On the Convergence of the Multi-Directional Search Algorithm

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ON THE CONVERGENCE OF THE MULTI-DIRECTIONAL SEARCH
ALGORITHM*

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Abstract. This paper presents the convergence analysis for the multi-directional search algorithm, a direct search method developed by Dennis and Torczon [5], [13], for unconstrained minimization. The analysis follows the classic lines of proofs of convergence for gradient-related methods. The novelty of the argument lies in the fact that explicit calculation of the gradient is unnecessary, although it is assumed that the function is continuously differentiable over some subset of the domain. The proof can be extended to handle most nonsmooth cases of interest; the argument breaks down only at points where the derivative exists but is not continuous. Finally, we describe how a general convergence theory can be developed for an entire class of direct search methods — which includes such methods as the factorial design algorithm of Box [2] and the pattern search algorithm of Hooke and Jeeves [7] — that share a key feature of the multi-directional search algorithm.

Key Words. unconstrained optimization, convergence analysis, direct search methods, Nelder-Mead simplex algorithm, parallel optimization

1. Introduction. In this paper we shall give the convergence analysis for the multi-directional search algorithm developed by Dennis and Torczon [5], [13]. The multi-directional search algorithm is a direct search method designed to solve the unconstrained minimization problem:

\[ \min_{x \in \mathbb{R}^n} f(x), \]

where \( f : \mathbb{R}^n \to \mathbb{R} \).

Direct search algorithms presume little of the function — typically only that the function is continuous — since they do not require, or even directly estimate, gradient information. It has long been recognized that these methods are gradient-related, but the convergence analysis for a large class of these algorithms has been incomplete, as we shall discuss in the next section.

Our proof of convergence for the multi-directional search algorithm will follow the classic lines of proofs for gradient-related methods. First we will show that the multi-directional search algorithm is a descent method. Then we will show that the search directions do not deteriorate. Finally we will show that the algorithm satisfies a notion of sufficient decrease in the value of the objective function for the size of the step taken. While we assume that the function is continuously differentiable over some subset of the domain, we never explicitly compute the gradient. The novelty in this argument lies in the fact that the algorithm provides enough structure to make explicit information about the gradient unnecessary. The multi-directional search algorithm will be introduced in

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Section 3. The convergence analysis for the differentiable case will be developed in Sections 4, 5, and 6.

The result for the smooth case can also be extended to handle most nonsmooth cases of interest. This extension will be given in Section 7. Finally, we will close by reviewing both what the convergence analysis tells us about how the multi-directional search algorithm works and what it also suggests about a more general convergence theory for an entire class of direct search algorithms, a subject of our current research.

2. Direct search methods. Direct search methods are characterized by the fact that they do not use derivatives. They forgo this very useful information for very practical reasons. Often, particularly in experimental settings, analytic derivatives are simply unavailable. Finite-difference approximations to the gradient could be used, but the cost of computing the function values on a sequential machine often makes this option prohibitively expensive. Furthermore, in an experimental setting it is not at all unusual to have function values that can only be trusted to a few decimal places so that finite-difference approximations to the gradient may prove unreliable. Another possibility is that the experimental apparatus itself may make finite-difference approximations to the gradient difficult, if not impossible.

Having relinquished explicit derivative information, the direct search methods typically consider a natural alternative: at every iteration they explore each direction in a linearly independent set of \( n \) search directions. As we shall see, if this set of search directions has the right structure, it is possible to derive convergence results for these algorithms. Our interest in direct search methods arose from the observation that at every iteration the algorithms typically perform searches in each of \( n \) directions. Thus, it certainly seems reasonable to assume that in most, if not all, of these algorithms the \( n \) searches required for a single iteration can be conducted independently. This, in turn, suggests a natural way to develop new optimization algorithms for parallel machines [5], [13].

The direct search algorithms are distinguished both by the way in which the set of \( n \) search directions is chosen and maintained and by the way “exploratory” steps are taken in each of the \( n \) directions. The most important distinction, for theoretical purposes, is between those methods for which the set of search directions is modified at the end of each iteration and those methods for which the set of search directions remains fixed across all iterations. Examples of algorithms in the first class include Rosenbrock’s method [11], Powell’s method [10], and Zangwill’s method [16]. In the second class of direct search methods one finds such examples as the factorial design algorithm of Box [2], the pattern search algorithm of Hooke and Jeeves [7], and the simplex algorithm of Spendley, Hext, and Himsworth [12] (the method upon which the simplex algorithm of Nelder and Mead [8] is based). The Nelder-Mead simplex algorithm [8], perhaps the most popular of the direct search methods, does not search in each of \( n \) linearly independent search directions at every iteration. It is worth noting that there has been no satisfactory convergence analysis for the Nelder-Mead simplex algorithm and, in fact, there is experimental evidence to suggest such analysis may not be possible [5], [13].
The methods that modify the set of search directions at the end of each iteration use the result of the exploratory searches along each of \( n \) linearly independent search directions to compute a new search direction — that defined by the point used to start the iteration and the point found at the conclusion of the \( n \) exploratory steps. The methods are distinguished by the way in which the new set of search directions is then determined. As Zangwill [16] points out, care must be taken to ensure that the set of search directions remains linearly independent. However, once proper precautions are observed, several nice results can be derived as shown by both Powell [10] and Zangwill [16] in their original papers, as well as those found in later works. (See [1], [9].)

The direct search methods for which the search directions remain fixed across all iterations have been analyzed with varying degrees of success. One of the best known algorithms of this sort is the pattern search algorithm of Hooke and Jeeves. Céa [3] gives a concise proof of convergence that uses few of the features of the pattern search algorithm. His analysis does, however, rely on the fact that the algorithm requires the step sizes to be monotonically decreasing. The multi-directional search algorithm allows the steps to increase in size if there is a corresponding decrease in the value of the objective function. Thus, Céa's result cannot be extended to the multi-directional search algorithm. Until recently, this has been the only convergence result of which we were aware for this class of direct search methods. We have since discovered a more ambitious convergence analysis undertaken by Yu Wen-ci [14], [15]. He, too, noted that the pattern search algorithm of Hooke and Jeeves and the original simplex algorithm of Spendley, Hext, and Himsworth share the features of fixed search directions and fixed rescaling factors. Using these observations, and the notion of a positive basis, he derived a general convergence result for modified versions of both these algorithms.

