Chapter 8

Simplicial direct-search methods

The Nelder–Mead algorithm [177] is one of the most popular derivative-free methods. It has been extensively used in the engineering community and is probably the most widely cited of the direct-search methods (the 1965 paper by Nelder and Mead [177] is officially a *Science Citation Classic*). Among the reasons for its success are its simplicity and its ability to adapt to the curvature of the function being minimized. In this chapter we will describe the original Nelder–Mead method for solving (1.1) and some of its features. We will show why it can fail and how it can be fixed to globally converge to stationary points.

8.1 The Nelder–Mead simplex method

The Nelder–Mead algorithm [177] is a direct-search method in the sense that it evaluates the objective function at a finite number of points per iteration and decides which action to take next solely based on those function values and without any explicit or implicit derivative approximation or model building. Every iteration in $\mathbb{R}^n$ is based on a simplex of $n+1$ vertices $Y = \{y^0, y^1, \ldots, y^n\}$ ordered by increasing values of f. See Section 2.5 for the definition and basic properties of simplices.

The most common Nelder–Mead iterations perform a reflection, an expansion, or a contraction (the latter can be inside or outside the simplex). In such iterations the worst vertex y^n is replaced by a point in the line that connects y^n and y^c,

$$y \;=\; y^c + \delta(y^c - y^n), \quad \delta \in \mathbb{R},$$

where $y^c = \sum_{i=0}^{n-1} y^i/n$ is the centroid of the best n vertices. The value of δ indicates the type of iteration. For instance, when $\delta = 1$ we have a (genuine or isometric) reflection, when $\delta = 2$ an expansion, when $\delta = 1/2$ an outside contraction, and when $\delta = -1/2$ an inside contraction. In Figure 8.1, we plot these four situations.

A Nelder–Mead iteration can also perform a simplex shrink, which rarely occurs in practice. When a shrink is performed all the vertices in Y are thrown away except the best one y^0. Then n new vertices are computed by shrinking the simplex at y^0, i.e., by computing, for instance, $y^0 + 1/2(y^i - y^0)$, $i = 1,\ldots,n$. See Figure 8.2. We note that the "shape" of the resulting simplices can change by being stretched or contracted, unless a shrink occurs—as we will study later in detail.

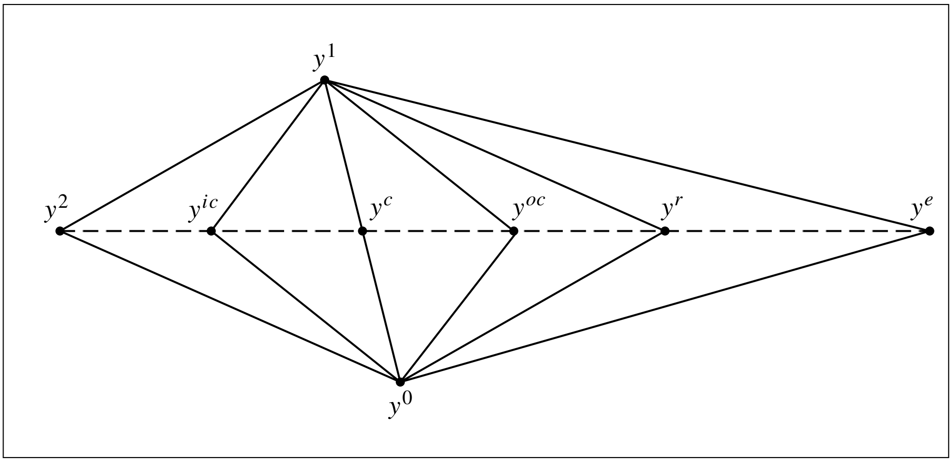

Figure 8.1. *Reflection, expansion, outside contraction, and inside contraction of a simplex, used by the Nelder–Mead method.*

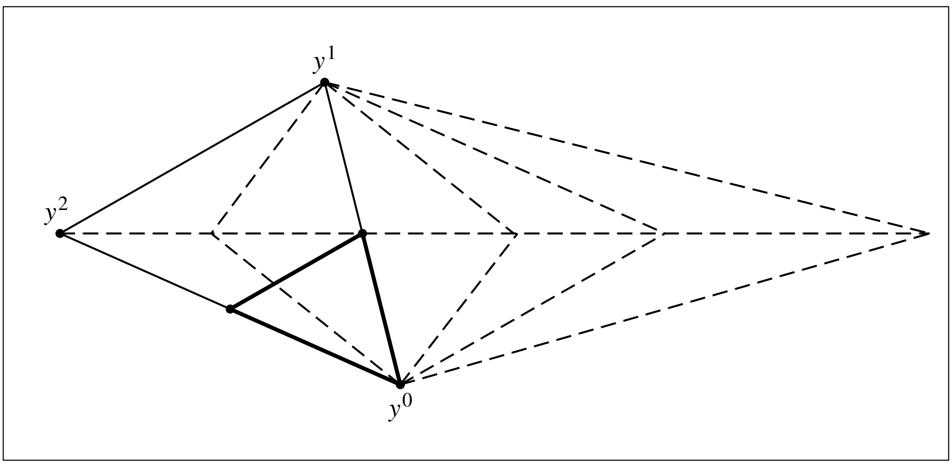

Figure 8.2. *Shrink of a simplex, used by the Nelder–Mead method.*

The Nelder–Mead method is described in Algorithm 8.1. The standard choices for the coefficients used are

$$\gamma^s = \frac{1}{2}, \quad \delta^{ic} = -\frac{1}{2}, \quad \delta^{oc} = \frac{1}{2}, \quad \delta^r = 1, \quad \text{and} \quad \delta^e = 2. \tag{8.1}$$

Note that, except for shrinks, the emphasis is on replacing the worse vertex rather than improving the best. It is also worth mentioning that the Nelder–Mead method does not parallelize well since the sampling procedure is necessarily sequential (except at a shrink).

Algorithm 8.1 (The Nelder–Mead method).

Initialization: Choose an initial simplex of vertices $Y_0 = \{y_0^0, y_0^1, \ldots, y_0^n\}$. Evaluate f at the points in Y_0. Choose constants:

$$0 < \gamma^s < 1, \qquad -1 < \delta^{ic} < 0 < \delta^{oc} < \delta^r < \delta^e.$$

For $k = 0, 1, 2, \ldots$

0. Set $Y = Y_k$.
1. **Order:** Order the $n+1$ vertices of $Y = \{y^0, y^1, \ldots, y^n\}$ so that

$$f^0 = f(y^0) \;\le\; f^1 = f(y^1) \;\le\; \cdots \;\le\; f^n = f(y^n).$$

2. **Reflect:** Reflect the worst vertex y^n over the centroid $y^c = \sum_{i=0}^{n-1} y^i/n$ of the remaining n vertices:

$$y^r = y^c + \delta^r (y^c - y^n).$$

   Evaluate $f^r = f(y^r)$. If $f^0 \le f^r < f^{n-1}$, then replace y^n by the reflected point y^r and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y^{n-1}, y^r\}$.

3. **Expand:** If $f^r < f^0$, then calculate the expansion point

$$y^e = y^c + \delta^e (y^c - y^n)$$

   and evaluate $f^e = f(y^e)$. If $f^e \le f^r$, replace y^n by the expansion point y^e and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y^{n-1}, y^e\}$. Otherwise, replace y^n by the reflected point y^r and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y^{n-1}, y^r\}$.

4. **Contract:** If $f^r \ge f^{n-1}$, then a contraction is performed between the best of y^r and y^n.

   (a) **Outside contraction:** If $f^r < f^n$, perform an outside contraction

$$y^{oc} = y^c + \delta^{oc} (y^c - y^n)$$

   and evaluate $f^{oc} = f(y^{oc})$. If $f^{oc} \le f^r$, then replace y^n by the outside contraction point y_k^{oc} and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y^{n-1}, y^{oc}\}$. Otherwise, perform a shrink.

   (b) **Inside contraction:** If $f^r \ge f^n$, perform an inside contraction

$$y^{ic} = y^c + \delta^{ic} (y^c - y^n)$$

   and evaluate $f^{ic} = f(y^{ic})$. If $f^{ic} < f^n$, then replace y^n by the inside contraction point y^{ic} and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y^{n-1}, y^{ic}\}$. Otherwise, perform a shrink.

5. **Shrink:** Evaluate f at the n points $y^0 + \gamma^s (y^i - y^0)$, $i = 1, \ldots, n$, and replace $y^1, \ldots, y^n$ by these points, terminating the iteration: $Y_{k+1} = \{y^0 + \gamma^s (y^i - y^0),\ i = 0, \ldots, n\}$.

A stopping criterion could consist of terminating the run when the diameter of the simplex becomes smaller than a chosen tolerance $\Delta_{tol} > 0$ (for instance, $\Delta_{tol} = 10^{-5}$).

