end{aligned}$$

4. The relationship in (3) must hold for $i+1$, that is

$$\frac{x_2^{i+1} - a_{i+1}}{b_{i+1} - a_{i+1}} = \frac{b_{i+1} - x_1^{i+1}}{b_{i+1} - a_{i+1}} = \tau \tag{6}$$

Based on the above observation, we can derive τ. Suppose $f(x_2^i) > f(x_1^i)$. Substituting x_2^{i+1}, a_{i+1}, b_{i+1} from (4) and (5) into the left side of (6), we obtain

$$\frac{x_2^{i+1} - a_{i+1}}{b_{i+1} - a_{i+1}} = \frac{x_1^i - a_i}{x_2^i - a_i} = \tau.$$

Since

$$x_1^i - a_i = b_i - a_i - (x_2^i - a_i)$$

We have from (3) and (6)

$$\tau = \frac{x_1^i - a_i}{x_2^i - a_i} = \frac{b_i - a_i}{x_2^i - a_i} - 1 = \frac{1}{\tau} - 1$$

from which we can solve

$$\tau = \frac{\sqrt{5} - 1}{2} = 0.618\cdots.$$

Example 2.1 Consider the minimization problem

$$\begin{array}{ll} \min & f(x) := -\frac{1}{(x-1)^2}\left(\log x - 2\frac{x-1}{x+1}\right) \\ \text{s.t.} & x \in [1.5, 4.5]. \end{array}$$

(a) Estimate the number of function evaluations needed for the Golden Section method to reduce the size of interval to be less or equal to 0.2 (Do not carry out actual computation).

(b) Use the golden section algorithm to find an approximate minimum and minimizer of the problem (Stop if the interval size is reduced to be less or equal to 0.2).

Computational results.

i		a_i	x_1^i	x_2^i	b_i	update
1	x	1.5	2.65	3.35	4.5	$x_1^1 = b_1 - \tau(b_1 - a_1)$
	$100f(x)$	-2.188	-2.588	-2.327	-1.899	$x_2^1 = a_1 + \tau(b_1 - a_1)$
2	x					
	$100f(x)$	-2.188	-2.671	-2.588	-2.327	
3	x					
	$100f(x)$	-2.188	-2.633	-2.671	-2.588	
4	x	1.95	2.20		2.65	
	$100f(x)$	-2.633	-2.671	-2.650	-2.588	
5	x			2.20	2.40	
	$100f(x)$	-2.633	-2.670	-2.671	-2.650	
6	x	2.15		2.35	2.40	
	$100f(x)$	-2.670	-2.671	-2.658	-2.650	

Example 2.2 Consider the following minimization problem

$$\begin{aligned} \min \quad & f(x) \equiv e^{-x} - \cos x \\ \text{s.t.} \quad & x \in [0, 1]. \end{aligned}$$

(a) Prove that f is a unimodal function and there is a unique global minimizer in the interior of $[0, 1]$.

(b) Reduce the size of the interval containing the global minimizer to less or equal to 0.5 using Golden section method.

2.2 Fibonacci method

In this subsection, We continue to discuss the minimization problem (2) where $f(x)$ is unimodal on $[a, b]$.

In the golden search method, two function evaluations are made at the first iteration and then only one function evaluation is made for each subsequent iteration. The ratio for the reduction of intervals at each iteration remains constant.

The Fibonacci method differs from the golden ratio method in that the ratio for the reduction of intervals is not constant. Additionally, the number of subintervals (iterations) is predetermined and based on the specified tolerance.

2.2.1 Fibonacci numbers

The Fibonacci search is based on the sequence of Fibonacci numbers which are defined by the equations

$$\begin{aligned} F_0 &= 1 \\ F_1 &= 1 \\ F_{N+1} &= F_N + F_{N-1}, \text{for} N = 1, 2, \cdots \end{aligned}$$

Thus the Fibonacci numbers are $1, 1, 2, 3, 5, 8, 13, 21, 34 \cdots$.

