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An alternative globalization strategy for unconstrained optimization

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ABSTRACT

We propose a new globalization strategy that can be used in unconstrained optimization algorithms to support rapid convergence from remote starting points. Our approach is based on using multiple points at each iteration to build a sequence of representative models of the objective function. Using the new information gathered from those multiple points, a local step is gradually improved by updating its direction as well as its length. We give a global convergence result and also provide the parallel implementation details accompanied with a numerical study. Our numerical study shows that the proposed algorithm is a promising alternative as a globalization strategy.

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1. Introduction

In unconstrained optimization, frequently used algorithms, like quasi-Newton or trust-region methods, need to involve mechanisms that ensure convergence to local solutions from remote starting points. Roughly speaking, these *globalization strategies* guarantee that the improvement obtained by the algorithm is comparable to the improvement obtained with a gradient step [1].

In this paper, we present a new globalization strategy that can be used in unconstrained optimization methods for solving problems of the form

$$\min_{x\in\Re^n} \; f(x), \tag{1}$$

where f is a first-order differentiable function. Conventional methods for solving this problem mostly use local approximations that are very powerful once the algorithm arrives at the close proximity of a stationary point. The main idea behind the proposed strategy is based on using additional information collected from multiple points to construct an adaptive approximation of the function f in (1). In particular, we update our approximate model constructed around the current iterate and a sequence of trial points. Our objective is to come up with a better local model than the one obtained by the current iterate only. We observe that the collection of this additional information can have a noteworthy effect on the performance of the method. Before moving to the next iterate, the step is improved by updating its direction as well as its length simultaneously. This step computation involves only the inner products of vectors. Therefore, each iteration of the algorithm is amenable to a parallel implementation. Our numerical experiments demonstrate that the additional computations at each step may reduce the total number of iterations, since we learn more about the function structure.

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Parallel execution of linear algebra operations is common in the parallel optimization literature generally in designing parallel implementations of the existing methods. One of the earliest work is given by [2], who discuss the parallelization of linear algebra steps and the function evaluations in the BFGS quasi-Newton method. Around the same time, [3] propose to use truncated-Newton methods combined with the computation of the search direction via the block iterative methods. In particular, they focus on the block conjugate direction method. Using the block iterative methods, they parallelize some steps of the algorithm, in particular, the linear algebra operations. For extensive reviews of the topic, we refer to [4–6].

The use of multiple trial points or directions is also a recurring idea in the field of parallel nonlinear optimization. However, unlike our case, these mostly depend on the concurrent information collection or generation. [7] proposes an algorithm based on evaluating multiple points in parallel to determine the next iterate. In the parallel line search implementation of [8], multiple step sizes are tried in parallel. [9] discusses three parallel quasi-Newton algorithms that are also based on considering multiple directions to extend the rank-one updates. To solve the original problem by solving a series of independent subproblems, [10] suggests using conjugate subspaces for quasi-Newton updates. Thus, the resulting method can be applied in a parallel computing environment.

The rest of this paper is organized as follows. In Section 2, we discuss the derivation and the theoretical properties of the proposed strategy. In Section 3, the success of the main idea of the method is numerically tested, and its parallel implementation is discussed in Section 4. Conlusion of the study is presented in Section 5.

2. Proposed globalization strategy

At the core of the proposed strategy lies an *extended* model function, which is constructed using two linear models at two reference points. The first of these points is the current iterate and the second one is a trial point. When one of these trials leads to a successful step, then the algorithm moves to a new iterate. To make our discussion more concrete, we start by describing an iteration of the algorithm.

Let x_k and s_k denote the current iterate and the kth step of the algorithm, respectively. Then, the next iterate becomes $x_{k+1} = x_k + s_k$. These are the outer iterations. The vector s_k is obtained by executing a series of inner iterations and computing the trial steps s_k^t, $t = 0, 1, \ldots$. We can further simplify our exposition by defining

$$f_k := f(x_k),\ g_k := \nabla f(x_k),\ x_k^t := x_k + s_k^t,$$
$$f_k^t := f(x_k^t),\ g_k^t := \nabla f(x_k^t),\ y_k^t := g_k^t - g_k.$$

The trial step s_k^t is accepted as new s_k, if it provides sufficient decrease in the sense

$$f_k^t - f_k \leq \rho g_k^\intercal s_k^t \quad \text{for some } \rho \in (0, 1). \tag{2}$$

This is nothing but the well-known Armijo condition [1].

Up to this point, the algorithm behaves like a typical unconstrained minimization procedure. However, to come up with the proposed globalization strategy, we design a new subprocedure for computing the trial steps, s_k^t. The inner step computation is done by solving a subproblem that consists of an extended model function updated at every inner iteration and a constraint restricting the length of the steps. The extended model function is an approximation to the objective function, f. It is constructed using the information gathered around the region bordered by x_k and x_k^t. Actually, the extended model function is a combination of the linear models of f at x_k and x_k^t. That is,

$$m_k^t(s) := \alpha_k^0(s) l_k^0(s) + \alpha_k^t(s) l_k^t(s - s_k^t),$$

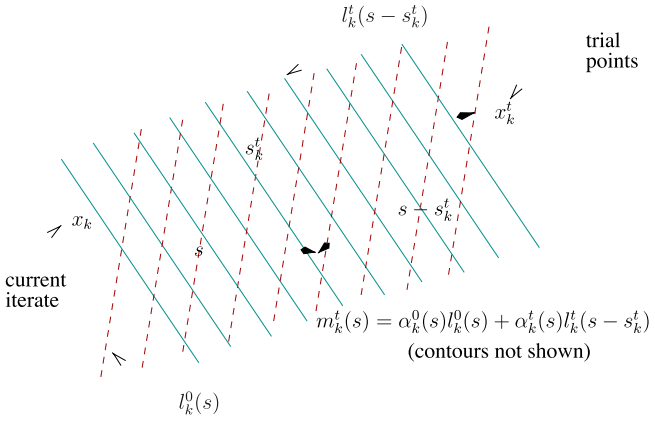


Figure 1. Construction of the model function $m_k^t(s)$ around x_k and x_k^t.

where

$$l_k^0(s) := f_k + g_k^\mathsf{T} s \quad \text{and} \quad l_k^t(s - s_k^t) := f_k^t + (g_k^t)^\mathsf{T}(s - s_k^t). \tag{3}$$

This construction is illustrated in Figure 1. Note that both weights, $\alpha_k^0(s)$ and $\alpha_k^t(s)$ are functions of s. We want to make sure that if s is closer to s_k^t, then the weight $\alpha_k^t(s)$ of the linear model around x_k increases. Similarly, $\alpha_k^t(0)$ should increase as $(s - s_k^t)$ gets closer to $(-s_k^t)$. This is achieved by measuring the length of the projections of $(s - s_k^t)$ and s on s_k^t by

$$\alpha_k^0(s) = \frac{(s - s_k^t)^\mathsf{T}(-s_k^t)}{(-s_k^t)^\mathsf{T}(-s_k^t)} \text{ and } \alpha_k^t(s) = \frac{s^\mathsf{T} s_k^t}{(s_k^t)^\mathsf{T} s_k^t}, \tag{4}$$

respectively.