This algorithmic description is what we can refer to as the "modern interpretation" of the original Nelder–Mead algorithm [177], which had several ambiguities about strictness of inequalities and tie breaking. The only significant difference between Algorithm 8.1 and the original Nelder–Mead method [177] is that in the original version the expansion point y^e is accepted if $f^e < f^0$ (otherwise, the reflection point y^r is accepted). The standard practice nowadays [149, 169] is to accept the best of y^r and y^e if both improve over y^0, as is done in Algorithm 8.1.

The Nelder–Mead algorithm performs the following number of function evaluations per iteration:

1	if the iteration is a reflection,
2	if the iteration is an expansion or contraction,
$n+2$	if the iteration is a shrink.

Lexicographic decrease at nonshrink iterations

We focus our attention now on how ties are broken in Algorithm 8.1 when equal function values occur. The way in which the initial points are originally ordered when ties occur is not relevant to what comes next. It also makes no difference how these ties are broken among the n new points calculated in the shrink step.

However, we need tie-breaking rules if we want to well define the smallest index k^* of a vertex that differs between iterations k and $k+1$,

$$k^* \;=\; \min\left\{ i \in \{0,1,\ldots,n\} : \; y_k^i \neq y_{k+1}^i \right\}.$$

It is a simple matter to see that such tie-breaking rules involve only the situations reported in the next two paragraphs.

When a new point is brought to the simplex in the reflection, expansion, or contraction steps, there might be a point in the simplex which already has the same objective function value. We need to define tie-breaking rules to avoid unnecessary modifications to the change index k^*. We adopt here the natural rule suggested in [149]. If a new accepted point (y_k^r, y_k^e, y_k^{oc}, or y_k^{ic}) produces an objective function value equal to the value of one (or more than one) of the points $y_k^0, \ldots, y_k^{n-1}$, then it is inserted into Y^{k+1} with an index larger than that of such a point (or points). In this way the change index k^* remains the same whenever points with identical function values are generated in consecutive iterations.

Another situation where tie breaking is necessary to avoid modifications by chance on the change index k^* occurs at a shrink step when the lowest of the values $f(y_k^0 + \gamma^s(y_k^i - y_k^0))$, $i = 1,\ldots,n$, is equal to $f(y_k^0)$. In such a case, we set y_{k+1}^0 to y_k^0.

Thus, k^* takes the following values:

$1 \le k^* \le n-1$	if the iteration ends at a reflection step,
$k^* = 0$	if the iteration ends at an expansion step,
$0 \le k^* \le n$	if the iteration ends at a contraction step,
$k^* = 0$ or 1	if the iteration ends at a shrink step.

In addition, the definition of the change index k^*, under the two above-mentioned tie-breaking rules, implies that at a nonshrink iteration

$$\begin{array}{lcll} f_{k+1}^j = f_k^j & \text{and} & y_{k+1}^j = y_k^j & \text{if } j < k^*, \\ f_{k+1}^j < f_k^j & \text{and} & y_{k+1}^j \neq y_k^j & \text{if } j = k^*, \\ f_{k+1}^j = f_k^{j-1} & \text{and} & y_{k+1}^j = y_k^{j-1} & \text{if } j > k^*. \end{array}$$

We observe that the vector $(f_k^0, \ldots, f_k^n)$ decreases lexicographically at nonshrink iterations. It follows from these statements that, at nonshrink iterations,

$$\sum_{j=0}^{n} f_{k+1}^j \; < \; \sum_{j=0}^{n} f_k^j .$$

This property of the Nelder–Mead algorithm has been explored by several authors. Kelley [140] used it to detect and remedy stagnation in the context of the Nelder–Mead method. Tseng [220] suggested a class of simplex-type methods that includes a modified Nelder–Mead method where this inequality plays a relevant role (see Section 8.3).

Note that the worst vertex function value might not necessarily decrease after a nonshrink iteration. For instance, suppose that $n = 4$ and that the vertex function values are $(f_k^0, f_k^1, f_k^2, f_k^3, f_k^4) = (1,2,2,3,3)$ at the nonshrink iteration k. Suppose also that the new vertex has function value 2. Then the vertex function values at iteration $k+1$ are $(f_{k+1}^0, f_{k+1}^1, f_{k+1}^2, f_{k+1}^3, f_{k+1}^4) = (1,2,2,2,3)$. It is clear from this example that the worst vertex function has not improved. However, one can easily see that the worst function value will necessarily decrease after at most $n+1$ consecutive nonshrink iterations, unless an optimal value has already been attained.

Nelder–Mead simplices

The Nelder–Mead algorithm was designed with the idea that the simplices would adapt themselves to “the local landscape” [177]. In fact, we can see that the Nelder–Mead moves allow any simplex shape to be approximated. The good practical performance of the Nelder–Mead algorithm, when it works, is directly related to this capability of fitting well the curvature of the function.

However, the simplices can become arbitrarily flat or needle shaped, which is the reason why it is not possible to establish global convergence to stationary points for the Nelder–Mead algorithm (as the example by McKinnon given in Section 8.2 demonstrates). A common procedure used by today’s practitioners is to restart Nelder–Mead whenever the geometry or well poisedness of the simplex vertices deteriorates.

One way to monitor the geometry of $Y = \{y^0, y^1, \ldots, y^n\}$ is to check if it is Λ-poised (for some prefixed constant $\Lambda > 0$), i.e., to check if

$$\|\hat{L}(Y)^{-1}\| \; \leq \; \Lambda, \tag{8.2}$$

where

$$\hat{L}(Y) \; = \; \frac{1}{\Delta(Y)} L(Y) \; = \; \frac{1}{\Delta(Y)} \left[y^1 - y^0 \cdots y^n - y^0 \right] \tag{8.3}$$

and $\Delta(Y) = \max_{1 \le i \le n} \|y^i - y^0\|$. It is easy to see that such a simplex measure is consistent with the definition of linear Λ-poisedness (see Sections 2.5, 3.3, and 4.3).

Now recall from Section 2.5 the definition of the diameter of a simplex: $\mathrm{diam}(Y) = \max_{0 \le i < j \le n} \|y^i - y^j\|$. Since $\Delta(Y) \le \mathrm{diam}(Y) \le 2\Delta(Y)$ (see also Section 2.5), it is irrelevant both in practice and in a convergence analysis whether the measure of the scaling of Y is given by $\Delta(Y)$ or by $\mathrm{diam}(Y)$. We choose to work with $\mathrm{diam}(Y)$ in simplex-type methods like Nelder–Mead because it does not depend on a centering point like $\Delta(Y)$ does. Instead of Λ-poisedness, we will work with the normalized volume (see Section 2.5)

$$\mathrm{von}(Y) \;=\; \mathrm{vol}\left(\frac{1}{\mathrm{diam}(Y)} Y\right) \;=\; \frac{|\det(L(Y))|}{n!\,\mathrm{diam}(Y)^n}.$$

The choices of $\mathrm{diam}(Y)$ and $\mathrm{von}(Y)$ will be mathematically convenient when manipulating a simplex by reflection or shrinkage. Tseng [220] ignores the factor $n!$ in the denominator, which we could also do here.

We end this section with a few basic facts about the volume and normalized volume of Nelder–Mead simplices [149]. Recall from Section 2.5 that the volume of the simplex of vertices $Y_k = \{y_k^0, y_k^1, \ldots, y_k^n\}$ is defined by the (always positive) quantity

$$\mathrm{vol}(Y_k) \;=\; \frac{|\det(L_k)|}{n!},$$

where

$$L_k \;=\; \left[y_k^0 - y_k^n \cdots y_k^{n-1} - y_k^n \right].$$

Theorem 8.1.

- *If iteration k performs a nonshrink step (reflection, expansion, or contraction), then*

$$\mathrm{vol}(Y_{k+1}) \;=\; |\delta|\,\mathrm{vol}(Y_k).$$

- *If iteration k performs a shrink step, then*

$$\mathrm{vol}(Y_{k+1}) \;=\; (\gamma^s)^n\,\mathrm{vol}(Y_k).$$

Proof. Let us prove the first statement only. The second statement can be proved trivially.

Let us assume without loss of generality that $y_k^n = 0$. In this case, the vertex computed at a nonshrink step can be written in the form

$$L_k\, t_k(\delta), \quad \text{where} \quad t_k(\delta) \;=\; \left[\frac{1+\delta}{n}, \ldots, \frac{1+\delta}{n}\right]^\top.$$

Since the volume of the new simplex Y_{k+1} is independent of the ordering of the vertices, let us assume that the new vertex $L_k t_k(\delta)$ is the last in Y_{k+1}. Thus, recalling that $y_k^n = 0$,

$$|\det(L_{k+1})| \;=\; \left|\det\left(L_k - L_k t_k(\delta) e^\top\right)\right| \;=\; |\det(L_k)| \left|\det\left(I - t_k(\delta) e^\top\right)\right|,$$

Table 8.1. *Number of times where the diameter of a simplex increased and the normalized volume decreased by isometric reflection. Experiments made on* 10^5 *simplices in* $\mathbb{R}^3$ *with* $y^0 = 0$ *and remaining vertex components randomly generated in* $[-1,1]$*, using MATLAB®* [1] *software. The notation used is such that* $Y = \{y^0, y^1, y^2, y^3\}$ *and* $Y^r = \{y^0, y^1, y^2, y^r\}$.

