A Finite-Difference Trust-Region Method for Convexly Constrained Smooth Optimization

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Abstract

We propose a derivative-free trust-region method based on finite-difference gradient approximations for smooth optimization problems with convex constraints. The proposed method does not require computing an approximate stationarity measure. For nonconvex problems, we establish a worst-case complexity bound of $\mathcal{O}\Big(n\left(\frac{L}{\sigma}\epsilon\right)^{-2}\Big)$ function evaluations for the method to reach an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate stationary point, where n is the number of variables, L is the Lipschitz constant of the gradient, and σ is a user-defined estimate of L. If the objective function is convex, the complexity to reduce the functional residual below $(L/\sigma)\epsilon$ is shown to be of $\mathcal{O}\Big(n\left(\frac{L}{\sigma}\epsilon\right)^{-1}\Big)$ function evaluations, while for Polyak–Łojasiewicz functions on unconstrained domains, the bound further improves to $\mathcal{O}\left(n\log\left(\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)\right)$. Numerical experiments on benchmark problems and a model-fitting application demonstrate the method's efficiency relative to state-of-the-art derivative-free solvers for both unconstrained and bound-constrained problems.

1 Introduction

1.1 Problem and Contributions

We are interested to solve optimization problems of the form

$$\text{Minimize } f(x) \text{ subject to } x\in\Omega, \tag{1}$$

where $f:\mathbb{R}^n\to\mathbb{R}$ is assumed to be a continuously differentiable function with Lipschitz continuous gradient, and Ω is a nonempty closed convex set. Specifically, we consider the scenario where $f(\cdot)$ is a black-box function, i.e., given x, all we can compute is $f(x)$. Problems of this type appear in several applications (see, e.g., [1]), and require the use of *Derivative-Free Optimization* (DFO) methods [13, 5, 22].

In DFO, there exist two main classes of methods: *direct-search methods* and *model-based trust-region methods*. At each iteration of a direct-search method, a mesh of trial points is built around the current iterate. If one of them decreases sufficiently the objective function, then the point is accepted

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as the next iterate. Otherwise, the method remains at the current point and a new set of trial points is built. Regarding model-based trust-region methods, the aim at each iteration is to minimize an interpolation-based model inside a region around the current iterate. If the trial point resulting from the minimization of the model produces a sufficient decrease for the objective function, then the point is accepted as the next iterate, and the trust-region radius can be increased. Otherwise, the method stays at the same point, the radius is shrunk and the model is possibly rebuilt, before being minimized inside the new region.

For smooth optimization with convex constraints, the model-based trust-region methods BOBYQA and CDFO-TR were designed by Powell [26] and by Hough and Roberts [21], respectively. In the latter work, a worst-case evaluation complexity of $\mathcal{O}(n^3\epsilon^{-2})$ is proved for linear interpolation models of the objective function to bring the stationarity measure below ϵ. For unconstrained smooth and composite nonsmooth optimization, Garmanjani, Júdice and Vicente [17] proposed a model-based trust-region method enjoying a worst-case complexity bound of $\mathcal{O}\left(n^2\epsilon^{-2}\right)$ function evaluations to reach an ϵ-approximate stationary point.

Recently, improved worst-case evaluation complexities have been established in deterministic DFO by considering *finite-difference based methods*. For functions with Lipschitz continuous gradient, Grapiglia [18, 19] proposed methods based on finite differences with a quadratic regularization term for smooth unconstrained problems, enjoying the bounds of $\mathcal{O}\left(n\epsilon^{-2}\right)$, $\mathcal{O}\left(n\epsilon^{-1}\right)$ and $\mathcal{O}\left(n\log\left(\epsilon^{-1}\right)\right)$ evaluations when the function is possibly nonconvex, convex and strongly convex, respectively. For composite nonsmooth functions of the form $f(x) = h\left(F(x)\right)$ with convex constraints, worst-case evaluation complexity bounds have been established for TRFD [16], a derivative-free trust-region method based on finite differences. For specific instances, it was shown that TRFD requires no more than $\mathcal{O}\left(n\epsilon^{-2}\right)$ evaluations of $F\left(\,\cdot\,\right)$ to bring the stationarity measure below ϵ, and no more than $\mathcal{O}\left(n\epsilon^{-1}\right)$ evaluations to put the functional residual below ϵ when $h\left(F(\,\cdot\,)\right)$ is convex. However, TRFD requires to solve two trust-region subproblems: one to compute the approximate stationarity measure, and one to compute the trial step. Moreover, TRFD only relies on first-order approximations of the inner function by approximating the Jacobian of $F(\,\cdot\,)$ at x with forward finite differences. This makes TRFD uncompetitive with respect to methods that use second-order approximations for smooth problems, i.e., problems where $F:\mathbb{R}^n \to \mathbb{R}$ and $h(z) = z$, $\forall z \in \mathbb{R}$.

Therefore, in this paper we propose TRFD-S, a derivative-free trust-region method based on finite differences for smooth problems with convex feasible sets. Compared to the method proposed in [16], TRFD-S relies on quadratic models and assumes a weaker sufficient model decrease, which is expressed through a Cauchy decrease. Moreover, TRFD-S does not require the computation of the approximate stationarity measure, thereby reducing the cost per iteration to a single subproblem solve. Of course, such a reduction in the cost per iteration comes at the expense of slightly weaker worst-case complexity guarantees. Specifically, we prove that TRFD-S takes at most $\mathcal{O}\left(n\left(\frac{L}{\sigma}\epsilon\right)^{-2}\right)$ function evaluations to find an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate stationary point of $f\left(\,\cdot\,\right)$ in Ω for nonconvex problems, where σ is a user-defined estimate of the Lipschitz constant L. This bound is improved to $\mathcal{O}\left(n\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)$ to find an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate minimizer of $f\left(\,\cdot\,\right)$ in Ω, by assuming the objective function to be convex. In addition, a bound of $\mathcal{O}\left(n\log\left(\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)\right)$ is obtained for Polyak-Lojasiewicz functions to reach an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate minimizer of $f\left(\,\cdot\,\right)$, in the particular case where $\Omega = \mathbb{R}^n$. The appearance of the factor L/σ in our complexity bounds highlights a tradeoff determined by the choice of σ. When σ overestimates L, the method can ensure that the resulting stationarity measure lies below ϵ, though this may increase the number of function evaluations required in the worst-case. In contrast, when σ underestimates L, the oracle complexity decreases, but the method can only guarantee convergence to an approximate stationary point with reduced accuracy. Finally, we present numerical results, illustrating the relative efficiency of TRFD-S with respect to state-of-the-art derivative-free solvers such as NEWUOA [31], DFQRM [19], BOBYQA [31] and NOMAD [6]. We conducted experiments on both unconstrained test problems and constrained test problems with unrelaxable box constraints. Additionally, we evaluated the performance of TRFD-S on the calibration of an Ordinary Differential Equations (ODEs) model.

1.2 Contents

The paper is structured as follows. In Section 2, we give the assumptions and auxiliary results. In Section 3 we present TRFD-S for problems with relaxable convex constraints and prove worst-case evaluation complexity bounds for nonconvex, convex and Polyak-Lojasiewicz objective functions. In Section 4, we propose an adaptation of TRFD-S to unrelaxable bound constraints. Finally, in Section 5, we provide numerical results on benchmark problems for unconstrained and bound constraints sets, in addition to showing a model fitting application.

2 Assumptions and Auxiliary Results

Through the paper, we will consider the following assumptions:

A1. $\Omega \subset \mathbb{R}^n$ is a nonempty closed convex set.
A2. $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable and its gradient ∇f is L-Lipschitz with respect to the Euclidean norm.

In addition, the following definition of stationarity will be used.

Definition 2.1. *A point $x^* \in \Omega$ is a stationary point of f when*

$$\langle \nabla f(x^*), s \rangle \geq 0, \quad \forall s \in \Omega - \{x^*\}.$$

Definition 2.1 motivates the use of the following stationarity measure. Given $r > 0$, let us denote

$$\psi_r(x) = \frac{1}{r}\left(- \min_{\substack{s \in \Omega - \{x\} \\ \|s\| \leq r}} \langle \nabla f(x), s \rangle \right). \tag{2}$$

The lemma below provides some properties on this stationarity measure.