Next, we introduce a constraint to handle the possibly hard quadratic function m_k^t as well as control the step length. Recall that our model function is constructed around the previous trial step s_k^t by considering the area lying between x_k and $x_k + s_k^t$. Thus, we impose the constraint

$$\|s\|^2 + \|s - s_k^t\|^2 \leq \|s_k^t\|^2. \tag{5}$$

Clearly, this constraint controls not only the length of s but also its deviation from the previous trial point s_k^t. In addition, this choice of the constraint ensures that both weight functions $\alpha_k^0(s)$ and $\alpha_k^t(s)$ are in $[0, 1]$, and they add up to 1. Hence, our model function m_k^t is the convex combination of the linear functions l_k^0 and l_k^t. This observation is formally presented in Lemma 2.1 and its proof is given in Appendix 1.

Lemma 2.1: *If constraint (5) holds at inner iteration $t + 1$ of iteration k, then both $\alpha_k^0(s)$ and $\alpha_k^t(s)$ are nonnegative, and they satisfy $\alpha_k^0(s) + \alpha^t(s) = 1$.*

We also make the following observations about the region defined by constraint (5). First, this region is never empty, since any step $s = \gamma s_k^t$ for $\gamma \in (0, 1]$ is in the region. This implies in a sense that a backtracking operation on the previous trial step, s_k^t would give a new feasible trial step, s_k^{t+1}. Second, there are always feasible steps in the steepest descent direction *whenever* $g_k^\mathsf{T} s_k^t \leq 0$ holds. That is, the steps $s = -\xi g_k$ are feasible for $0 \leq \xi \leq -\frac{g_k^\mathsf{T} s_k^t}{\|g_k\|^2}$. Thus, as long as the first trial step s_k^0 is gradient related, each feasible region constructed around a subsequent trial step involves a feasible point, which is also gradient related.

Algorithm 1 gives the outline of the proposed method. The stopping condition is the usual check whether the current iterate, x_k is a stationary point. We start the inner iterations by computing the

first trial step, s_k^0. We shall elaborate on how to select this initial trial step in Section 4. As long as the trial steps s_k^t, $t = 0, 1, 2, \ldots$ are not acceptable, we carry on with constructing and minimizing the model functions. Once an acceptable step is obtained by the inner iteration, we evaluate the next iterate x_{k+1} and continue with solving the overall problem.

Algorithm 1: Outline

Input: x_0; $\rho \in (0,1)$; $k = 0$
while x_k *is not a stationary point* **do**
  $t = 0$;
  Compute the first trial step s_k^0;
  while $f_k^t - f_k > \rho g_k^\intercal s_k^t$ **do**
    Compute the trial step s_k^{t+1} by solving

$$\begin{aligned} &\text{minimize} && m_k^t(s) = \alpha_k^0(s) l_k^0(s) + \alpha_k^t(s) l_k^t(s - s_k^t) \\ &\text{subject to} && \|s\|^2 + \|s - s_k^t\|^2 \leq \|s_k^t\|^2, \end{aligned} \tag{6}$$

    where l^0, l^t, α^0, and α^t are given by (3) and (4), respectively;
    t = t + 1;
  end
  $x_{k+1} = x_k + s_k^t$;
end

In Algorithm 1, the crucial part is solving subproblem (6), which has a quadratic objective function and a quadratic constraint. After some derivation, the objective function of this subproblem simplifies to

$$m_k^t(s) = f_k + (\bar{g}_k^t)^\intercal s + s^\intercal B_k^t s,$$

where

$$\bar{g}_k^t := g_k + \frac{1}{\|s_k^t\|^2}(f_k^t - (g_k^t)^\intercal s_k^t - f_k) s_k^t$$

and

$$B_k^t := \frac{1}{\|s_k^t\|^2} s_k^t (g_k^t - g_k)^\intercal.$$

The Hessian of this quadratic objective function is the rank-one matrix B_k^t. Its only nonzero eigenvalue is $(s_k^t)^\intercal y_k^t$, and the eigenvectors corresponding to this eigenvalue are s_k^t and $-s_k^t$. Furthermore, its eigenvectors corresponding to the zero eigenvalues are perpendicular to y_k^t. Let us note at this point that the gradient of the model $m_k^t(s)$ is given by

$$\nabla m_k^t(s) = g_k + \frac{1}{\|s_k^t\|^2}(f_k^t - (g_k^t)^\intercal s_k^t - f_k) s_k^t + \frac{1}{\|s_k^t\|^2}[s_k^t (y_k^t)^\intercal + y_k^t (s_k^t)^\intercal] s. \tag{7}$$

2.1. Convex objective function

Before considering the general case, we discuss in this section how subproblem (6) can be solved when the objective function is convex. We shall soon observe that it is not straightforward to obtain trial steps that yield sufficient descent with this initial design. Thus, we shall propose modifications over this first attempt in Section 2.2 to guarantee convergence. However, we still present here our observations with the convex case as it constitutes the basis of our approach for general functions given in the next section.

We first check whether the subproblem always provides a nonzero step at every inner iteration. It turns out that if the most recent trial step, s_k^t is gradient related, then the next trial step, s_k^{t+1} cannot

be the zero vector. Furthermore, if the objective function value of the recent trial step is strictly greater than the current objective function value, then the optimal solution of the subproblem is in the interior of the region defined by the constraint (5). Lemma 2.2 summarizes this discussion. The proof of this lemma is given in Appendix 1.

Lemma 2.2: *Let f be a convex function and consider the inner iteration $t+1$ of iteration k with $\|s_k^t\| \neq 0$. If $g_k^\intercal s_k^t \leq 0$, then $\|s_k^{t+1}\| \neq 0$ and*

$$\alpha^* := \underset{0\leq\alpha\leq 1}{\arg\min}\, m_k^t(\alpha s_k^t) = \min\left\{\frac{(y_k^t)^\intercal s_k^t - f_k^t + f_k}{2(y_k^t)^\intercal s_k^t}, 1\right\}.$$

If we additionally have $f_k^t > f_k$, then $\alpha^* < 1$.

Note that we require condition $g_k^\intercal s_k^t \leq 0$ hold for all trial steps to guarantee nonzero trial steps. So, a convergence argument for the proposed algorithm is not clear unless it ensures this condition. We shall visit this issue later in this section.