Difference (power k)	0	2	4	6	8
$\mathrm{diam}(Y^r) > \mathrm{diam}(Y) + 10^{-k}$	0%	24%	26%	26%	26%
$\mathrm{von}(Y^r) < \mathrm{von}(Y) - 10^{-k}$	0%	1%	23%	26%	26%

where e is a vector of ones of dimension n. The eigenvalues of $I - t_k(\delta)e^\top$ are 1 (with multiplicity $n-1$) and $-\delta$. Thus, $|\det(I - t_k(\delta)e^\top)| = |\delta|$, and the proof is completed. □

A simple consequence of this result is that all iterations of the Nelder–Mead algorithm generate simplices, i.e., $\mathrm{vol}(Y_k) > 0$, for all k (provided that the vertices of Y_0 form a simplex). Theorem 8.1 also allows us to say, algebraically, that isometric reflections ($\delta = 1$) preserve the volume of the simplices, that contractions and shrinks are volume decreasing, and that expansions are volume increasing.

It is also important to understand how these operations affect the normalized volume of the simplices. When a shrink step occurs one has

$$\mathrm{von}(Y_{k+1}) \;=\; \mathrm{von}(Y_k). \tag{8.4}$$

This is also true for isometric reflections ($\delta = 1$) when $n = 2$ or when n is arbitrary but the simplices are equilateral. We leave these simple facts as exercises. Although counterintuitive, isometric reflections do not preserve the normalized volume in general when $n > 2$, and in particular they can lead to a decrease of this measure.[13] We know from above that the volume is kept constant in isometric reflections. However, the diameter can increase and therefore the normalized volume can decrease. The reader can be convinced, for instance, by taking the simplex of vertices $y^0 = (0,0,0)$, $y^1 = (1,1,0)$, $y^2 = (0,1,0)$, and $y^3 = (0,0,1)$. The diameter increases from 1.7321 to 1.7951, and the normalized volume decreases from 0.0321 to 0.0288. We conducted a simple experiment using MATLAB [1] software, reported in Table 8.1, to see how often the normalized volume can change.

One can prove that the decrease in the normalized volume caused by isometric reflections is no worse than

$$\mathrm{von}(Y_{k+1}) \;\geq\; \frac{\mathrm{von}(Y_k)}{2^n}. \tag{8.5}$$

In practice, the decrease in the normalized volume after isometric reflections is not significant throughout an optimization run and rarely affects the performance of the Nelder–Mead method.

[13] It is unclear whether one could perform an isometric reflection using a centroid point of the form $y^c = \sum_{i=0}^{n-1} \alpha^i y^i$, with $\sum_{i=0}^{n-1} \alpha^i = 1$ and $\alpha^i > 0$, $i = 0, \ldots, n-1$, that would preserve the normalized volume for values of α^i, $i = 0, \ldots, n-1$, bounded away from zero.

8.2 Properties of the Nelder–Mead simplex method

The most general properties of the Nelder–Mead algorithm are stated in the next theorem.

Theorem 8.2. *Consider the application of the Nelder–Mead method (Algorithm* 8.1*) to a function f which is bounded from below on $\mathbb{R}^n$.*

1. *The sequence $\{f_k^0\}$ is convergent.*

2. *If only a finite number of shrinks occur, then all the $n+1$ sequences $\{f_k^i\}$, $i = 0,\ldots,n$, converge and their limits satisfy $f_*^0 \le f_*^1 \le \cdots \le f_*^n$.*

   Moreover, if there is an integer $j \in \{0,\ldots,n-1\}$ for which $f_*^j < f_*^{j+1}$ (a property called broken convergence), then for sufficiently large k the change index is such that $k^* > j$.

3. *If only a finite number of nonshrinks occur, then all the simplex vertices converge to a single point.*

Proof. The proof of the first and second assertions is essentially based on the fact that monotonically decreasing sequences bounded from below are convergent. The proof of the third assertion is also straightforward and left as an exercise. □

Note that the fact that $\{f_k^0\}$ converges does not mean that it converges to the value of f at a stationary point. A consequence of *broken convergence* is that if the change index is equal to zero an infinite number of times, then $f_*^0 = f_*^1 = \cdots = f_*^n$ (assuming that f is bounded from below and no shrinks steps are taken).

If the function is strictly convex, one can show that no shrink steps occur.

Theorem 8.3. *No shrink steps are performed when the Nelder–Mead method (Algorithm* 8.1*) is applied to a strictly convex function f.*

Proof. Shrink steps are taken only when outside or inside contractions are tried and fail. Let us focus on an outside contraction, which is tried only when $f_k^{n-1} \le f_k^r < f_k^n$. Now, from the strict convexity of f and the fact that y_k^{oc} is a convex combination of y_k^c and y_k^r for some parameter $\lambda \in (0,1)$,

$$f(y_k^{oc}) \;=\; f(\lambda y_k^c + (1-\lambda) y_k^r) \;<\; \lambda f(y_k^c) + (1-\lambda) f(y_k^r) \;\le\; \max\left\{f_k^c, f_k^r\right\}.$$

But $\max\left\{f_k^c, f_k^r\right\} = f_k^r$ since $f_k^{n-1} \le f_k^r$ and $f_k^c \le f_k^{n-1}$ (the latter is, again, a consequence of the strict convexity of f). Thus, $f_k^{oc} < f_k^r$ and the outside contraction is applied (and the shrink step is not taken).

If, instead, an inside contraction is to be considered, then a similar argument would be applied, based on the fact that y_k^{ic} is a convex combination of y_k^n and y_k^c. Note that strict convexity is required for this argument. □

Lagarias et al. [149] proved that the Nelder–Mead method (Algorithm 8.1) is globally convergent when $n = 1$. An alternative and much shorter proof, mentioned in [145] for the standard choices (8.1), is sketched in the exercises.

Convergence of the Nelder–Mead method to nonstationary points

Woods [230] constructed a nonconvex differentiable function in two variables for which the Nelder–Mead method is claimed to fail. The reason for this failure is that the method applies consecutive shrinks towards a point that is not a minimizer.

McKinnon [169] has derived a family of strictly convex examples for which the Nelder–Mead method (Algorithm 8.1) converges to a nonstationary point. From Theorem 8.3, shrink steps are immediately ruled out. In these examples the inside contraction step is applied repeatedly with the best vertex remaining fixed. McKinnon referred to this behavior as *repeated focused inside contraction* (RFIC). It is shown in [169] that no other type of step is taken in these examples. The simplices generated by the Nelder–Mead method collapse along a direction orthogonal to the steepest descent direction. The functions are defined in $\mathbb{R}^2$ as follows:

$$f(x_1,x_2) = \begin{cases} \theta\phi|x_1|^\tau + x_2 + x_2^2 & \text{if } x_1 \le 0, \\ \theta x_1^\tau + x_2 + x_2^2 & \text{if } x_1 > 0. \end{cases} \tag{8.6}$$

The function is strictly convex if $\tau > 1$. It has continuous first derivatives if $\tau > 1$, continuous second derivatives if $\tau > 2$, and continuous third derivatives if $\tau > 3$. Note that $(0,-1)$ is a descent direction from the origin. The Nelder–Mead algorithm is started with the simplex of vertices

$$y_0^0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad y_0^1 = \begin{bmatrix} \lambda_1^0 \\ \lambda_2^0 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \text{and} \quad y_0^2 = \begin{bmatrix} \lambda_1^1 \\ \lambda_2^1 \end{bmatrix}, \tag{8.7}$$

where $\lambda_1^1 = (1+\sqrt{33})/8 \simeq 0.84$ and $\lambda_2^1 = (1-\sqrt{33})/8 \simeq -0.59$. For values of τ, θ, and ϕ satisfying certain conditions, the method can be shown to converge to the origin which is not a stationary point. An example of values of τ, θ, and ϕ that satisfy these conditions is $\tau = 2$, $\theta = 6$, and $\phi = 60$. The contours of the function (8.6) are shown in Figure 8.3 for these values of τ, θ, and ϕ. Another set of parameter values for which this type of counterexample works is $\tau = 3$, $\theta = 6$, and $\phi = 400$. The RFIC behavior generates a sequence of simplices whose vertices are not uniformly Λ-poised (for any fixed $\Lambda > 0$).

We ran the MATLAB [1] implementation of the Nelder–Mead method to minimize the McKinnon function (8.6) for the choices $\tau = 2$, $\theta = 6$, and $\phi = 60$. First, we selected the initial simplex as in (8.7). As expected, we can see from Figure 8.3 that the method never moved the best vertex from the origin. Then we changed the initial simplex to

$$y_0^0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad y_0^1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \text{and} \quad y_0^2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \tag{8.8}$$

and it can be observed that the Nelder–Mead method was able to move away from the origin and to converge to the minimizer ($x_* = (0,-0.5)$, $f(x_*) = -0.25$).