Our analysis differs from that of Yu Wen-ci in two important respects. First, Yu Wen-ci, like Céa, must assume that the step sizes are monotonically decreasing. Again, this means that his analysis cannot be extended to cover the multi-directional search algorithm. Our analysis allows the step sizes to increase if decreases are seen in the corresponding objective function values.

Second, to show that these algorithms cannot take steps that are too long relative to the amount of decrease in the value of the objective function — in other words, that there is sufficient decrease in the value of the objective function for the size of the step taken — Yu Wen-ci introduces the notion of an "error-controlling" sequence. Unfortunately, it is not clear how such a sequence can be constructed and maintained in practice. In fact, one of the difficulties in applying the classical analysis for descent methods to these algorithms is that an explicit calculation of the initial descent slope is used to enforce the Armijo-Goldstein-Wolfe conditions for sufficient decrease (see [4], [9]). Direct search methods, by definition, do not compute such information. Our result places no such burden on the multi-directional search algorithm. We can guarantee that the algorithm cannot take steps that are too long, relative to the amount of decrease in the object function value, without enforcing the Armijo-Goldstein-Wolfe conditions or introducing any other such measure of sufficient decrease. Furthermore, the aim of
our current research is to extend the results presented here for the multi-directional search algorithm to the direct search methods that share the key feature of the multi-directional search algorithm that makes this analysis possible, namely, that both the search directions and the scaling factors which determine the step sizes are fixed across all iterations of the algorithm. The only limitation imposed is that the scaling factors used to determine the size of the steps taken must be rational. This mild restriction is easily satisfied by all the algorithms in this class; the values typically recommended for the scaling factors are \( \frac{1}{2} \) and 2.

We are now ready to introduce the multi-directional search algorithm.

3. Algorithm. We start with a formal statement of the multi-directional search algorithm and then proceed to a brief description.

Given an initial simplex \( S_0 \) with vertices < \( v_0^0, v_1^0, \ldots, v_n^0 \)>, choose \( \mu, \theta \in Q \) such that

\[ \mu \in (1, +\infty) \], and
\[ \theta \in (0, 1) \].

for \( i = 0, \ldots, n \)

- calculate \( f(v_i^0) \)

end

for \( k = 0, 1, \ldots \)

- \( j \leftarrow \arg \min \{ f(v_i^k) : i = 0, \ldots, n \} \)
- swap \( v_j^k \) and \( v_0^k \)

repeat

- Check the stopping criterion.

  for \( i = 1, \ldots, n \)
  - \( r_i^k \leftarrow 2v_i^k - v_0^k \)
  - calculate \( f(r_i^k) \)

end

- \( replaced \leftarrow (\min \{ f(r_i^k) : i = 1, \ldots, n \} < f(v_i^0)) \)

if \( replaced \) then

  for \( i = 1, \ldots, n \)
  - \( e_i^k \leftarrow (1 - \mu) v_i^0 + \mu r_i^k \)
  - calculate \( f(e_i^k) \)

end

if \( (\min \{ f(e_i^k) : i = 1, \ldots, n \} < \min \{ f(r_i^k) : i = 1, \ldots, n \}) \) then

- \( v_i^k \leftarrow e_i^k \) for \( i = 1, \ldots, n \)
  /* accept expansion */

else

  \( v_i^k \leftarrow r_i^k \) for \( i = 1, \ldots, n \)
  /* accept rotation */
endif

else

  for \( i = 1, \ldots, n \)
  - \( c_i^k \leftarrow (1 + \theta) v_i^0 - \theta r_i^k \)
  - calculate \( f(c_i^k) \)

end
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\[ \text{replaced} = \left( \min \{ f(c_i^k) : i = 1, \ldots, n \} < f(v^k_0) \right) \]
\[ v^k_i \leftarrow c_i^k \text{ for } i = 1, \ldots, n \]
\[ /\star \text{ accept contraction } \star/ \]
end
until \text{replaced}
end

/**** end repeat loop ****/
/******* end for loop******* /

In order to understand the algorithm, consider the sequence of "best" vertices \{v^k_0\}, where by "best" we mean that at every iteration \( k \),

\[ f(v^k_0) \leq f(v^k_i) \text{ for } i = 1, \ldots n. \]

At each iteration \( k \) a search is conducted from the current best vertex \( v^k_0 \) in each of the \( n \) directions determined by the \( n \) edges adjacent to \( v^k_0 \). The goal of the search is to replace \( v^k_0 \), i.e., to find a new vertex with a function value that is strictly less than the function value at \( v^k_0 \).

![Diagram](image)

**Fig. 1.** The three possible steps given the simplex \( S_k \) with vertices \(< v^k_0, v^k_1, v^k_2 >\)

There are three possible trial steps: the rotation step, the expansion step, and the contraction step, which are illustrated in Figure 1. Note that the algorithm always computes the rotation step and then tests to see if a new best vertex has been found. If a new best vertex has been identified, an expansion step is computed. Otherwise, the algorithm computes, and automatically accepts, the contraction step.

The algorithm can thus be viewed in terms of its two primary loops: the outer for loop, which determines a new set of search directions by considering a new best vertex, and the inner \textbf{repeat} loop, which determines the length of the steps to be taken.
The expansion factor $\mu$ and the contraction factor $\theta$ determine the lengths, relative to the original edges in the simplex, of the steps to be considered. In our implementation $\mu$ is set equal to 2 and $\theta$ is set equal to $\frac{1}{2}$, as in the example shown in Figure 1. Further discussion of the choice of scaling factors, as well as additional implementation details, can be found in [13].

4. Key lemmas. Two important results follow directly from the description of the multi-directional search algorithm. First, the multi-directional search algorithm is a descent method since

$$f(v_0^{k+1}) < f(v_0^k).$$

For this to be true we need only show that if the best vertex $v_0^k$ is at a point where the function is differentiable, and $\nabla f(v_0^k)$ is not equal to zero, then the inner repeat loop terminates in a finite number of iterations. Second, the search directions determined by the multi-directional search algorithm are uniformly linearly independent. This means that there exists a constant $\gamma > 0$ such that for all $k \geq 0$ and $x \neq 0$,

$$\max \left\{ \frac{|x^T(v_i^k - v_0^k)|}{\|x\| \|v_i^k - v_0^k\|}, i = 1, \ldots, n \right\} \geq \gamma.$$

This follows from the observation that while the algorithm may translate and rotate the simplex, or change its scale, the angles in the original simplex $S_0$ are preserved across all iterations of the algorithm. Both results are given in the next two lemmas. We begin by introducing the following notation.