2.2.2 Fibonacci method

1. Determine the number of function evaluations, $N - 1$.

2. Divide the initial interval $[a_1, b_1]$ evenly into F_N subintervals and hence the length of each suinterval is $\frac{1}{F_N}(b_1 - a_1)$. Grid point P_i, $i = 1, \cdots, F_N - 1$, in the interval can be expressed as

$$P_i = a_1 + \frac{i}{F_N}(b_1 - a_1).$$

3. In the first iteration, take the F_{N-2}-th grid point from left as x_1^1 and the

F_{N-1}-th grid point from left as x_2^1, that is,

$$x_1^1 = \frac{F_{N-2}}{F_N}(b_1 - a_1) + a_1$$

and

$$x_2^1 = \frac{F_{N-1}}{F_N}(b_1 - a_1) + a_1.$$

Compare the function values at these two points and decide a_2 and b_2 as in the Golden search method. Repeat the process with $N := N - 1$ to obtain x_1^2, x_2^2, $\cdots$.

You will find that $N - 1$ function evaluations are made at $N - 1$ of the $F_N - 1$ grid points. Try $N = 3, 4$ with $a_1 = 0, b_1 = 1$.

2.2.3 Fibanacci algorithm

Algorithm 2.2 *(Fibonacci algorithm) Let initial interval* $[a_1, b_1]$ *be given and the number of function evaluations* $N-1$ *(*$N \geq 3$*) be preset.*

For $i = 1, \cdots, N-2$*, do*

$$x_1^i = \frac{F_{N-i-1}}{F_{N-i+1}}(b_i - a_i) + a_i$$

and

$$x_2^i = \frac{F_{N-i}}{F_{N-i+1}}(b_i - a_i) + a_i$$

If $f(x_2^i) > f(x_1^i)$,

$$\begin{aligned} a_{i+1} &= a_i \\ b_{i+1} &= x_2^i \end{aligned}$$

If $f(x_2^i) \leq f(x_1^i)$,

$$\begin{aligned} a_{i+1} &= x_1^i \\ b_{i+1} &= b_i \end{aligned}$$

Remark 2.2 1. Number of function evaluations. First note that if $f(x_2^i) > f(x_1^i)$,

$$x_2^{i+1} = x_1^i$$

if $f(x_2^i) \leq f(x_1^i)$,

$$x_1^{i+1} = x_2^i$$

Summary: at first step, 2-evaluations are needed, 1-evaluation is needed for each

of later $N-2$ iterations. Total number of evaluations is $2+N-2(=N-1)$.

2. Reduction of interval size. Since

$$b_{i+1}-a_{i+1}=x_2^i-a_i=b_i-x_1^i=\frac{F_{N-i}}{F_{N-i+1}}(b_i-a_i),$$

after $N-1$ evaluations the length of the interval is

$$\delta=\frac{F_{N-1}}{F_N}\frac{F_{N-2}}{F_{N-1}}\cdots\frac{F_3}{F_4}\frac{F_2}{F_3}(b_1-a_1)=\frac{2(b_1-a_1)}{F_N}$$

3. Properties of Fibonacci algorithm.

- Fibonacci algorithm is optimum in the sense that it gives the largest ratio of initial to final interval for a fixed number of function evaluations.
- the relationship between Fibnacci algorithm and Golden section algorithm can be observed by

$$\lim_{N\to\infty}\frac{F_{N-1}}{F_N}=\frac{\sqrt{5}-1}{2}=0.618\cdots.$$

Example 2.3 Use Fibonacci algorithm to minimize

$$f(x) = -\frac{1}{(x-1)^2}\left(\log x - 2\frac{x-1}{x+1}\right).$$

It is known that the minimizer is in the range $[1.5, 4.5]$. Reduce the interval to 2/21 of the original.