8.3 A globally convergent variant of the Nelder–Mead method

There are a number of issues that must be taken care of in the Nelder–Mead method (Algorithm 8.1) to make it globally convergent to stationary points.

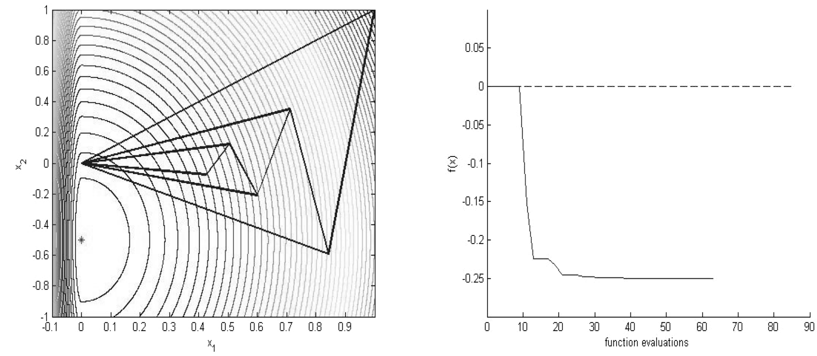

Figure 8.3. *The left plot depicts the contours of the McKinnon function* (8.6) *for* $\tau = 2$, $\theta = 6$, *and* $\phi = 60$ *and illustrates the RFIC when starting from the initial simplex* (8.7). *The right plot describes the application of the Nelder–Mead method to this function. The dashed line corresponds to the initial simplex* (8.7) *and the solid line to* (8.8).

First, the quality of the geometry of the simplices must be monitored for all operations, with the exception of shrinks for which we know that the normalized volume is preserved (see (8.4)). Thus, when a shrink occurs, if the normalized volume of Y_k satisfies $\mathrm{von}(Y_k) \geq \xi$ for some constant $\xi > 0$ independent of k, so does the normalized volume of Y_{k+1}. However, there is no guarantee that this will happen for reflections (even isometric ones), expansions, and contractions. A threshold condition like $\mathrm{von}(Y_{k+1}) \geq \xi$ must therefore be imposed in these steps.

Expansions or contractions might then be skipped because of failure in determining expansion or contraction simplices that pass the geometry threshold. However, special provision must be taken for reflections since these are essential for ensuring global convergence, due to their positive spanning effect. One must guarantee that some form of reflection is always feasible in the sense that it does not deteriorate the geometry of the simplices (i.e., does not lead to a decrease in their normalized volumes). Unfortunately, isometric reflections are not enough for this purpose because they might decrease the normalized volume. Several strategies are then possible. To simplify matters, we will assume that an isometric reflection is always tried first. If the isometric reflected point satisfies $\mathrm{diam}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^r\}\right) \leq \gamma^e \Delta$ and $\mathrm{von}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^r\}\right) \geq \xi$, then no special provision is taken and the method proceeds by evaluating the function at y^r. Otherwise, we attempt a safeguard step, by rotating the vertices y^i, $i = 1, \ldots, n$, $180°$ around y^0. This rotation is the same as the one applied by the MDS method (see the end of Chapter 7). As in MDS, we could also consider an expansion step by enlarging this rotated simplex, but we will skip it for the sake of brevity.

On the other hand, we know from Chapter 7 that avoiding degeneracy in the geometry is not sufficient for direct-search methods which accept new iterates solely based on simple decrease. In Chapter 7 we described two possibilities to fortify the decrease in the objective function: (i) to ask the iterates to lie on a sequence of meshes defined as integer lattices, where the minimal separation of the mesh points is proportional to the step size α_k; (ii) to ask the iterates to satisfy a sufficient decrease condition of the type $f(x_{k+1}) < f(x_k) - \rho(\alpha_k)$. (Recall that $\rho : (0,+\infty) \to \mathbb{R}_+$ was called a *forcing function* and was asked to be continuous and positive and to satisfy

$$\lim_{t \longrightarrow 0^+} \frac{\rho(t)}{t} = 0 \qquad \text{and} \qquad \rho(t_1) \leq \rho(t_2) \quad \text{if} \quad t_1 < t_2.$$

A simple example of a forcing function presented was $\rho(t) = t^2$.)

Forcing the iterates to lie on integer lattices seems an intractable task in the Nelder–Mead context for $n > 1$, given the diversity of steps that operate on the simplices. Thus, the approach we follow in this book for a modified Nelder–Mead method is based on the imposition of sufficient decrease. However, in the Nelder–Mead context we do not have a situation like the one we have in the directional direct-search methods of Chapter 7, where the current iterate is the best point found so far. In the Nelder–Mead algorithm, one makes comparisons among several objective function values, and sufficient decrease must be applied to the different situations. Also, the step size parameter α_k used in the sufficient decrease condition of Chapter 7 is now replaced by the diameter of the current simplex $\Delta_k = \mathrm{diam}(Y_k)$—but, as we have mentioned before, we could had chosen $\Delta_k = \Delta(Y_k)$.

The modified Nelder–Mead method described in Algorithm 8.2 is essentially one of the instances suggested and analyzed by Tseng [220]. To simplify matters, the two contraction steps (inside and outside) have been restated as a single contraction step. There is also a relevant difference in the shrink step compared to the original Nelder–Mead method. We have seen that the shrink step in Algorithm 8.1 is guaranteed not to increase the minimal simplex value ($f^0_{k+1} \leq f^0_k$), which follows trivially from the fact that the best vertex of Y_k is kept in Y_{k+1}. This is not enough now because we need sufficient decrease; in other words, we need something like $f^0_{k+1} \leq f^0_k - \rho(\Delta_k)$, where $\Delta_k = \mathrm{diam}(Y_k)$. When this sufficient decrease condition is not satisfied, the iteration is repeated but using the shrunken simplex. Thus, we must take into account the possibility of having an infinite number of cycles within an iteration by repeatedly applying shrink steps. When that happens we will show that the algorithm returns a stationary limit point.

Algorithm 8.2 (A modified Nelder–Mead method).

Initialization: Choose $\xi > 0$. Choose an initial simplex of vertices $Y_0 = \{y^0_0, y^1_0, \ldots, y^n_0\}$ such that $\mathrm{von}(Y_0) \geq \xi$. Evaluate f at the points in Y_0. Choose constants:

$$0 < \gamma^s < 1 < \gamma^e, \qquad -1 < \delta^{ic} < 0 < \delta^{oc} < \delta^r < \delta^e.$$

For $k = 0, 1, 2, \ldots$

0. Set $Y = Y_k$.
1. **Order:** Order the $n+1$ vertices of $Y = \{y^0, y^1, \ldots, y^n\}$ so that

$$f^0 = f(y^0) \leq f^1 = f(y^1) \leq \cdots \leq f^n = f(y^n).$$

Set $\Delta = \mathrm{diam}(Y)$.

2. **Reflect:** Calculate an isometric reflected point y^r (as in Algorithm 8.1 with $\delta^r = 1$). If
$$\begin{aligned} \operatorname{diam}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^r\}\right) &\le \gamma^e \Delta, \\ \operatorname{von}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^r\}\right) &\ge \xi, \end{aligned} \tag{8.9}$$
then evaluate $f^r = f(y^r)$. If $f^r \le f^{n-1} - \rho(\Delta)$, then attempt an expansion (and then accept either the reflected or the expanded point). Otherwise, attempt a contraction.

   Safeguard rotation: If the isometric reflection failed to satisfy (8.9), then rotate the simplex around the best vertex y^0:
$$y^{rot,i} = y^0 - (y^i - y^0), \quad i = 1, \ldots, n.$$
Evaluate $f(y^{rot,i})$, $i = 1, \ldots, n$, and set $f^{rot} = \min\{f(y^{rot,i}) : i = 1, \ldots, n\}$. If $f^{rot} \le f^0 - \rho(\Delta)$, then terminate the iteration and take the rotated simplex: $Y_{k+1} = \{y^0, y^{rot,1}, \ldots, y^{rot,n}\}$. Otherwise, attempt a contraction.

3. **Expand:** Calculate an expansion point y^e (for instance, as in Algorithm 8.1). If
$$\begin{aligned} \operatorname{diam}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^e\}\right) &\le \gamma^e \Delta, \\ \operatorname{von}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^e\}\right) &\ge \xi, \end{aligned}$$
then evaluate $f^e = f(y^e)$, and if $f^e \le f^r$, replace y^n by the expansion point y^e, and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y^{n-1}, y^e\}$. Otherwise, replace y^n by the reflected point y^r, and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y_k^{n-1}, y^r\}$.