We next show how subproblem (6) can be solved, if the conditions given in Lemma 2.2 hold. This subproblem can be rewritten as

$$\begin{array}{ll}\text{minimize} & [(f_k^t - (g_k^t)^\intercal s_k^t - f_k)s_k^t + \|s_k^t\|^2 g_k]^\intercal s + s^\intercal[s_k^t(g_k^t - g_k)^\intercal]s \\ \text{subject to} & s^\intercal(s - s_k^t) \leq 0.\end{array}$$

Note that this is a convex program as $(s_k^t)^\intercal(g_k^t - g_k) \geq 0$ by the convexity assumption on f. Let s_k^{t+1} denote the optimal solution of the above problem and $\beta \geq 0$ be the Lagrange multiplier corresponding to the constraint. The Karush–Kuhn–Tucker optimality conditions imply

$$(f_k^t - (g_k^t)^\intercal s_k^t - f_k - \beta)s_k^t + \|s_k^t\|^2 g_k + s_k^t(y_k^t)^\intercal s_k^{t+1} + y_k^t(s_k^t)^\intercal s_k^{t+1} + 2\beta s_k^{t+1} = 0, \tag{8}$$

$$\beta(s_k^{t+1} - s_k^t)^\intercal s_k^{t+1} = 0. \tag{9}$$

Simplifying (8) leads to

$$s_k^{t+1} = c_g(\beta)g_k + c_s(\beta)s_k^t + c_y(\beta)y_k^t, \tag{10}$$

where

$$c_g(\beta) = -\tfrac{\|s_k^t\|^2}{2\beta},$$

$$c_s(\beta) = -\tfrac{\|s_k^t\|^2}{2\beta}\left(\tfrac{\delta}{\|s_k^t\|^2} - \tfrac{(y_k^t)^\intercal s_k^t + 2\beta}{\theta}((y_k^t)^\intercal g_k + \tfrac{\delta}{\|s_k^t\|^2}(y_k^t)^\intercal s_k^t) + \tfrac{\|y_k^t\|^2}{\theta}((s_k^t)^\intercal g_k + \delta)\right),$$

$$c_y(\beta) = -\tfrac{\|s_k^t\|^2}{2\beta}\left(-\tfrac{(y_k^t)^\intercal s_k^t + 2\beta}{\theta}((s_k^t)^\intercal g_k + \delta) + \tfrac{\|s_k^t\|^2}{\theta}((y_k^t)^\intercal g_k + \tfrac{\delta}{\|s_k^t\|^2}(y_k^t)^\intercal s_k^t)\right)$$

with

$$\delta = f_k^t - f_k - (g_k^t)^\intercal s_k^t - \beta \text{ and } \theta = \left((y_k^t)^\intercal s_k^t + 2\beta\right)^2 - \|s_k^t\|^2\|y_k^t\|.$$

Consider first the case when $\beta = 0$. Then, using Lemma 2.2, we have $s_k^{t+1} = \alpha^* s_k^t$. When $\beta > 0$, the optimal solution is at the boundary of the constraint. If we now use (10) with (9), then after some derivation we obtain

$$\frac{1}{4\beta\theta^2}P(\beta) = 0,$$

where $P(\beta)$ is a sixth order polynomial function of β (see the online supplement[1] for the details). Thus, the subproblem can be solved by computing the roots of this polynomial.

In fact, it is not hard to show that if the inner iteration step s_k^t satisfies $s_k^t = -M^t g_k$ for some matrix M^t, then at the next inner iteration we have $s_k^{t+1} = -M^{t+1}g_k$. However, it is not possible to guarantee that the matrix M^{t+1} will be positive definite given M^t is. That is because the gradient of

the model function is given as the conical combination of g_k and $-s_k^t$. First of all, the model gradient can be zero for $s = 0$ at a point x_k with $g_k \neq 0$. Also, when the deviation of the objective function f from linearity is relatively large, then the model gradient can point a *backward* direction; *i.e.* the reverse direction of s_k^t. Since the constraint of the model does not allow such a backward step, this can cause s_k^{t+1} to be *zero*. Moreover, the model gradient is scaled with a matrix, and the scaled step adds a third component along y_k to the linear combination whose coefficient is not necessarily positive. So, the resulting s_k^{t+1} might not satisfy $g_k^T s_k^{t+1} \leq 0$ even if s_k^t does.

2.2. General objective function

Using our observations on the convex case, we next concentrate on a construction where the model function m_k^t has the same gradient value at $s = 0$ as the original objective function, f. Then, we also add a regularization term so that the subproblem can be made convex even if f is not.

We start by relaxing the constraint (5) and moving it to the objective function. That is

$$\min_{s\in\mathbb{R}^n}\{m_k^t(s) + \sigma_1(s - s_k^t)^\intercal s\}.$$

We choose

$$\sigma_1 = \frac{1}{\|s_k^t\|^2}(f_k^t - (g_k^t)^\intercal s_k^t - f_k),$$

so that $\nabla m_k^t(0) = g_k$. Observe that the above choice of σ_1 can be negative (for f nonconvex), in which case the constraint operates the reverse way; that is, it tries to keep s away from s_k^t. Since that causes us to loose our control on the size of s, we add a regularization term and the subproblem becomes

$$\min_{s\in\mathbb{R}^n}\{m_k^t(s) + \sigma_1(s - s_k^t)^\intercal s + \sigma_2 s^\intercal s\}.$$

After simplifying the objective function, we obtain our new subproblem for the general case

$$\min_{s\in\mathbb{R}^n}\{g_k^T s + s^\intercal \frac{1}{\|s_k^t\|^2}[\sigma I + s_k^t(y_k^t)^\intercal]s\}, \tag{11}$$

where

$$\sigma = (\sigma_1 + \sigma_2)\|s_k^t\|^2 = (f_k^t - (g_k^t)^\intercal s_k^t - f_k) + \sigma_2\|s_k^t\|^2.$$

Note that the model function (11) is always convex provided that the regularization parameter σ_2 is chosen sufficiently large. Beyond the convexity of m_k^t, we want to guarantee for some $\eta \in (0, 1)$ that the step length condition

$$\|s_k^{t+1}\| \leq \eta\|s_k^t\| \tag{12}$$

holds. Suppose s_k^{t+1} is such a step, and it is the optimal solution for problem (11) with a convex objective function. Then, the first-order optimality condition implies

$$s_k^{t+1} = -\|s_k^t\|^2(\bar{B}_k^t)^{-1}g_k, \tag{13}$$

where

$$\bar{B}_k^t = 2\sigma I + s_k^t(y_k^t)^\intercal + y_k^t(s_k^t)^\intercal.$$

Thus, we obtain

$$\|s_k^{t+1}\| \leq \|s_k^t\|^2 \left\|(\bar{B}_k^t)^{-1}\right\| \|g_k\| = \left(\|s_k^t\|\|g_k\|\lambda_{\min}(\bar{B}_k^t)^{-1}\right)\|s_k^t\|,$$

where $\lambda_{\min}$ denotes the smallest eigenvalue of its matrix parameter. It is not difficult to see that 2σ is an eigenvalue of $\bar{B}_k^t$ with multiplicity $n-2$, and the remaining two eigenvalues are the extreme eigenvalues of $\bar{B}_k^t$ given by

$$\lambda_{\max}(\bar{B}_k^t) = 2\sigma + \|y_k^t\|\|s_k^t\| + (y_k^t)^\intercal s_k^t \quad \text{and} \quad \lambda_{\min}(\bar{B}_k^t) = 2\sigma - \|y_k^t\|\|s_k^t\| + (y_k^t)^\intercal s_k^t,$$

where $\lambda_{\max}$ denotes the largest eigenvalue of its matrix parameter.

