THE SEARCH PROCEDURE OF NELDER AND MEADE

The multi-dimensional optimisation procedure of Nelder and Meade attempts to minimise a scalar-valued function of n real variables using only function values, without any information regarding the derivatives of the function. It looks for the minimum amongst the $n+1$ vertices of a non-degenerate simplex, which is a solid figure within an n-dimensional space; and it adapts the shape of the simplex when a neigbouring point is found with a function value lower than those of the vertices. Eventually, a close approximation to the minimum should be found amongst the vertices of the simplex, after it has shrunk to a negligable size.

The logic of the method can be understood by considering the minimisation of a function of two variables. Then, the simplex becomes a triangle. By finding their associated function values, we can fix the vertices of the triangle to points on the surface of the function to be minimised, thereby providing information on its inclination. Using this information, an attempt is made to descend towards the minimum of the function. This entails finding a new point with which to replace the vertex associated with highest function value; and, in the process, a new simplex or triangle is formed on which to base a further step.

In general, the simplex is a set of $n+1$ points $x_j; j = 0, \ldots, n$ within an n-dimensional space. Each point is associated with a value $f_j = f(x_j)$ of the function for which the minimum is being sought. We shall denote the index of the point associated with the highest function value by $j = w$ (*worst*), that associated with next highest value by $j = p$ (*poor*) and the index associated with the lowest value by $j = b$ (*best*). The ordering of these function values is

$$f_w > f_p > \cdots > f_b. \tag{1}$$

We attempt to find a point where the function value represents an improvement on some or all of the values above, and we react in various ways according to the quality of the point. The function value f_r of the trial point r can fall either between the listed values or outside their range. The potential outcomes are represented in the diagram below, which indicates, by the numbers in parenthesis, the possible positions of f_r relative to the listed values:

$$(4) > f_w > (3) > f_p > (2) > f_b > (1). \tag{2}$$

The initial trial point r is computed by projecting a line running from the worst point x_w, which is associated with the highest function value, through the centroid of the remaining points of the simplex, which is given by

$$\bar{x} = \frac{1}{n} \sum_{j \neq w} x_j.$$

The trial point, which is described as the *reflection point,* is given by

$$r = (1+\alpha)\bar{x} - \alpha x_w, \tag{3}$$

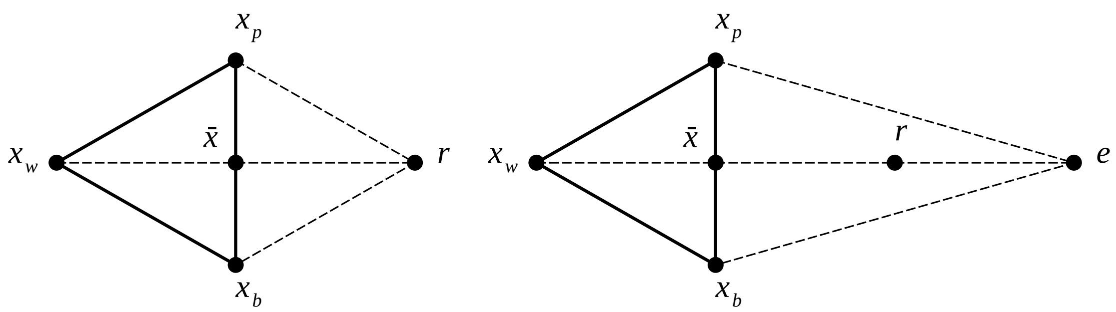

Figure 1. The reflection point r and the extension point e both lie of a line running from the worst point x_w through the centroid $\bar{x}$ of the remaining points of the simplex.

where $\alpha > 0$ is typically $\alpha = 1$. Observe that, if $\alpha \in (-1, 0)$, then (3) would stand for a convex combination of $\bar{x}$ and x_w, producing a point within the simplex lying somewhere on the line segment joining the two. With $\alpha > 0$, it represents an extrapolation of the line beyond $\bar{x}$.

We shall examine, in succession, the various outcomes that are represented by the display of (2).

(1) We might find that $f_b > f_r$. This is a favourable circumstance; and we are tempted to push our luck by investigating a point further along the line, which is the so-called *extension point* given by

$$e = (1 + \gamma)\bar{x} - \gamma x_w, \tag{4}$$

where $\gamma > \alpha$ is typically $\gamma = 2$. The associated function value is $f_e = f(e)$. If $f_b > f_r > f_e$, then e can become a new point of the simplex; and it can be written in place of the worst point x_w. Otherwise, if $f_e > f_r$, we replace x_w by r instead.

(2) Having established that (1) is not the case, we might find that $f_p > f_r > f_b$. In this case, we simply replace x_w by r.

(3) Given that neither (1) nor (2) is the case, we might find that $f_w > f_r > f_p$. The supposition is that the trial point r has been placed at too great a distance from the simplex. Therefore, we are inclined to find a new point, external to the simplex, described as an *outside contraction* point, given by

$$c = (1 + \beta)\bar{x} - \beta x_w, \tag{5}$$

where $\beta \in (0, 1)$ is typically $\beta = 0.5$. The associated function value is $f_c = f(c)$. Observe that, when $\beta = 0.5$, this contraction point can also be expressed as

$$c = (1 - \beta)\bar{x} + \beta r, \tag{6}$$

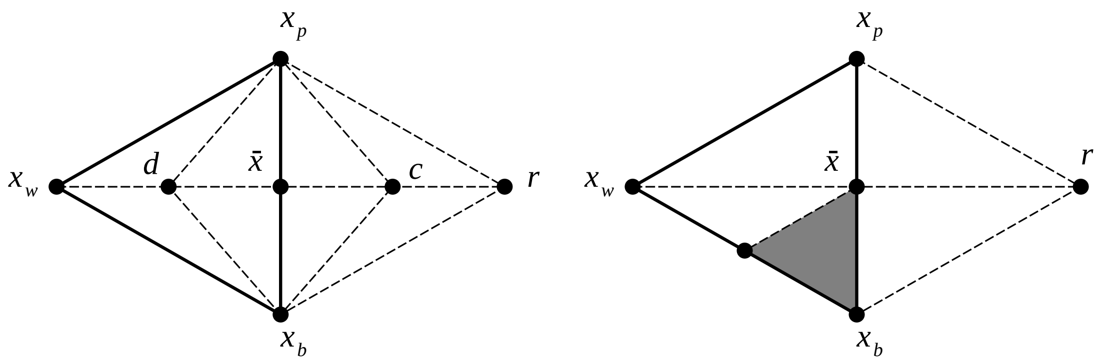

Figure 2. The external contraction point c and the internal contraction point d (left). The shrinkage of the simplex towards the best point x_b (right).

which is to say that it is a point internal to the reflected simplex derived by replacing x_w by r. If $f_w > f_c$, then we replace x_w by c. However, if $f_c > f_w$ then we have not succeeded in finding a point that is better than the worst point. Therefore, we decide to shrink the simplex towards the best point by reducing the length of its sides. Thus, we replace all points x_j other than the best point x_b by

$$v_j = \beta x_j + (1 - \beta)x_b. \tag{7}$$

(4) If $f_r > f_w$, then the trial point r has a function value greater than that of the worst point. Then, we should find a find a new trial value, internal to the simplex, described as an *inside contraction* point

$$d = (1 - \beta)\bar{x} + \beta x_w. \tag{8}$$

If this does not secure a better function value, then we perform a shrinkage according to equation (7).

References

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