4. **Contract:** Calculate a contraction point y^{cc} (such as an outside or inside contraction in Algorithm 8.1). If
$$\begin{aligned} \operatorname{diam}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^{cc}\}\right) &\le \Delta, \\ \operatorname{von}\left(\{y^0, y^1, \ldots, y^{n-1}\} \cup \{y^{cc}\}\right) &\ge \xi, \end{aligned}$$
then evaluate $f^{cc} = f(y^{cc})$, and if $f^{cc} \le f^n - \rho(\Delta)$, then replace y^n by the contraction point y^{cc} and terminate the iteration: $Y_{k+1} = \{y^0, y^1, \ldots, y^{n-1}, y^{cc}\}$. Otherwise, perform a shrink.

5. **Shrink:** Evaluate f at the n points $y^0 + \gamma^s(y^i - y^0)$, $i = 1, \ldots, n$, and let f^s be the lowest of these values. If $f^s \le f^0 - \rho(\Delta)$, then accept the shrunken simplex and terminate the iteration: $Y_{k+1} = \{y^0 + \gamma^s(y^i - y^0),\ i = 0, \ldots, n\}$. Otherwise, go back to Step 0 with $Y = \{y^0 + \gamma^s(y^i - y^0),\ i = 0, \ldots, n\}$.

In practice we could choose γ^e close to 1 for reflections and around 2 for expansions, similarly as in the original Nelder–Mead method. Note also that the normalized volume of the simplices does not change after safeguard rotations and shrinks. In safeguard rotations the diameter of the simplex is unaltered, whereas for shrinks it is reduced by a factor of γ^s. Once again, a stopping criterion could consist of terminating the run when the diameter Δ_k of the simplex becomes smaller than a chosen tolerance $\Delta_{tol} > 0$ (for instance, $\Delta_{tol} = 10^{-5}$).

We define an index n_k depending on the operation in which the iteration has terminated:

$n_k = n$ for (isometric) reflections, expansions, and contractions,

$n_k = 0$ for shrinks and safeguard rotations.

Then the sequence of simplices generated by the modified Nelder–Mead method (Algorithm 8.2) satisfies

$$f_{k+1}^i \;\le\; f_k^i, \quad i = 0,\ldots,n_k, \tag{8.10}$$

and

$$\sum_{i=0}^{n_k} f_{k+1}^i \;\le\; \sum_{i=0}^{n_k} f_k^i - \rho(\Delta_k). \tag{8.11}$$

Theorem 8.4 below, which plays a central role in the analysis of the modified Nelder–Mead method, is essentially based on conditions (8.10)–(8.11) and thus is valid for other (possibly more elaborated) simplex-based direct-search methods as long as they satisfy these conditions for any $n_k \in \{0,\ldots,n\}$.

What is typically done in the convergence analysis of algorithms for nonlinear optimization is to impose smoothness and boundedness requirements for f on a level set of the form

$$L(x_0) \;=\; \{x \in \mathbb{R}^n :\; f(x) \le f(x_0)\}.$$

A natural candidate for x_0 in the context of the modified Nelder–Mead method would be y_0^n. However, although (isometric) reflection, rotation, expansion, and contraction steps generate simplex vertices for which the objective function values are below f_0^n, a shrink might not necessarily do so. It is possible to define a value f^{max} such that all the simplex vertices lie in $\{x \in \mathbb{R}^n : f(x) \le f^{max}\}$, but such a definition would unnecessarily complicate the presentation. We will impose our assumptions on f in $\mathbb{R}^n$; in particular, in what comes next, we assume that f is bounded from below and uniformly continuous in $\mathbb{R}^n$.

The next theorem states under these assumptions on f that the diameter of the simplices generated by the Nelder–Mead algorithm converges to zero. Its proof is due to Tseng [220]—and it is surprisingly complicated. The difficulty comes from the fact that, for steps like isometric reflection, expansion, or contraction, the sufficient decrease condition is imposed at simplex vertices different from the one with the best objective function value. Note that such a result would be proved in a relatively straightforward way for an algorithm that generates a sequence of points $\{x_k\}$ for which $f(x_{k+1}) < f(x_k) - \rho(\Delta_k)$. In the context of simplex-type methods that would correspond, for instance, to having $x_k = y_k^0$ and $f(y_{k+1}^0) < f(y_k^0) - \rho(\Delta_k)$ (a condition we impose only for shrinks and safeguard rotations in the modified Nelder–Mead method).

Theorem 8.4. *If f is bounded from below and uniformly continuous in $\mathbb{R}^n$, then the modified Nelder–Mead method (Algorithm* 8.2*) generates a sequence $\{Y_k\}$ of simplices whose diameters converge to zero:*

$$\lim_{k \longrightarrow +\infty} \operatorname{diam}(Y_k) \;=\; 0.$$

Proof. The proof is done by contradiction, assuming that Δ_k does not converge to zero. For each $i \in \{0,1,\ldots,n\}$, we define

$$K_i \;=\; \left\{k \in \{0,1,\ldots\} :\; f_{k+1}^i \le f_k^i - \rho(\Delta_k)/(n_k+1)\right\}.$$

The fact that both $n_k \le n$ and (8.11) hold at every iteration guarantees, for all k, that there exists at least one $i \in \{0,1,\ldots,n\}$ such that $k \in K_i$. Thus, $\cup_{i=0}^{n} K_i = \{0,1,\ldots\}$ and the following index is well defined:

$$i_{min} \;=\; \min\left\{ i \in \{0,1,\ldots,n\} : \, |K_i| = +\infty, \, \lim_{k \in K_i} \Delta_k \neq 0 \right\}.$$

Now, since $\Delta_k \nrightarrow 0$ in $K_{i_{min}}$, there exists a subsequence $K \subset K_{i_{min}}$ and a positive constant κ such that $\rho(\Delta_k) \ge \kappa$ for all $k \in K$. As a result of this,

$$f_{k+1}^{0} \;\le\; f_{k+1}^{i_{min}} \;\le\; f_{k}^{i_{min}} - \kappa/(n+1) \quad \forall k \in K. \tag{8.12}$$

For each k now let ℓ_k be the largest index $\ell \in \{1,\ldots,k\}$ for which $f_{\ell}^{i_{min}} > f_{\ell-1}^{i_{min}}$ (with $\ell_k = 0$ if no such ℓ exists). Note that ℓ_k must tend to infinity; otherwise, $\{f_k^{i_{min}}\}$ would have a nonincreasing tail; i.e., there would be an index k_{tail} such that $\{f_k^{i_{min}}\}_{k \ge k_{tail}}$ is nonincreasing. Then $\{f_k^{i_{min}}\}_{k \ge k_{tail}, k \in K}$ would also be nonincreasing and thus convergent (since f is bounded from below). By taking limits in (8.12) a contradiction would be reached.

The relation (8.12) and the definition ℓ_k trivially imply

$$f_{k+1}^{0} \;\le\; f_{\ell_k}^{i_{min}} - \kappa/(n+1) \quad \forall k \in K. \tag{8.13}$$

The definition of ℓ_k also implies that $f_{\ell_k}^{i_{min}} > f_{\ell_k - 1}^{i_{min}}$ (for k sufficiently large such that $\ell_k > 0$). Thus $\ell_k - 1 \notin K_{i_{min}}$. On the other hand, we have seen before that $\ell_k - 1$ must be in K_j for some j, which must satisfy $j < i_{min}$. Since $\ell_k \to +\infty$ when $k \to +\infty$, by passing at a subsequence if necessary, we can assume that this index j is the same for all indices $\ell_k - 1$. We also have, for the same reason, that $|K_j| = +\infty$. From the choice of i_{min} and the fact that $i_{min} \neq j$, we necessarily have that $\Delta_{\ell_k - 1} \to 0$ for $k \in K$. Since $\Delta_{k+1} \le \gamma^e \Delta_k$ for all k, it turns out that $\Delta_{\ell_k} = \mathrm{diam}(Y_{\ell_k}) \to 0$ for $k \in K$.

One can now conclude the proof by arriving at a statement that contradicts (8.13). First, we write

$$f_{k+1}^{0} - f_{\ell_k}^{i_{min}} \;=\; \left(f_{k+1}^{0} - f_{\ell_k}^{0} \right) + \left(f_{\ell_k}^{0} - f_{\ell_k}^{i_{min}} \right).$$

Note that the first term converges to zero since both f_{k+1}^{0} and $f_{\ell_k}^{0}$ converge to the same value (here we use the fact that $\{f_k^0\}$ is decreasing and f is bounded from below but also that ℓ_k tends to infinity). The second term also converges to zero since f is uniformly continuous and $\mathrm{diam}(Y_k) \to 0$ for $k \in K$. Thus, $f_{k+1}^{0} - f_{\ell_k}^{i_{min}}$ converges to zero in K, which contradicts (8.13). □

In the next theorem we prove that if the sequence of simplex vertices is bounded, then it has at least one limit point which is stationary. The proof of this result relies on the fact that the set of vectors $y^n - y^i$, $i = 0,\ldots,n-1$, and $y^r - y^i$, $i = 0,\ldots,n-1$, taken together form a positive spanning set (in fact, a maximal positive basis; see Figure 8.4.) It is simple to see that this set (linearly) spans $\mathbb{R}^n$. It can be also trivially verified that

$$\sum_{i=0}^{n-1} (y^n - y^i) + \sum_{i=0}^{n-1} (y^r - y^i) \;=\; 0, \tag{8.14}$$

and, hence, from Theorem 2.3(iii), we conclude that this set spans $\mathbb{R}^n$ positively.