Lemma 2.2. *(Lemma 2.6 in [16]). Suppose that A1 and A2 hold, and let ψ_r be defined by (2). Then,*

(a) $\psi_r(x) \geq 0, \quad \forall x \in \Omega$;
(b) $\psi_r(x^*) = 0$ if, and only if, x^* is a stationary point of f in Ω.

In view of Lemma 2.2, we say that a point $x \in \Omega$ is an ϵ-approximate stationary point of f in Ω with respect to $r > 0$, when $\psi_r(x) \leq \epsilon$.

Since the gradient is supposed not to be accessible, the stationarity measure defined in (2) will be approached by

$$\eta_r(x) = \frac{1}{r}\left(-\min_{\substack{s\in\Omega-\{x\}\\ \|s\|\leq r}}\langle g, s\rangle\right), \tag{3}$$

where $g \in \mathbb{R}^n$ is an approximation to the gradient of f at x.

The following lemma gives a bound for $\|\nabla f(x) - g\|$ when g is a forward finite-difference approximation of $\nabla f(x)$.

Lemma 2.3. *(Lemma 2.8 in [16]). Suppose that A2 holds. Given $x \in \mathbb{R}^n$ and $\tau > 0$, let $g \in \mathbb{R}^n$ be defined by*

$$[g]_i = \frac{f(x+\tau e_i) - f(x)}{\tau}, \quad i = 1, ..., n.$$

Then,

$$\|\nabla f(x) - g\| \leq \frac{L}{2}\tau\sqrt{n}.$$

3 Trust-Region Method for Relaxable Convex Constraints

In what follows, we present TRFD-S, a derivative-free **T**rust-**R**egion method based on **F**inite **D**ifferences for **S**mooth problems with relaxable convex constraints, that is, problems in which function values can be computed at points outside the feasible set. At the k-th iteration of TRFD-S, an approximation g_k of $\nabla f(x_k)$ is built by using finite differences. Then, a step d_k is computed by solving approximately a trust-region subproblem, where the model to minimize is given by

$$m_k(d) = f(x_k) + \langle g_k, d\rangle + \frac{1}{2}\langle H_k d, d\rangle,$$

with H_k being an approximation to the Hessian of f at x_k. After, we assess the quality of the step d_k. If

$$\frac{f(x_k) - f(x_k + d_k)}{m_k(0) - m_k(d_k)} \geq \alpha,$$

with $\alpha \in (0, 1)$, then we define $x_{k+1} = x_k + d_k$, the trust-region radius can grow, and the finite-difference stepsize remains constant by defining $\tau_{k+1} = \tau_k$. Otherwise, the method sets $x_{k+1} = x_k$, the trust-region radius is halved, while the finite-difference stepsize is possibly reduced to ensure the following bound (see Assumption 4 in Conejo et al. [11] and (7)):

$$\|\nabla f(x_k) - g_k\| \leq \frac{L}{2}\Delta_k.$$

The trust-region radius keeps decreasing until the step is accepted. In what follows, we describe precisely the steps of our new method.

Algorithm 1: TRFD-S for relaxable convex constraints

Step 0. Given a feasible set Ω, an initial point $x_0 \in \Omega$, a parameter $\epsilon > 0$, an estimate $\sigma > 0$ of L, and a threshold $\alpha \in (0,1)$ for accepting trial points, define

$$\tau_0 = \frac{\epsilon}{\sigma\sqrt{n}}.$$

Choose an initial trust-region radius Δ_0 and an upper bound on the trust-region radii $\Delta_{\max}$ such that $\tau_0\sqrt{n} \leq \Delta_0 \leq \Delta_{\max}$, and set $k := 0$.

Step 1. Construct $g_k \in \mathbb{R}^n$ with

$$[g_k]_i = \frac{f(x_k + \tau_k e_i) - f(x_k)}{\tau_k}, \quad i = 1, ..., n,$$

and choose a nonzero symmetric matrix $H_k \in \mathbb{R}^{n\times n}$.

Step 2. Compute an approximate solution d_k of the trust-region subproblem

$$\begin{aligned} \min_{d\in\mathbb{R}^n} \quad & m_k(d) = f(x_k) + \langle g_k, d\rangle + \frac{1}{2}\langle H_k d, d\rangle \\ \text{s.t.} \quad & \|d\| \leq \Delta_k \\ & x_k + d \in \Omega \end{aligned}$$

such that

$$m_k(0) - m_k(d_k) \geq \kappa\eta_{\Delta_{\max}}(x_k) \min\left\{\Delta_k, \frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}\right\}, \tag{4}$$

where $\kappa \in (0,1)$ is a constant independent of k.

Step 3. Compute

$$\rho_k = \frac{f(x_k) - f(x_k + d_k)}{m_k(0) - m_k(d_k)}. \tag{5}$$

If $\rho_k \geq \alpha$, define $x_{k+1} = x_k + d_k$, $\Delta_{k+1} = \min\{2\Delta_k, \Delta_{\max}\}$, $\tau_{k+1} = \tau_k$, set $k := k+1$ and go to Step 1.

Step 4 Define $x_{k+1} = x_k$ and $\Delta_{k+1} = \frac{1}{2}\Delta_k$. If $\tau_k\sqrt{n} \leq \Delta_{k+1}$, define $\tau_{k+1} = \tau_k$, $g_{k+1} = g_k$, $H_{k+1} = H_k$, set $k := k+1$ and go to Step 2. Otherwise, define $\tau_{k+1} = \frac{1}{2}\tau_k$, set $k := k+1$ and go to Step 1.

Remark 3.1. *In contrast with TRFD [16] when applied to smooth optimization (i.e., the case $F : \mathbb{R}^n \to \mathbb{R}$ and $h(z) = z, \forall z \in \mathbb{R}$), TRFD-S approximates second-order information through H_k, which may be constructed from approximate first-order information using various strategies, such as the safeguarded BFGS update outlined in Subsection 5.1.1. In addition, TRFD requires to compute two trust-region subproblems per iteration, while TRFD-S only needs to solve one. Finally, TRFD assumes that the model decrease is at least proportional to a fraction of the exact model decrease, while TRFD-S assumes inequality* (4)*. In the case where $\Omega = \mathbb{R}^n$, condition* (4) *is naturally satisfied by any step at least as good as the Cauchy step. In the case where $\Omega \neq \mathbb{R}^n$ and A1 holds, condition* (4) *is also guaranteed by any step at least as good as the Generalized Cauchy step, which can be* *computed by Algorithm 12.2.2 in [12]. Notice that despite condition* (4)*, TRFD-S never computes* $\eta_{\Delta_{\max}}(x_k)$*.*

In TRFD-S, we have the following sets of iterations:

1. **Successful iterations** ($\mathcal{S}$): those where $\rho_k \geq \alpha$.
2. **Unsuccessful iterations of type I** ($\mathcal{U}^{(1)}$): those where $\rho_k < \alpha$ and $\tau_k\sqrt{n} \leq \Delta_{k+1}$.
3. **Unsuccessful iterations of type II** ($\mathcal{U}^{(2)}$): those where $\rho_k < \alpha$ and $\tau_k\sqrt{n} > \Delta_{k+1}$.

The lemma below shows that the finite-difference stepsize τ_k is always bounded from above by $\Delta_k/\sqrt{n}$.

Lemma 3.2. *Given* $T \geq 1$*, let* $\{\tau_k\}_{k=0}^{T}$ *and* $\{\Delta_k\}_{k=0}^{T}$ *be generated by TRFD-S. Then*

$$\tau_k\sqrt{n} \leq \Delta_k, \quad \textit{for} \quad k = 0, ..., T. \tag{6}$$

Proof. Let us work through an induction argument. By Step 0 of TRFD-S, we have that (6) holds for $k = 0$. By assuming (6) to be true for some $k \in \{0, ..., T-1\}$, let us show that (6) also holds for $k+1$. With our sets of iterations, we have three possible cases:

Case I: $k \in \mathcal{S}$.

By Step 3 of TRFD-S, we have $\tau_{k+1} = \tau_k$ and $\Delta_{k+1} \geq \Delta_k$. Thus, by the induction assumption,

$$\tau_{k+1}\sqrt{n} = \tau_k\sqrt{n} \leq \Delta_k \leq \Delta_{k+1},$$

which means that (6) is true for $k+1$.

Case II: $k \in \mathcal{U}^{(1)}$.

