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REVISITING ASYNCHRONOUS PARALLEL PATTERN SEARCH FOR NONLINEAR OPTIMIZATION*

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Abstract. We present a new asynchronous parallel pattern search (APPS) method which is different from that developed previously by Hough, Kolda, and Torczon. APPS efficiently uses parallel and distributed computing platforms to solve science and engineering design optimization problems where derivatives are unavailable and cannot be approximated. The original APPS was designed to be fault-tolerant as well as asynchronous and was based on a peer-to-peer design. Each process was in charge of a single, fixed search direction. Our new version is based instead on a manager-worker paradigm. Though less fault-tolerant, the resulting algorithm is more flexible in its use of distributed computing resources. We further describe how to incorporate a zero-order sufficient decrease condition and handle bound constraints. Convergence theory for all situations (unconstrained and bound constrained as well as simple and sufficient decrease) is developed. We close with a discussion of how the new APPS will better facilitate the future incorporation of linear and nonlinear constraints.

Key words. asynchronous parallel optimization, pattern search, direct search, distributed computing, generating set search

AMS subject classifications. 65K05, 90C56, 65Y05, 68W15, 90C90

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1. Introduction.

Asynchronous parallel pattern search (APPS) is a variation on parallel pattern search that uses parallel resources more efficiently by eliminating synchronization [12]. Pattern search methods [18, 20, 21, 26] and, more generally, generating set search (GSS) methods [14, 15] are geared toward solving science and engineering optimization problems that lack explicit derivative information. These problems are typically characterized by objective functions based on complex and expensive computer simulations. GSS methods are provably convergent to a stationary point if the underlying objective function is suitably smooth; further, GSS methods often work well in practice (with some theoretical justification; see, e.g., [1]) even on nonsmooth problems; see, e.g., [8] and references therein.

The original APPS algorithm is described in [12], and analysis follows in [16, 17]. The motivation for an asynchronous version of parallel pattern search has not changed from that described in [12]:

> A single synchronization step at the end of every iteration... is neither appropriate nor effective when any of the following factors holds: function evaluations finish in varying amounts of time (even on equivalent processors), the processors employed in the computation possess different performance characteristics, or the processors have varying loads.

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However, another driving motivation for the original APPS was the need for a method that was tolerant to various types of failures that might cause synchronous parallel pattern search to completely fail or be extremely slow to converge. To facilitate fault-tolerance, the original APPS algorithm was based on a peer-to-peer model and used PVM [7] as the communication architecture. The new APPS is based instead on a manager-worker paradigm, sacrificing some fault-tolerance in exchange for greater simplicity and flexibility. Further, the new version is based on MPI [25], which many users seem to prefer to PVM. (Is should be noted that some fault-tolerant versions of MPI do exist [4] but such functionality is still rare.)

The sacrifices in terms of fault-tolerance are minimal since checkpointing to disk in the manager-worker version can be used in lieu of a peer-to-peer design. The checkpoint data is small, consisting of only the current best point and corresponding function value. The primary difference between peer-to-peer and checkpointing manager-worker implementations is that the checkpoint version requires some mechanism for restarting (either manual or automated) after a failure, whereas the peer-to-peer continues without any intervention.

In the original APPS, there were multiple agents (i.e., the peers), each of which owned part of the logic of the search. These agents had to correspond with one another regarding algorithmic events (a better point, single direction convergence, and overall convergence), not to mention different types of faults; see [12] for more details. With a single manager process controlling all the logic of the search, these complexities are eliminated. Since the number of worker processes is typically very small (1 to 100 workers) and each communicates infrequently and asynchronously with the manager, it is unlikely that there will be any sort of communication bottleneck at the manager process.

In our description of the new APPS, we present additional modifications for a zero-order (i.e., does not use gradient information) sufficient decrease condition and for bound constraints. The adaptation of a zero-order sufficient decrease condition to pattern search has been discussed in several contexts [14, 23], including a different take on peer-to-peer asynchronous parallel pattern search [6]. In particular, the generalization of pattern search to GSS in [14] was motivated by the desire to incorporate generic globalization strategies, including sufficient decrease, into the framework. The use of a sufficient decrease condition yields greater flexibility in the selection of search directions at each iteration. Handling bound constraints for pattern search has also been the subject of several papers [19, 22, 14]. Some problematic numerical results in the original APPS paper [12, Table 5.6] are the result of not appropriately handling the bound constraints.

The organization of this paper is as follows. In section 2, we review the parallel pattern search algorithm and variants that can be used for sufficient decrease and/or bound constraints; known convergence results are summarized in section 2.4. The new APPS algorithm is presented in section 3, along with its own corresponding variants. An illustrative example of the new APPS algorithm is presented in section 4. Convergence theory follows in section 5. Numerical results comparing the synchronous and asynchronous versions are presented in section 6. We conclude with commentary on the algorithm and associated theory, pointers to its implementation and more numerical results, and ideas for future work in section 7. Table 1.1 summarizes the differences between the new and original versions of APPS. For those familiar with the original APPS, a discussion of the evolution from that one to this one is discussed in Appendix A.

For the purposes of this text, we consider both the unconstrained and bound-

TABLE 1.1
Comparison of new and original APPS.

	New APPS	**Original APPS**
Parallel model	Manager-worker	Peer-to-peer
Load Balancing	Each evaluation is assigned dynamically to a worker process.	Each evaluation is assigned to the agent process that owns the corresponding direction.
Communication architecture	MPI (or PVM)	PVM, or any *fault-tolerant* architecture
Fault-tolerance achieved by...	Checkpointing to disk	Automatic run-time recovery
Provably convergent in unconstrained case	Yes	Yes [17]
... in bound constrained case	Yes	Possible, but has not been published
... using zero-order sufficient decrease condition	Yes	Possible, but has not been published
Can be modified to run in synchronous mode?	Yes, very easily	Not easily
Can the directions change?	Yes, at successful iterations. Also possible at unsuccessful iterations, but more difficult to implement.	Possible at successful iterations, but very difficult to implement.

constrained nonlinear optimizations problems. The unconstrained problem is given by

$$\min_{x \in \mathbb{R}^n} \quad f(x). \tag{1.1}$$

Here $f : \mathbb{R}^n \to \mathbb{R}$ and $x \in \mathbb{R}^n$. The bound constrained problem is given by

$$\begin{array}{ll} \min & f(x) \\ \text{subject to} & \ell \leq x \leq u. \end{array} \tag{1.2}$$

The function f is the same as for the unconstrained problem. The upper and/or lower bounds are optional on an element-by-element basis; specifically, ℓ is an n-vector with entries in $\mathbb{R} \cup \{-\infty\}$ and u is an n-vector with entries in $\mathbb{R} \cup \{+\infty\}$. The set Ω denotes the feasible region; i.e.,

$$\Omega = \{x \in \mathbb{R}^n : \ell \leq x \leq u\}.$$

The unconstrained problem can be thought of as a special case of the bound constrained problem; in other words, $\Omega = \mathbb{R}^n$ in the unconstrained problem.

2. Review of parallel pattern search. We briefly review parallel pattern search (PPS) with simple decrease and its extensions for sufficient decrease and bound constraints. We refer throughout to pattern search, although it might be more accurate to refer to GSS; recall that the generalization of pattern search to GSS was motivated by the desire to bring in different globalization strategies, including sufficient decrease [14]. We conclude by presenting unified convergence results. This review lays the groundwork for the description of the asynchronous methods.

Initialization.

Let $\Delta_{\text{tol}} > 0$ be the step length convergence tolerance.

Set $x_0 \in \Omega$ to be some feasible initial guess.

Set $\mathcal{D}_0 = \left\{ d_0^{(1)}, \ldots, d_0^{(p_0)} \right\}$ to be the initial set of search directions.

Set $\Delta_0 > \Delta_{\text{tol}}$ to be the initial value of the step length.

Iteration. For $k = 0, 1, \ldots$

STEP 1. Generate a set of trial points corresponding to the search directions; i.e.,

$$\mathbf{X}_k = \left\{ x_k + \tilde{\Delta}_k^{(i)} d_k^{(i)} : 1 \leq i \leq p_k \text{ and } \tilde{\Delta}_k^{(i)} \geq \Delta_{\text{tol}} \right\}.$$

Send all points in $\mathbf{X}_k$ to the evaluation queue.

STEP 2. Wait until all trial points in the evaluation queue have been evaluated. Collect those points in the set $\mathbf{Y}_k$.

STEP 3. If there exists a trial point in $y_k \in \mathbf{Y}_k$ such that $f(y_k) < f(x_k) - \rho(\Delta_k)$, then goto Step 4; else goto Step 5.

STEP 4. The iteration is successful:

- Set $x_{k+1} = y_k$.
- Choose a new $\mathcal{D}_{k+1} = \left\{ d_{k+1}^{(1)}, \ldots, d_{k+1}^{(p_{k+1})} \right\}$.
- Set $\Delta_{k+1} = \Delta_k$.
- Go to Step 1.

STEP 5. The iteration is unsuccessful:

- Set $x_{k+1} = x_k$.
- Set $\mathcal{D}_{k+1} = \mathcal{D}_k$ (and $p_{k+1} = p_k$).
- Set $\Delta_{k+1} = \frac{1}{2}\Delta_k$
- If $\Delta_{k+1} < \Delta_{\text{tol}}$, **terminate**; else, goto Step 1.