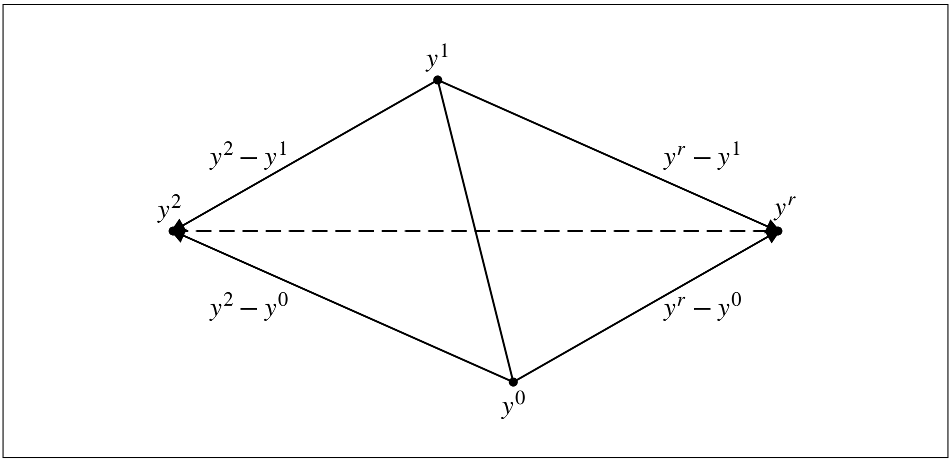

Figure 8.4. *The vectors $y^r - y^0, y^r - y^1$ (right) and $y^2 - y^0, y^2 - y^1$ (left). (This picture is misleading in the sense that isometric reflections are guaranteed only to preserve the diameter and the normalized volume of simplices when $n = 2$ or the simplices are equilateral.)*

When we say that the sequence of simplex vertices $\{Y_k\}$ has a limit point x_* we mean that there is a sequence of vertices of the form $\{x_k\}$, with $x_k \in Y_k$, which has a subsequence converging to x_*.

Theorem 8.5. *Let f be bounded from below, uniformly continuous, and continuously differentiable in $\mathbb{R}^n$. Assume that the sequence of simplex vertices $\{Y_k\}$ generated by the modified Nelder–Mead method (Algorithm* 8.2*) lies in a compact set. Then $\{Y_k\}$ has at least one stationary limit point x_*.*

Proof. From the hypotheses of the theorem and the fact that $\Delta_k \to 0$ (see Theorem 8.4), there exists a subsequence K_1 of iterations consisting of contraction or shrink steps for which all the vertices of Y_k converge to a point x_*.

From the ordering of the vertices in the simplices, we know that

$$f(y_k^n) \;\geq\; f(y_k^i), \quad i = 0, \ldots, n-1,$$

which in turn implies

$$\nabla f(a_k^i)^\top (y_k^n - y_k^i) \;\geq\; 0, \quad i = 0, \ldots, n-1, \tag{8.15}$$

for some a_k^i in the line segment connecting y_k^n and y_k^i. Since the sequences $\{(y_k^n - y_k^i)/\Delta_k\}$ are bounded, by passing to nested subsequences if necessary we can assure the existence of a subsequence $K_2 \subseteq K_1$ such that $(y_k^n - y_k^i)/\Delta_k \to z^i$, $i = 0, \ldots, n-1$. Thus, dividing (8.15) by Δ_k and taking limits in K_2 leads to

$$\nabla f(x_*)^\top z^i \;\geq\; 0, \quad i = 0, \ldots, n-1. \tag{8.16}$$

On the other hand, contraction or shrink steps are attempted only when either

$$f(y_k^r) \; > \; f(y_k^{n-1}) - \rho(\Delta_k) \tag{8.17}$$

or

$$f_k^{rot} \; > \; f(y_k^0) - \rho(\Delta_k). \tag{8.18}$$

Thus, there exists a subsequence K_3 of K_2 such that either (8.17) or (8.18) holds.

In the (8.17) case, we get for $k \in K_3$

$$f(y_k^r) \; > \; f(y_k^i) - \rho(\Delta_k), \quad i = 0,\ldots,n-1. \tag{8.19}$$

Thus, for $k \in K_3$,

$$\nabla f(b_k^i)^\top (y_k^r - y_k^i) \; > \; -\rho(\Delta_k), \quad i = 0,\ldots,n-1,$$

for some b_k^i in the line segment connecting y_k^r and y_k^i. Once again, since the sequences $\{(y_k^r - y_k^i)/\Delta_k\}$ are bounded, by passing to nested subsequences if necessary we can assure the existence of a subsequence $K_4 \subseteq K_3$ such that $(y_k^r - y_k^i)/\Delta_k \to w^i$, $i = 0,\ldots,n-1$. Also, from the properties of the forcing function ρ we know that $\rho(\Delta_k)/\Delta_k$ tends to zero in K_4. If we now divide (8.19) by Δ_k and take limits in K_4, we get

$$\nabla f(x_*)^\top w^i \; \geq \; 0, \quad i = 0,\ldots,n-1. \tag{8.20}$$

We now remark that $[z^0 \cdots z^{n-1} w^0 \cdots w^{n-1}]$ is a positive spanning set. One possible argument is the following. First, we point out that both $[z^0 \cdots z^{n-1}]$ and $[w^0 \cdots w^{n-1}]$ (linearly) span $\mathbb{R}^n$, since they are limits of uniform linearly independent sets. Then we divide (8.14) by Δ_k and take limits, resulting in

$$z^0 + \cdots + z^{n-1} + w^0 + \cdots + w^{n-1} \; = \; 0.$$

Thus, from Theorem 2.3(iii), $[z^0 \cdots z^{n-1} w^0 \cdots w^{n-1}]$ is a positive spanning set. The property about spanning sets given in Theorem 2.3(iv) and inequalities (8.16) and (8.20) then imply that $\nabla f(x_*) = 0$.

In the (8.18) case, we have that, for all $k \in K_3$,

$$f(y_k^{rot,i}) \; > \; f(y_k^0) - \rho(\Delta_k), \quad i = 1,\ldots,n.$$

From the ordering of the vertices in the simplices, we also known that, for all $k \in K_3$,

$$f(y_k^i) \; > \; f(y_k^0), \quad i = 1,\ldots,n.$$

Thus, for $k \in K_3$,

$$\nabla f(c_k^i)^\top (y_k^{rot,i} - y_k^0) \; > \; -\rho(\Delta_k), \quad i = 1,\ldots,n, \tag{8.21}$$

and

$$\nabla f(c_k^i)^\top (y_k^i - y_k^0) \; \geq \; 0, \quad i = 1,\ldots,n, \tag{8.22}$$

for some c_k^i in the line segment connecting $y_k^{rot,i}$ and y_k^0, and for some d_k^i in the line segment connecting y_k^i and y_k^0. Since the sequences $\{(y_k^{rot,i} - y_k^0)/\Delta_k\}$ and $\{(y_k^i - y_k^0)/\Delta_k\}$

are bounded, by passing to nested subsequences if necessary we can assure the existence of a subsequence $K_4 \subseteq K_3$ such that $(y_k^{rot,i} - y_k^0)/\Delta_k \to -u^i$, $i = 1,\ldots,n$, and $(y_k^i - y_k^0)/\Delta_k \to u^i$, $i = 1,\ldots,n$. Thus, dividing (8.21) and (8.22) by Δ_k and taking limits in K_3 yields

$$\nabla f(x_*)^\top(-u^i) \geq 0 \quad \text{and} \quad \nabla f(x_*)^\top u^i \geq 0, \quad i = 1,\ldots,n. \tag{8.23}$$

Now note that $[u^1 \cdots u^n]$ (linearly) spans $\mathbb{R}^n$, since it is a limit of uniform linearly independent sets. Thus, from what has been said after Theorem 2.4, we know that $[u^1 \cdots u^n \; -u^1 \cdots -u^n]$ is a positive spanning set. Theorem 2.3(iv) and inequalities (8.23) together imply that $\nabla f(x_*) = 0$.