By Step 4 of TRFD-S, we have $\tau_{k+1} = \tau_k$ and $\tau_k\sqrt{n} \leq \Delta_{k+1}$. Then,

$$\tau_{k+1}\sqrt{n} = \tau_k\sqrt{n} \leq \Delta_{k+1},$$

so (6) is true for $k+1$.

Case III: $k \in \mathcal{U}^{(2)}$.

By Step 4 of TRFD-S, we have $\tau_{k+1} = \frac{1}{2}\tau_k$ and $\Delta_{k+1} = \frac{1}{2}\Delta_k$. Thus, by using the induction assumption, we have

$$\tau_{k+1}\sqrt{n} = \frac{1}{2}\tau_k\sqrt{n} \leq \frac{1}{2}\Delta_k = \Delta_{k+1},$$

that is, (6) is true for $k+1$, which concludes the proof. □

In view of Lemmas 2.3 and 3.2, the finite-difference approximation g_k in TRFD-S satisfies

$$\|\nabla f(x_k) - g_k\| \leq \frac{L}{2}\Delta_k, \quad \forall k \geq 0. \tag{7}$$

Using the previous inequality, the next lemma proves that if the trust-region radius is sufficiently small, then $k \in \mathcal{S}$.

Lemma 3.3. *Suppose that A1 and A2 hold, and let x_k be generated by TRFD-S. If*

$$\Delta_k \leq \frac{(1-\alpha)\kappa\eta_{\Delta_{\max}}(x_k)}{2L+\|H_k\|}, \tag{8}$$

then $k \in \mathcal{S}$, where κ is the constant in (4).

Proof. By (5), A2, (4) and (7), we have

$$\begin{aligned}
1-\rho_k &= \frac{m_k(0)-m_k(d_k)-(f(x_k)-f(x_k+d_k))}{m_k(0)-m_k(d_k)} \\
&\leq \frac{f(x_k+d_k)-f(x_k)-\langle\nabla f(x_k),d_k\rangle+\langle\nabla f(x_k),d_k\rangle-\langle g_k,d_k\rangle-\frac{1}{2}\langle H_kd_k,d_k\rangle}{m_k(0)-m_k(d_k)} \\
&\leq \frac{|f(x_k+d_k)-f(x_k)-\langle\nabla f(x_k),d_k\rangle|+|\langle\nabla f(x_k),d_k\rangle-\langle g_k,d_k\rangle|+\left|\frac{1}{2}\langle H_kd_k,d_k\rangle\right|}{\kappa\eta_{\Delta_{\max}}(x_k)\min\left\{\Delta_k,\frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}\right\}} \\
&\leq \frac{\frac{L}{2}\|d_k\|^2+\|\nabla f(x_k)-g_k\|\|d_k\|+\frac{1}{2}\|H_k\|\|d_k\|^2}{\kappa\eta_{\Delta_{\max}}(x_k)\min\left\{\Delta_k,\frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}\right\}} \\
&\leq \frac{\frac{L}{2}\Delta_k^2+\frac{L}{2}\Delta_k^2+\frac{\|H_k\|}{2}\Delta_k^2}{\kappa\eta_{\Delta_{\max}}(x_k)\min\left\{\Delta_k,\frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}\right\}} \\
&< \frac{(2L+\|H_k\|)\Delta_k^2}{\kappa\eta_{\Delta_{\max}}(x_k)\min\left\{\Delta_k,\frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}\right\}}.
\end{aligned}$$

Since $\alpha \in (0,1)$, $\kappa \in (0,1)$ and $2L > 0$, by (8) we get

$$\Delta_k < \frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}.$$

So, it follows that

$$1-\rho_k \leq \frac{(2L+\|H_k\|)\Delta_k}{\kappa\eta_{\Delta_{\max}}(x_k)}.$$

Finally, by (8) we have

$$1-\rho_k \leq 1-\alpha.$$

Thus, we get $\rho_k \geq \alpha$, meaning that $k \in \mathcal{S}$, which concludes the proof. □

The next lemma bounds the error $|\psi_{\Delta_{\max}}(x_k)-\eta_{\Delta_{\max}}(x_k)|$ with the same quantity as for $\|\nabla f(x_k)-g_k\|$.

Lemma 3.4. *(Lemma 2.10 in [16]). Suppose that A1 and A2 hold, and let x_k be generated by TRFD-S. Then,*

$$|\psi_{\Delta_{\max}}(x_k)-\eta_{\Delta_{\max}}(x_k)| \leq \frac{L}{2}\tau_k\sqrt{n}. \tag{9}$$

By using the tolerance $\left(\frac{L}{\sigma}\epsilon\right)$, the following lemma provides a lower bound on the approximate stationarity measure $\eta_{\Delta_{\max}}(x_k)$.

Lemma 3.5. *Suppose that A1 and A2 hold, and let x_k be generated by TRFD-S. If*

$$\psi_{\Delta_{\max}}(x_k) > \left(\frac{L}{\sigma}\epsilon\right), \tag{10}$$

then

$$\eta_{\Delta_{\max}}(x_k) > \frac{1}{2}\left(\frac{L}{\sigma}\epsilon\right). \tag{11}$$

Proof. By the update rules of TRFD-S, we have

$$\tau_k \leq \tau_0, \quad \forall k \geq 0. \tag{12}$$

Then, by Lemma 3.4, (12), the definition of τ_0 in Step 0 of TRFD-S and (10), it follows that

$$\begin{aligned}\psi_{\Delta_{\max}}(x_k) &\leq |\psi_{\Delta_{\max}}(x_k) - \eta_{\Delta_{\max}}(x_k)| + \eta_{\Delta_{\max}}(x_k) \leq \frac{L}{2}\tau_k\sqrt{n} + \eta_{\Delta_{\max}}(x_k) \\ &\leq \frac{L}{2}\tau_0\sqrt{n} + \eta_{\Delta_{\max}}(x_k) = \frac{L}{2}\frac{\epsilon}{\sigma} + \eta_{\Delta_{\max}}(x_k) \\ &< \frac{1}{2}\psi_{\Delta_{\max}}(x_k) + \eta_{\Delta_{\max}}(x_k).\end{aligned}$$

Thus, we get

$$\eta_{\Delta_{\max}}(x_k) > \frac{1}{2}\psi_{\Delta_{\max}}(x_k). \tag{13}$$

Therefore, by (10), it follows that (11) is true. □

Now let us consider the following assumption on the matrix H_k:

A3. There exists a nonzero positive constant M such that $\|H_k\| \leq M$, for all $k \geq 0$.

The next lemma gives a lower bound on the trust-region radius Δ_k.

Lemma 3.6. *Suppose that A1-A3 hold. Given $T \geq 1$, let $\{\Delta_k\}_{k=0}^{T}$ be generated by TRFD-S. If*

$$\psi_{\Delta_{\max}}(x_k) > \left(\frac{L}{\sigma}\epsilon\right), \quad \textit{for} \quad k = 0, ..., T-1,$$

then

$$\Delta_k \geq \frac{(1-\alpha)\kappa}{8L+4M}\left(\frac{L}{\sigma}\epsilon\right) \equiv \Delta_{\min}(\epsilon), \quad \textit{for} \quad k = 0, \ldots, T, \tag{14}$$

where κ is the constant in (4).

Proof. For $k = 0$, by Step 0 of TRFD-S, since $\alpha \in (0,1)$, $\kappa \in (0,1)$ and $\frac{L}{8L+4M} \in (0,1)$, we have

$$\Delta_0 \geq \tau_0\sqrt{n} = \frac{\epsilon}{\sigma} > \frac{(1-\alpha)\kappa}{8L+4M}\left(\frac{L}{\sigma}\epsilon\right) = \Delta_{\min}(\epsilon).$$

So, (14) is true for $k = 0$. Now, let us assume that (14) is true for some $k \in \{0, \ldots, T-1\}$. On one hand, if $\rho_k \geq \alpha$, then Step 3 of TRFD-S and the induction assumption imply that

$$\Delta_{k+1} \geq \Delta_k \geq \Delta_{\min}(\epsilon).$$

On the other hand, if $\rho_k < \alpha$, then by Lemmas 3.3, 3.5 and A3, we must have

$$\Delta_k > \frac{(1-\alpha)\kappa}{2L+M}\frac{1}{2}\left(\frac{L}{\sigma}\epsilon\right), \tag{15}$$

since otherwise we would have $\rho_k \geq \alpha$, contradicting the assumption that $\rho_k < \alpha$. Then, by the update rule in Step 4 of TRFD-S and (15), it follows that

$$\Delta_{k+1} = \frac{1}{2}\Delta_k > \frac{(1-\alpha)\kappa}{8L+4M}\left(\frac{L}{\sigma}\epsilon\right) = \Delta_{\min}(\epsilon),$$

which shows that (14) is true. □

3.1 Worst-Case Complexity Bound for Nonconvex Problems

Given $j \in \{0, 1, \ldots\}$, let

$$\begin{aligned} \mathcal{S}_j &= \{0,\ldots,j\} \cap \mathcal{S}, \\ \mathcal{U}_j^{(1)} &= \{0,\ldots,j\} \cap \mathcal{U}^{(1)}, \\ \mathcal{U}_j^{(2)} &= \{0,\ldots,j\} \cap \mathcal{U}^{(2)}. \end{aligned}$$