FIG. 2.1. *PPS algorithm (with synchronization).*

The generic algorithm is presented in Figure 2.1, and the notation used is as follows. Subscripts denote the iteration index. The vector $x_k \in \mathbb{R}^n$ denotes the *best point* (i.e., the point with the smallest known function value) at the beginning of iteration k. The set

$$\mathcal{D}_k = \left\{ d_k^{(1)}, \ldots, d_k^{(p_k)} \right\}$$

denotes the set of *search directions* at iteration k, and the number of search directions in $\mathcal{D}_k$ is denoted by p_k. Superscripts denote the *direction index*, which ranges between 1 and p_k at iteration k. The value Δ_k denotes the *step length* at iteration k, and the values $\tilde{\Delta}_k^{(i)} \in [0, \Delta_k]$, for $i = 1, \ldots, p_k$, denote the corresponding *pseudo step lengths*. The function $\rho(\cdot)$ denotes the *forcing function*.

In Step 1 of Figure 2.1, a set of trial points is generated, denoted by $\mathbf{X}_k$. The method for choosing the pseudo step lengths is discussed in detail in the subsections that follow. In general, $\tilde{\Delta}_k^{(i)} = \Delta_k$ unless bound constraints are involved.

In Step 2 of Figure 2.1, the trial points are evaluated, and the results are collected in $\mathbf{Y}_k$. For PPS, $\mathbf{Y}_k = \mathbf{X}_k$ for all k; however, this will not be the case for the asynchronous version in section 3. Step 2 is where parallelism may be employed, in which case the p_k function evaluations are executed in parallel. The algorithm does not go on to the next step until all evaluations have completed, so this is the point of synchronization. Furthermore, this is typically the most computationally expensive step because p_k function evaluations must be computed.

In Step 3 of Figure 2.1, the decrease condition is evaluated. The choice of the function $\rho(\cdot)$ is discussed in detail in section 2.1 and section 2.2. If the decrease condition is satisfied, then the iteration is termed *successful*; otherwise, it is *unsuccessful*.

As an aside, we make the following remark. If multiple points in $\mathbf{Y}_k$ produce decrease, any one can be chosen as y_k without impacting the convergence theory in section 2.4. However, from a practical perspective, a point that yields the smallest function value should be selected.

The algorithm executes Step 4 of Figure 2.1 if the iteration is successful. The next iterate x_{k+1} is updated to be the trial point that produced decrease in the function, y_k. A new set of search directions may also be selected at this point. The search directions must be chosen in a particular way to guarantee that the algorithm will converge. The criteria are detailed in the subsections that follow. For simplicity, a choice that always works is the set of plus and minus unit vectors, i.e., $\mathcal{D}_k = \{\pm e_1, \pm e_2, \ldots, \pm e_n\}$ and $p_k = 2n$ for $k = 1, 2, \ldots$.

The algorithm executes Step 5 of Figure 2.1 if the iteration is unsuccessful. In this case, the step length Δ_k is reduced by a factor of two. In practice, termination occurs when the step length is less then $\Delta_{\text{tol}} > 0$. However, for the purposes of studying the asymptotic behavior of the algorithm, $\Delta_{\text{tol}} = 0$.

2.1. PPS with simple decrease. Let us consider PPS with simple decrease for the unconstrained optimization problem (1.1). The term *simple decrease* means that only $f(y_k) < f(x_k)$ is required in Step 3. In other words, the function $\rho(\cdot)$ is assumed to be identically zero.

Below, we describe the four conditions that specialize the algorithm in Figure 2.1 to be PPS with simple decrease (in the unconstrained case).

The first two conditions have to do with the selection of the search directions, $\mathcal{D}_k$. It is useful to decompose the set of search directions as $\mathcal{D}_k = \mathcal{G}_k \cup \mathcal{H}_k$. The subset $\mathcal{G}_k$ is the core set of search directions (the poll set), while the subset $\mathcal{H}_k$ is a possibly empty set of additional search directions (the search set) [3, 14]. The two subsets play different roles in the analysis and are constructed according to different rules. The subset $\mathcal{G}_k$ is key to the convergence analysis and must satisfy very specific properties as outlined below. On the other hand, the subset $\mathcal{H}_k$ is subject to only those requirements that ensures it does not interfere with convergence. This means the subset $\mathcal{H}_k$ can be populated with directions that might accelerate the search by, for example, allowing very long steps.

Condition 1 requires that the *cosine measure* of the subset $\mathcal{G}_k$ be uniformly bounded; see [14] for a discussion of cosine measure.

Condition 1. Every $\mathcal{G}_k$ positively spans $\mathbb{R}^n$. Furthermore, there exists a constant $c_{\min} > 0$, both independent of k, such that $\kappa(\mathcal{G}_k) \geq c_{\min}$ for all k, where

$$\kappa(\mathcal{G}_k) \equiv \min_{v \in \mathbb{R}^n} \max_{d \in \mathcal{G}_k} \frac{v^T d}{\| v \| \, \| d \|}.$$

Condition 2 requires that the search directions in $\mathcal{G}_k$ be uniformly bounded in length.

Condition 2. There exist $\beta_{\min} > 0$ and $\beta_{\max} > 0$, independent of k, such that for all k the following holds:

$$\beta_{\min} \leq \| d \| \leq \beta_{\max} \qquad \text{for all } d \in \mathcal{G}_k.$$

Parts (a)–(c) of Condition 3 set more specific conditions for selecting the search directions; these conditions are important in the simple decrease case. Essentially, all search directions must be derived from a fixed, finite set $\mathbf{G}$. Part (c) explains how the optional set $\mathcal{H}_k$ must be formed. Condition 3 also requires that the forcing function is identically zero in part (d) and that the pseudo step lengths are chosen appropriately in part (e).

Condition 3 *(rational lattice).*

(a) There exists a finite set $\mathbf{G} = \{d^{(1)}, \ldots, d^{(p)}\}$ such that every vector $d^{(i)} \in \mathbf{G}$ is of the form $d^{(i)} = Bc^{(i)}$, where $B \in \mathbb{R}^{n \times n}$ is a nonsingular matrix and $c^{(i)} \in \mathbb{Q}^n$.
(b) All search directions in $\mathcal{G}_k$ are chosen from $\mathbf{G}$; i.e., $\mathcal{G}_k \subseteq \mathbf{G}$ for all k.
(c) All search directions in $\mathcal{H}_k$ are nonnegative integer combinations of the elements of $\mathbf{G}$;. i.e., $\mathcal{H}_k \subset \left\{ \sum_{i=0}^{p} \xi^{(i)} d^{(i)} \mid \xi^{(i)} \in \{0, 1, 2, \ldots\} \right\}$ for all k.
(d) The forcing function is identically zero, i.e., $\rho(t) \equiv 0$.
(e) All pseudo step lengths satisfy $\tilde{\Delta}_k^{(i)} \in \{0, \Delta_k\}$.

Conditions 1–3 are not difficult to satisfy; consider, for example,

$$\mathcal{D}_k = \{\pm e_1, \pm e_2, \ldots, \pm e_n\} \text{ for all } k.$$

Since we are only considering the unconstrained problem in this subsection, we further assume that the pseudo step lengths are always equal to the step length, i.e.,

$$\tilde{\Delta}_k^{(i)} = \Delta_k \text{ for } i = 1, \ldots, p_k, \ k = 1, 2, \ldots.$$

This is Condition 6, formalized in the discussion of bound constraints.

2.2. PPS with sufficient decrease. Let us consider PPS with sufficient decrease for the unconstrained optimization problem (1.1). In this case, $\rho(\cdot)$ is a nonzero function, in contrast to the simple decrease case.

There are four conditions that specialize the algorithm in Figure 2.1 to be PPS with sufficient decrease (in the unconstrained case). As before, Conditions 1, 2, and 6 are imposed. Condition 3 is replaced instead by the following.

Condition 4 *(forcing function).*
(a) The function $\rho(\Delta)$ is a nonnegative continuous function on $\Delta \in [0, +\infty)$.
(b) The function $\rho(\Delta)/\Delta$ monotonically decreases to zero as $\Delta \downarrow 0$.

A common choice that satisfies Condition 4 is

$$\rho(\Delta) = \alpha\Delta^2,$$

where α is some fixed, positive constant. For a complete discussion of forcing functions for GSS, see [14] and references therein.

2.3. PPS with bound constraints. Let us consider PPS for the bound constrained optimization problem (1.2). Adapting PPS for bound constraints affects the choice of search directions and the choice of the pseudo step lengths. The adaptation is largely independent of the choice of simple or sufficient decrease, except for the particulars of choosing the pseudo step lengths.

Three conditions specialize the algorithm in Figure 2.1 to be PPS with bound constraints.

In the bound constrained case, the search directions must conform to the geometry of the nearby boundary, so Condition 5 requires that $\mathcal{G}_k$ be the coordinate search directions [19]. Condition 5 replaces Condition 1 and Condition 2 since these conditions are trivially satisfied by this choice of $\mathcal{G}_k$. Condition 5 is more restrictive than absolutely necessary and more general selection criteria may be employed; e.g., see the requirements on choosing search directions for general linear constraints in [14, 15].

Condition 5. For all k, we have $\mathcal{G}_k = \{\pm e_1, \ldots, \pm e_n\}$.