To obtain a convex model, we need

$$2\sigma - \|y_k^t\|\|s_k^t\| + (y_k^t)^\intercal s_k^t > 0. \tag{14}$$

On the other hand, the step length condition (12) requires

$$\|s_k^t\|\|g_k\|\lambda_{\min}(\bar{B}_k^t)^{-1} \le \eta \quad \Rightarrow \quad 2\sigma - \|y_k^t\|\|s_k^t\| + (y_k^t)^\intercal s_k^t \ge \frac{\|s_k^t\|\|g_k\|}{\eta} \tag{15}$$

Since the latter bound is larger, using relation (15) for choosing σ_2 provides the convexity requirement and satisfies the step length condition. That is

$$\sigma = \|s_k^t\|^2(\sigma_2 + \sigma_1) \ge \frac{1}{2}\left(\|s_k^t\|\left(\|y_k^t\| + \frac{1}{\eta}\|g_k\|\right) - (y_k^t)^\intercal s_k^t\right).$$

Our last step is to state the minimizer s_k^{t+1} of (11) with selected σ_1 and σ_2 values. Following similar steps as in Section 2.1 and after some derivation, we obtain

$$s_k^{t+1} = c_g(\sigma)g_k + c_y(\sigma)y_k^t + c_s(\sigma)s_k^t, \tag{16}$$

where

$$c_g(\sigma) = -\frac{\|s_k^t\|^2}{2\sigma}, \quad c_y(\sigma) = -\frac{\|s_k^t\|^2}{2\sigma\theta}[-((y_k^t)^\intercal s_k^t + 2\sigma)((s_k^t)^\intercal g_k) + \|s_k^t\|^2((y_k^t)^\intercal g_k)],$$

$$c_s(\sigma) = -\frac{\|s_k^t\|^2}{2\sigma\theta}[-((y_k^t)^\intercal s_k^t + 2\sigma)((y_k^t)^\intercal g_k) + \|y_k^t\|^2((s_k^t)^\intercal g_k)],$$

with

$$\theta = \left((y_k^t)^\intercal s_k^t + 2\sigma\right)^2 - \|s_k^t\|^2\|y_k^t\|^2,$$

and

$$\sigma = \tfrac{1}{2}\left(\|s_k^t\|\left(\|y_k^t\| + \frac{1}{\eta}\|g_k\|\right) - (y_k^t)^\intercal s_k^t\right). \tag{17}$$

It is important to observe that the solution of the subproblem does not require storing any matrices and the main computational burden is only due to inner products, which could be done in parallel (see Section 4 for implementation details).

When it comes to the convergence of the proposed algorithm, we are saved basically by keeping the directions of its steps *gradient related*. However, we could not directly refer to the existing convergence results, since the directions in our algorithm change during inner iterations and the step length is not computed using a one-dimensional function. In the following convergence note, we only assume additionally that the objective function f is bounded below and its gradient ∇f is Lipschitz continuous with parameter L.

Lemma 2.3: *Suppose that the first trial step s_k^0 satisfies $m_0\|g_k\| \le \|s_k^0\| \le M_0\|g_k\|$ and $0 \ge s_k^0 g_k \ge -\lambda_0\|g_k\|^2$ for some $m_0, M_0, \lambda_0 \in (0,\infty)$. Then, at any iteration k, the optimal solution s_k^{t+1} in (16)*

becomes an acceptable step satisfying (2) *in finite number of inner iterations at a nonstationary point* x_k.

***Proof*:** Consider any iteration k. Since s_k^{t+1} is obtained by (13), the steps computed at each inner iteration satisfy $-g_k^\intercal s_k^{t+1} \geq \lambda_{t+1}\|g_k\|^2$, $t = 0, 1, 2, \ldots$ for $\lambda_{t+1} = \|s_k^t\|^2(\lambda_{\max}(\bar{B}_k^t))^{-1}$. Note for $t = 0, 1, \ldots$ that $\lambda_t > 0$ by the choice of λ_0 and the relation (14). We have

$$\begin{aligned}
\lambda_{t+1}\frac{\|g_k\|^2}{\|s_k^{t+1}\|^2} &\geq \lambda_{t+1}\frac{\|g_k\|^2}{\eta^2\|s_k^t\|^2} \\
&= \|s_k^t\|^2\left(\|s_k^t\|\left(\|y_k^t\| + \frac{1}{\eta}\|g_k\|\right) - (y_k^t)^\intercal s_k^t + \|y_k^t\|\|s_k^t\| + (y_k^t)^\intercal s_k^t\right)^{-1}\frac{\|g_k\|^2}{\eta^2\|s_k^t\|^2} \\
&= \frac{\|g_k\|^2}{\|s_k^t\|\left(2\|y_k^t\| + \eta^{-1}\|g_k\|\right)\eta^2} \geq \frac{\|g_k\|^2}{\|s_k^t\|\left(2L\|s_k^t\| + \eta^{-1}\|g_k\|\right)\eta^2}.
\end{aligned}$$

Using (12), we have $\|s_k^t\| \leq \eta_t M_0\|g_k\|$. Then,

$$\lambda_{t+1}\frac{\|g_k\|^2}{\|s_k^{t+1}\|^2} \geq \frac{\|g_k\|^2}{\left(2L\eta^{2t}M_0^2 + \eta^t M_0\eta^{-1}\right)\|g_k\|^2\eta^2} = \frac{1}{2L\eta^{2t+2}M_0^2 + \eta^{t+1}M_0}.$$

Therefore, we obtain

$$\lambda_t\frac{\|g_k\|^2}{\|s_k^t\|^2} \geq \frac{1}{2L\eta^{2t+1}M_0^2 + \eta^t M_0}. \tag{18}$$

Suppose that the acceptance criterion (2) is never satisfied as $t \to \infty$. Then,

$$f_k^t - f_k > \rho g_k^\intercal s_k^t, \quad \text{for all } t.$$

This implies

$$g_k^\intercal s_k^t + \frac{L}{2}\|s_k^t\|^2 > \rho.$$

Next, the desired inequality is obtained by

$$\frac{L}{2} > (1-\rho)\frac{(-g_k^\intercal s_k^t)}{\|s_k^t\|^2} \geq (1-\rho)\lambda_t\frac{\|g_k\|^2}{\|s_k^t\|^2} \geq (1-\rho)\frac{1}{2L\eta^{2t+1}M_0^2 + \eta^t M_0}.$$

Since $\eta \in (0, 1)$, the right-hand side of the last inequality increases without a bound as $t \to \infty$. This gives a contradiction as L is bounded. So, an acceptable $\|s_k^t\|$ should be obtained in finite number of inner iterations. □

Note that the conditions on the initial step, s_k^0 in Lemma 2.3 are simply satisfied, if we choose $s_k^0 = -\epsilon g_k$ for any $\epsilon \in (0, 1]$. This implies $m_0 = M_0 = \lambda_0 = \epsilon$.

Theorem 2.1: *Let* $\{x_k\}$ *be the sequence of iterates generated by Algorithm 2 and* $\{s_k^0\}$ *satisfy the requirements in Lemma 2.3. Then, any limit point of the sequence* $\{x_k\}$ *is a stationary point of the objective function* f.