We want

$$\frac{2(4.5-1.5)}{F_N} \leq \frac{2}{7}$$

Thus $F_N \geq 21$.

Computational results.

i		a_i	x_1^i	x_2^i	b_i	update
1	x	1.5	2.64	3.36	4.5	
	$100f(x)$	-2.188	-2.591	-2.323	-1.899	
2	x	1.5			3.36	
	$100f(x)$	-2.188	-2.670	-2.591	-2.323	
3	x	1.5			2.64	
	$100f(x)$	-2.188	-2.621	-2.670	-2.591	
4	x	1.92			2.64	
	$100f(x)$	-2.621	-2.670	-2.660	-2.591	
5	x	1.92			2.34	
	$100f(x)$	-2.621	-2.57	-2.670	-2.660	

Example 2.4 Consider Example 2.2. Reduce the size of the interval containing the global minimizer to less or equal to 0.5 using Fibonacc method.

2.3 Hooke and Jeeves' method

We consider minimization problem

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & x \in \mathbb{R}^n \end{aligned}$$

Hook and Jeeves' method, which dates from 1961, is one of the most widely used search methods. The method proceeds by a sequence of *exploratory* and *pattern moves* from a base point. If an exploratory move leads to a decrease of the value of $f(\mathbf{x})$ it is called a *success*; otherwise it is called a *failure*.

Exploratory moves

Step 1. Choose a base point $\mathbf{b}_1$ and step length h_1.

Step 2. Evaluate $f(\mathbf{b}_1 + h_1\mathbf{e}_1)$ where the first unit coordinate vector, that is, $\mathbf{e}_1 = (1, 0, \cdots, 0)^T$. If

$$f(\mathbf{b}_1 + h_1\mathbf{e}_1) < f(\mathbf{b}_1),$$

replace $\mathbf{b}_1$ by $\mathbf{b}_1 + h_1\mathbf{e}_1$. Otherwise evaluate $f(\mathbf{b}_1 - h_1\mathbf{e}_1)$. If

$$f(\mathbf{b}_1 - h_1\mathbf{e}_1) < f(\mathbf{b}_1),$$

replace $\mathbf{b}_1$ by $\mathbf{b}_1 - h_1\mathbf{e}_1$. Otherwise retain $\mathbf{b}_1$.

Step 3. Repeat the procedure in Step 2 for the second variable x_2 (note that $f(\mathbf{x})$ has n variables) by considering variations $+(-)h_2\mathbf{e}_2$ from the base point which results from Step 2. Apply the procedure to each variable in turn, finally arriving at a new base point $\mathbf{b}_2$ (after at most $(2n + 1)$ function evaluations).

Step 4. If $\mathbf{b}_2 = \mathbf{b}_1$, halve each of the step lengths h_j and return to Step 1. Terminate when the lengths have been reduced to the prescribed precision.

If $\mathbf{b}_2 \neq \mathbf{b}_1$, make the following **pattern moves**:

Step 1. Move from $\mathbf{b}_2$ to $\mathbf{p}_1 = 2\mathbf{b}_2 - \mathbf{b}_1$ and continue with a new sequence of exploratory moves about $\mathbf{p}_1$.

Step 2. If the lowest function value obtained during the pattern and exploratory moves of Step 1 is less than $f(\mathbf{b}_2)$, then a new base point $\mathbf{b}_3$ has been reached. Return to Step 1 with all suffices increased by 1. Otherwise, abandon the pattern move from $\mathbf{b}_2$ and continue with a new sequence of exploratory moves.

Example 2.5 Use Hooke and Jeeves' method to minimize

$$f(\mathbf{x}) = 3x_1^2 - 2x_1x_2 + x_2^2 + 4x_1 + 3x_2.$$

Take $\mathbf{b}_1 = (0, 0)^T$ as the initial base point, $h_1 = h_2 = 1$ as initial step lengths and $h_1 = h_2 = 0.25$ as the stopping criterion.