The second condition is either Condition 3 or Condition 4, depending on the choice of simple or sufficient decrease.

The final condition is the one we have already referred to, having to do with the choice for pseudo step lengths. Special choices for these values are required in the case of bound constraints. There are several ways that $\tilde{\Delta}_k^{(i)}$ can be chosen so long as Condition 6, which states that the full step is used if possible, is satisfied.

Condition 6. If $x_k + \Delta_k d_k^{(i)} \in \Omega$, then $\tilde{\Delta}_k^{(i)} = \Delta_k$.

Three possible strategies for choosing admissible values for $\tilde{\Delta}_k^{(i)}$ are described in [15] for the case of general linear constraints; we present two here. The simplest choice is the following:

$$\tilde{\Delta}_k^{(i)} = \begin{cases} \Delta_k & \text{if } x_k + \Delta_k d_k^{(i)} \in \Omega, \\ 0 & \text{otherwise.} \end{cases} \tag{2.1}$$

A more sophisticated choice may be employed in the sufficient decrease case: taking the longest possible feasible step. Define $\tilde{\Delta}_k^{(i)}$ as the solution to

$$\begin{array}{ll} \max & \tilde{\Delta} \\ \text{subject to} & 0 \le \tilde{\Delta} \le \Delta_k, \\ & x_k + \tilde{\Delta}\, d_k^{(i)} \in \Omega. \end{array} \tag{2.2}$$

Note that only elementary algebra is required to solve (3.2)

2.4. PPS convergence theory. Before discussing convergence theory, we present some useful definitions and assumptions.

In any practical situation, $\Delta_{\text{tol}} > 0$. However, for the purposes of studying the asymptotic behavior of the algorithm, $\Delta_{\text{tol}} = 0$.

The following assumptions on the function are employed later theorems.

Assumption 1. The set $\mathcal{L}_f(x_0) = \{x \in \Omega : f(x) \leq f(x_0)\}$ is bounded.

Assumption 2. The function f is bounded below on Ω.

Assumption 3. The function f is continuously differentiable on $\mathcal{L}_f(x_0)$.

Assumption 4. The gradient ∇f is Lipschitz continuous with constant M on $\mathcal{L}_f(x_0)$.

Assumption 4 is stronger than necessary and can be replaced by assuming only continuous differentiability. (See the note at the end of section 3.6 in [14].) In that case, we let $M = \omega(x, r)$, where ω denotes the modulus of continuity, i.e.,

$$\omega(x, r) = \max\{\|\nabla f(y) - \nabla f(x)\| \mid \|y - x\| \leq r\}.$$

In constrained optimization, we can measure progress to a KKT point using the following analogue of $\| \nabla f(x) \|$. For $x \in \Omega$, define

$$\chi(x) = \max_{\substack{x+w \in \Omega \\ \| w \| \leq 1}} -\nabla f(x)^T w.$$

The function χ is particularly suitable for the analysis of pattern search (and GSS) methods [14, 15]. It has the following three properties [2]: $\chi(x)$ is continuous, $\chi(x) \geq 0$, and $\chi(x) = 0$ if and only if x is a KKT point. Note that $\chi(x) \equiv \| \nabla f(x) \|$ if $\Omega = \mathbb{R}^n$.

Now that the assumptions and notation have been established, we can present the convergence results for PPS.

THEOREM 2.1 (see [14] and references therein). *Consider the optimization problem* (1.1)*, satisfying Assumptions* 1–4*. Let the PPS algorithm in Figure* 2.1 *satisfy Conditions* 1*,* 2*, either* 3 *or* 4*, and* 6*. Then*

$$\liminf_{k \to +\infty} \| \nabla f(x_k) \| = 0.$$

THEOREM 2.2 (see [14, 15] and references therein). *Consider the optimization problem* (1.2)*, satisfying Assumptions* 1–4*. Let the PPS algorithm in Figure* 2.1 *satisfy Conditions either* 3 *or* 4*,* 5*, and* 6*. Then*

$$\liminf_{k \to +\infty} \chi(x_k) = 0.$$

The next sections describe an asynchronous version of parallel pattern search and its convergence theory.

3. APPS. The premise of APPS is that greater efficiency in parallel processor utilization will enable faster solution in comparison with synchronous pattern search. The original peer-to-peer version has indeed demonstrated faster execution times [12]. The new version is based on a manager-worker design, and that it also demonstrates faster execution times in section 6. A comparison between the manager-worker and peer-to-peer approaches is presented in Table 1.1 and Appendix A.

As mentioned in section 2, the synchronization point in pattern search occurs in Step 2 of Figure 2.1, where the algorithm is required to wait until the evaluation of every trial point is complete before continuing. The difference between the synchronous and asynchronous versions is that the asynchronous version need not wait until all function evaluations complete before moving on to the decision step (Step 3). Instead, the points with incomplete function evaluations are stored in a queue, and the algorithm moves ahead based on the best information available to it.

The flexibility of APPS necessitates a small amount of additional bookkeeping, as observed in [12]. Each trial point must "remember" how it was generated. More specifically, let y be a trial point generated at Step 1 in iteration k using direction i; then the following information is also stored:

- $\textsc{Parent}(y)$ = its parent, x_k,
- $\textsc{ParentFx}(y)$ = its parent's function value, $f(x_k)$,
- $\textsc{Dir}(y)$ = its direction index, i, and
- $\textsc{Step}(y)$ = its step length, $\Delta_k^{(i)}$ (defined below).

It is not necessary that the actual parent be stored; instead, a unique identifier is sufficient. In terms of implementation, the additional storage is for this bookkeeping negligible.

The manager-worker APPS algorithm, presented in in Figure 3.1, has the same structure as PPS in Figure 2.1. We discuss the major differences.

The notation is the same as for PPS, with the following exceptions and additions. There is no longer a single step length Δ_k at step k; instead, there is a step length associated with each direction, denoted by $\Delta_k^{(i)}$. As before, we assume that $\tilde{\Delta}_k^{(i)} = \Delta_k^{(i)}$ in the unconstrained case. We introduce a minimum step length, $\Delta_{\min}$, defined by the integer $\Gamma_{\min}$. There is an evaluation queue which may not be completely emptied in each iteration. Correspondingly, we introduce the set $\mathcal{A}_k$ containing the indices of the search directions that, at the start of iteration k, are "active"; in other words, those directions that have an associated trial point in the evaluation queue. Further, we define $q_{\max}$ to be the maximum number of points the queue holds.

In Step 1 of Figure 3.1, the trial points are generated. The selection criteria for generating new trial points have changed slightly and now take into account whether a given search direction is active. The set $\mathcal{A}_{k+1}$ is set during this step, and it may be reset or modified in Step 4 or Step 5.

In Step 2 of Figure 3.1, a set of evaluated trial points, denoted $\mathbf{Y}_k$, is collected. In contrast to Step 2 of Figure 2.1, this step does not wait until all trial points have been evaluated before moving on. Thus, it may be the case that $\mathbf{Y}_k \neq \mathbf{X}_k$ and further that $\mathbf{Y}_k \not\subseteq \mathbf{X}_k$. Note that if it is always the case that $\mathbf{Y}_k = \mathbf{X}_k$, then the APPS algorithm in Figure 3.1 is equivalent to the PPS algorithm in Figure 2.1 with the exception of how Δ_{k+1} is reset in Step 4, which is inconsequential in practice as discussed below.

Step 3 of Figure 3.1 now selects a *subset* of the trial points to consider for a simple decrease comparison with respect to the current best point. The subset includes those points that satisfy a sufficient decrease condition *with respect to their corresponding*

Initialization.

Set $x_0 \in \Omega$ be some feasible initial guess.
Set $\mathcal{D}_0 = \left\{ d_0^{(1)}, \ldots, d_0^{(p_0)} \right\}$ to be the initial set of search directions.
Let $\Delta_{\text{tol}} > 0$ be the step length convergence tolerance.
Set $\Delta_0^{(i)} = \Delta_0 > \Delta_{\text{tol}}$ for $i = 1, \ldots, p_0$ to be the initial step lengths.
Let $\Gamma_{\min} \in \mathbb{Z}$ with $\Gamma_{\min} \geq 0$. Set $\Delta_{\min} = 2^{-\Gamma_{\min}} \Delta_0$.
Set $\mathcal{A}_0 = \emptyset$. Let $q_{\max}$ be the evaluation queue size.

Iteration. For $k = 0, 1, \ldots$

STEP 1. Generate a (possibly empty) set of trial points

$$\mathbf{X}_k = \left\{ x_k + \tilde{\Delta}_k^{(i)} d_k^{(i)} \ : \ 1 \leq i \leq p_k, \ \ i \notin \mathcal{A}_k, \text{ and } \tilde{\Delta}_k^{(i)} > \Delta_{\text{tol}} \right\}.$$

Then, send the set of points $\mathbf{X}_k$ to the evaluation queue.
Set $\mathcal{A}_{k+1} = \{ i \ : \ \tilde{\Delta}_k^{(i)} > \Delta_{\text{tol}} \}$.

STEP 2. Collect a nonempty set $\mathbf{Y}_k$ of evaluated trial points.

STEP 3. Let $\bar{\mathbf{Y}}_k \subseteq \mathbf{Y}_k$ be the subset of trial points that satisfy the sufficient decrease condition (see Figure 3.2). If there exists a trial point $y_k \in \bar{\mathbf{Y}}_k$ such that $f(y_k) < f(x_k)$, then goto Step 4; else goto Step 5.