Let $v_0^k$ be the best vertex of the simplex $S_k$ used to start the $k^{th}$ iteration of the algorithm. Define the level set of $f$ at $v_0^k$ to be

$$L(v_0^k) = \{ x : f(x) \leq f(v_0^k) \}.$$

Given $y \in IR^n$, let the contour $C(y)$ be

$$C(y) = \{ x : f(x) = f(y) \}.$$

Let $X_*$ be the set of stationary points of the function $f$ in $L(v_0^0)$.

We will assume, for now, that $f$ is continuously differentiable on $L(v_0^0)$; however, as we will discuss in Section 7, if we redefine $X_*$, this assumption can be weakened. We next show that the multi-directional search algorithm is a descent method.

**Lemma 4.1.** If $f$ is continuously differentiable on $L(v_0^0)$, then for all $k$

$$f(v_0^{k+1}) < f(v_0^k).$$

**Proof.** In the multi-directional search algorithm, the best vertex of the current simplex $v_0^k$ is replaced only if the algorithm finds another vertex which has a function value that is strictly less than the function value at $v_0^k$. The question now becomes, if $v_0^k \notin X_*$, will the inner repeat loop terminate in a finite number of iterations?
The set of edges adjacent to any vertex in a simplex is linearly independent. Thus, the set of $n$ edges adjacent to the current best vertex $v_0^k$,

$$\{(v_i^k - v_0^k) : i = 1, \ldots, n\},$$

spans $\mathbb{R}^n$.

If $v_0^k \notin X_*$, then $\nabla f(v_0^k)$ is nonzero. Consequently, there exists at least one $i$, for $i = 1, \ldots, n$, such that

$$\nabla f(v_0^k)^T(v_i^k - v_0^k) \neq 0.$$

There are then two cases to consider.

**CASE 1.** $\nabla f(v_0^k)^T(v_i^k - v_0^k) > 0$

Note that since $(v_i^k - v_0^k) = -(r_i^k - v_0^k)$,

$$\nabla f(v_0^k)^T(r_i^k - v_0^k) < 0.$$

Consider the right-hand directional derivative of $f$ at $v_0^k$ in the direction $(r_i^k - v_0^k)$:

$$f'(v_0^k)^T(r_i^k - v_0^k) = \lim_{h \to 0^+} \frac{f(v_0^k + h(r_i^k - v_0^k)) - f(v_0^k)}{h} < 0.$$

Thus, there exists an $h_k > 0$ such that for $0 < t \leq h_k$

$$f(v_0^k + t(r_i^k - v_0^k)) < f(v_0^k).$$

**CASE 2.** $\nabla f(v_0^k)^T(v_i^k - v_0^k) < 0$

Consider the right-hand directional derivative of $f$ at $v_0^k$ in the direction $(v_i^k - v_0^k)$:

$$f'(v_0^k)^T(v_i^k - v_0^k) = \lim_{h \to 0^+} \frac{f(v_0^k + h(v_i^k - v_0^k)) - f(v_0^k)}{h} < 0.$$

Thus, there exists an $\bar{h}_k \in (0, h_k]$ such that for $0 < t \leq \bar{h}_k$

$$f(v_0^k + t(v_i^k - v_0^k)) < f(v_0^k).$$

**CONCLUSION.** The vertices of the contracted simplex are defined to be

$$c_i^k = v_0^k + \theta(v_i^k - v_0^k),$$

for $i = 1, \ldots, n$, where $\theta \in (0, 1)$ is the fixed contraction factor. If the contracted step is accepted at the current iteration of the inner repeat loop, and a new best vertex has not been found, then at the next iteration of the inner loop, the rotated step can be defined in terms of the contracted vertices as

$$r_i^k = 2v_0^k - c_i^k = 2v_0^k - (v_0^k + \theta(v_i^k - v_0^k)) = v_0^k - \theta(v_i^k - v_0^k).$$
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Therefore, for any $k$, if $v^k_i \notin X_*$, then there exists a positive integer $p_k$, such that $\vartheta^{p_k} < \bar{h}_k$ and so the inner repeat loop terminates in a finite number of iterations as required. □

**Lemma 4.2.** The search directions determined by the multi-directional search algorithm are uniformly linearly independent.

*Proof.* Consider each of the three possible steps the multi-directional search algorithm may take.

The rotation step rotates the given initial simplex about the best vertex. This could be viewed as first translating the given initial simplex by $-v^0_i$, applying the transformation $-I$, and then translating the simplex by $v^0_i$. Since $-I$ is an orthogonal transformation, the Euclidean inner product is preserved. Thus, neither the translations nor the rotation affect the angles in the given initial simplex.

The expansion step rescales the rotated simplex by a factor of $\mu$, which again leaves the angles of the given initial simplex unchanged.

The contraction simplex is formed by first translating the rotated simplex by $-v^0_i$, applying the orthogonal transformation $-I$, and then translating the simplex by $v^0_i$, which simply restores the initial simplex. The simplex is then rescaled by a factor of $\theta$. Thus, the angles of the given initial simplex are unchanged.

Since none of the three possible steps affect the angles in the initial simplex, the angles of the simplex used to start the algorithm $S_0$ remain constant across all iterations of the multi-directional search algorithm. Therefore, there exists a $\gamma > 0$, which does not depend on $k$, such that

$$
\max \left\{ \frac{|x^T(v^k_i - v^0_i)|}{||x|| \cdot ||v^k_i - v^0_i||}, i = 1, \ldots, n \right\} \geq \gamma
$$

for all $x \in \mathbb{R}^n$, $x \neq 0$, as required. □

**5. The smooth case.** We are now ready for a formal statement of the theorem.

**Theorem 5.1.** Assume that $L(v^0_i)$ is compact and that $f$ is continuously differentiable on $L(v^0_i)$. Then some subsequence of $\{v^0_i\}$ converges to a point $x_* \in X_*$. Furthermore, $\{v^0_i\}$ converges to $C_* = C(x_*)$ in the sense that

$$
\lim_{k \to \infty} \left[ \inf_{x \in C_*} ||v^k_i - x|| \right] = 0.
$$

**Corollary 5.2.** Assume that $f$ is continuously differentiable, $L(v^0_i)$ is compact, and $f$ is strictly convex on $L(v^0_i)$. Then

$$
\lim_{k \to \infty} v^k_i = x_*,
$$

where $x_*$ is the unique minimizer of $f$ in $L(v^0_i)$.