Also, let

$$T_g(\epsilon) = \inf\left\{k \in \mathbb{N} \,:\, \psi_{\Delta_{\max}}(x_k) \leq \left(\frac{L}{\sigma}\epsilon\right)\right\} \tag{16}$$

be the first iteration index reaching an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate stationary point of f in Ω, if it exists. Our goal is to obtain a finite upper bound for $T_g(\epsilon)$. If $T_g(\epsilon) \geq 1$, it follows from the notation above that

$$T_g(\epsilon) = \left|\mathcal{S}_{T_g(\epsilon)-1}\right| + \left|\mathcal{U}^{(1)}_{T_g(\epsilon)-1} \cup \mathcal{U}^{(2)}_{T_g(\epsilon)-1}\right|. \tag{17}$$

In the next two lemmas, we will provide upper bounds for the two terms in (17). To that end, let us consider the following additional assumption:

A4. There exists $f_{low} \in \mathbb{R}$ such that $f(x) \geq f_{low}$, for all $x \in \Omega$.

The next lemma provides an upper bound on $\left|\mathcal{S}_{T_g(\epsilon)-1}\right|$.

Lemma 3.7. *Suppose that A1-A4 hold, and assume that $T_g(\epsilon) \geq 1$. Then*

$$\left|\mathcal{S}_{T_g(\epsilon)-1}\right| \leq \frac{(16L+8M)(f(x_0)-f_{low})}{\alpha(1-\alpha)\kappa^2}\left(\frac{L}{\sigma}\epsilon\right)^{-2},$$

where κ is the constant in (4).

Proof. Given $k \in \mathcal{S}_{T_g(\epsilon)-1}$, by (5), (4), Lemmas 3.5, 3.6 and A3, we have

$$f(x_k) - f(x_{k+1}) \geq \alpha\kappa\eta_{\Delta_{\max}}(x_k)\min\left\{\Delta_k, \frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}\right\}$$

$$> \frac{\alpha\kappa}{2}\left(\frac{L}{\sigma}\epsilon\right)\min\left\{\frac{(1-\alpha)\kappa}{8L+4M}\left(\frac{L}{\sigma}\epsilon\right),\frac{1}{2M}\left(\frac{L}{\sigma}\epsilon\right)\right\}.$$

Since $\alpha \in (0,1)$, $\kappa \in (0,1)$ and $L > 0$, it follows that

$$f(x_k) - f(x_{k+1}) \geq \frac{\alpha(1-\alpha)\kappa^2}{16L+8M}\left(\frac{L}{\sigma}\epsilon\right)^2, \quad \text{when } k \in \mathcal{S}_{T_g(\epsilon)-1}. \tag{18}$$

Notice that when $k \notin \mathcal{S}_{T_g(\epsilon)-1}$, then $f(x_k) = f(x_{k+1})$. So, by A4 and (18) we get

$$\begin{aligned} f(x_0) - f_{low} &\geq f(x_0) - f(x_{T_g(\epsilon)}) = \sum_{k=0}^{T_g(\epsilon)-1} f(x_k) - f(x_{k+1}) = \sum_{k \in \mathcal{S}_{T_g(\epsilon)-1}} f(x_k) - f(x_{k+1}) \\ &\geq \left|\mathcal{S}_{T_g(\epsilon)-1}\right| \frac{\alpha(1-\alpha)\kappa^2}{16L+8M}\left(\frac{L}{\sigma}\epsilon\right)^2, \end{aligned}$$

which concludes the proof. □

The lemma below provides an upper bound on $\left|\mathcal{U}^{(1)}_{T_g(\epsilon)-1} \cup \mathcal{U}^{(2)}_{T_g(\epsilon)-1}\right|$.

Lemma 3.8. *Suppose that A1-A3 hold, and assume that $T_g(\epsilon) \geq 1$. If $T \in \{1,\ldots,T_g(\epsilon)\}$, then*

$$\left|\mathcal{U}^{(1)}_{T-1} \cup \mathcal{U}^{(2)}_{T-1}\right| \leq \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right) + |\mathcal{S}_{T-1}|, \tag{19}$$

where κ is the constant in (4)*.*

Proof. By the update rules for Δ_k in TRFD-S, we have

$$\Delta_{k+1} \leq 2\Delta_k, \quad \text{if} \quad k \in \mathcal{S}_{T-1}, \tag{20}$$

$$\Delta_{k+1} = \frac{1}{2}\Delta_k, \quad \text{if} \quad k \in \mathcal{U}^{(1)}_{T-1} \cup \mathcal{U}^{(2)}_{T-1}. \tag{21}$$

In addition, by Lemma 3.6 we have

$$\Delta_k \geq \Delta_{\min}(\epsilon), \quad \text{for} \quad k = 0,\ldots,T, \tag{22}$$

where $\Delta_{\min}(\epsilon)$ is defined in (14). So, in view of (20)-(22), it follows that

$$2^{|\mathcal{S}_{T-1}| - \left|\mathcal{U}^{(1)}_{T-1} \cup \mathcal{U}^{(2)}_{T-1}\right|}\Delta_0 \geq \Delta_T \geq \Delta_{\min}(\epsilon),$$

which gives

$$2^{|\mathcal{S}_{T-1}| - \left|\mathcal{U}^{(1)}_{T-1} \cup \mathcal{U}^{(2)}_{T-1}\right|} \geq \frac{\Delta_{\min}(\epsilon)}{\Delta_0}.$$

Then, taking the logarithm on both sides, we get

$$|\mathcal{S}_{T-1}| - \left|\mathcal{U}^{(1)}_{T-1} \cup \mathcal{U}^{(2)}_{T-1}\right| \geq \log_2\left(\frac{\Delta_{\min}(\epsilon)}{\Delta_0}\right),$$

which is equivalent to

$$\left|\mathcal{U}^{(1)}_{T-1} \cup \mathcal{U}^{(2)}_{T-1}\right| \leq \log_2\left(\frac{\Delta_0}{\Delta_{\min}(\epsilon)}\right) + |\mathcal{S}_{T-1}|. \tag{23}$$

Therefore, by the definition of $\Delta_{\min}(\epsilon)$ in (14), we conclude that (19) is true. □

Combining the previous results, we obtain the following worst-case iteration complexity bound of TRFD-S to find an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate stationary point of f in Ω.

Theorem 3.9. *Suppose that A1-A4 hold, and let $T_g(\epsilon)$ be defined by* (16). *Then*

$$T_g(\epsilon) \leq \frac{(32L + 16M)(f(x_0) - f_{low})}{\alpha(1-\alpha)\kappa^2} \left(\frac{L}{\sigma}\epsilon\right)^{-2} + \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right) + 1, \tag{24}$$

where κ is the constant in (4).

Proof. If $T_g(\epsilon) \leq 1$, then we have that (24) is true. Let us assume that $T_g(\epsilon) \geq 2$. By (17),

$$T_g(\epsilon) = \left|\mathcal{S}_{T_g(\epsilon)-1}\right| + \left|\mathcal{U}^{(1)}_{T_g(\epsilon)-1} \cup \mathcal{U}^{(2)}_{T_g(\epsilon)-1}\right|.$$

Then, (24) follows from Lemmas 3.7 and 3.8. □

Since each iteration of TRFD-S requires at most $(n+1)$ evaluations of f, from Theorem 3.9 we obtain the following upper bound on the number of function evaluations required by TRFD-S to find an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate stationary point of f in Ω.