(Example 2.5 continued)

2.4 Spendley, Hext and Himsworth's method

Spendley, Hext and Himsworth's (1962) devised a method based on the geometrical design known as a *regular simplex*. A *simplex* in $\mathbb{R}^n$ consists of $n+1$ points which do not lie on a hyperplane, together with every convex combination of these points. The simplex is *regular* if the vertices are equally spaced.

Examples of regular simplices: an equilateral triangle in $\mathbb{R}^2$ and a regular tetrahedron in $\mathbb{R}^3$.

Two dimensional case. Consider the minimization of $f(\mathbf{x})$. The idea of the simplex method can be explained as follows.

Let $\mathbf{x}_1$ be an initial estimate of $\mathbf{x}^*$, a minimizer. Let $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ be the vertices of a regular simplex.

Calculate the reflection of the vertex $\mathbf{x}_1$ with respect to the line segment joining $\mathbf{x}_2$ and $\mathbf{x}_3$ as

$$\mathbf{x}_4 =$$

If $f(\mathbf{x})$ is a linear function, then

$$f(\mathbf{x}_4) = f(\mathbf{x}_2) + f(\mathbf{x}_3) - f(\mathbf{x}_1)$$

Suppose that $f(\mathbf{x}_1) > \max(f(\mathbf{x}_2), f(\mathbf{x}_3))$. Then

$$f(\mathbf{x}_4) < \min(f(\mathbf{x}_2), f(\mathbf{x}_3)).$$

We therefore replace $\mathbf{x}_1$ with $\mathbf{x}_4$ and obtain a new simplex, and repeat the process described above.

The idea is used to minimize a general nonlinear function. The procedure can be stated as follows.

Step 1. Given an initial estimate $\mathbf{x}_1$ of $\mathbf{x}^*$ and find $\mathbf{x}_2$ and $\mathbf{x}_3$ to form a regular simplex.

Step 2. Evaluate f at these points and identify the point with highest function value.

Step 3. Calculate the reflection of the point with respect to the line segment joining the rest two points.

Step 4. Evaluate the value of f at the reflected point.

Step 5. If the highest value occurs at the new vertex in the new simplex, reflect the vertex with second highest function value to avoid oscillations.

Step 6. If one vertex persists for four iterations, reduce the size of the most recently simplex by halving the distances of the remaining vertices from that vertex. This step is called a *contraction*.

Step 7. Stop after a prescribed number of contractions have been carried out.

The method can be generalized to n-dimensional case. Let $\mathbf{x}_1, \cdots, \mathbf{x}_{n+1}$ be the vertices of a regular simplex in $\mathbb{R}^n$. The reflection of the vertex $\mathbf{x}_p$ is defined by

$$\mathbf{x}_q = 2\mathbf{x}_c - \mathbf{x}_p$$

where

$$\mathbf{x}_c = \frac{1}{n}(\mathbf{x}_1 + \cdots + \mathbf{x}_{p-1} + \mathbf{x}_{p+1} + \cdots + \mathbf{x}_{n+1})$$

is the centroid of the remaining vertices.

2.5 Nelder and Mead's method

Nelder and Mead increased the efficiency of Spendley, Hext and Himsworth's method by allowing the simplices to become non-regular.

Let $\mathbf{x}_1$ be initial estimate of $\mathbf{x}^*$ and let the vertices of the initial simplex be $\mathbf{x}_1, \cdots, \mathbf{x}_{n+1}$, where

$$\mathbf{x}_{j+1} + \mathbf{x}_1 + h_j \mathbf{e}_j,\ j = 1, \cdots, n,$$

the $\mathbf{e}_j$ are the usual coordinate vectors and h_j are scalars choses to equalize, as far as possible, the quantities

$$|f(\mathbf{x}_1 + h_j \mathbf{e}_j) - f(\mathbf{x}_1)|.$$

In the current simplex, let

- $\mathbf{x}_h$ be the vertex with the highest function value
- $\mathbf{x}_s$ be the vertex with the second highest function value
- $\mathbf{x}_l$ be the vertex with the lowest function value
- $\mathbf{x}_c$ be the centroid of all vertices except $\mathbf{x}_h$, that is,

$$\mathbf{x}_c = \frac{1}{n} \sum_{j=1, j \neq h}^{n+1} \mathbf{x}_j.$$

Also, for the simplicity of notation, let $\mathbf{y} = f(\mathbf{x})$ and $\mathbf{y}_h = f(\mathbf{x}_h)$.