The proof of Theorem 5.1 will be given in Section 6. First we will build the machinery necessary to prove the convergence result.
5.1. Enforcing step length control. Together, Lemmas 4.1 and 4.2 guarantee that if \( f \) is continuously differentiable on \( L(v^0) \), then the multi-directional search algorithm generates at least one direction of descent that is uniformly bounded away from orthogonality with the gradient. However, we still need to ensure that the steps the algorithm takes are neither too long nor too short relative to the amount of decrease seen in the value of the objective function. In most other descent methods, step length control is guaranteed by enforcing the Armijo-Goldstein-Wolfe conditions. The multi-directional search algorithm cannot enforce the Armijo-Goldstein-Wolfe conditions because it does not have explicit knowledge of the gradient. There is enough structure in the algorithm, however, to enforce step length control without enforcing the Armijo-Goldstein-Wolfe conditions.

We begin by proving the existence of an upper bound on the lengths of the edges of the simplex.

**Proposition 5.3.** Assume that \( L(v^0) \) is compact and that \( f \) is continuously differentiable on \( L(v^0) \). Then there exists a constant \( M > 0 \) such that

\[
\| v^k_i - v^0_i \| \leq M \quad \forall \ i, k.
\]

**Proof.** Assume that \( v^0 \notin X_r \). If so, in the proof of Lemma 4.1 we showed that the multi-directional search algorithm will produce a new best vertex in a finite number of iterations of the inner repeat loop. Since \( L(v^0) \) is compact, for all \( k \geq 1 \) there exists at least one vertex \( v^k_i \) such that the vertices \( v^k_i, v^k_l \in L(v^0) \). Since \( L(v^0) \) is bounded, this implies a bound on the length of the edge \( (v^k_i - v^k_l) \). Since the rescaling factors \( \mu \) and \( \theta \) are constant across all edges of the simplex for all iterations of the multi-directional search algorithm, the relative lengths of all edges in the simplex remain the same across all iterations of the algorithm. This implies the existence of \( M > 0 \) as required.

If \( v^0 \in X_r \), we can no longer argue that the inner repeat loop will produce a new best vertex in a finite number of iterations. There are then two possibilities. The first is that the multi-directional search algorithm produces a new best vertex. If so, the argument given above still holds. The other possibility is that the multi-directional search does not find a new best vertex, i.e., the inner repeat loop does not terminate. If so, then the contraction step has been accepted, because the rotation step and the expansion step are accepted only when they produce a new best vertex. Since the contraction factor \( \theta \) is strictly less than one, this means that the length of every edge in the simplex is strictly monotonically decreasing. Thus, the maximum length across all edges in the initial simplex \( S_0 \) provides an upper bound on the length of all edges in all subsequent simplices, as required.

The existence of an upper bound on the lengths of the edges of the simplex implies the existence of a compact set, which we shall call \( \mathcal{M} \), that contains \( L(v^0) \) and all the simplices generated by the multi-directional search algorithm from a given initial simplex \( S_0 \).

Next we will prove the existence of a lower bound on the lengths of the edges in the simplices the algorithm generates under the hypothesis that the best vertices stay
uniformly bounded away from $X_*$. It is important to note that this is a null hypothesis — it is not true — or the multi-directional search algorithm would certainly not be of use. We posit the null hypothesis, and then prove the existence of a lower bound for the lengths of the edges of the simplex, to set up a proof, by contradiction, of convergence for the multi-directional search algorithm.

To show that under the null hypothesis a lower bound on the lengths of the edges in the simplex does exist, we will show that once the edges in the simplex become small enough, the rotation step will always be acceptable. Note that this does not necessarily mean that the rotation step will be accepted. If the rotation step is acceptable the multi-directional search algorithm automatically considers the expansion step; however, we are guaranteed that the contraction step will not be considered. Since the lengths of the edges in the simplex are reduced only when the simplex is contracted, this argument ensures no further reduction in the size of the simplex.

**Proposition 5.4.** Assume that $L(v_0^0)$ is compact and $f$ is continuously differentiable on $L(v_0^0)$. Suppose that the best vertices stay uniformly bounded away from $X_*$; i.e., for a fixed $\varepsilon > 0$, independent of $k$,

$$\|v_k^k - x_*\| \geq \varepsilon \quad \forall x_* \in X_*, \forall k \geq 0.$$  

Then there exists a constant $m > 0$ such that for all $k \geq 1$

$$m \leq \|v_j^k - v_l^k\| \quad \forall 0 \leq j, l \leq n, j \neq l.$$  

**Proof.**
Define the set $X_*$ as follows:

$$X_* = \left\{ x \in L(v_0^0) : \|x - x_*\| < \frac{\varepsilon}{2} \text{ for some } x_* \in X_* \right\}.$$  

Consider its complement $\Omega$ in $L(v_0^0)$:

$$\Omega = L(v_0^0) \setminus X_*.$$  

Note that $\Omega$ is compact. Furthermore, $f$ is continuously differentiable on $\Omega$, so

1. $\|\nabla f\|$ achieves a minimum $\sigma > 0$ on $\Omega$, and
2. $\nabla f$ is uniformly continuous on $\Omega$.

This leads to two observations. First, for all $k$,

$$\|\nabla f(v_k^k)\| \geq \sigma > 0,$$  

and $\sigma$ does not depend on $k$. Second, the uniform linear independence of the set of search directions at each iteration gives us the constant $\gamma > 0$ seen in (1). From the uniform continuity of $\nabla f$ on $\Omega$ there exists a $\delta > 0$, depending only on $\sigma$, $\gamma$, and $\Omega$, such that

$$\|\nabla f(x) - \nabla f(v_k^k)\| < \sigma \gamma / 2 \text{ whenever } \|x - v_k^k\| < \delta \quad (\text{and } x \in \Omega).$$
Now we will show that once the edges of the simplex become "small enough," the rotation step is always acceptable so that the simplex will not contract; hence the simplex cannot become any smaller.