STEP 4. The iteration is successful.

- Set $x_{k+1} = y_k$.
- Choose a new $\mathcal{D}_{k+1} = \left\{ d_{k+1}^{(1)}, \ldots, d_{k+1}^{(p_{k+1})} \right\}$.
- Let $\hat{\Delta} = \text{STEP}(y_k)$, i.e., the step length that produced y_k.
- Set $\Delta_{k+1}^{(i)} = \max\{\hat{\Delta}, \Delta_{\min}\}$ for $i = 1, \ldots, p_{k+1}$.
- Reset $\mathcal{A}_{k+1} = \emptyset$.
- Prune the evaluation queue to $(q_{\max} - p_{k+1})$ or fewer entries.
- Go to Step 1.

STEP 5. The iteration is unsuccessful.

- Set $x_{k+1} = x_k$.
- Set $\mathcal{D}_{k+1} = \mathcal{D}_k$ (and $p_{k+1} = p_k$).
- Let $\mathcal{I}_k = \{\text{DIR}(y) : y \in \mathbf{Y}_k \text{ and } \text{PARENT}(y) = x_k\}$, i.e., the directions that generated the points that have x_k as their parent.
- Update $\mathcal{A}_{k+1} \leftarrow \mathcal{A}_{k+1} \setminus \mathcal{I}_k$ where $\mathcal{A}_{k+1}$ is defined in Step 1.
- Set $\Delta_{k+1}^{(i)} = \begin{cases} \frac{1}{2}\Delta_k^{(i)}, & \text{if } i \in \mathcal{I}_k \\ \Delta_k^{(i)}, & \text{if } i \notin \mathcal{I}_k \end{cases}$ for $i = 1, \ldots, p_{k+1}$.
- If $\Delta_{k+1}^{(i)} < \Delta_{\text{tol}}$ for $i = 1, \ldots, p_{k+1}$, **terminate**. Else, goto Step 1.

FIG. 3.1. *Manager-worker APPS algorithm.*

For each $y \in \mathbf{Y}_k$
- Let $f(\hat{y}) = \textsc{ParentFx}(y)$, i.e., the function value of the parent of y.
- Let $\hat{\Delta} = \textsc{Step}(y)$, i.e., the step length that produced y.
- Define the set $\bar{\mathbf{Y}}_k = \left\{ y \in \mathbf{Y}_k \ : \ f(y) < f(\hat{y}) - \rho(\hat{\Delta}) \right\}$.

FIG. 3.2. *Sufficient decrease condition for Step* 3 *in APPS (Figure* 3.1*).*

parent function values. The specific criteria are presented in Figure 3.2 and discussed in more detail in section 3.1 and section 3.2.

In the case of a successful iteration (Step 4), the primary difference between APPS (Figure 3.1) and PPS (Figure 2.1) is the step length update. In both cases, the step length is updated to be the same as the step length that produced y_k. In PPS, this is simply Δ_k. However, in APPS, the step used to produce y_k is stored as $\textsc{Step}(y_k)$, part of the extra bookkeeping described above. All p_{k+1} step lengths are reset to the larger of either $\textsc{Step}(y_k)$ or the quantity $\Delta_{\min}$. If $\Delta_{\min} \leq \Delta_{\text{tol}}$, this has no affect in practice, but it is important in the convergence theory (where it cannot be less than Δ_{tol} since $\Delta_{\text{tol}} = 0$). A successful iteration clears the active directions, so $\mathcal{A}_{k+1}$ is reset to the empty set. At this point, the evaluation queue needs to be pruned to prevent it from growing too large; such a measure has analytical (see Condition 9) as well as practical benefits. Any or all points may be pruned.

In the case of an unsuccessful iteration (Step 5 in Figure 3.1), the step lengths are reduced individually depending on the trial points in $\mathbf{Y}_k$. Specifically, each evaluated trial point is considered, and if the trial point's parent is not x_k, then it is discarded. (Recall that keeping track of the parent is part of the bookkeeping described above.) Otherwise, the corresponding step is reduced by a factor of two. The correct step is identified by the direction index that was used to generate the trial point (also part of the bookkeeping). Termination is essentially the same, except that there are now p_{k+1} steps, all of which must be less than the specified tolerance before the algorithm terminates.

3.1. APPS with simple decrease. In the simple decrease version of APPS, Conditions 1–3 are imposed as in the synchronous version discussed in section 2.1. Condition 6 is replaced with Condition 7 (see section 3.3); the new condition handles the multiple, possibly different step lengths.

In the simple decrease case, we can assume, without loss of generality, that $\bar{\mathbf{Y}}_k = \mathbf{Y}_k$ in Step 3. The reasoning is that it cannot be the case that a trial point y satisfies $f(y) < f(x_k)$ but not $f(y) < f(\hat{y})$ (where $\hat{y}$ is the parent of y). Since $\hat{y}$ is a previous best point, it must be true that $f(x_k) \leq f(\hat{y})$.

3.2. APPS with sufficient decrease. In the sufficient decrease version of APPS, Conditions 1, 2, 4, and 7 (the replacement for Condition 6) are enforced.

Implementing sufficient decrease in an asynchronous environment adds a layer of difficulty because the sufficiency condition is with respect to the parent of the trial point. There is no assurance that x_k is the parent of the trial point, as in the synchronous case. Consequently, in the asynchronous case, determining whether or not an evaluated trial point is a new best point becomes a two-step process. First, the point is checked to see if it satisfies a sufficient decrease condition with respect

to its parent's function value (see Figure 3.2). Second, it is assessed to see if simple decrease with respect to the current x_k is satisfied.

For example, consider an evaluated trial point y at iteration k. Let $f(\hat{y}) = \textsc{ParentFx}(y)$ be the parent function value, and let $\hat{\Delta} = \textsc{Step}(y)$ be the step length that produced y. To be a candidate for new best point, y must satisfy

$$f(y) < \min\{f(\hat{y}) - \rho(\hat{\Delta}), f(x_k)\}.$$

3.3. APPS with bound constraints. Bound constraints are handled essentially the same as before. Now, however, Condition 6 must be modified to reflect the p_k independent step lengths. Condition 7 results.

Condition 7. If $x_k + \Delta_k^{(i)} d_k^{(i)} \in \Omega$, then $\tilde{\Delta}_k^{(i)} = \Delta_k^{(i)}$.

Similarly, the step calculations in (2.1) and (2.2) need to be modified. The following choice is suitable for either simple or sufficient decrease [15]:

$$\tilde{\Delta}_k^{(i)} = \begin{cases} \Delta_k^{(i)} & \text{if } x_k + \Delta_k^{(i)} d_k^{(i)} \in \Omega, \\ 0 & \text{otherwise.} \end{cases} \tag{3.1}$$

In the sufficient decrease case, taking the longest possible feasible step is an alternative [15]. Define $\tilde{\Delta}_k^{(i)}$ as the solution to

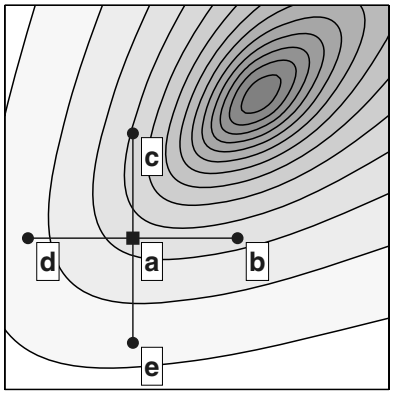
$$\begin{array}{ll} \max & \tilde{\Delta} \\ \text{subject to} & 0 \le \tilde{\Delta} \le \Delta_k^{(i)}, \\ & x_k + \tilde{\Delta}\, d_k^{(i)} \in \Omega. \end{array} \tag{3.2}$$

4. An illustrated example of APPS. A two-dimensional example is presented in Figures 4.1 and 4.2. The contour plot of the objective function uses darker shading to indicate lower function values. Each figure represents the state of the algorithm at an iteration. The square denotes the best point (i.e., x_k) at that iteration, and the circles denote points in the evaluation queue after Step 1 is completed. The lines denote the search directions. For simplicity, we use the same set of search directions throughout: $\mathcal{D}_k = \{e_1, e_2, -e_1, -e_2\}$. The points are labeled with letters, and the algorithm is initialized with the starting point $x_0 = \mathbf{a}$ and an initial step length of $\Delta_0 = 1$.

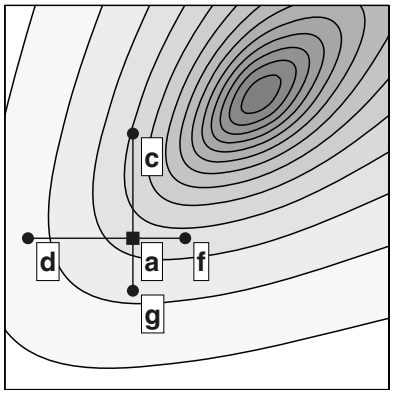
Before we continue, it is important to note the following. At each iteration, the set of evaluated trial points returned in Step 2 could be any nonempty subset of points in the evaluation queue—the choice of this subset is not controlled by the APPS algorithm. Thus, the set $\mathbf{Y}_k$ at each iteration can be interpreted as the result of random chance. (In truth, we have crafted the selection in this example to demonstrate certain features of the algorithm.) The algorithm makes no assumption that the points in the evaluation queue finish being evaluated in any particular order.