It remains to analyze what happens when an infinite number of cycles occur within an iteration (by consecutive application of shrink steps). Using the same arguments as those above, it is possible to prove that the vertices of the shrunken simplices converge to a stationary point. $\square$

It is actually possible to prove that all limit points of the sequence of vertices are stationary. In [220] this result is proved for a broader class of simplicial direct-search methods. For this purpose, one needs to impose one additional condition to accept isometric reflections or expansions.[14] As in [220], one performs isometric reflections or expansions if both conditions are satisfied:

$$f^r \leq f^{n-1} - \rho(\Delta) \quad \text{and} \quad f^r \leq f^{n-1} - \left(f^n - \frac{1}{n}\sum_{i=0}^{n-1} f^i \right) + \rho(\Delta). \tag{8.24}$$

Thus, in the isometric reflection or expansion cases we have both (8.11) for $n_k = n$ and

$$\sum_{i=0}^{n} f_{k+1}^i \leq \sum_{i=0}^{n} f_k^i - \left(f_k^n - \frac{1}{n}\sum_{i=0}^{n-1} f_k^i \right) + \rho(\Delta_k). \tag{8.25}$$

Theorem 8.6. *Let f be bounded from below, uniformly continuous, and continuously differentiable in $\mathbb{R}^n$. Assume that the sequence of simplex vertices $\{Y_k\}$ generated by the modified Nelder–Mead method (Algorithm* 8.2, *further modified to accept only isometric reflections or expansions if* (8.24) *occurs) lies in a compact set. Assume that isometric reflections always satisfy* (8.9). *Then all the limit points of $\{Y_k\}$ are stationary.*

Proof. The first part of the proof consists of showing that Theorem 8.5 is still valid under the modification introduced by (8.24). Now contraction or shrink steps can be attempted because of either (8.17) or

$$f_k^r > f_k^{n-1} - \left(f_k^n - \frac{1}{n}\sum_{i=0}^{n-1} f_k^i \right) + \rho(\Delta_k). \tag{8.26}$$

If we have an infinite subsequence of K_2 for which the condition (8.17) is true, then the proof of Theorem 8.5 remains valid by passing first to a subsequence of K_2 if necessary.

[14] The need for additional conditions arises in other direct-search methods too (see, for instance, Section 7.5, where it is pointed out that it is possible to prove (7.10) for complete polling).

Thus, we just need to consider the case where K_2, or a subsequence of K_2, satisfies (8.26). However, this case is treated similarly. First, we write

$$f(y_k^r) \;>\; f(y_k^i) - \left(f_k^n - \frac{1}{n}\sum_{i=0}^{n-1} f_k^i \right) + \rho(\Delta_k), \quad i = 0,\ldots,n-1.$$

Thus, for $k \in K_2$,

$$\nabla f(b_k^i)^\top (y_k^r - y_k^i) \;>\; \frac{1}{n}\left(\sum_{i=0}^{n-1} \nabla f(a_k^i)^\top (y_k^i - y_k^n) \right) + \rho(\Delta_k), \quad i = 0,\ldots,n-1, \tag{8.27}$$

where a_k^i is in the line segment connecting y_k^n and y_k^i, and b_k^i is in the line segment connecting y_k^r and y_k^i. We already know that $\{(y_k^n - y_k^i)/\Delta_k\}$ converges to z_i in K_2 for $i = 0,\ldots,n-1$. Once again, since the sequences $\{(y_k^r - y_k^i)/\Delta_k\}$ are bounded, by passing to nested subsequences if necessary we can assure the existence of a subsequence $K_3 \subseteq K_2$ such that $(y_k^r - y_k^i)/\Delta_k \to w^i$, $i = 0,\ldots,n-1$. So, by taking limits in (8.27) for $k \in K_3$, we obtain

$$\nabla f(x_*)^\top w^i \;\geq\; \nabla f(x_*)^\top \left(\frac{1}{n}\sum_{i=0}^{n-1} (-z_i) \right), \quad i = 0,\ldots,n-1,$$

or, equivalently,

$$\nabla f(x_*)^\top \left(w_i + \frac{1}{n}\sum_{i=0}^{n-1} z_i \right) \;\geq\; 0, \quad i = 0,\ldots,n-1. \tag{8.28}$$

From (8.16) and (8.28), we conclude that $\nabla f(x_*) = 0$ (the argument used here is similar to the one presented before).

Now suppose that there is a limit point x_∞ which is not stationary. Then, from the continuous differentiability of f, there exists a ball $B(x_\infty;\Delta_\infty)$ of radius $\Delta_\infty > 0$ centered at x_∞ where there are no stationary points.

We focus our attention on one (necessarily infinite) subsequence $\{x_k\}_{k\in K_\infty}$, with $x_k \in Y_k$, that lies in this ball. Note that we can guarantee that for sufficiently large k there are no contraction or shrink iterations in K_∞, since otherwise we would apply a line of thought similar to that of the proof of Theorem 8.5 and conclude that there would be a stationary point in $B(x_\infty;\Delta_\infty)$. So, we can assume without loss of generality that K_∞ is formed by iterations where an isometric reflection or an expansion necessarily occurs. Thus, we can assume, for all $k \in K_\infty$, that inequality (8.25) holds.

We point out that there must exist a constant $\kappa > 0$ such that, for $k \in K_\infty$ sufficiently large,

$$\frac{f_k^n - \frac{1}{n}\sum_{i=0}^{n-1} f_k^i}{\Delta_k} \;\geq\; 2\kappa. \tag{8.29}$$

(Otherwise, we would apply an argument similar to the one of Theorem 8.5 and conclude that $\nabla f(x_\infty)^\top(-z_i) \geq 0$, $i = 0,\ldots,n-1$, which, together with $\nabla f(x_\infty)^\top z_i \geq 0$, $i = 0,\ldots,n-1$, would imply $\nabla f(x_\infty) = 0$.) Thus, by applying inequality (8.29) and the properties of the forcing function ρ to (8.25), we can assure, for k sufficiently large, that

$$\sum_{i=0}^{n} f_{k+1}^i - \sum_{i=0}^{n} f_k^i \;\leq\; -\kappa\,\Delta_k.$$

Now we divide the ball $B(x_\infty;\Delta_\infty)$ into three mutually exclusive sets:

$$\begin{aligned} R_1 &= \{x \in \mathbb{R}^n :\ 2\Delta_\infty/3 < \|x - x_\infty\| \leq \Delta_\infty\},\\ R_2 &= \{x \in \mathbb{R}^n :\ \Delta_\infty/3 < \|x - x_\infty\| \leq 2\Delta_\infty/3\},\\ R_3 &= \{x \in \mathbb{R}^n :\ \|x - x_\infty\| \leq \Delta_\infty/3\}. \end{aligned}$$

Since, from Theorem 8.4, $\Delta_k \to 0$, we know that the number of contractions or shrinks must be infinite. Thus, the sequence of vertices $\{x_k\}$ enters and leaves the ball $B(x_\infty;\Delta_\infty)$ an infinite number of times. Because $\Delta_k \to 0$ this implies that the sequence of vertices $\{x_k\}$ must cross between R_1 and R_3 through R_2 also an infinite number of times. So, there must be subsequences $\{k_j\}$ and $\{k_\ell\}$ of K_∞ such that

$$x_{k_j} \in R_1, \quad x_{k_j+1} \in R_2, \ldots, x_{k_\ell-1} \in R_2, \quad \text{and} \quad x_{k_\ell} \in R_3.$$

Then, from the fact that $\|x_{k+1} - x_k\| \leq \Delta_{k+1} + \Delta_k \leq (1+\gamma^e)\Delta_k$ and that the distance between points in R_1 and R_3 is at least $\Delta_\infty/3$, we obtain

$$\begin{aligned} \sum_{i=0}^{n} f_{k_\ell}^i - \sum_{i=0}^{n} f_{k_j}^i &= \left\{\sum_{i=0}^{n} f_{k_\ell}^i - \sum_{i=0}^{n} f_{k_\ell-1}^i\right\} + \cdots + \left\{\sum_{i=0}^{n} f_{k_j+1}^i - \sum_{i=0}^{n} f_{k_j}^i\right\}\\ &\leq -\kappa\left(\Delta_{k_\ell-1} + \cdots + \Delta_{k_j}\right)\\ &\leq -\tfrac{\kappa}{1+\gamma^e}\left(\|x_{k_\ell} - x_{k_\ell-1}\| + \cdots + \|x_{k_j+1} - x_{k_j}\|\right)\\ &\leq -\tfrac{\kappa}{1+\gamma^e}\|x_{k_\ell} - x_{k_j}\|\\ &\leq -\tfrac{\kappa\Delta_\infty}{3(1+\gamma^e)}. \end{aligned}$$

One can now arrive at a contradiction. From the above inequality, the monotone decreasing subsequence $\{\sum_{i=0}^n f_k^i\}_{k\in K_\infty}$ cannot converge, which is a contradiction. In fact, we know from (8.10)–(8.11) that $\{f_k^0\}_{k\in K_\infty}$, under the boundedness of f, must be convergent. Since $\Delta_k \to 0$ and f is uniformly continuous, then the subsequences $\{f_k^i\}_{k\in K_\infty}$ are also convergent for $i = 1,\ldots,n$, and $\{\sum_{i=0}^n f_k^i\}_{k\in K_\infty}$ is convergent. $\square$

A similar result can be proved when safeguard rotations are always attempted (see the exercises).