"Small enough" will mean that the simplex and its rotation are contained in $\Omega$ and $\|v_j^k - v_0^k\| < \delta$ for any choice of $j = 1, \ldots, n$. These conditions will determine our choice of $m$.

We need first some measure of the relative lengths of the edges in the simplex. We define $\kappa$ as follows:

$$\kappa = \frac{\|e^k\|}{\|E^k\|},$$

where

$$e^k = \min_{0 \leq i, j \leq n, j \neq l} \|v_j^k - v_l^k\|,$$

and

$$E^k = \max_{0 \leq i, j \leq n, j \neq l} \|v_j^k - v_l^k\|.$$

Thus, for any $1 \leq j, l \leq n$,

$$\|v_j^k - v_l^k\| \leq \|E^k\| = \frac{1}{\kappa} \|e^k\| \leq \frac{1}{\kappa} \|v_i^k - v_0^k\|.$$

Note that $\kappa$ is independent of $k$ since, as we demonstrated in Lemma 4.2, the relative lengths of the edges in the simplex remain fixed across all iterations of the algorithm. Finally, observe that $0 < \kappa \leq 1$.

We also define $d$ to be the distance between the contour defined by $v_0^k$ and the level set defined by $v_1^k$:

$$d = \text{dist } \left( L(v_0^k), C(v_0^k) \right).$$

Note that Lemma 4.1, together with the assumption that the best vertices are uniformly bounded away from $X_*$, assures us that $d > 0$. We now make the following two claims.

**Claim 1.** Suppose $k \geq 1$. If, for some $i = 1, \ldots, n$, $\|v_i^k - v_0^k\| \leq \kappa d$, then $S_k \subset L(v_0^k)$.

**Proof.** The triangle inequality gives us

$$\text{dist } \left( v_j^k, L(v_0^k) \right) \leq \text{dist } \left( v_j^k, L(v_0^k) \right) + \text{dist } \left( L(v_0^k), L(v_0^k) \right)$$

$$= \text{dist } \left( v_j^k, L(v_0^k) \right)$$

$$\leq \|v_j^k - v_0^k\|$$

$$\leq \frac{1}{\kappa} \|v_i^k - v_0^k\|$$

$$\leq d,$$

for any choice of $j = 1, \ldots, n$. Therefore, $S_k \subset L(v_0^k)$ as required.  

**Claim 2.** If, for some $i = 1, \ldots, n$, $\|v_i^k - v_0^k\| \leq \kappa \frac{\delta}{3}$, then none of the vertices in the rotated simplex are contained in $X_*$, i.e., $r_j^k \notin X_*$ for any $j = 1, \ldots, n$.  

Proof. Recall that \( \|r_j^k - v_0^k\| = \|v_j^k - v_0^k\| \) for any \( j = 1, \ldots, n \).
Let \( x_* \in X_* \). We appeal to the "reverse" form of the triangle inequality to obtain
\[
\|r_j^k - x_*\| \geq \|r_j^k - v_0^k\| - \|v_0^k - x_*\| > \frac{\epsilon}{2}.
\]

We define \( a \) as follows:
\[
a = \kappa \min \left\{ d, \frac{\epsilon}{3}, \delta \right\}.
\]
We are now assured that if
\[
\max_{j=1,\ldots,n} \|v_j^k - v_0^k\| \leq a,
\]
then \( S_k \) and its rotation are contained in \( \Omega \) and that \( \|\nabla f(v_j^k) - \nabla f(v_0^k)\| < \sigma \gamma / 2 \) for all \( j = 1, \ldots, n \). We are ready to argue that if, at any iteration \( k \), (2) is satisfied, then the rotation step will always be acceptable. Again, we have two cases to consider.

**CASE 1.** \( \nabla f(v_0^k)^T(v_i^k - v_0^k) > 0 \)
Choose a vertex \( v_i^k, i \neq 0 \), which satisfies
\[
\frac{|\nabla f(v_0^k)^T(v_i^k - v_0^k)|}{\|\nabla f(v_0^k)\| \|v_i^k - v_0^k\|} \geq \gamma.
\]

Lemma 4.2 guarantees the existence of at least one such vertex.

By definition
\[
r_i^k = v_0^k + (v_i^k - v_i^k) \quad \text{so} \quad v_i^k - v_0^k = -(r_i^k - v_0).
\]

Our choice of \( a \) guarantees that the edge \( v_0 v_i^k \) is contained in \( \Omega \). We can then invoke the Mean Value Theorem to obtain
\[
f(r_i^k) - f(v_0^k) = \nabla f(\xi)^T (r_i^k - v_0^k)
\]
for some \( \xi \in \overline{v_0 v_i^k} \), whence
\[
f(r_i^k) - f(v_0^k) = \nabla f(v_0^k)^T(r_i^k - v_0^k)
\]
\[
+ \left( \nabla f(\xi) - \nabla f(v_0^k) \right)^T (r_i^k - v_0^k).
\]

Consider the first term on the right-hand side of (3), \( \nabla f(v_0^k)^T(r_i^k - v_0^k) \). Our choice of \( v_i^k \) gives us
\[
|\nabla f(v_0^k)^T (v_i^k - v_0^k)| \geq \gamma \|\nabla f(v_0^k)\| \|v_i^k - v_0^k\|.
\]
Since $\nabla f(v_0^k)^T (v_i^k - v_0^k) > 0$ we have

$$\nabla f(v_0^k)^T (v_i^k - v_0^k) \geq \gamma \|\nabla f(v_0^k)\| \|v_i^k - v_0^k\|.$$

By construction, $\|r_i^k - v_0^k\| = \|v_i^k - v_0^k\|$. Thus,

$$\nabla f(v_0^k)^T (v_i^k - v_0^k) \geq \gamma \|\nabla f(v_0^k)\| \|r_i^k - v_0^k\|.$$