***Proof*:** By Lemma 2.3, for any k, (2) is satisfied after a finite number of inner iterations, say $t(k)$. Also, note that relation (13) implies $\|s_k^t\| \geq \lambda_t\|g_k\|$ with the same λ_t as in (18). We next derive a lower bound for $\lambda_{t(k)}$:

$$\lambda_{t+1} = \|s_k^t\|^2 \left(\|s_k^t\| \left(\|y_k^t\| + \frac{1}{\eta}\|g_k\| \right) - (y_k^t)^\mathsf{T} s_k^t + \|y_k^t\| \|s_k^t\| + (y_k^t)^\mathsf{T} s_k^t \right)^{-1}$$
$$= \frac{\eta \|s_k^t\|}{\|g_k\| + 2\eta \|y_k^t\|} \geq \frac{\eta \|s_k^t\|}{\|g_k\| + 2L\eta \|s_k^t\|} \geq \frac{\eta}{\|g_k\| + 2L\eta^{t+1} M_0 \|g_k\|} \|s_k^t\|.$$

So,

$$\lambda_1 \geq \frac{\eta}{1 + 2L\eta M_0} m_0 \quad \text{and} \quad \lambda_t \geq \frac{\eta}{1 + 2L\eta^t M_0} \lambda_{t-1}$$
$$\geq \frac{\eta}{1 + 2L\eta M_0} \lambda_{t-1} \geq \left(\frac{\eta}{1 + 2L\eta M_0} \right)^t m_0, \ t = 2, 3, \ldots$$

Recall that for the accepted step s_k of iteration k we have $-s_k^\mathsf{T} g_k \geq \lambda_{t(k)} \|g_k\|^2$. Clearly, $\lambda_{t(k)} > 0$ is bounded away from zero as $t(k)$ is finite. Consider now any subsequence of $\{x_k\}$ with indices $k \in \mathcal{K}$ such that

$$\lim_{k \in \mathcal{K}} x_k = \hat{x}.$$

Then, for any $k, k' \in \mathcal{K}$ with $k' > k$ we have

$$f_k - f_{k'} \geq f_k - f_k^t \geq -\rho g_k^\mathsf{T} s_k \geq \rho \lambda_{t(k)} \|g_k\|^2. \tag{19}$$

Since $\{x_k\}_{k \in \mathcal{K}}$ converges to $\hat{x}$, the continuity of f implies that $f_k \to \hat{f}$ as $k \in \mathcal{K}$. Therefore, $f_k - f_{k'} \to 0$ as $k, k' \to \infty$. Thus, we obtain $\nabla f(\hat{x}) = 0$ by (19) since $\lambda_{t(k)}$ is bounded away from zero. □

2.3. Relationship with quasi-newton updates

Observing the formula in (13), we next question the relationship between the step computation of the proposed algorithm and the quasi-Newton updates, in particular the DFP formula [1]. The key to understanding this relationship is to treat the current iterate x_k as the previous iterate, whereas our trial step x_k^t becomes the next iterate in standard quasi-Newton updates.

Let D_k denote the quasi-Newton approximation to the Hessian at iterate x_k. Then, the infamous DFP formula yields the new approximation to the Hessian in the next iterate x_{k+1} as

$$D_{k+1} = \left(I - \frac{y_k s_k^\mathsf{T}}{y_k^\mathsf{T} s_k} \right) D_k \left(I - \frac{s_k y_k^\mathsf{T}}{y_k^\mathsf{T} s_k} \right) + \frac{y_k y_k^\mathsf{T}}{y_k^\mathsf{T} s_k},$$

where $s_k = x_{k+1} - x_k$ and $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$. We first substitute s_k^t for s_k and y_k^t for y_k in the above equation. Then, by setting

$$D_k = -\frac{(y_k^t) s_k^t}{\|s_k^t\|^2} I,$$

we obtain

$$D_{k+1} = \frac{1}{\|s_k^t\|^2} \left((-y_k^t)^\mathsf{T} s_k^t I + s_k^t (y_k^t)^\mathsf{T} + y_k^t (s_k^t)^\mathsf{T} \right).$$

Let us now denote the Hessian of the objective our model function given in relation (11) by H_k^t. Then, we have

$$H_k^t = \frac{1}{\|s_k^t\|^2} \left(2\sigma I + s_k^t (y_k^t)^\mathsf{T} + y_k^t (s_k^t)^\mathsf{T} \right).$$

Next, we plug in the value of σ from (17) and obtain

$$H_k^t = \frac{1}{\|s_k^t\|^2} \left((-y_k^t)^\mathsf{T} s_k^t I + s_k^t (y_k^t)^\mathsf{T} + y_k^t (s_k^t)^\mathsf{T} \right) + \left(\frac{\|y_k^t\| + \eta^{-1} \|g_k\|}{\|s_k^t\|} \right) I.$$

The last term above, in a sense, serves the purpose of obtaining a positive definite matrix. Thus, the objective function becomes convex. Looking at our approach from the quasi-Newton approximation point of view, we again confirm that the additional information collected from the trial iterate x_k^t is used to come up with a better model around the current iterate x_k. Our derivation above also shows that the construction of the model function $m^{t+1}(s)$ from one inner iteration to the next is completely independent.

3. Practical performance

In this section, we shall conduct a numerical study to demonstrate the novel features of the proposed globalization strategy. We have compiled a set of unconstrained optimization problems from the well-known CUTEst collection [11]. We have also embedded the proposed strategy (PS) into the L-BFGS package [12] as a new globalization alternative to the existing two line search routines; backtracking (BT) and More-Thuente line search (MT).

First, let us give a two-dimensional example to illustrate how the proposed strategy can be beneficial. Figure 2 shows the contours of the Rosenbrock function. The inner iterates of PS are denoted by + markers, the inner iterates of BT are denoted by ∘ markers and the inner iterates of MT are denoted by × markers. All three globalization strategies start from the same initial point. The numbers next to the trial points denote the inner iterations. The corresponding objective function values are given in the subplot at the southeast corner of the figure.

Figure 2 illustrates the main point of the proposed strategy: PS can change the direction of the trial step as well as its length. It is important to note that PS is *not* a trust-region method because it builds a new model function using the current trial step for computing the next trial step at *every* inner iteration. However, in a trust-region method the model function is not updated within the same iteration and the current trial step does not contribute to the computation of the next trial step. For this particular two-dimensional problem, PS performs better than the other two globalization strategies as it attains the lowest objective function value after three inner iterations.