Corollary 3.10. *Suppose that A1-A4 hold, and let $FE_{T_g(\epsilon)}$ be the number of function evaluations executed by TRFD-S up to the $(T_g(\epsilon)-1)$-st iteration. Then*

$$FE_{T_g(\epsilon)} \leq (n+1)\left[\frac{(32L + 16M)(f(x_0) - f_{low})}{\alpha(1-\alpha)\kappa^2} \left(\frac{L}{\sigma}\epsilon\right)^{-2} + \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right) + 1\right]. \tag{25}$$

In view of (25), TRFD-S needs no more than

$$\mathcal{O}\left(n\left(\frac{\sigma}{L}\right)^2 L\left(f(x_0) - f_{low}\right)\epsilon^{-2}\right) \tag{26}$$

function evaluations to reach a point $x_k \in \Omega$ such that $\psi_{\Delta_{\max}}(x_k) \leq \frac{L}{\sigma}\epsilon$. Therefore, in the case where the user-defined parameter σ equals the Lipschitz constant L, we get a worst-case evaluation complexity of

$$\mathcal{O}\left(nL\left(f(x_0) - f_{low}\right)\epsilon^{-2}\right) \tag{27}$$

to satisfy $\psi_{\Delta_{\max}}(x_k) \leq \epsilon$. Otherwise, when $\sigma \neq L$, Table 1 shows the different impacts of σ.

Value of σ	Impact on (26)	Impact on the target accuracy $(\frac{L}{\sigma}\epsilon)$
$\sigma < L$	(26) lower than (27) by a quadratic factor $\left(\frac{\sigma}{L}\right)^2$	Accuracy weaker than ϵ by a factor $\left(\frac{L}{\sigma}\right)$
$\sigma > L$	(26) larger than (27) by a quadratic factor $\left(\frac{\sigma}{L}\right)^2$	Accuracy stricter than ϵ by a factor $\left(\frac{L}{\sigma}\right)$

Table 1: Impacts of the user-defined parameter σ for nonconvex problems

3.2 Worst-Case Complexity Bound for Convex Problems

Let us consider two additional assumptions:

A5. f is convex.

A6. f has a global minimizer x^* in Ω and

$$D_0 \equiv \sup_{x\in\mathcal{L}_f(x_0)} \{\|x - x^*\|\} < +\infty,$$

for $\mathcal{L}_f(x_0) = \{x \in \Omega \, : \, f(x) \leq f(x_0)\}$.

The lemma below establishes the relationship between the stationarity measure and the functional residual when the reference radius r is sufficiently large.

Lemma 3.11. *(Lemma 3.14 in [16]). Suppose that A1, A2, A5 and A6 hold, and let $x_k \in \mathcal{L}_f(x_0)$. If $r \geq D_0$, then*

$$\psi_r(x_k) \geq \frac{f(x_k) - f(x^*)}{r}.$$

The next lemma provides a lower bound on the approximate stationarity measure $\eta_{\Delta_{\max}}(x_k)$ in terms of the functional residual.

Lemma 3.12. *Suppose that A1, A2, A5 and A6 hold, and let x_k be generated by TRFD-S. If $\Delta_{\max} \geq D_0$ and*

$$f(x_k) - f(x^*) > \Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right), \tag{28}$$

then

$$\eta_{\Delta_{\max}}(x_k) > \frac{f(x_k) - f(x^*)}{2\Delta_{\max}}. \tag{29}$$

Proof. By Lemma 3.11 and (28), it follows that

$$\psi_{\Delta_{\max}}(x_k) > \left(\frac{L}{\sigma}\epsilon\right). \tag{30}$$

Therefore, by (13) and Lemma 3.11, we obtain (29), which concludes the proof. □

Next, we establish an upper bound for $\frac{f(x_k)-f(x^*)}{\Delta_k}$.

Lemma 3.13. *Suppose that A1-A3, A5 and A6 hold. Given $T \geq 1$, let $\{x_k\}_{k=0}^T$ and $\{\Delta_k\}_{k=0}^T$ be generated by TRFD-S. If $\Delta_{\max} \geq D_0$ and*

$$f(x_k) - f(x^*) > \Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right), \quad \textit{for} \quad k = 0, ..., T-1,$$

then

$$\left(\frac{1}{\Delta_k}\right)(f(x_k) - f(x^*)) \leq \max\left\{\left(\frac{1}{\Delta_0}\right)(f(x_0) - f(x^*)), \frac{(8L+4M)\Delta_{\max}}{(1-\alpha)\kappa}\right\} \equiv \beta, \tag{31}$$

for $k = 0, \ldots, T$, where κ is the constant in (4).

Proof. By the definition of β, (31) is true for $k = 0$. Suppose that (31) is true for some $k \in \{0, \ldots, T-1\}$. Let us show that it is also true for $k+1$.

In the case where $\rho_k \geq \alpha$, by Step 3 of TRFD-S we have $\Delta_{k+1} \geq \Delta_k$. Since $f(x_{k+1}) \leq f(x_k)$, it follows that

$$\left(\frac{1}{\Delta_{k+1}}\right)(f(x_{k+1}) - f(x^*)) \leq \left(\frac{1}{\Delta_k}\right)(f(x_k) - f(x^*)) \leq \beta,$$

where the last inequality is the induction assumption. Therefore, (31) holds for $k+1$ in this case. In the case where $\rho_k < \alpha$, by Step 4 of TRFD-S we have

$$\Delta_{k+1} = \frac{1}{2}\Delta_k. \tag{32}$$

In addition, in view of Lemma 3.3 and A3, we must have

$$\Delta_k > \frac{(1-\alpha)\kappa\eta_{\Delta_{\max}}(x_k)}{2L+M}, \tag{33}$$

since otherwise, by Lemma 3.3, we would have $\rho_k \geq \alpha$, contradicting our assumption that $\rho_k < \alpha$. Notice that (33) is equivalent to

$$\left(\frac{1}{\Delta_k}\right)\eta_{\Delta_{\max}}(x_k) < \frac{2L+M}{(1-\alpha)\kappa}. \tag{34}$$

Finally, it follows from (32), Lemma 3.12 and (34) that

$$\begin{aligned}\left(\frac{1}{\Delta_{k+1}}\right)(f(x_{k+1}) - f(x^*)) &= \left(\frac{2}{\Delta_k}\right)(f(x_{k+1}) - f(x^*)) = \left(\frac{2}{\Delta_k}\right)(f(x_k) - f(x^*)) \\ &< \frac{4\Delta_{\max}}{\Delta_k}\eta_{\Delta_{\max}}(x_k) < 4\Delta_{\max}\frac{2L+M}{(1-\alpha)\kappa} \\ &\leq \beta,\end{aligned}$$

that is, (31) also holds for $k+1$ in this case, which concludes the proof. □

Let

$$T_f(\epsilon) = \inf\left\{k \in \mathbb{N} \,:\, f(x_k) - f(x^*) \leq \Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right)\right\} \tag{35}$$

be the first iteration index reaching a $\Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right)$-approximate solution of (1) in Ω, if it exists. Our goal is to establish a finite upper bound for $T_f(\epsilon)$. In this context, the lemma below provides an upper bound on $\left|\mathcal{S}_{T_f(\epsilon)-1}\right|$.

Lemma 3.14. *Suppose that A1-A3, A5 and A6 hold, and assume that $T_f(\epsilon) \geq 2$. If $\Delta_{\max} \geq D_0$, then*

$$\left|\mathcal{S}_{T_f(\epsilon)-1}\right| \leq 1 + \frac{2\beta}{\alpha\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}, \tag{36}$$

where β is defined in (31) *and κ is the constant in* (4)*.*

Proof. Let $k \in \mathcal{S}_{T_f(\epsilon)-2}$. By (5), (4), Lemmas 3.12, 3.13 and A3, we have

$$\begin{aligned} f(x_k) - f(x_{k+1}) &\geq \alpha\kappa\eta_{\Delta_{\max}}(x_k)\min\left\{\Delta_k, \frac{\eta_{\Delta_{\max}}(x_k)}{\|H_k\|}\right\} \\ &\geq \alpha\kappa\frac{f(x_k)-f(x^*)}{2\Delta_{\max}}\min\left\{\frac{f(x_k)-f(x^*)}{\beta}, \frac{f(x_k)-f(x^*)}{2\Delta_{\max}M}\right\} \\ &= \frac{\alpha\kappa(f(x_k)-f(x^*))^2}{2\Delta_{\max}}\min\left\{\frac{1}{\beta}, \frac{1}{2\Delta_{\max}M}\right\}. \end{aligned}$$