Since $v_i^k - v_0^k = -(r_i^k - v_0^k)$, we obtain

(4)  \quad $\nabla f(v_0^k)^T (r_i^k - v_0^k) \leq -\gamma \|\nabla f(v_0^k)\| \|r_i^k - v_0^k\|.$

Now consider the second term on the right-hand side of (3). The Cauchy-Schwarz inequality gives us

(5)  \quad $|\nabla f(\xi) - \nabla f(v_0^k)^T (r_i^k - v_0^k)| \leq \|\nabla f(\xi) - \nabla f(v_0^k)\| \|r_i^k - v_0^k\|.$

Combine (4) and (5) to rewrite (3) as

$$f(r_i^k) - f(v_0^k) \leq -\gamma \|\nabla f(v_0^k)\| \|r_i^k - v_0^k\| + \|\nabla f(\xi) - \nabla f(v_0^k)\| \|r_i^k - v_0^k\|.$$

Since $\nabla f$ is uniformly continuous on $\Omega$ and $\|\xi - v_0^k\| \leq \|r_i^k - v_0^k\| = \|v_i^k - v_0^k\| \leq a$, the following holds:

$$f(r_i^k) - f(v_0^k) \leq (-\gamma \|\nabla f(v_0^k)\| + \|\nabla f(\xi) - \nabla f(v_0^k)\| \|r_i^k - v_0^k\|.$$

Thus,

Thus,

$$f(r_i^k) - f(v_0^k) < 0 \implies f(r_i^k) < f(v_0^k),$$

whenever $\max_{j=1,\ldots,n} \|v_j^k - v_0^k\| \leq a$. We can then conclude that the vertex $r_i^k$ can replace the best vertex $v_0^k$. Therefore, the simplex will not contract.

**CASE 2.**  $\nabla f(v_0^k)^T (v_i^k - v_0^k) < 0$

The proof for Case 2 follows that given for Case 1. The conclusion, however, is quite different. Since $\nabla f(v_0^k)^T (v_i^k - v_0^k) < 0$, we get, as in (4)

$$\nabla f(v_0^k)^T (v_i^k - v_0^k) \leq -\gamma \|\nabla f(v_0^k)\| \|v_i^k - v_0^k\|,$$

without substituting $-(r_i^k - v_0^k)$ for $v_i^k - v_0^k$. We continue the argument as in (5) but with $v_i^k$ rather than with $r_i^k$. Finishing the reductions, we are left with

$$f(v_i^k) < f(v_0^k).$$
whenever }\max_{j=1,\ldots,n} \|v_j^k - v_0^k\| \leq a. \) But this leads to a contradiction! We have chosen \( v_i^k \) so that \( i \neq 0 \) and the multi-directional search algorithm requires that
\[
f(v_i^k) \leq f(v_1^k) \quad \forall i = 1, \ldots, n.
\]
Therefore, Case 2 cannot happen.

**Conclusion.** We have now established that once every edge of the simplex has length less than \( a \) then the rotation step will always be acceptable. Since the algorithm reduces the lengths of the edges of the simplex by at most \( \theta \) at any iteration of the inner \textbf{repeat} loop, it follows that the length of every edge of the simplex will be between \( \kappa \theta a \) and \( a \). Thus we choose \( m = \kappa \theta a \). \( \square \)

We emphasize that the existence of a lower bound for the lengths for the edges in the simplex is guaranteed \emph{only} under the null hypothesis that the best vertices are uniformly bounded away from \( X_\ast \). However, now that we have established both lower and upper bounds for the lengths of the edges in the simplex, we are ready to show that given these lower and upper bounds, the multi-directional search algorithm can only visit a finite number of points. Again, this does not occur, but it does follow from the hypothesis that the best vertices are uniformly bounded away from \( X_\ast \).

To see how the argument works, we begin by considering how the algorithm decides which points to visit. In Figure 1 we are given an initial simplex with a designated "best" vertex. The algorithm automatically generates the rotated simplex. The result of the acceptance test then dictates whether the expanded or the contracted simplex will be constructed. In either event, given an initial simplex and the best vertex in that simplex, we can determine, in advance, all the simplices that can be generated during the first iteration of the inner \textbf{repeat} loop. This means we can enumerate, \emph{a priori}, all the points that can possibly be visited during the first iteration through the \textbf{repeat} loop.

Now assume that we are given an initial simplex, but do not know any information about the function values at any of the vertices in the simplex. This means that we have no way of identifying the "best" vertex in the simplex. Even without this information, we can still determine all the simplices that might be generated during the first iteration of the inner \textbf{repeat} loop and we can still enumerate all the points that might be visited during this iteration. To do this, we simply allow each of the vertices in the original simplex to be "best" and consider all the possibilities, as shown in Figure 3.

We now extend this speculation further. After one pass through the inner \textbf{repeat} loop there are two possibilities: either the best vertex has been replaced, and we go to the next iteration of the outer \textbf{for} loop, or the best vertex has not been replaced and we pass once more through the inner \textbf{repeat} loop. Again, we assume no knowledge of the function value at any of the vertices. We can still consider, \emph{a priori}, all the possibilities by allowing each vertex, including the original best vertex, in each of the trial simplices generated at the previous iteration to be "best" and generate all possible new simplices. For our example, seen in Figure 4, we begin to enforce a lower bound on the lengths of the edges in any of the simplices. Furthermore, we require our simplices
to be contained in a compact set. Both of these restrictions are important because they
eliminate several of the simplices that might otherwise have been considered.

Consider yet another iteration of either the outer for loop or the inner repeat loop.
Again we allow each vertex in each of the trial simplices generated at the previous
iteration to be “best,” but again we apply our restrictions to eliminate even more
simplices. The result can be seen in Figure 5.

Finally, if we remove all the edges, we see in Figure 6 that the multi-directional
search algorithm is, in fact, generating a grid. Since the grid must be contained in
a compact set, and since its mesh size is fixed, this means that there are only a finite
number of points that the algorithm can visit. We require the lower bound on the lengths
of the edges in the simplex to fix the mesh size of the grid. We require the upper bound
on the lengths of the edges in the simplex to give us a compact set over which to search.
However, once we accept these two restrictions, this means we can compute — without
any knowledge of function information — all the points the algorithm can possibly visit
from any given initial simplex.

Now we will prove that given any initial simplex, if we assume that the best vertices
are uniformly bounded away from the set $X_*$, then the multi-directional search algorithm
can visit only a finite number of points.