A couple of algorithmic choices also influence our example. In Step 2, we assume that no sufficient decrease criteria is employed (i.e., $\rho \equiv 0$) so that $\bar{\mathbf{Y}}_k \equiv \mathbf{Y}_k$ for all k. In Step 4, we assume that $q_{\max} = 6$.

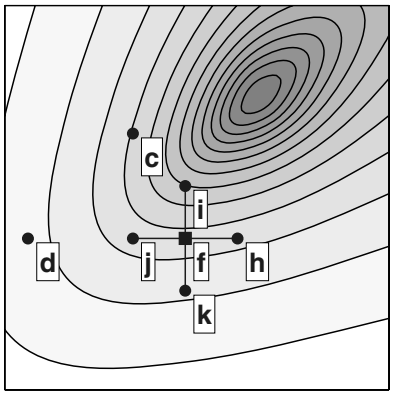
Iteration 0 illustrates an unsuccessful iteration. We assume that only two evaluations ($\mathbf{b}$ and $\mathbf{e}$) are returned in Step 2. Neither $\mathbf{b}$ nor $\mathbf{e}$ improves the function value, so the iteration is unsuccessful. The parent of both $\mathbf{b}$ and $\mathbf{e}$ is $x_0 = \mathbf{a}$ and their corresponding direction indices are 0 and 3, thus $\mathcal{I}_0 = \{0, 3\}$ in Step 5. The



Iteration 0
$x_0 = \mathrm{a}$
$\Delta_0^{(0)} = \Delta_0^{(1)} = \Delta_0^{(2)} = \Delta_0^{(3)} = 1$
$\mathcal{A}_0 = \emptyset$
$X_0 = \{\mathrm{b}, \mathrm{c}, \mathrm{d}, \mathrm{e}\}$ Queue $= \{\mathrm{b}, \mathrm{c}, \mathrm{d}, \mathrm{e}\}$
$Y_0 = \{\mathrm{b}, \mathrm{e}\}$ Queue $= \{\mathrm{c}, \mathrm{d}\}$
Unsuccessful ($\mathcal{I}_0 = \{0, 3\}$)



Iteration 1
$x_1 = \mathrm{a}$
$\Delta_1^{(0)} = \Delta_1^{(3)} = \frac{1}{2}, \Delta_1^{(1)} = \Delta_1^{(2)} = 1$
$\mathcal{A}_1 = \{1, 2\}$
$X_1 = \{\mathrm{f}, \mathrm{g}\}$ Queue $= \{\mathrm{c}, \mathrm{d}, \mathrm{f}, \mathrm{g}\}$
$Y_1 = \{\mathrm{f}, \mathrm{g}\}$ Queue $= \{\mathrm{c}, \mathrm{d}\}$
Successful (f) Pruned Queue $= \{\mathrm{c}, \mathrm{d}\}$

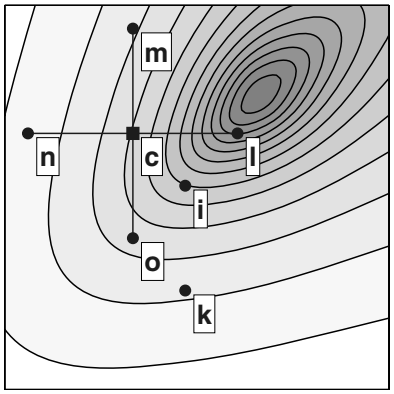


Iteration 2
$x_2 = \mathrm{f}$
$\Delta_2^{(0)} = \Delta_2^{(1)} = \Delta_2^{(2)} = \Delta_2^{(3)} = \frac{1}{2}$
$\mathcal{A}_2 = \emptyset$
$X_2 = \{\mathrm{h}, \mathrm{i}, \mathrm{j}, \mathrm{k}\}$ Queue $= \{\mathrm{c}, \mathrm{d}, \mathrm{h}, \mathrm{i}, \mathrm{j}, \mathrm{k}\}$
$Y_2 = \{\mathrm{c}, \mathrm{j}, \mathrm{h}\}$ Queue $= \{\mathrm{d}, \mathrm{i}, \mathrm{k}\}$
Successful (c) Pruned Queue $= \{\mathrm{i}, \mathrm{k}\}$

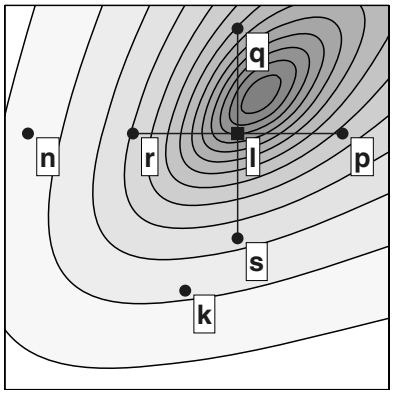
FIG. 4.1. *Example APPS iterations: part* 1.

step lengths corresponding to those directions are reduced by a factor of 2. Note that points **c** and **d** remain in the evaluation queue.

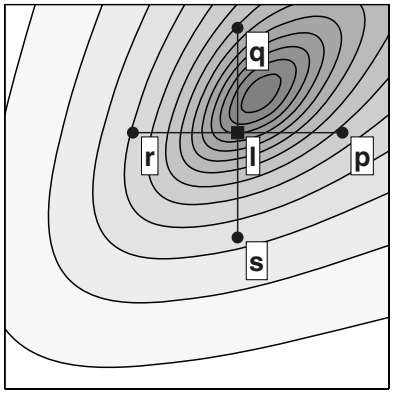
Iteration 1 illustrates a successful iteration. In Step 1, this iteration generates only two new trial points (**f** and **g**) because Directions 1 and 2 are already active (i.e., $\mathcal{A}_1 = \{1, 2\}$). In Step 2, we assume points **f** and **g** are returned. Since **f** reduces the function value, this iteration is successful. All step lengths for the next iteration are



Iteration 3
$x_3 = \mathrm{c}$
$\Delta_3^{(0)} = \Delta_3^{(1)} = \Delta_3^{(2)} = \Delta_3^{(3)} = 1$
$\mathcal{A}_3 = \emptyset$
$X_3 = \{\mathrm{l}, \mathrm{m}, \mathrm{n}, \mathrm{o}\}$ Queue $= \{\mathrm{i}, \mathrm{k}, \mathrm{l}, \mathrm{m}, \mathrm{n}, \mathrm{o}\}$
$Y_3 = \{\mathrm{i}, \mathrm{l}, \mathrm{m}, \mathrm{o}\}$ Queue $= \{\mathrm{k}, \mathrm{n}\}$
Successful (l) Pruned Queue $= \{\mathrm{k}, \mathrm{n}\}$



Iteration 4
$x_4 = \mathrm{l}$
$\Delta_4^{(0)} = \Delta_4^{(1)} = \Delta_4^{(2)} = \Delta_4^{(3)} = 1$
$\mathcal{A}_4 = \emptyset$
$X_4 = \{\mathrm{p}, \mathrm{q}, \mathrm{r}, \mathrm{s}\}$ Queue $= \{\mathrm{k}, \mathrm{n}, \mathrm{p}, \mathrm{q}, \mathrm{r}, \mathrm{s}\}$
$Y_4 = \{\mathrm{k}, \mathrm{n}\}$ Queue $= \{\mathrm{p}, \mathrm{q}, \mathrm{r}, \mathrm{s}\}$
Unsuccessful ($\mathcal{I}_4 = \emptyset$)



Iteration 5
$x_5 = \mathrm{l}$
$\Delta_5^{(0)} = \Delta_5^{(1)} = \Delta_5^{(2)} = \Delta_5^{(3)} = 1$
$\mathcal{A}_5 = \{0, 1, 2, 3\}$
$X_5 = \emptyset$ Queue $= \{\mathrm{p}, \mathrm{q}, \mathrm{r}, \mathrm{s}\}$
...

FIG. 4.2. *Example APPS iterations: part* 2.

reset to the length of the step length that produced $\mathbf{f}$ (i.e., $\hat{\Delta} = \frac{1}{2}$). No pruning of the queue is necessary.

Iteration 2 illustrates "disconnected" points in the evaluation queue and a successful iteration that results from one of these disconnected points. Two points remain in the evaluation queue, and four new trial points are generated and added in Step 1. Because $x_2 \neq x_1$, the older points in the queue are no longer connected to the current

best point and so are referred to as disconnected. In Step 2, we assume the evaluation for the point **c** is finally returned (along with **j** and **h**) and results in another successful step. All step lengths for the next iteration are set to the step length that produced **c** (i.e., $\hat{\Delta} = 1$), and this step is from Iteration 0. This time, the evaluation queue is pruned by removing the oldest point, **d**.

Iteration 3 illustrates two points with improved function values returning simultaneously (**i** and **l**). As with synchronous parallel pattern search, we will assume that we take the best one, although this is not strictly necessary in terms of the theory.

Iteration 4 illustrates an unsuccessful iteration that results in no changes and thus no new trial points in the next iteration. Here, points **k** and **n** finish their evaluations and the result is an unsuccessful iteration. However, since both points are disconnected (i.e., neither has **l** as its parent), no step lengths are reduced in Step 5.