By the definition of β in (31), since $\alpha \in (0,1)$, $\kappa \in (0,1)$ and $L > 0$, we get

$$f(x_k) - f(x_{k+1}) \geq \frac{\alpha\kappa(f(x_k)-f(x^*))^2}{2\Delta_{\max}\beta}. \tag{37}$$

Denoting $\delta_k = f(x_k) - f(x^*)$, (37) becomes

$$\delta_k - \delta_{k+1} \geq \frac{\alpha\kappa}{2\Delta_{\max}\beta}\delta_k^2.$$

Consequently,

$$\frac{1}{\delta_{k+1}} - \frac{1}{\delta_k} = \frac{\delta_k - \delta_{k+1}}{\delta_k\delta_{k+1}} \geq \frac{\frac{\alpha\kappa}{2\Delta_{\max}\beta}\delta_k^2}{\delta_k^2} = \frac{\alpha\kappa}{2\Delta_{\max}\beta}, \quad \text{when } k \in \mathcal{S}_{T_f(\epsilon)-2}. \tag{38}$$

Since $\delta_{k+1} = \delta_k$ for any $k \notin \mathcal{S}_{T_f(\epsilon)-2}$, it follows from (38) that

$$\frac{1}{\delta_{T_f(\epsilon)-1}} - \frac{1}{\delta_0} = \sum_{k=0}^{T_f(\epsilon)-2}\frac{1}{\delta_{k+1}} - \frac{1}{\delta_k} = \sum_{k\in\mathcal{S}_{T_f(\epsilon)-2}}\frac{1}{\delta_{k+1}} - \frac{1}{\delta_k} \geq \left|\mathcal{S}_{T_f(\epsilon)-2}\right|\frac{\alpha\kappa}{2\Delta_{\max}\beta}.$$

Therefore, as $\delta_0 > 0$, we have

$$\Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right) < f(x_{T_f(\epsilon)-1}) - f(x^*) = \delta_{T_f(\epsilon)-1} \leq \frac{2\Delta_{\max}\beta}{\alpha\kappa\left|\mathcal{S}_{T_f(\epsilon)-2}\right|},$$

which implies

$$\left|\mathcal{S}_{T_f(\epsilon)-1}\right| \leq 1 + \left|\mathcal{S}_{T_f(\epsilon)-2}\right| < 1 + \frac{2\beta}{\alpha\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1},$$

that is, (36) is true. □

The next lemma establishes the relationship between $T_f(\epsilon)$ and $T_g(\epsilon)$.

Lemma 3.15. *Suppose that A1, A2, A5 and A6 hold, and let $T_f(\epsilon)$ and $T_g(\epsilon)$ be defined by* (35) *and* (16)*, respectively. If $\Delta_{\max} \geq D_0$, then $T_f(\epsilon) \leq T_g(\epsilon)$.*

Proof. Suppose by contradiction that $T_f(\epsilon) > T_g(\epsilon)$. Then, by $\Delta_{\max} \geq D_0$, Lemma 3.11 and the definition of $T_g(\epsilon)$, we would have the contradiction

$$\left(\frac{L}{\sigma}\epsilon\right) < \frac{f(x_{T_g(\epsilon)}) - f(x^*)}{\Delta_{\max}} \leq \psi_{\Delta_{\max}}(x_{T_g(\epsilon)}) \leq \left(\frac{L}{\sigma}\epsilon\right).$$

So, we conclude that $T_f(\epsilon) \leq T_g(\epsilon)$. □

The following theorem gives an upper bound on the number of iterations required by TRFD-S to reach a $\Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right)$-approximate solution of (1) in Ω, when f is a convex function.

Theorem 3.16. *Suppose that A1-A3, A5 and A6 hold, and let $T_f(\epsilon)$ be defined by* (35)*. If $\Delta_{\max} \geq D_0$, then*

$$T_f(\epsilon) \;\leq\; \frac{4\beta}{\alpha\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1} \;+\; \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right) + 2, \tag{39}$$

where β is defined in (31) *and κ is the constant in* (4)*.*

Proof. If $T_f(\epsilon) \leq 1$, then (39) is true. Let us assume that $T_f(\epsilon) \geq 2$. Similarly as in (17), we have

$$T_f(\epsilon) = \left|\mathcal{S}_{T_f(\epsilon)-1}\right| + \left|\mathcal{U}^{(1)}_{T_f(\epsilon)-1} \cup \mathcal{U}^{(2)}_{T_f(\epsilon)-1}\right|. \tag{40}$$

By Lemma 3.15, we have $T_f(\epsilon) \leq T_g(\epsilon)$. Thus, by considering $T = T_f(\epsilon)$ in Lemma 3.8, it follows that

$$\left|\mathcal{U}^{(1)}_{T_f(\epsilon)-1} \cup \mathcal{U}^{(2)}_{T_f(\epsilon)-1}\right| \leq \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right) + \left|\mathcal{S}_{T_f(\epsilon)-1}\right|. \tag{41}$$

Then, by combining (40), Lemma 3.14 and (41), we conclude that (39) is true. □

Since each iteration of TRFD-S requires at most $(n+1)$ function evaluations, from Theorem 3.16 we obtain the following upper bound on the number of function evaluations required by TRFD-S to find a $\Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right)$-approximate solution of (1) in Ω, when f is a convex function.

Corollary 3.17. *Suppose that A1-A3, A5 and A6 hold, and let $FE_{T_f(\epsilon)}$ be the number of function evaluations executed by TRFD-S up to the $(T_f(\epsilon)-1)$-st iteration. If $\Delta_{\max} \geq D_0$, then*

$$FE_{T_f(\epsilon)} \;\leq\; (n+1)\left[\frac{4\beta}{\alpha\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1} \;+\; \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right) + 2\right]. \tag{42}$$

In view of (42) and the definition of β in (31), TRFD-S needs no more than

$$\mathcal{O}\left(n\left(\frac{\sigma}{L}\right)L\Delta_{\max}\epsilon^{-1}\right)$$

function evaluations to find $x_k \in \Omega$ such that $f(x_k) - f(x^*) \le \Delta_{\max}\left(\frac{L}{\sigma}\epsilon\right)$. Thus, given $\epsilon_f > 0$, if we use TRFD-S with $\epsilon = \epsilon_f/\Delta_{\max}$, then it will need no more than

$$\mathcal{O}\left(n\left(\frac{\sigma}{L}\right)L\Delta_{\max}^2\epsilon_f^{-1}\right) \tag{43}$$

function evaluations to find $x_k \in \Omega$ such that $f(x_k) - f(x^*) \le \frac{L}{\sigma}\epsilon_f$. So, in the case where $\sigma = L$, we get a worst-case evaluation complexity of

$$\mathcal{O}\left(nL\Delta_{\max}^2\epsilon_f^{-1}\right) \tag{44}$$

to satisfy $f(x_k) - f(x^*) \le \epsilon_f$. Otherwise, when $\sigma \ne L$, Table 2 gives the different scenarios depending on the value of σ.

Value of σ	**Impact on** (43)	**Impact on the target accuracy** $\left(\frac{L}{\sigma}\epsilon_f\right)$
$\sigma < L$	(43) lower than (44) by a linear factor $\left(\frac{\sigma}{L}\right)$	Accuracy weaker than ϵ_f by a factor $\left(\frac{L}{\sigma}\right)$
$\sigma > L$	(43) larger than (44) by a linear factor $\left(\frac{\sigma}{L}\right)$	Accuracy stricter than ϵ_f by a factor $\left(\frac{L}{\sigma}\right)$

Table 2: Impacts of the user-defined parameter σ for convex problems

3.3 Worst-Case Complexity Bound for P-L functions

For the case where f is a Polyak-Lojasiewicz (P-L) function [25], we will assume that the feasible set is unconstrained, i.e., $\Omega = \mathbb{R}^n$. Therefore, given $x_k \in \mathbb{R}^n$, the stationarity measure $\psi_{\Delta_{\max}}(x_k)$ reduces to $\|\nabla f(x_k)\|$, while the approximate stationarity measure $\eta_{\Delta_{\max}}(x_k)$ reduces to $\|g_k\|$.

Now, let us consider the following assumption:

A7. f is a P-L function, i.e., it has a global minimizer $x^* \in \mathbb{R}^n$, and

$$\|\nabla f(x)\|^2 \ge 2\mu\left(f(x) - f(x^*)\right), \quad \forall x \in \mathbb{R}^n. \tag{45}$$

The following lemma relates the approximate stationarity measure $\|g_k\|$ with the functional residual.