Next, we test the effect of the direction updates introduced by the proposed strategy. We solve the CUTEst problems by employing the backtracking line search with Wolfe conditions using the default reduction factor of 0.5 given in the L-BFGS package. For the proposed strategy, we also set the

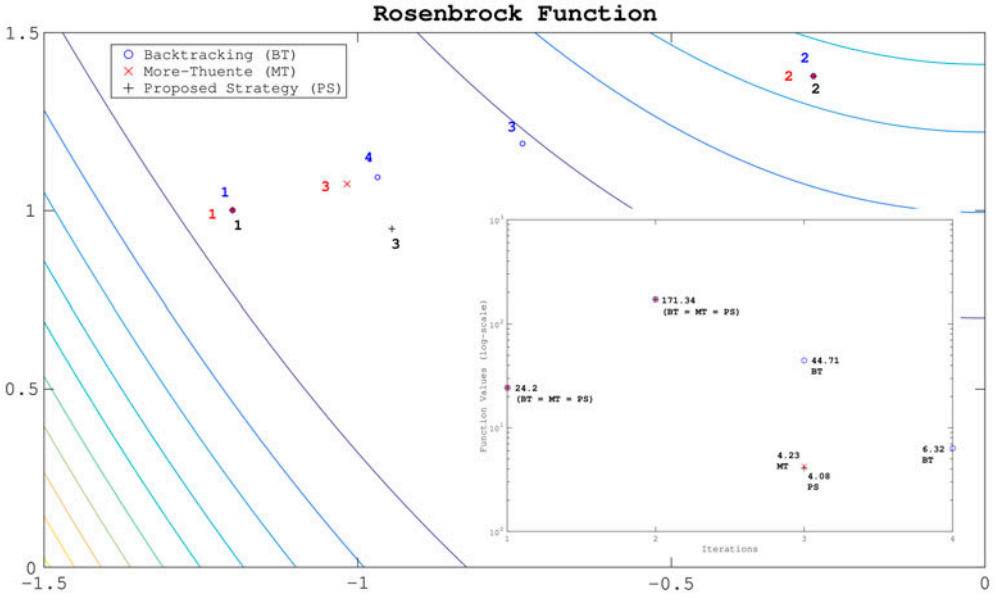


Figure 2. The inner iterations obtained with the two line search methods and the proposed strategy for the Rosenbrock function.

Table 1. Comparison of the proposed strategy against the line search method in terms of total number of function evaluations.

	PS < BT(%)	PS > BT(%)	PS = BT(%)
$m = 0$ (30 problems)	60.00	36.67	3.33
$m = 5$ (63 problems)	50.94	22.64	26.42

parameter η to 0.5. Therefore, the new strategy requires the same amount of step length decrease (but it may additionally alter the search direction). In our tests, we start with both the L-BFGS step with memory set to 5 ($m = 5$) and the gradient step ($m = 0$). The maximum number of iterations is set to 500 for the L-BFGS step, and to 1,000 for the gradient step. The comparison is carried out for those problems, where both methods obtained the same local solution (which is assessed by comparing the objective function values and the first two components of the solution vectors). The results are reported for 30 problems when $m = 0$, and for 63 problems when $m = 5$.

Table 1 summarizes our observations. We compare two strategies in terms of the total number of function evaluations required to solve the problems. When $m = 0$, the proposed strategy has used less number of function evaluations than the line search for 60% of the problems. The same figure becomes 50.94% when $m = 5$, and solving 26.42% of the problems has taken exactly the same number of function evaluations with both strategies. Overall, these results show that the direction updates of the new strategy can indeed provide improvements.

We have also implemented the proposed strategy for different programming languages. These codes and additional results on several other problems are available online,[2] where we again use the L-BFGS approach for preconditioning the first trial step.

4. Parallel implementation

In this section, we shall provide an outline of the subproblem solution operations while we discuss their parallel execution. Then, we conduct some numerical experiments to illustrate the parallel performance of the proposed algorithm.

As relation (16) shows, the basic trial step at inner iteration $t + 1$ is in the subspace spanned by g_k, g_k^t, and the previous trial step s_k^t. We should also emphasize that the computation of s_k^{t+1} requires just a few floating point operations, once the necessary inner products are completed. In particular, the computation of (16) requires the following inner products.

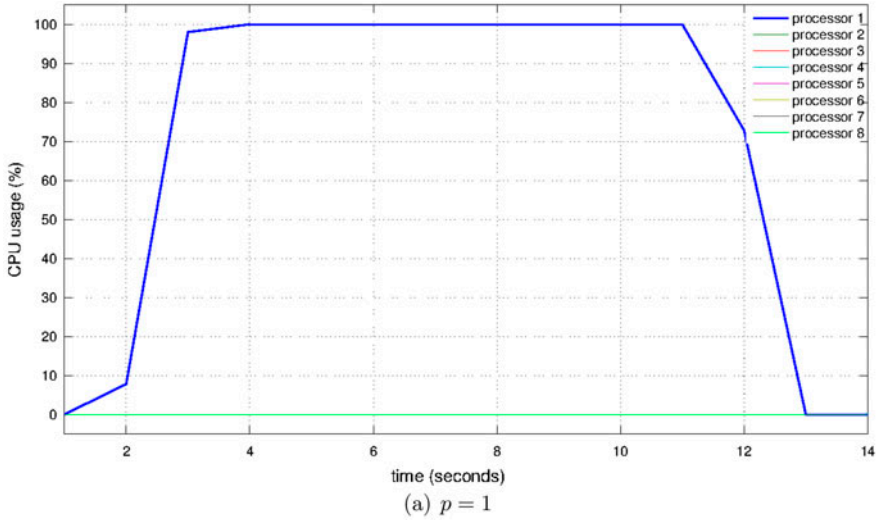
$$\begin{array}{lll} v_1 = (s_k^t)^\intercal y_k^t, & v_2 = (s_k^t)^\intercal s_k^t, & v_3 = (y_k^t)^\intercal y_k^t, \\ v_4 = (y_k^t)^\intercal g_k, & v_5 = g_k^\intercal g_k, & v_6 = (s_k^t)^\intercal g_k. \end{array} \tag{20}$$

Once the scalar values v_i, $i = 1, \ldots, 6$ are available, the multipliers $c_g(\sigma)$, $c_s(\sigma)$, $c_y(\sigma)$ in (16) can be computed in a total of 32 floating point operations as follows:

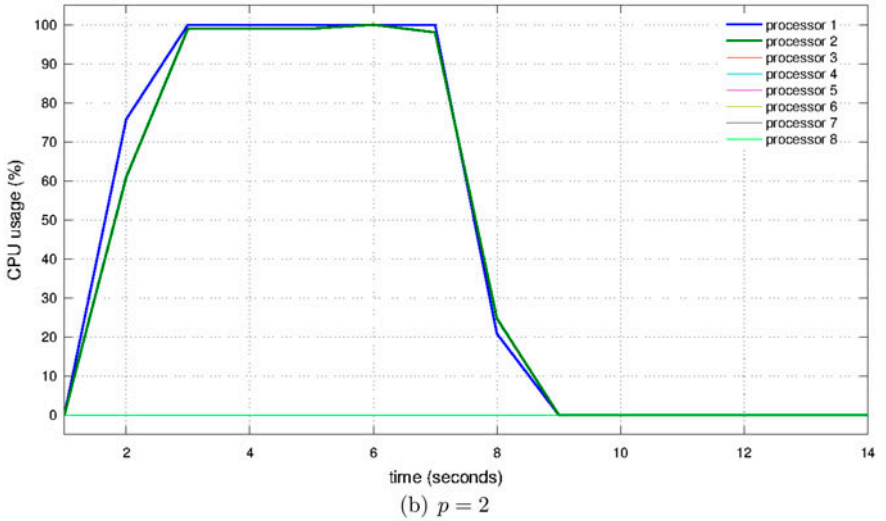
$$\begin{array}{lll} \sigma = \frac{1}{2}(\sqrt{v_2}(\sqrt{v_3} + \frac{1}{\eta}\sqrt{v_5}) - v_1), & \theta = (v_1 + 2\sigma)^2 - v_2 v_3, & c_g(\sigma) = \frac{-v_2}{2\sigma}, \\ c_s(\sigma) = c_g(\sigma)\left(-\frac{v_2+2\sigma}{\theta} v_4 + \frac{v_3}{\theta} v_6\right), & c_y(\sigma) = c_g(\sigma)\left(-\frac{v_2+2\sigma}{\theta} v_6 + \frac{v_2}{\theta} v_4\right). & \end{array} \tag{21}$$