Nelder and Mead's algorithm.

Step 1. Choose the vertices of the initial simplex as described above and evaluate $f(\mathbf{x})$ at the vertices.

Step 2. Reflection. Reflect $\mathbf{x}_h$ using a reflection factor

$$\mathbf{x}_0 = \mathbf{x}_c + \alpha(\mathbf{x}_c - \mathbf{x}_h),$$

where $\alpha > 0$.

Step 3. If

$$f(\mathbf{x}_l) \leq f(\mathbf{x}_0) \leq f(\mathbf{x}_s)$$

replace $\mathbf{x}_h$ by $\mathbf{x}_0$ and return to Step 2.

Step 4. *Expansion.* If $f(\mathbf{x}_0) < f(\mathbf{x}_l)$, expand the simplex using an expansion factor $\gamma > 1$,

$$\mathbf{x}_{00} - \mathbf{x}_c = \gamma(\mathbf{x}_0 - \mathbf{x}_c)$$

where $\gamma > 1$.

(a) if $f(\mathbf{x}_{00}) < f(\mathbf{x}_l)$, replace $\mathbf{x}_h$ by $\mathbf{x}_{00}$ and return to Step 2.

(b) If $f(\mathbf{x}_{00}) \geq f(\mathbf{x}_l)$, replace $\mathbf{x}_h$ by $\mathbf{x}_0$ and return to Step 2.

Step 5. *Contraction.* If $f(\mathbf{x}_0) > f(\mathbf{x}_s)$, contract the simplex using an contraction factor $\beta \in (0, 1)$,

(a) if $f(\mathbf{x}_0) < f(\mathbf{x}_h)$, find $\mathbf{x}_{00}$ such that

$$\mathbf{x}_{00} - \mathbf{x}_c = \beta(\mathbf{x}_0 - \mathbf{x}_c)$$

where $0 < \beta < 1$.

(b) If $f(\mathbf{x}_0) \geq f(\mathbf{x}_h)$, find $\mathbf{x}_{00}$ such that

$$\mathbf{x}_{00} - \mathbf{x}_c = \beta(\mathbf{x}_h - \mathbf{x}_c)$$

(c) If $f(\mathbf{x}_{00}) < f(\mathbf{x}_h)$ and $f(\mathbf{x}_{00}) < f(\mathbf{x}_0)$, replace $\mathbf{x}_h$ by $\mathbf{x}_{00}$ and return to Step 2.

(d) If $f(\mathbf{x}_{00}) \geq f(\mathbf{x}_h)$ or $f(\mathbf{x}_{00}) > f(\mathbf{x}_0)$, reduce the size of the simplex by halving the distances from $\mathbf{x}_l$ and return to Step 2.

Nelder and Mead suggest values of $\alpha = 1$, $\beta = 0.5$ and $\gamma = 2$ for reflection.

Example 2.6 Use the method of Nelder and Mead to minimize

$$f(x_1, x_2) = 4(x_1 - 5)^2 + 6(x_2 - 6)^2$$

The initial simplex has the following three vertices

$$A(8, 9),\ B(10, 11),\ C(8, 11)$$

Carry out 4 iterations.

Solution.