Lemma 3.18. *Suppose that A2 and A7 hold, and assume that $\Omega = \mathbb{R}^n$. Moreover, let x_k be generated by TRFD-S. If*

$$f(x_k) - f(x^*) > \frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2, \tag{46}$$

then

$$\|g_k\| \ge \sqrt{\frac{\mu}{2}}(f(x_k) - f(x^*))^{1/2}. \tag{47}$$

Proof. By (46) and A7, we have

$$\left(\frac{L}{\sigma}\epsilon\right) < \sqrt{\mu}(f(x_k) - f(x^*))^{1/2} < \sqrt{2\mu}(f(x_k) - f(x^*))^{1/2} \le \|\nabla f(x_k)\|.$$

Then, by Lemma 3.5, we have that (13) holds. Therefore, by combining (13) and (45), we conclude that (47) is true. □

The next lemma provides an upper bound on $\frac{(f(x_k)-f(x^*))^{1/2}}{\Delta_k}$.

Lemma 3.19. *Suppose that A2, A3 and A7 hold, and assume that $\Omega = \mathbb{R}^n$. Moreover, given $T \geq 1$, let $\{x_k\}_{k=0}^T$ and $\{\Delta_k\}_{k=0}^T$ be generated by TRFD-S. If*

$$f(x_k) - f(x^*) > \frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2, \quad \textit{for} \quad k = 0, ..., T-1,$$

then

$$\left(\frac{1}{\Delta_k}\right)(f(x_k) - f(x^*))^{1/2} \leq \max\left\{\left(\frac{1}{\Delta_0}\right)(f(x_0) - f(x^*))^{1/2}, \sqrt{\frac{2}{\mu}}\frac{(4L+2M)}{(1-\alpha)\kappa}\right\} \equiv \gamma, \tag{48}$$

for $k = 0, \ldots, T$, where κ is the constant in (4).

Proof. Let us work through an induction argument. For $k = 0$, (48) clearly holds. Now, let us assume that (48) is true for some $k \in \{0, ..., T-1\}$. In the case where $\rho_k \geq \alpha$, similarly as in Lemma 3.13, we get

$$\left(\frac{1}{\Delta_{k+1}}\right)(f(x_{k+1}) - f(x^*))^{1/2} \leq \left(\frac{1}{\Delta_k}\right)(f(x_k) - f(x^*))^{1/2} \leq \gamma.$$

So, (48) holds in this case. Let us now consider the case where $\rho_k < \alpha$. Similarly as in Lemma 3.13, we have

$$\frac{\|g_k\|}{\Delta_k} < \frac{2L+M}{(1-\alpha)\kappa}. \tag{49}$$

Then, since $\Delta_{k+1} = \frac{1}{2}\Delta_k$ and $f(x_{k+1}) = f(x_k)$, by combining Lemma 3.18 and (49), we get

$$\begin{aligned}\left(\frac{1}{\Delta_{k+1}}\right)(f(x_{k+1}) - f(x^*))^{1/2} &= \left(\frac{2}{\Delta_k}\right)(f(x_k) - f(x^*))^{1/2} \leq 2\sqrt{\frac{2}{\mu}}\frac{\|g_k\|}{\Delta_k} < \sqrt{\frac{2}{\mu}}\frac{4L+2M}{(1-\alpha)\kappa} \\ &\leq \gamma.\end{aligned}$$

So, (48) is also true in this case, which concludes the proof. □

Now, let

$$T_{PL}(\epsilon) = \inf\left\{k \in \mathbb{N} \,:\, f(x_k) - f(x^*) \leq \frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2\right\} \tag{50}$$

be the first iteration index reaching a $\frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2$-approximate solution of (1) in $\mathbb{R}^n$, if it exists. Our goal is to establish a finite upper bound for $T_{PL}(\epsilon)$. In this context, the following lemma gives an upper bound for $\left|S_{T_{PL}(\epsilon)-1}\right|$.

Lemma 3.20. *Suppose that A2, A3 and A7 hold, and assume that $\Omega = \mathbb{R}^n$. If $T_{PL}(\epsilon) \geq 2$, then*

$$\left|S_{T_{PL}(\epsilon)-1}\right| \leq 1 + \frac{\log\left(\mu(f(x_0) - f(x^*))\left(\frac{L}{\sigma}\epsilon\right)^{-2}\right)}{\left|\log\left(1 - \frac{\alpha\kappa(4L+2M)}{\gamma^2}\right)\right|}, \tag{51}$$

where γ is defined in (48) *and κ is the constant in* (4).

Proof. Let $k \in \mathcal{S}_{T_{PL}(\epsilon)-2}$. By (5), (4), Lemmas 3.18, 3.19 and A3, we have

$$\begin{aligned} f(x_k) - f(x_{k+1}) &\geq \alpha\kappa \|g_k\| \min\left\{\Delta_k, \frac{\|g_k\|}{\|H_k\|}\right\} \\ &\geq \alpha\kappa \sqrt{\frac{\mu}{2}} \left(f(x_k) - f(x^*)\right)^{1/2} \min\left\{\frac{\left(f(x_k) - f(x^*)\right)^{1/2}}{\gamma}, \sqrt{\frac{\mu}{2}} \frac{\left(f(x_k) - f(x^*)\right)^{1/2}}{M}\right\} \\ &= \alpha\kappa \sqrt{\frac{\mu}{2}} \left(f(x_k) - f(x^*)\right) \min\left\{\frac{1}{\gamma}, \sqrt{\frac{\mu}{2}} \frac{1}{M}\right\}. \end{aligned}$$

By the definition of γ in (48), we have $\gamma \geq \sqrt{\frac{2}{\mu}} \frac{4L+2M}{(1-\alpha)\kappa}$. So, since $\alpha \in (0,1)$ and $\kappa \in (0,1)$, we get

$$\sqrt{\frac{\mu}{2}} \geq \frac{4L + 2M}{\gamma}, \tag{52}$$

which implies

$$\frac{1}{\gamma} \leq \sqrt{\frac{\mu}{2}} \frac{1}{M}. \tag{53}$$

Therefore, by (52) and (53), it follows that

$$f(x_k) - f(x_{k+1}) \geq \frac{\alpha\kappa(4L + 2M)}{\gamma^2} \left(f(x_k) - f(x^*)\right). \tag{54}$$

Denoting $\delta_k = f(x_k) - f(x^*)$, (54) becomes

$$\delta_k - \delta_{k+1} \geq \frac{\alpha\kappa(4L + 2M)}{\gamma^2} \delta_k,$$

which gives

$$\delta_{k+1} \leq \left(1 - \frac{\alpha\kappa(4L + 2M)}{\gamma^2}\right) \delta_k, \quad \text{when } k \in \mathcal{S}_{T_{PL}(\epsilon)-2},$$

where $\frac{\alpha\kappa(4L+2M)}{\gamma^2} < 1$ by the definition of γ in (48) and by $\mu \leq L$. Then, since $\delta_{k+1} = \delta_k$ when $k \notin \mathcal{S}_{T_{PL}(\epsilon)-2}$, we have

$$\begin{aligned} \frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2 < f(x_{T_{PL}(\epsilon)-1}) - f(x^*) = \delta_{T_{PL}(\epsilon)-1} &\leq \prod_{k \in \mathcal{S}_{T_{PL}(\epsilon)-2}} \left(1 - \frac{\alpha\kappa(4L + 2M)}{\gamma^2}\right) \delta_0 \\ &= \left(1 - \frac{\alpha\kappa(4L + 2M)}{\gamma^2}\right)^{\left|\mathcal{S}_{T_{PL}(\epsilon)-2}\right|} (f(x_0) - f(x^*)), \end{aligned}$$

which is equivalent to

$$\left(1 - \frac{\alpha\kappa(4L + 2M)}{\gamma^2}\right)^{\left|\mathcal{S}_{T_{PL}(\epsilon)-2}\right|} > \frac{1}{\mu(f(x_0) - f(x^*))} \left(\frac{L}{\sigma}\epsilon\right)^2.$$

Then, taking the logarithm on both sides,

$$\left|\mathcal{S}_{T_{PL}(\epsilon)-2}\right| \log\left(1 - \frac{\alpha\kappa(4L + 2M)}{\gamma^2}\right) > \log\left(\frac{1}{\mu(f(x_0) - f(x^*))} \left(\frac{L}{\sigma}\epsilon\right)^2\right).$$

So,

$$\left|\mathcal{S}_{T_{PL}(\epsilon)-1}\right| \leq 1+\left|\mathcal{S}_{T_{PL}(\epsilon)-2}\right| < 1+\frac{\log\left(\mu(f(x_0)-f(x^*))\left(\frac{L}{\sigma}\epsilon\right)^{-2}\right)}{\left|\log\left(1-\frac{\alpha\kappa(4L+2M)}{\gamma^2}\right)\right|},$$

which shows that (51) is true. $\square$

The next lemma shows that $T_{PL}(\epsilon) \leq T_g(\epsilon)$.