Other modifications to the Nelder–Mead method

We know that the Nelder–Mead method can stagnate and fail to converge to a stationary point due to the deterioration of the simplex geometry or lack of sufficient decrease. One approach followed by some authors is to let Nelder–Mead run relatively freely, as long as it provides some form of sufficient decrease, and to take action only when failure to satisfy such a condition is identified.

For instance, the modified Nelder–Mead method of Price, Coope, and Byatt [194] is in this category. Basically, they let Nelder–Mead run (without shrinks) as long as the worst vertex results in sufficient decrease relatively to the size of Y_k, e.g., $f^n_{k+1} < f^n_k - \rho(\mathrm{diam}(Y_k))$, where ρ is a forcing function. These internal Nelder–Mead iterations are not counted as regular iterations. After a finite number of these internal Nelder–Mead steps either a new simplex of vertices Y_{k+1} is found yielding sufficient decrease $f^0_{k+1} < f^0_k - \rho(\mathrm{diam}(Y_k))$, in which case a new iteration is started from Y_{k+1}, or else the algorithm attempts to form a *quasi-minimal frame* (see below) around the vertex y^0_{k+1}, for which we know that $f^0_{k+1} \le f^0_k$.

It is the process of identifying this quasi-minimal frame that deviates from the Nelder–Mead course of action. A quasi-minimal frame in the Coope and Price terminology is a polling set of the form

$$P_k = \{x_k + \alpha_k d : d \in D_k\},$$

where D_k is a positive basis or positive spanning set, and $f(x_k + \alpha_k d) + \rho(\alpha_k) \ge f(x_k)$, for all $d \in D_k$. In the above context we have that $x_k = y^0_{k+1}$ and α_k is of the order of diam(Y_k). One choice for D_k would be a maximal positive basis formed by positive multiples of $y^i_{k+1} - y^0_{k+1}$, $i = 1,\ldots,n$, and their negative counterparts, if the cosine measure cm(D_k) is above a uniform positive threshold, or a suitable replacement otherwise. Other choices are possible in the Nelder–Mead simplex geometry. Note that the process of attempting to identify a *quasi-minimal frame* either succeeds or generates a new point y^0_{k+1} for which $f^0_{k+1} < f^0_k - \rho(\mathrm{diam}(Y_k))$. It is shown in [194], based on previous work by Coope and Price [65], that the resulting algorithm generates a sequence of iterates for which all the limit points are stationary, provided the iterates are contained in an appropriate level set in which f is continuously differentiable and has a Lipschitz continuous gradient. However, their analysis requires one to algorithmically enforce $\alpha_k \to 0$, which in the Nelder–Mead environment is equivalent to enforcing diam(Y_k) $\to 0$.

In the context of the Nelder–Mead method, Kelley [140] used the simplex gradient in a sufficient decrease-type condition to detect stagnation as well as in determining the orientation of the new simplices to restart the process. More precisely, he suggested restarting Nelder–Mead when

$$\sum_{j=0}^{n} f^j_{k+1} < \sum_{j=0}^{n} f^j_k$$

holds but

$$\sum_{j=0}^{n} f^j_{k+1} < \sum_{j=0}^{n} f^j_k - \eta \|\nabla_s f(y^0_k)\|^2$$

fails, where η is a small positive number and $\nabla_s f(y^0_k)$ is the simplex gradient (see Section 2.6) calculated using Y_k. For the restarts, the vertices $y^1_k,\ldots,y^n_k$ are replaced by $y^0_k \pm (0.5 \min_{1\le i\le n} \|y^i_k - y^0_k\|)e_i$, $i = 1,\ldots,n$, where e_i is the ith column of the identity matrix of order n. The signs $\pm$ are chosen depending of the sign of the ith component of $\nabla_s f(y^0_k)$. (In the same spirit but in a different context, Mifflin [171] had suggested using the signs of the centered simplex gradients as descent indicators.)

8.4 Other notes and references

The work by Nelder and Mead [177] profited by the earlier contribution of Spendley, Hext, and Himsworth [210] in 1962, where simplex-based operations were first introduced for the purpose of optimization. In their approach, Spendley, Hext, and Himsworth tried to improve the worst vertex of a simplex (in terms of the values of the objective function) by isometrically reflecting it with respect to the centroid of the other n vertices or else by repeating such operations but now reflecting the second worst vertex. The Nelder–Mead algorithm [177] incorporates similar types of reflections but "improves" over the Spendley–Hext–Himsworth, by allowing nonisometric reflections, which can be regarded as expansions and contractions, and thus permitting arbitrary simplex shapes. Of course, it is this additional flexibility that makes convergence more difficult to consider. In the year of the publication of the Nelder–Mead paper, Box [45] published a "simplicial" method based on reflecting the worst vertex over the centroid of the remaining vertices. The method allowed a number of points between $n+1$ and $2n$ and took simple bounds on the variables into consideration.

Several other variants of the original methods by Nelder and Mead [177] and Spendley, Hext, and Himsworth [210] have been proposed and analyzed, in particular in the Russian literature. Dambrauskas [71] suggested an extension of the Spendley–Hext–Himsworth method in which the simplex may also contract toward its centroid. Yu [234] proved global convergence to a stationary point of a modified version of the Spendley–Hext–Himsworth method (where the condition to accept reflections was already based on a sufficient decrease condition). Rykov (see [202] and the references therein) proposed direct-search algorithms based on reflections, expansions, and contractions of simplices. Tseng [220] lists in detail the differences between his general simplex-based framework and Rykov's. One fundamental difference is that Rykov's analysis requires the objective function to be convex. Woods [230] and Nazareth and Tseng [176] also proved properties for modified Nelder–Mead algorithms under forms of convexity.

Hvattum and Glover [135] developed a method inspired by several direct-search methods of simplicial and directional types which works with sample sets of various sizes and is enhanced by techniques from scatter search to handle the selection of the sample sets.

The MDS method was tested and applied by a number of authors. Hough and Meza [133], for instance, applied the MDS method to the derivative-free solution of a modified trust-region subproblem within a derivative-based trust-region framework. Buckley and Ma [48] studied practical improvements of MDS by quadratic interpolation over sample sets generated by the algorithm.

8.5 Exercises

1. The Nelder–Mead method is invariant under affine transformations [149]. To prove this property consider $g(x) = Ax + b$, where $b \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n \times n}$ is a nonsingular matrix. Show that the Nelder–Mead method (Algorithm 8.1) applied to $f(x)$ from the starting simplex Y_0 and to $f(g(x))$ from the starting simplex $g^{-1}(Y_0) = A^{-1}Y_0 - b$ generate the same sequence of simplex vertices.

2. Show that shrink steps preserve the normalized volume of simplices.

3. Prove that isometric reflections preserve the normalized volume of simplices when either $n = 2$ or the simplices are equilateral (meaning that the distance between the vertices is constant).

4. Prove that isometric reflections in general yield
$$\mathrm{diam}(Y_{k+1}) \le \left(\frac{2n-1}{n}\right) \mathrm{diam}(Y_k).$$
Use this bound to show (8.5).

5. Show that the rotations and expansions of the MDS method (see the end of Chapter 7) preserve the normalized volume of simplices.

6. Show that the three assertions of Theorem 8.2 are true.

7. Frame the Nelder–Mead method (Algorithm 8.1), when $n = 1$ and the parameters are given by the standard values (8.1), as a directional direct-search method of the type of Algorithm 7.2. By showing that Assumptions 7.8, 7.9, and 7.10 are satisfied (globalization by simple decrease with integer lattices) the Nelder–Mead method produces a sequence of iterates $\{x_k\}$ for which a subsequence of $\{\|\nabla f(x_k)\|\} = \{|f'(x_k)|\}$ converges to zero.

8. Why do the sequences $\{a_k^i\}$, $\{b_k^i\}$, and $\{c_k^i\}$ converge to x_* (proof of Theorem 8.5)?

9. Using similar arguments as in the proof of Theorem 8.5, prove that if an infinite loop occurs at a given iteration of Algorithm 8.2, then the vertices of the shrunken simplices converge to a stationary point.

10. In the context of the proof of Theorem 8.6, show that (8.16) and (8.28) imply that $\nabla f(x_*) = 0$.

11. Explain why a simplified version of the modified Nelder–Mead method that considers only isometric reflections and shrinks is globally convergent (in the sense of Theorems 8.5 and 8.6) if it starts from an equilateral simplex.

12. Prove the following alternative for Theorem 8.6: Let f be bounded from below, uniformly continuous, and continuously differentiable in $\mathbb{R}^n$. Assume that the sequence of simplex vertices $\{Y_k\}$ generated by the modified Nelder–Mead method (Algorithm 8.2) lies in a compact set. Assume that safeguarded rotations are always attempted (meaning that the reflection step would consist only of safeguard rotations). Then all the limit points of $\{Y_k\}$ are stationary. (The proof follows the lines of the proof of Theorem 8.6 but is simpler since (8.24) is not needed and $f(y_{k+1}^0) > f(y_k^0) - \rho(\Delta_k)$ can be used directly in the contradicting argument.)