Iteration =1

$f(8, 9) = 90.0$

$f(10, 11) = 250.0$

$f(8, 11) = 186.0$

Therefore

$X_h = (10, 11)$,

$X_s = (8, 11)$,

$X_l = (8, 9)$

$X_c = \frac{1}{2}((8, 9) + (8, 11)) = (8.0, 10.0)$

Reflection

$X_0 = 2\,(8, 10) - (10, 11) = (6.0, 9.0)$

We need to check if an expansion or a contraction is needed. Since

$f\,(6.0, 9.0) = 58.0$

$$f\,(6.0, 9.0) = 58.0 < f(x_l),$$

an expansion is needed.

$(8.0, 10.0) + 2((6.0, 9.0) - (8.0, 10.0)) = (4.0, 8.0)$

$$\begin{aligned} X_{00} &= (8.0, 10.0) + 2((6.0, 9.0) - (8.0, 10.0)) \\ &= (4.0, 8.0) \end{aligned}$$

Since

$f(4,8) = 28.0$

$$f\left(x_{00}\right) = 28 < f(X_l),$$

the expansion is accepted and we update the simplex vertices

$X_h = (8,11)$,

$X_s = (8,9)$,

$X_l = (4,8)$

Iteration =2

Reflection

$X_c = \frac{1}{2}((8,9) + (4,8)) = (6.0, 8.5)$

$X_0 = 2\,(6.0, 8.5) - (8,11) = (4.0, 6.0)$

$f\,(4.0, 6.0) = 4.0$

therefore $f(X_0) < f(X_l)$ An expansion is needed.

$(6.0, 8.5) + 2((4.0, 6.0) - (6.0, 8.5)) = (2.0, 3.5)$

$f(2, 3.5) = 73.5$

replace X_h by X_0, we obtain a new simplex with vertices

$X_h = (8,9)$,

$X_s = (4,8)$

$X_l = (4.0, 6.0)$

Iteration =3

Reflection

$X_c = \frac{1}{2}((4,8) + (4.0, 6.0)) = (4.0, 7.0)$

$X_0 = 2\,(4.0, 7.0) - (8, 9) = (0, 5.0)$

$f\,(0, 5.0) = 106.0 > f(X_h) = 90$ A contraction is needed

$X_{00} = (4.0, 7.0) + 0.5((8, 9) - (4.0, 7.0)) = (6.0, 8.0)$

$f(6.0, 8.0) = 28.0 = f(X_s)$

Since

$$f\,(1.578\,3, .871\,16) = -14.49 < \min(f(X_0), f(X_h))$$

we replace X_h by X_{00} and obtain a new simplex with vertices

$X_h = (6.0, 8.0)$

$X_s = (4, 8)$

$X_l = (4.0, 6.0)$

Iteration =4

Reflection

$X_c = \frac{1}{2}((4, 8) + (4.0, 6.0)) = (4.0, 7.0)$

$X_0 = 2\,(4.0, 7.0) - (6.0, 8.0) = (2.0, 6.0)$

Since

$f(2.0, 6.0) = 36.0 > f(X_h)$

$$f\,(.871\,2, 1.578\,3) = -11.201 > f(X_h) = -13.585$$

a contraction is needed.

$(4.0, 7.0) + 0.5((6.0, 8.0) - (4.0, 7.0)) = (5.0, 7.\,5)$

$$X_{00} = (4.0, 7.0) + 0.5((6.0, 8.0) - (4.0, 7.0)) = (5.0, 7.\,5)$$

Since

$f\,(5.0, 7.\,5) = 13.\,5$

$$f\,(2.126, 1.242) = -15.266 < \min(f(X_h), f(x_0))$$

X_{00} is accepted. We obtain a new simplex with vertices

$X_h = (4.0, 8.0)$

$X_s = (5.0, 7.5)$

$X_l = (4.0, 6.0)$

2.6 References

1. J. Nocedal and S.J. Wright (1999), *Numerical Optimisation*, Springer-Verlag.

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3. G.R. Walsh (1975), Methods of Optimization, John Wiley & Sons.