At the beginning of Iteration 5, no new trial points are generated, and four points remain in the evaluation queue. The process continues from there, marching toward a local minimizer.

5. APPS convergence theory. We develop convergence theory for APPS, concluding with results analogous to Theorems 2.1 and 2.2. The analysis borrows heavily from [14, 15, 17]. We begin in section 5.1 by determining bounds on $\| \nabla f(x_k) \|$ and $\chi(x_k)$ in terms of the step lengths. Next, in section 5.2, we present some results showing that a subsequence of the step lengths go to zero. Finally, in section 5.3, we give the convergence results.

It is implicitly assumed in the discussion of the asymptotic behavior that $\Delta_{\text{tol}} = 0$ in Figure 3.1.

We make explicit the bound on the number p_k of search directions in $\mathcal{D}_k$ in Condition 8. This is an implicit assumption in PPS.

> *Condition* 8. There exists $p_{\max}$, independent of k, such that for all k, $p_k \leq p_{\max}$.

We also need to ensure that a trial point cannot languish in the evaluation queue indefinitely. This is also an implicit assumption in PPS.

> *Condition* 9. If a trial point is submitted to the evaluation queue at iteration k, either its evaluation will have completed or it will have been pruned from the evaluation queue by iteration $k + \eta$.

Condition 9 is not saying that every function evaluation requires η iterations; instead, this is an upper bound on the number of iterations. In fact, the value of η may be quite large. A sticky point here is that an iteration does not necessarily correspond to a unit of time, so it is difficult to specify a maximum number of iterations for a function evaluation. However, if we assume that a unit of time is associated with an iteration, this assumption can be enforced as follows. Without loss of generality, let the minimum iteration time correspond to 1 time unit. Now, suppose that there are w workers available for computing function evaluations and that the maximum number of time units required to compute a single function evaluation on a single worker is ϕ. Next, assume that trial points submitted to the evaluation queue are sent to the workers in order (although there is no assumption that the function evaluations finish in order). Finally, assume the maximum queue size is $q_{\max} \geq p_{\max}$ and is always pruned to a size no greater than $(q_{\max} - p_{k+1})$ for any successful iteration. Then, η

can explicitly be computed as

$$\eta = \phi \left\lceil \frac{q_{\max}}{w} \right\rceil .$$

From an implementation point of view, the critical requirement is that the evaluation queue cannot be allowed to grow too large, and so the pruning in Step 4 is necessary for enforcing Condition 9.

5.1. Bounding the measure of stationarity. Theorem 5.1, below, applies to the unconstrained case and bounds the norm of the gradient as a function of the step length. This result and its proof are nearly identical to Theorem 3.3 in [14]. The difference is identifying those iterations for which such a bound can be shown. The necessary condition is that there must have been at least one contraction in every direction since the last successful iteration.

THEOREM 5.1. *Consider the optimization problem* (1.1)*, satisfying Assumptions* 3–Lipschitz*. Let the APPS algorithm in Figure* 3.1 *satisfy Conditions* 1*,* 2*, either* 3 *or* 4*, and* 7*. For every* k *such that*

$$\hat{\Delta}_k \equiv \max_{1 \le i \le p_k} \left\{ 2\Delta_k^{(i)} \right\} \le \Delta_{\min}, \tag{5.1}$$

we have

$$\| \nabla f(x_k) \| \le \frac{1}{c_{\min}} \left[M \hat{\Delta}_k \beta_{\max} + \frac{\rho(\hat{\Delta}_k)}{\hat{\Delta}_k \beta_{\min}} \right]. \tag{5.2}$$

Proof. By hypothesis (5.1), $\Delta_k^{(i)} < \Delta_{\min}$ for all $i = 1, \ldots, p_k$. This implies that there has been at least one contraction along each direction since that last successful iteration, so

$$0 \le f(x_k + 2\Delta_k^{(i)} d_k^{(i)}) - f(x_k) + \rho(2\Delta_k^{(i)}) \text{ for } i = 1, \ldots, p_k. \tag{5.3}$$

The value of $2\Delta_k^{(i)}$ comes in because the current value of $\Delta_k^{(i)}$ is half of that for which the contraction was done. Also note that it is assumed $\tilde{\Delta}_k^{(i)} = \Delta_k^{(i)}$ by Condition 7.

Since, by hypothesis, Condition 1 is satisfied, there exists an $\bar{\imath} \in \{1, \ldots, p_k\}$ such that

$$c_{\min} \| \nabla f(x_k) \| \| d_k^{(\bar{\imath})} \| \le -\nabla f(x_k)^T d_k^{(\bar{\imath})}. \tag{5.4}$$

Employing Assumption 3, the mean value theorem can be applied to (5.3) for $i = \bar{\imath}$ to conclude that there exists $\bar{\alpha} \in [0, 1]$ such that

$$f(x_k + 2\Delta_k^{(\bar{\imath})} d_k^{(\bar{\imath})}) - f(x_k) = 2\Delta_k^{(\bar{\imath})} \nabla f(x_k + \bar{\alpha} 2\Delta_k^{(\bar{\imath})} d_k^{(\bar{\imath})})^T d_k^{(\bar{\imath})}. \tag{5.5}$$

Combining (5.3) and (5.5), dividing through by $2\Delta_k^{(\bar{\imath})}$, and subtracting $\nabla f(x_k)^T d_k^{(\bar{\imath})}$ from both sides yields

$$\begin{aligned} -\nabla f(x_k)^T d_k^{(\bar{\imath})} &\le \left(\nabla f(x_k + \bar{\alpha}\, 2\Delta_k^{(\bar{\imath})} d_k^{(\bar{\imath})}) - \nabla f(x_k) \right)^T d_k^{(\bar{\imath})} + \frac{\rho(2\Delta_k^{(\bar{\imath})})}{2\Delta_k^{(\bar{\imath})}} \\ &\le \| \nabla f(x_k + \bar{\alpha}\, 2\Delta_k^{(\bar{\imath})} d_k^{(\bar{\imath})}) - \nabla f(x_k) \| \| d_k^{(\bar{\imath})} \| + \frac{\rho(2\Delta_k^{(\bar{\imath})})}{2\Delta_k^{(\bar{\imath})}}. \end{aligned}$$

Using (5.4) to replace the left-hand side and dividing through by $\| d_k^{(\bar{\imath})} \|$, we now have

$$c_{\min} \| \nabla f(x_k) \| \leq \| \nabla f(x_k + \bar{\alpha} 2\Delta_k^{(\bar{\imath})} d_k^{(\bar{\imath})}) - \nabla f(x_k) \| + \frac{1}{\| d_k^{(\bar{\imath})} \|} \frac{\rho(2\Delta_k^{(\bar{\imath})})}{2\Delta_k^{(\bar{\imath})}}. \tag{5.6}$$

Since ∇f is Lipschitz (Assumption 4), the norm of any search direction is bounded (Condition 2), and $\bar{\alpha} \in [0, 1]$, it follows that

$$\| \nabla f(x_k + \bar{\alpha} 2\Delta_k^{(\bar{\imath})} d_k^{(\bar{\imath})}) - \nabla f(x_k) \| \leq M \left(\bar{\alpha}\, 2\Delta_k^{(\bar{\imath})} \| d_k^{(\bar{\imath})} \| \right) \leq M \hat{\Delta}_k \beta_{\max}. \tag{5.7}$$

Now, either ρ is identically zero (Condition 3) or $\rho(t)/t$ is monotonically decreasing as $t \downarrow 0$ (Condition 4). In either case,

$$\frac{1}{\| d_k^{(\bar{\imath})} \|} \frac{\rho(2\Delta_k^{(\bar{\imath})})}{2\Delta_k^{(\bar{\imath})}} \leq \frac{1}{\beta_{\min}} \frac{\rho(\hat{\Delta}_k)}{\hat{\Delta}_k}. \tag{5.8}$$

Note that the lower bound in Condition 2 is also employed in the above inequality.

Finally, combining (5.6), (5.7), and (5.8) and dividing by $c_{\min}$ yields (5.2). Hence, the claim. ∎

A similar result can be proved in the constrained case that is nearly identical to Theorem 4.4 in [15]. The same adaptations are used as in the unconstrained case, so the proof is left to the reader.

THEOREM 5.2. *Consider the optimization problem* (1.2)*, satisfying Assumptions* 1, 3*, and* 4*. Let the APPS algorithm in Figure* 3.1 *satisfy Conditions either* 3 *or* 4*,* 5*, and* 7*. Let* $\epsilon_\star > 0$ *be given. Then there exists a constant* c *such that, for every* k *that satisfies*

$$\hat{\Delta}_k \equiv \max_{1 \leq i \leq p_k} \left\{ 2\Delta_k^{(i)} \right\} \leq \max \left\{ \Delta_{\min}, \frac{\epsilon_\star}{\beta_{\max}} \right\}, \tag{5.9}$$

we have

$$\chi(x_k) \leq c \left[M \hat{\Delta}_k \beta_{\max} + \frac{\rho(\hat{\Delta}_k)}{\hat{\Delta}_k \beta_{\min}} \right]. \tag{5.10}$$

5.2. Globalization. Before we proceed to the globalization results, it is necessary to introduce some additional notation and assumptions.