Clearly, the total cost of synchronization operations is negligible. Thus, the parallel execution of the above inner products determine the parallel performance as well as the two remaining components of the algorithm: the computation of initial trial step s_k^0 and function/gradient evaluations. We require that s_k^0 is computed without introducing too much sequential work to the overall algorithm, and satisfy the conditions in Section 2. A simple choice could be the gradient step, which we have also preferred in our own parallel implementation.

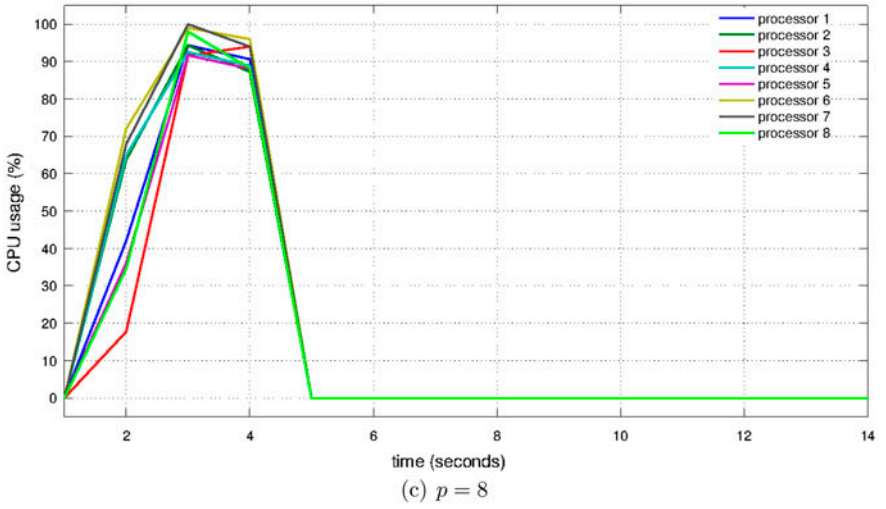
Algorithm 2 is considered for a shared memory environment with p physical cores (threads). Note that we have dropped the superscript t from s_k^t and used simply s_k. The parallel implementa-



(a) $p = 1$



(b) $p = 2$



(c) $p = 8$

Figure 3. CPU usage (per second) during the solution processes with 1,2, and 8 threads.

Table 2. Run times (in seconds) for varying values of n and p.

Problem	n	$p = 1$	$p = 2$	$p = 4$	$p = 8$	$p = 16$
COSINE	5M	8.80	4.41	2.24	1.29	0.89
	25M	43.98	22.07	11.19	6.33	4.35
	125M	219.77	111.74	57.98	31.62	21.47
NONCVXUN	5M	25.19	12.57	6.49	4.08	2.88
	25M	118.59	58.63	30.44	18.39	13.29
	125M	496.45	249.43	127.38	75.43	55.07
ROSENBR	5M	45.93	22.69	11.89	7.91	6.11
	25M	219.52	111.16	57.02	35.74	28.31
	125M	1113.83	554.07	283.83	178.41	140.60

tion of function/gradient computations is clearly problem-dependent. However – at least partial – separability is likely to occur for large-scale problems. This issue, we assume, is taken care of by the user.

Algorithm 2: Parallel Implementation

Input: x_0; $\rho \in (0, 1)$; $k = 0$
Compute f_0, g_0 (Parallel);
while x_k *is not a stationary point* **do**
  Compute the first trial step s_k;
  for $t = 0, 1, 2, \ldots$ **do**
    $x_k^t = x_k + s_k$ (Parallel);
    Compute f_k^t, g_k^t (Parallel);
    $v_6 = g_k^{\mathsf{T}} s_k$ (Parallel, $O(n/p)$);
    if $f_k - f_k^t \geq -\rho v_6$ **then**
      $x_{k+1} = x_k^t, f_{k+1} = f_k^t, g_{k+1} = g_k^t$;
      $k = k + 1$;
      break;
    end
    Compute $v_i, i = 1, 2, \ldots, 5$ as in (20) (Parallel, $O(n/p)$);
    Compute c_g, c_s, c_y as in (21) (Sequential, $O(1)$);
    $s_k \leftarrow c_g g_k + c_y y_k^t + c_s s_k$ (Parallel);
  end
end

We have implemented the algorithm in C using OpenMP. We have selected three test problems from the CUTEst collection [11], whose dimensions can be varied to obtain small- to large-scale problems, namely COSINE, NONCVXUN and ROSENBR. The objective functions of the problems, and the initial points used in our tests are as follows:

$$f(x) = \sum_{i=1}^{n-1} \cos(-0.5x_{i+1} + x_i^2), \qquad x_i^0 = 1.0, \qquad \text{(COSINE)}$$

$$f(x) = \sum_{i=1}^{n} x_i^2 + 4\cos(x_i), \qquad x_i^0 = \log(1.0 + i), \qquad \text{(NONCVXUN)}$$

$$f(x) = \sum_{i=1}^{n-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2, \qquad x_i^0 = 1.2, \qquad \text{(ROSENBR)}$$

where x_i denotes the ith component of point x and x^0 is the initial point. We note that the function and the gradient evaluations of all three test problems are in the order of $O(n)$. So, the function evaluation does not dominate the computations required for he new strategy. Moreover, the evaluations of all three functions can be done in parallel with one synchronization.

To test the parallelization performance of the algorithm, we set the dimension of the problems to 5 million, 25 million and 125 million, and solve each of the resulting instances for various values of the total number of threads, $p \in \{1, 2, 4, 8, 16\}$. We run the algorithm by setting $\eta = 0.5$, and the step acceptability is checked using condition (2) with $\rho = 0.1$. We set both the maximum number of inner iterations and the maximum number of outer iterations to 100. If the algorithm cannot reach a solution with the desired accuracy

$$\frac{\|\nabla f(x_k)\|}{\max\{||x_k||, 1\}} < 10^{-5},$$

then we report the clock time elapsed until the maximum number of outer iterations is reached. We summarize these results in Table 2. We observe that the speed-up is close to linear for up to eight cores. Since there is no data reuse, if we further increase the number of cores, the main memory bandwidth becomes the bottleneck. This is a common issue when memory-bounded computations, like inner product evaluations, are parallelized.