**PROPOSITION 5.5.** Assume that $L(v_0^k)$ is compact and that $f$ is continuously dif-
ferrable on $L(v_0^k)$. Further, suppose that the best vertices stay uniformly bounded
away from $X_*$, i.e., for a fixed $\epsilon > 0$, independent of $k$,

$$
\|v_0^k - x_*\| \geq \epsilon \quad \forall \; x_* \in X_*, \; \forall \; k \geq 0.
$$

Then the multi-directional search algorithm can visit only a finite number of points.

**Proof.** The proof is by construction.

Rescale the initial simplex $S_0$, using the contraction factor $\theta$, until every edge in
the simplex satisfies the condition

$$
\kappa \theta a \leq \|v_j^0 - v_l^0\| \leq a,
$$

for all $0 \leq j, l \leq n$, $j \neq l$, where $\kappa$ and $a$ are as defined in Proposition 5.4.

Find the least common denominator for the scale factors $\theta$ and $\mu$. This makes sense
since $\theta$ and $\mu$ are restricted to the set of rational numbers.

Divide the least common denominator by the reduction factor $\theta$. Reduce the simp-
lex one last time by this factor.

Designate any one of the vertices in the rescaled simplex as “best.” (There is no
need to consider function information.) Take the set of edges adjacent to the best vertex

$$
\{(v_i^0 - v_0^0) : i = 1, \ldots, n\}
$$

as a basis for the grid. Now take all integer multiples of the basis that generate points
inside the compact set $M$. (Recall that Proposition 5.3 implies the existence of a com-
 pact set $M$ which contains all the simplices generated from $S_0$ by the multi-directional
search algorithm.)
This will give a grid with fixed mesh size inside a compact set. Thus the number of points in the grid will be finite. Furthermore, every possible simplex, given the initial simplex \( S_0 \), will be mapped onto the grid since all possible step sizes are integer multiples of the mesh size.

Therefore, the multi-directional search algorithm can visit only a finite number of points. \( \square \)

5.2. Technical results. We now introduce one last technical result before giving the proof of Theorem 5.1.

Lemma 4.1 shows that the multi-directional search algorithm is a descent method with a strictly monotonically decreasing sequence of function values at the best vertices. The following proposition and its corollary demonstrate that this sequence of function values converges and that the sequence of best vertices converges to the corresponding level set.

Proposition 5.6. Assume that \( \{x^k\} \) is a sequence contained in a compact set \( S \), that \( f \) is continuous, and that \( \{f(x^k)\} \) is a monotone non-increasing sequence. Then there is some \( \hat{f} \) such that

\[
\lim_{k \to \infty} f(x^k) = \hat{f}.
\]

Furthermore, assume that \( \hat{x} \) is any limit point of \( \{x^k\} \). Then \( f(\hat{x}) = \hat{f} \) and \( \{x^k\} \) converges to \( C(\hat{x}) \) in the sense that

\[
\lim_{k \to \infty} \left[ \inf_{y \in C(\hat{x})} \|x^k - y\| \right] = 0.
\]

Proof. The proof of the first statement is immediate: \( \hat{f} \) exists because \( \{f(x^k)\} \) is a monotone non-increasing sequence that is bounded below.

To prove the second statement, consider the following: since \( S \) is compact, \( \{x^k\} \) contains a convergent subsequence. We will denote this convergent subsequence by \( \{x^{k_i}\} \) and say that \( x^{k_i} \to \hat{x} \). By continuity, \( f(\hat{x}) = \lim_{i \to \infty} f(x^{k_i}) = \hat{f} \).

Define

\[
\delta_k = \inf_{y \in C(\hat{x})} \|x^k - y\|.
\]

But \( \lim_{i \to \infty} \delta_{k_i} = 0 \), which implies that

\[
\liminf_{k \to \infty} \delta_k = 0.
\]

Next, suppose that \( \{\delta_{k_i}\} \) is any convergent subsequence of \( \{\delta_k\} \). There is a corresponding sequence of \( \{x^{k_i}\} \). This sequence has a convergent subsequence which we denote also by \( \{x^{k_i}\} \) and say that \( x^{k_i} \to \hat{x} \). Again, \( f(\hat{x}) = \lim_{i \to \infty} f(x^{k_i}) = \hat{f} \), so \( \hat{x} \in C(\hat{x}) \). Thus, \( \delta_{k_i} \to 0 \). Hence, the only possible accumulation points of \( \{\delta_k\} \) are 0.
and \( \infty \). Note that since \( S \) is compact, \( \{ \delta_k \} \) is bounded, i.e., there exists a \( b \geq 0 \) such that \( 0 \leq \delta_k \leq b \). Thus,

\[
\limsup_{k \to \infty} \delta_k = 0.
\]

Since \( \liminf_{k \to \infty} \delta_k = \limsup_{k \to \infty} \delta_k = 0 \),

\[
\lim_{k \to \infty} \delta_k = 0
\]
as required. \( \square \)

**Corollary 5.7.** Assume that \( L(v_0) \) is compact and that \( f \) is continuously differentiable on \( L(v_0) \). Then for the sequence of best vertices \( v_k \) generated by the multi-directional search algorithm there is some \( \hat{f} \) such that

\[
\lim_{k \to \infty} f(v_k) = \hat{f}.
\]

Furthermore, assume that \( \hat{x} \) is any limit point of \( \{ v_0 \} \), then \( f(\hat{x}) = \hat{f} \) and \( \{ v_0 \} \) converges to \( C(\hat{x}) \) in the sense that

\[
\lim_{k \to \infty} \left[ \inf_{x \in C(\hat{x})} \| v_k - x \| \right] = 0.
\]

**Proof.** Lemma 4.1 established that \( \{ f(v_0) \} \) is a monotone decreasing sequence. We appeal to Proposition 5.6 to complete the proof. \( \square \)

6. **Proof of convergence.** We have established that the multi-directional search algorithm is a descent method. In addition, we can guarantee first, that the search directions will not deteriorate, and second, that the steps taken by the algorithm cannot become too long or too short. Finally, we have shown that the sequence of function values at the best vertices converges and the sequence of best vertices converges to the corresponding level set. Thus we are now ready to prove Theorem 5.1.