We define $\Gamma_k^{(i)}$ for all k and $i = 1, \ldots, p_k$ as

$$\Gamma_k^{(i)} = \log_2 \left(\frac{\Delta_0}{\Delta_k^{(i)}} \right). \tag{5.11}$$

We can conclude that $\Gamma_k^{(i)} \in \mathbb{Z}$ because any $\Delta_k^{(i)}$ is an integral power of 2 times the initial step size, i.e.,

$$\Delta_{k+1}^{(i)} = 2^{-\Gamma_k^{(i)}} \Delta_0.$$

The following Lemma 5.3 applies to APPS with a sufficient decrease condition. Because x_k is not necessarily the parent of x_{k+1}, the proof is somewhat different than its synchronous analogue, Theorem 3.4 in [14].

Additional notation is required for the proof. For any successful iteration k, a set of ancestors may be constructed for the point x_{k+1}. Let Π_k denote the iteration indices of the ancestors of x_{k+1} as well as $(k+1)$ itself, and let ℓ_k denote the number of ancestors. (The size of Π_k will be ℓ_k+1). To illustrate, consider again the example of section 4. Iterations 1, 2, and 3 are successful and yield the following ancestor sets:

$$\begin{array}{ll} \Pi_1 = \{0,2\}, & \ell_1 = 1, \\ \Pi_2 = \{0,3\}, & \ell_2 = 1, \\ \Pi_3 = \{0,1,4\} & \ell_3 = 2. \end{array}$$

It is important to note that 0 is necessarily in every set Π_k since x_0 is an ancestor to every point.

LEMMA 5.3. *Consider the optimization problem* (1.1) *or* (1.2)*, satisfying Assumption* 2*. Let the APPS algorithm in Figure* 3.1 *satisfy Conditions* 4*,* 8*, and* 9*. Then there exists an index j and a set $\mathcal{K} \subset \{1,2,\ldots\}$ such that*

$$\lim_{k\in\mathcal{K}} \Gamma_k^{(j)} = +\infty.$$

Proof. Suppose the lemma is false. Then there exists $\Gamma_\star$ such that $\Gamma_k^{(i)} < \Gamma_\star$ for all k and $i = 1,\ldots,p_k$. Consequently, the step lengths are bounded below:

$$\Delta_k^{(i)} \geq \Delta_\star = 2^{-\Gamma_\star}\Delta_0 \text{ for all } k \text{ and } i = 1,\ldots,p_k. \tag{5.12}$$

Then, by Condition 4, the forcing term is bounded below as well:

$$\rho(\Delta_k^{(i)}) \geq \rho_\star = \rho(\Delta_\star) \text{ for all } k \text{ and } i = 1,\ldots,p_k. \tag{5.13}$$

Suppose k is a successful iteration, and let $\Pi_k = \{i_1, i_2, \ldots, i_{\ell_k+1}\}$. Since each child-parent pair satisfies the sufficient decrease condition, we can apply a telescoping sum argument and (5.13) to obtain

$$f(x_{k+1}) - f(x_0) = \sum_{j=1}^{\ell_k} \left\{ f\left(x_{i_{j+1}}\right) - f\left(x_{i_j}\right) \right\} \geq \ell_k\, \rho_\star. \tag{5.14}$$

Another consequence of the lower bound on the step lengths in (5.12) is that each parent can only have a finite number of children. Specifically, a parent can have no more than $c = p_{\max}(\Gamma_\star + 1)$ children where the bound $p_{\max}$ comes from Condition 8. Thus, if iteration k is successful, x_{k+1} must have at least $\lceil k/c \rceil$ ancestors. Combining this information with (5.14) yields

$$f(x_{k+1}) \geq k\left(\frac{\rho_\star}{c}\right) + f(x_0).$$

Let $\mathcal{S}$ denote the subsequence of successful iterates. By Condition 9, the maximum number of iterations to evaluate a single trial point is bounded. This coupled with the method by which step lengths are updated implies that there must be infinitely many successful steps, i.e., $\mathcal{S}$ is infinite. Thus,

$$\lim_{k\in\mathcal{S}} f(x_{k+1}) \geq \lim_{k\in\mathcal{S}} k\left(\frac{\rho_\star}{c}\right) + f(x_0) = +\infty.$$

This contradicts Assumption 2. Hence, the claim. ∎

Before we can establish a result analogous to Lemma 5.3 for the simple decrease case, we first state a result regarding the structure of the iterates. It is a standard result, so no proof is provided here; see instead, e.g., [14].

PROPOSITION 5.4 (see [17]). *Consider the optimization problem* (1.1) *or* (1.2). *Consider the APPS algorithm in Figure* 3.1 *satisfying Condition* 3. *Let* $\Gamma > 0$ *be a constant. Then, for any* k *with*

$$\Gamma \leq \Gamma_j^{(i)} \text{ for all } j \leq k, i = 1, \ldots, p_j,$$

the following holds:

$$x_{k+1} = x_0 + 2^{-\Gamma}\, \Delta_0 \sum_{i=1}^{p} \zeta_k(i, \Gamma)\, d^{(i)}, \tag{5.15}$$

where $\zeta_k(i, \Gamma) \in \mathbb{Z}$ *for each* $i = 1, \ldots, p$ *and* $k = 0, 1, 2, \ldots$.

Given this result, the fact that the $\zeta_k(i, \Gamma)$ are integral, and the set $\mathbf{G}$ is as described in Condition 3, all iterates lie on on the lattice

$$\mathcal{M}(x_0, \Delta_0, \mathbf{G}, \Gamma) = \left\{ x_0 + 2^{-\Gamma} \Delta_0 \sum_{i=1}^{p} \zeta^{(i)} d^{(i)} \ : \ i \in \mathbb{Z} \right\}.$$

We can now present our result.

LEMMA 5.5. *Consider the optimization problem* (1.1) *or* (1.2), *satisfying Assumption* 1. *Let the APPS algorithm in Figure* 3.1 *satisfy Conditions* 3 *and* 9. *Then, there exists an index* j *and a set* $\mathcal{K} \subset \{1, 2, \ldots\}$ *such that*

$$\lim_{k \in \mathcal{K}} \Gamma_k^{(j)} = +\infty.$$

Proof. Suppose not. Then there exists $\Gamma_\star$ such that $\Gamma_k^{(i)} < \Gamma_\star$ for all k and $i = 1, \ldots, p_k$. By Proposition 5.4, every iterate must lie on the lattice $\mathcal{M}(x_0, \Delta_0, \mathbf{G}, \Lambda_\star)$. On the other hand, by Assumption 1, every iterate must lie in the bounded set $\mathcal{L}_f(x_0)$. The intersection of $\mathcal{M}(x_0, \Delta_0, \mathbf{G}, \Gamma_\star)$ and $\mathcal{L}_f(x_0)$ is finite, so every successful iterate is drawn from a finite set. Next, observe that a successful point can be successful only once because Step 3 in Figure 3.1 requires strict improvement. Therefore, there can be only finitely many successful iterates; let $\hat{k}$ denote the last successful iterate.

After iteration $\hat{k}$, the set of search directions does not change. Further, by Condition 9, there is a contraction in the step length along each direction at least once per η iterations. Thus,

$$\lim_{k \to \infty} \max_{1 \leq i \leq p_k} \left\{ \Delta_k^{(i)} \right\} = 0.$$

So, necessarily, $\min\{\Gamma_k^{(i)}\} \to +\infty$. This contradicts our original assumption. Hence, the claim. ∎

Both Lemma 5.3 and Lemma 5.5 lead to the following general result regarding the step lengths. Additional notation is required for this proof. Define

$$\tilde{\Gamma}_k^{(i)} = \Gamma_k^{(i)} - \Gamma_{\min}.$$

This quantity is equal to the number of contractions required to go from $\Delta_{\min}$ to $\Delta_k^{(i)}$.

THEOREM 5.6. *Consider the optimization problem* (1.1) *or* (1.2)*, satisfying Assumptions* 1 *and* 2*. Let the APPS algorithm in Figure* 3.1 *satisfy Conditions either* 3 *or* 4*,* 8*, and* 9*, Then, there exists a set* $\mathcal{K} \subset \{1, 2, \ldots\}$ *such that*

$$\lim_{k \in \mathcal{K}} \left\{ \max_{1 \le i \le p_k} \Delta_k^{(i)} \right\} = 0.$$

Proof. By either Lemma 5.3 (using Assumption 2 and Conditions 4, 8, and 9) or Lemma 5.5 (using Assumption 1 and Conditions 3 and 9), we have that there exists an index j and set $\mathcal{K}$ such that

$$\lim_{k \in \mathcal{K}} \Gamma_k^{(j)} = +\infty.$$

Without loss of generality, assume that

$$\Gamma_k^{(j)} > \eta \, (\Gamma_{\min} + 1) \text{ for all } k \in \mathcal{K}, \tag{5.16}$$

where η is as defined in Condition 9.

Then if $k \in \mathcal{K}$, by (5.16), $\tilde{\Gamma}_k^{(i)} > 0$ and there has not been a success for at least $\tilde{\Gamma}_k^{(j)}$ iterations. On the other hand, by (5.16), $\lfloor \tilde{\Gamma}_k^{(j)} / \eta \rfloor > 0$ and there has been at least $\lfloor \tilde{\Gamma}_k^{(j)} / \eta \rfloor$ contractions in all other directions. Thus,

$$\tilde{\Gamma}_k^{(i)} \ge \lfloor \tilde{\Gamma}_k^{(j)} / \eta \rfloor \text{ for } k \in \mathcal{K}, 1, \le i \le p_k, i \ne j.$$

Thus,

$$\lim_{k \in \mathcal{K}} \left\{ \min_{1 \le i \le p_k} \Gamma_k^{(i)} \right\} = +\infty.$$

Hence, the claim. ∎

5.3. Convergence results. Using the machinery built in sections 5.1 and 5.2, results following Theorems 2.1 and 2.2 are immediate.