Finally, we consider the load balance issue. To observe the usage of capacity and the workload distribution, we plot the CPU usage during the solution of 1M-dimensional instance of the problem COSINE (see Figure 3). The plots are obtained by recording the CPU usage information per second via the `mpstat` command-line tool (see Linux manual pages). Figure 3(a) reveals the idle resources when the program runs sequentially. In fact, during the sequential run, the average resource usage stays at a level of 11.12%. This value is computed by taking the average usage of eight cores. When eight threads are used, this average raises up to 78.65%. Figure 3(c) shows the usage of all available resources as well as the distribution of the workload.

5. Conclusion and future research

The current study is a part of our research efforts that aim at harnessing parallel processing power for solving optimization problems. Our main motivation here was to present the design process that we went through to come up with an alternate globalization strategy for unconstrained optimization.

The proposed algorithm works with a model function and considers its optimization over an elliptical region. However, it does not employ a conventional trust-region approach, nor does it match with any one of the well-known quasi-Newton updates. The basic idea is to use multiple trial points for learning the function structure until a good point is obtained. These trials constitute the inner iterations. Fortunately, all these computations of the algorithm are domain-separable with two $O(1)$ synchronization points at each inner iteration.

Our numerical experience verifies that the direction updates of the resulting algorithm can reduce the total number of function evaluations required, and it is scalable to a degree allowed by the inner iterations with a balanced distribution of the workload among parallel processors. Like any parallel optimization method, the parallel performance of the proposed algorithm can be compromised if function evaluations are computationally intensive and unfit for parallelization.

We have only solved a set of examples with our algorithm. It is yet to be seen whether the algorithm is apt for solving other large-scale problems, especially those ones arising in different applications. In our implementation, we chose the initial trial point simply using the negative gradient step. One may try to integrate other, potentially more powerful but still parallelizable, steps to the algorithm. An example could be using a truncated Newton step; perhaps computed by a few iterations of the conjugate gradient on the initial quadratic model. Then switching to the globalization strategy, as described here, could adjust the direction and the length of the initial step. Finally, our observations

on the relationship of the new strategy with a quasi-Newton update method may be extended to other update methods. This point is in our future research agenda.

Notes

1. http://people.sabanciuniv.edu/sibirbil/glob_strat/OnlineSupplement.pdf.
2. https://github.com/sibirbil/PMBSolve.

Disclosure statement

No potential conflict of interest was reported by the authors.

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Appendix 1. Omitted proofs

The proofs that we have deferred in the main text are given in this section.

Lemma 1.1: *If constraint (5) holds at inner iteration $t+1$ of iteration k, then both $\alpha_k^0(s)$ and $\alpha_k^t(s)$ are nonnegative, and they satisfy $\alpha_k^0(s) + \alpha^t(s) = 1$.*

***Proof*:** We have

$$s^\mathsf{T} s_k^t - (s_k^t)^\mathsf{T} s_k^t = (s - s_k^t)^\mathsf{T}(-(s - s_k^t) + s) = -\|s - s_k^t\|^2 + s^\mathsf{T} s - s^\mathsf{T} s_k^t.$$

Since constraint (5) implies $s^\mathsf{T} s \leq s^\mathsf{T} s_k^t$, we obtain

$$0 \leq s^\mathsf{T} s_k^t \leq (s_k^t)^\mathsf{T} s_k^t.$$

The result follows from the definitions of $\alpha^0(s)$ and $\alpha^t(s)$. □

Lemma 1.2: *Let f be a convex function and consider the inner iteration $t+1$ of iteration k with $\|s_k^t\| \neq 0$. If $g_k^\mathsf{T} s_k^t \leq 0$, then $\|s_k^{t+1}\| \neq 0$ and*

$$\alpha^* := \arg\min_{0 \leq \alpha \leq 1} m_k^t(\alpha s_k^t) = \min\left\{ \frac{(y_k^t)^\mathsf{T} s_k^t - f_k^t + f_k}{2(y_k^t)^\mathsf{T} s_k^t}, 1 \right\}.$$

If we additionally have $f_k^t > f_k$, then $\alpha^* < 1$.

Proof: Using relation (7), we have

$$\nabla m_k^t(0) = g_k + \frac{1}{\|s_k^t\|^2}(f_k^t - (g_k^t)^\intercal s_k^t - f_k)s_k^t.$$

Since f is a convex function, we know that $f_k^t - (g_k^t)^\intercal s_k^t - f_k \leq 0$. If $f_k^t - (g_k^t)^\intercal s_k^t - f_k = 0$, then $\|\nabla m_k^t(0)\| = \|g_k\| \neq 0$ because x_k is not a stationary point. Now, consider the case $f_k^t - (g_k^t)^\intercal s_k^t - f_k < 0$, and suppose for contradiction that $\|\nabla m_k^t(0)\| = 0$. Then,

$$s_k^t = \frac{\|s_k^t\|^2}{f_k - f_k^t + (g_k^t)^\intercal s_k^t} g_k.$$

Multiplying both sides with g_k, we obtain

$$g_k^\intercal s_k^t = \frac{\|s_k^t\|^2}{f_k - f_k^t + (g_k^t)^\intercal s_k^t} \|g_k\|^2.$$

Since $g_k^\intercal s_k^t \leq 0$, we obtain a contradiction and hence $\|\nabla m_k^t(0)\| \neq 0$. This shows that $\|s_k^{t+1}\| \neq 0$. Note that

$$(s_k^t)^\intercal \nabla m_k^t(0) = g_k^\intercal s_k^t + f_k^t - (g_k^t)^\intercal s_k^t - f_k = f_k^t - f_k - (s_k^t)^\intercal (g_k^t - g_k) \leq 0.$$

This implies that s_k^t is a descent direction for $m_k^t(s)$ at $s = 0$. Then, it is easy to solve the one-dimensional convex optimization problem to obtain

$$\alpha^* = \arg\min_{0 \leq \alpha \leq 1} m_k^t(\alpha s_k^t) = \min\left\{ \frac{(y_k^t)^\intercal s_k^t - f_k^t + f_k}{2(y_k^t)^\intercal s_k^t}, 1 \right\}.$$

Again using relation (7), we have

$$\nabla m_k^t(s_k^t) = g_k^t - \frac{1}{\|s_k^t\|^2}(f_k + g_k{}^\intercal s_k^t - f_k^t)s_k^t,$$

which gives

$$-(s_k^t)^\intercal \nabla m_k^t(s_k^t) = -(g_k^t)^\intercal s_k^t + f_k + g_k^\intercal s_k^t - f_k^t = f_k - f_k^t - (s_k^t)^\intercal (g_k^t - g_k).$$

If $f_k^t < f_k$ along with $g_k^\intercal s_k^t \leq 0$, then

$$0 < f_k^t - f_k \leq (s_k^t)^\intercal (g_k^t - g_k)$$

holds. Therefore, we have $-(s_k^t)^\intercal \nabla m_k^t(s_k^t) \leq 0$, which implies that $(-s_k^t)$ is a descent direction for $m_k^t(s)$ at $s = s_k^t$. In this case, the minimizer along s_k^t should be in the interior. Thus, $\alpha^* < 1$. □