**Proof.** The proof is by contradiction.

Suppose for all but finitely many \( k \) there exists a fixed constant \( \epsilon > 0 \), which does not depend on \( k \), such that

\[
\| v_k - x_* \| \geq \epsilon \quad \forall x_* \in X_*.
\]

Then, taken together, the upper and lower bounds on the lengths of the edges in the simplex (Proposition 5.3 and Proposition 5.4) imply that the algorithm can visit only a finite number of points (Proposition 5.5). But this contradicts Lemma 4.1, which guarantees strict decrease in the function values at the best vertex in a finite number of iterations. Thus, the hypothesis cannot hold, which means that

\[
\liminf_{k \to \infty} \| v_k - x_* \| = 0.
\]

Then there exists some subsequence of the best vertices \( \{ v_k \} \) that converges to a point \( x_* \in X_* \).

We invoke Corollary 5.7 to complete the proof. \( \square \)
7. The nonsmooth case. To extend Theorem 5.1 to handle most cases when the function $f$ is nondifferentiable, we need only modify the set $X_*$. Let $X_*$ include the set of stationary points of the function $f$ in $L(v_0^*)$, the set of all points in $L(v_0^*)$ where $f$ is nondifferentiable, and the set of all points in $L(v_0^*)$ where the derivative of $f$ exists but is not continuous. Our construction of the set $\Omega$ in the proof of Proposition 5.4 then guarantees that $f$ is continuously differentiable on $\Omega$. We can now replace the assumption that $f$ is continuously differentiable on $L(v_0^*)$ with the assumption that $f$ is continuous on $L(v_0^*)$. Since the proofs given in the previous sections were constructed to require only that $\nabla f$ be continuous on $\Omega$, the results can be extended, without modification, to cover this new characterization of $X_*$. We can state the result as follows.

**Theorem 7.1.** Assume that $L(v_0^*)$ is compact and that $f$ is continuous on $L(v_0^*)$. Then some subsequence of $\{v_0^k\}$ converges to a point $x_0 \in X_*$. Furthermore, $\{v_0^k\}$ converges to $C_* = C(x_0)$ in the sense that

$$\lim_{k \to \infty} \left[ \inf_{x \in C_*} \|v_0^k - x\| \right] = 0.$$

**Proof.** The proof follows directly from the proof of Theorem 5.1. □

This is not a general result for the nonsmooth case; rather, it is an extension of the result for the smooth case. The proof of Proposition 5.4 requires that the derivative be continuous wherever it exists to give us the uniform continuity of $\nabla f$ on the set $\Omega$. The constant we derive from the uniform continuity of $\nabla f$ on $\Omega$ plays a key part in deriving a lower bound on the lengths of the edges in the simplex. Thus $X_*$ must include the set of all points in $L(v_0^*)$ where the derivative of $f$ exists but is not continuous.

While this restriction is unfortunate, it does not prevent us from considering most nonsmooth cases of practical interest. For instance, it means that our theory can handle the following example constructed by Dennis and Woods [6]. Consider the strictly convex function $f(x) = \frac{1}{2} \max \{ ||x - c_1||^2, ||x - c_2||^2 \}$, whose level sets are shown in Figure 2, where $c_1 = (0, 32)^T$ and $c_2 = (0, -32)^T$.

**Figure 2. Level sets for the Dennis-Woods function**

Our numerical experience has shown that given any initial simplex the multi-directional search algorithm converges unfallingly to a point of the form $(\alpha, 0)^T$ but not necessarily to the minimizer $(0, 0)^T$. Theorem 7.1 confirms that convergence to a critical point (i.e., either a point where the function is nondifferentiable or where the gradient is equal to zero) is the best that can be expected for this example.
8. Conclusions. The convergence analysis for the multi-directional search algorithm actually explains how — and why — the algorithm works. As we have seen, the fixed search directions and fixed rescaling factors used to determine the step sizes allow us to construct a grid underlying the progress of the algorithm. We should note, however, that once we remove the null hypothesis, which required the sequence of best vertices to be uniformly bounded away from the set $X_*$, we no longer have a lower bound on the lengths of the edges in the simplex. Thus, the algorithm allows for further and further grid refinement until a satisfactory solution is obtained.

Furthermore, once we add function information, we eliminate many of the points the algorithm might otherwise visit. This means that while there is an implicit grid structure underlying the search, the algorithm by no means visits every point on the grid. Rather, it uses function information to prune the number of grid points that are considered — and to dictate when the grid must be refined further.

The simplex that is used to start the multi-directional search algorithm determines the shape of the grid underlying the search. However, we could just as easily have used another fixed "shape," or "pattern," to determine the shape of the underlying grid. For example, the factorial design algorithm of Box [2], in its simplest form, constructs a hypercube centered at the current iterate and then computes the function values at the vertices in an effort to find a new iterate with a function value that is strictly less than the function value at the current iterate. If a new best point is found, the hypercube is then centered on the new best iterate and the search is restarted. If not, the size of the hypercube is reduced by halving the lengths of the edges. Again we have a pattern for the grid underlying the search. We also have all the necessary ingredients to argue for convergence of the method: fixed search directions, a fixed rescaling factor, and strict decrease in the function value at the sequence of best points.

We should be able to use the arguments presented here to analyze any algorithm that maintains this sort of underlying grid structure. This is the subject of our current research. There is, however, one additional caveat that should be added to the above discussion. The number of points required by the simplex "pattern" of the multi-directional search algorithm is $O(n)$. For the algorithms that do not use a simplex pattern, the number of points required to guarantee convergence, though not necessarily to execute the algorithm on a sequential machine, is exponential in $n$. (For example, the hypercube constructed in the factorial design algorithm of Box requires $O(2^n)$ new points at each iteration.) All of these algorithms share the same convergence analysis and yet the number of points required by the multi-directional search algorithm is linear, rather than exponential, in the size of the problem — which is why we believe the multi-directional search algorithm to be the most practical of these algorithms to implement on a parallel machine.

REFERENCES


Fig. 3. Enumerating the vertices when the best vertex is not known
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Fig. 4. Enumerating the vertices after one additional iteration.
Fig. 5. Enumerating the vertices after two additional iterations
Fig. 6. Enumerating the vertices after removing all the edges