THEOREM 5.7. *Consider the optimization problem* (1.1)*, satisfying Assumptions* 1–4*. Let the APPS algorithm in Figure* 3.1 *satisfy Conditions* 1*,* 2*, either* 3 *or* 4*,* 7*,* 8*,* 9*. Then*

$$\liminf_{k \to +\infty} \| \nabla f(x_k) \| = 0.$$

THEOREM 5.8. *Consider the optimization problem* (1.2)*, satisfying Assumptions* 1–4*. Let the APPS algorithm in Figure* 3.1 *satisfy Conditions either* 3 *or* 4*,* 5*,* 7*,* 8*,* 9*. Then*

$$\liminf_{k \to +\infty} \chi(x_k) = 0.$$

6. Numerical results. As compared to (synchronous) PPS, the advantage of APPS is more efficient use of computation resources. Using PVM, the original APPS was shown to be faster than PPS on several different examples [12]. In later experiments on a small collection of test problems, "single-agent" versions of APPS (very similar to the new APPS proposed here) using MPI and PVM were shown to be overall faster than the original version of APPS using PVM [11].

TABLE 6.1
Comparison of PPS and APPS: average results over parallel multiple runs.

PROBLEM	METHOD	FINAL F	TIME (S)	% IDLE	V1	V2	EVALS	CACHE
UNC5	APPS	1.24×10^5	63.9	1.11	10	74	274	36
	PPS	1.24×10^5	101.2	29.22	9	78	273	39
UNC6	APPS	1.24×10^5	73.1	0.85	86	66	306	36
	PPS	1.24×10^5	106.1	17.64	135	69	345	39
CON5	APPS	1.39×10^5	72.5	1.05	11	1	342	39
	PPS	1.39×10^5	106.8	28.24	7	3	325	37
CON6	APPS	1.39×10^5	97.1	0.82	129	2	435	43
	PPS	1.39×10^5	106.0	17.61	111	3	355	32
HC	APPS	2.38×10^4	207.1	1.65	2	80	152	24
	PPS	2.38×10^4	242.3	20.54	2	77	128	20

In this section, we present comparisons of the new version of APPS with PPS, both using MPI. We use APPSPACK 4.0 [8, 13] for our comparisons because it implements both PPS and APPS. The APPS implementation is identical to what is shown in Figure 3.1, and the PPS implementation is the same as APPS except that, in Step 2, we wait for all evaluations to be completed so that $\mathbf{Y}_k = \mathbf{X}_k$. We used the default settings for all parameters except that "Scaling" was set equal to the upper bounds and "Step Tolerance" was set to 0.02. Full details of the implementation can be found in [8].

The methods are compared on a set of five proposed benchmark test problems in well-field design (UNC5, UNC6, CON5, CON6) and hydraulic capture (HC), as described in detail in [5]. The problems are based on the MODFLOW [24] simulator from the U.S. Geological Survey. Problems UNC5 and CON5 each have 10 variables, UNC6 and CON6 each have 18 variables, and HC has 12 variables. The problems have bound constraints and three nonlinear constraints. The nonlinear constraints were treated by using an extreme barrier approach that sets $f(x) = +\infty$ whenever a constraint is violated. The nonlinear constraints are separated into two categories: Category 1 is constraints that can be checked before the simulator is called and are inexpensive to check; Category 2 is constraints that cannot be checked until after the simulator has been called and are therefore expensive to check.

Table 6.1 compares APPS and PPS on the test problems. We ran each problem 10 times on 11 nodes of Sandia's Catalyst Linux cluster, using MPICH [9, 10]. The Final F column lists the optimal function value, Time (s) lists the average parallel run time in seconds, % Idle lists the average per worker idle time, V1 lists the average number of constraint violations for Category 1 constraints, V2 lists the average number of constraints violations for Category 2 constraints, Evals lists the number of successful (i.e., feasible) evaluations, and Cache lists the total number of evaluations (including infeasible) that were looked up in the cache. Note that the sum of columns V2 and Evals gives the total number of calls to the simulator. Because APPS is asynchronous, the results can vary from run to run. In particular, it can converge to different local minima. This happened twice for problem UNC6 and twice for problem CON5. The function values were fairly close, but the other numbers (e.g., run times) were better, so those results were removed from the averages. Otherwise, all the methods converged to the same final value. We also had to discard one APPS run from the HC results because it had a bogus time reported.

Compared to PPS, APPS reduced the run time up to 37%. This can be attributed to better load balancing, resulting is substantially less idle time per worker process. The speculative nature of APPS can lead to more work: for problem CON6, APPS had 22% more calls to the simulator and was only 8% faster. On the other hand, it sometimes results in less work: for problem UNC6, APPS had 10% fewer calls to the simulator and ran 31% faster.

7. Conclusions. We presented a new version of APPS based on a manager-worker paradigm. This algorithm encapsulates either simple or sufficient decrease as well as the ability to handle bound constraints. A nice feature of this version of APPS is that it closely mirrors PPS (at least as described here).

In fact, neither PPS nor APPS has been presented in its most general form. For example, these algorithms handle updating the step lengths in a particular way. At unsuccessful iterations, the contraction factor in Step 5 is hardwired to $\frac{1}{2}$; in fact, this could be any fixed value in the interval $(0, 1)$, with the additional requirement that the value be rational in the simple decrease case. Similarly, an expansion factor could be used on successful iterations in Step 4. In both cases, these terms could be adaptive (i.e., different at each iteration). We also assume that the search directions are fixed between successful iterations. This is not required for PPS; however, we have presented it that way because it makes the description of APPS more straightforward. Finally, it is possible to modify APPS so that the search directions are allowed to change at even unsuccessful iterations provided that adequate controls are in place for globalization.

Likewise, some of the assumptions and conditions employed in the convergence analysis can be relaxed. We need not assume that the gradient is Lipschitz (Assumption 4); instead, continuous differentiability is sufficient. Part (d) in Condition 3 can be changed to say that either ρ is identically zero or it satisfies Condition 4; in other words, the argument based on lattice structure is independent of the decrease condition. Part (e) in Condition 3 can be generalized to say that the pseudo step can be anything of the form $2^{-\Gamma}\Delta_0$ for $\Gamma \in \mathbb{Z}$. Part (b) in Condition 4 is more restrictive than necessary for PPS (which only needs that $\rho(t)$ monotonically decreases), but this more restrictive assumption is needed by APPS. Condition 5 can be weakened, but the resulting condition is much more complex (see Condition 1 in [15]).

The convergence theory borrows heavily from the analysis of GSS in [14, 15] as well as the analysis of the original APPS [17]. The convergence results presented in section 5 are *weak* convergence results because it is possible that only a subsequence of the iterates will converge to a stationary point. Although strong convergence results are possible in the synchronous case [14], it is unclear whether such assurances can be made for the asynchronous algorithm because strong convergence requires that the algorithm always take the best direction at each iteration. Local convergence results exist for PPS [14] but are left as a topic for future study for APPS.

Just like the original version of APPS, the new version of APPS demonstrates faster execution times than its synchronous counterpart. More information on the test problems and a comparison of APPS with other derivative-free optimization methods can be found in [5]. We used APPSPACK 4.0 [13] for testing, full details of which are provided in [8].

We close by pointing toward the future. As we have already stated, one objective of the redesign of APPS is to enable easier incorporation of methods for handling linear constraints. In that case, the search directions must conform to the nearby boundary [20, 15], so the ability to change the search directions in Step 4 makes this relatively simple. This will be pursued in future research.

Appendix A. Evolution of peer-to-peer to manager-worker. The switch from the peer-to-peer version [12] to manager-worker was gradual and largely the result of user requests. As mentioned in the introduction, peer-to-peer APPS is based on the concept of what are called agents. Each agent handles a single direction (and up to one corresponding trial point) and launches its own workers to execute the function evaluation. Thus, there is one agent per search direction and the number of search directions is necessarily fixed. The working assumption is that there is one direction per processor and one processor per machine.

The first step in the evolution to the manager-worker design is motivated by multiprocessor (i.e., SMP) machines. On a cluster of machines that each have, say, four processors, it is more efficient to have one agent (as opposed to four) for every four search directions. The peer-to-peer design remained intact, but a single agent could handle multiple search directions. The directions sharing a common agent also shared one common best point. In fact, this is equivalent to the original peer-to-peer model with instantaneous communication between appropriate subsets of the agents. Once agents were designed and implemented to handle multiple directions, having one agent handle all directions was trivial.

The difference between this first manager-worker concept and the algorithm described here is the handling of the search directions. Having a fixed set of search directions is fairly crucial to the peer-to-peer design. In particular, it is implemented so that there is at most one function evaluation per search direction at any given time. The disconnected points described in section 4 cannot exist. Although it would certainly be possible to design a peer-to-peer APPS that allows the search directions to change as the optimization progresses, it is much simpler to do this in a manager-worker context.

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