Lemma 3.21. *Suppose that A2 and A7 hold, and assume that $\Omega = \mathbb{R}^n$. Moreover, let $T_{PL}(\epsilon)$ and $T_g(\epsilon)$ be defined by* (50) *and* (16)*, respectively. Then, $T_{PL}(\epsilon) \leq T_g(\epsilon)$.*

Proof. Suppose by contradiction that $T_{PL}(\epsilon) > T_g(\epsilon)$. Then, by (45) and the definition of $T_g(\epsilon)$, we would have

$$\left(\frac{L}{\sigma}\epsilon\right) < \sqrt{\mu}(f(x_{T_g(\epsilon)})-f(x^*))^{1/2} < \sqrt{2\mu}(f(x_{T_g(\epsilon)})-f(x^*))^{1/2} \leq \|\nabla f(x_{T_g(\epsilon)})\| \leq \left(\frac{L}{\sigma}\epsilon\right),$$

leading to a contradiction. So, we conclude that $T_{PL}(\epsilon) \leq T_g(\epsilon)$. $\square$

The next theorem gives an upper bound on the number of iterations required by TRFD-S to reach a $\frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2$-approximate solution of (1) in $\mathbb{R}^n$, when f is a P-L function.

Theorem 3.22. *Suppose that A2, A3 and A7 hold, and assume that $\Omega = \mathbb{R}^n$. Moreover, let $T_{PL}(\epsilon)$ be defined by* (50)*. Then*

$$T_{PL}(\epsilon) \;\leq\; \frac{2\log\left(\mu(f(x_0)-f(x^*))\left(\frac{L}{\sigma}\epsilon\right)^{-2}\right)}{\left|\log\left(1-\frac{\alpha\kappa(4L+2M)}{\gamma^2}\right)\right|} + \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)+2, \qquad (55)$$

where γ is defined in (48) *and κ is the constant in* (4).

Proof. If $T_{PL}(\epsilon) \leq 1$, then (55) is true. Let us assume that $T_{PL}(\epsilon) \geq 2$. As in (17), we have

$$T_{PL}(\epsilon) = \left|\mathcal{S}_{T_{PL}(\epsilon)-1}\right| + \left|\mathcal{U}^{(1)}_{T_{PL}(\epsilon)-1}\cup\mathcal{U}^{(2)}_{T_{PL}(\epsilon)-1}\right|. \qquad (56)$$

Moreover, by Lemma 3.21 we have $T_{PL}(\epsilon) \leq T_g(\epsilon)$. Thus, by considering $T = T_{PL}(\epsilon)$ in Lemma 3.8, it follows that

$$\left|\mathcal{U}^{(1)}_{T_{PL}(\epsilon)-1}\cup\mathcal{U}^{(2)}_{T_{PL}(\epsilon)-1}\right| \leq \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)+\left|\mathcal{S}_{T_{PL}(\epsilon)-1}\right| \qquad (57)$$

holds. Then, combining (56), Lemma 3.20 and (57), we conclude that (55) is true. $\square$

Since each iteration of TRFD-S requires at most $(n+1)$ function evaluations, from Theorem 3.22 we obtain the following upper bound on the number of function evaluations required by TRFD-S to find a $\frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2$-approximate solution of (1) in $\mathbb{R}^n$, when f is a P-L function.

Corollary 3.23. *Suppose that A2, A3 and A7 hold, and assume that $\Omega = \mathbb{R}^n$. Moreover, let $FE_{T_{PL}(\epsilon)}$ be the number of function evaluations executed by TRFD-S up to the $(T_{PL}(\epsilon)-1)$-st iteration. Then*

$$FE_{T_{PL}(\epsilon)} \ \leq \ (n+1)\left[\frac{2\log\left(\mu(f(x_0)-f(x^*))\left(\frac{L}{\sigma}\epsilon\right)^{-2}\right)}{\left|\log\left(1-\frac{\alpha\kappa(4L+2M)}{\gamma^2}\right)\right|} + \ \log_2\left(\frac{(8L+4M)\Delta_0}{(1-\alpha)\kappa}\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)+2\right]. \quad (58)$$

In view of (58) and the definition of γ in (48), TRFD-S requires at most

$$\mathcal{O}\left(n\frac{L}{\mu}\log\left(\left(\frac{\sigma}{L}\right)^2\mu(f(x_0)-f(x^*))\epsilon^{-2}\right)\right)$$

function evaluations to find $x_k \in \mathbb{R}^n$ such that $f(x_k)-f(x^*) \leq \frac{1}{\mu}\left(\frac{L}{\sigma}\epsilon\right)^2$. Thus, given $\epsilon_f > 0$, if $\epsilon = \sqrt{\left(\frac{\sigma}{L}\right)\mu\epsilon_f}$, then TRFD-S requires no more than

$$\mathcal{O}\left(n\frac{L}{\mu}\log\left(\left(\frac{\sigma}{L}\right)(f(x_0)-f(x^*))\epsilon_f^{-1}\right)\right) \quad (59)$$

function evaluations to find $x_k \in \mathbb{R}^n$ such that $f(x_k)-f(x^*) \leq \frac{L}{\sigma}\epsilon_f$. Therefore, when the user-defined parameter σ equals L, we obtain a worst-case evaluation complexity of

$$\mathcal{O}\left(n\frac{L}{\mu}\log\left((f(x_0)-f(x^*))\,\epsilon_f^{-1}\right)\right) \quad (60)$$

to satisfy $f(x_k)-f(x^*) \leq \epsilon_f$. Otherwise, when $\sigma \neq L$, Table 3 summarizes the different impacts of σ.

Value of σ	**Impact on** (59)	**Impact on the target accuracy** $\left(\frac{L}{\sigma}\epsilon_f\right)$
$\sigma < L$	(59) lower than (60) by an additive term $n\frac{L}{\mu}\log\left(\frac{\sigma}{L}\right)$	Accuracy weaker than ϵ_f by a factor $\left(\frac{L}{\sigma}\right)$
$\sigma > L$	(59) larger than (60) by an additive term $n\frac{L}{\mu}\log\left(\frac{\sigma}{L}\right)$	Accuracy stricter than ϵ_f by a factor $\left(\frac{L}{\sigma}\right)$

Table 3: Impacts of the user-defined parameter σ for strongly convex problems

4 Trust-Region Method for Unrelaxable Bound Constraints

In this section, we propose an adaptation of TRFD-S for unrelaxable bound constraints problems, i.e., the case where $\Omega = [\ell, u]$ with $\ell, u \in \mathbb{R}^n$ being lower and upper bounds on the variables, respectively, and where f cannot be evaluated outside Ω. Such scenario typically appears in parameters-tuning, where the parameters have a particular range of values for intrinsic reasons [1].

As it is, Step 1 of TRFD-S may require evaluating f at points outside Ω. For problems where this is not feasible, we modify the step as follows. For each component $i \in \{1, \ldots, n\}$ of g_k, forward and backward finite-difference stepsizes, $\tau^F_{k,i}$ and $\tau^B_{k,i}$, are initially set to a default τ_k. These stepsizes are reduced if necessary to ensure that $x_k + \tau^F_{k,i} e_i$ and $x_k - \tau^B_{k,i} e_i$ remain in Ω:

$$\tau^F_{k,i} = \min\{[u - x_k]_i, \tau_k\}, \quad \tau^B_{k,i} = \min\{[x_k - \ell]_i, \tau_k\}.$$

Since one of these stepsizes might become too small—or even zero—we take, for each i, the larger of $\tau^F_{k,i}$ and $\tau^B_{k,i}$ as the effective stepsize to avoid numerical errors. Figure 1 illustrates this procedure in a two-dimensional box.

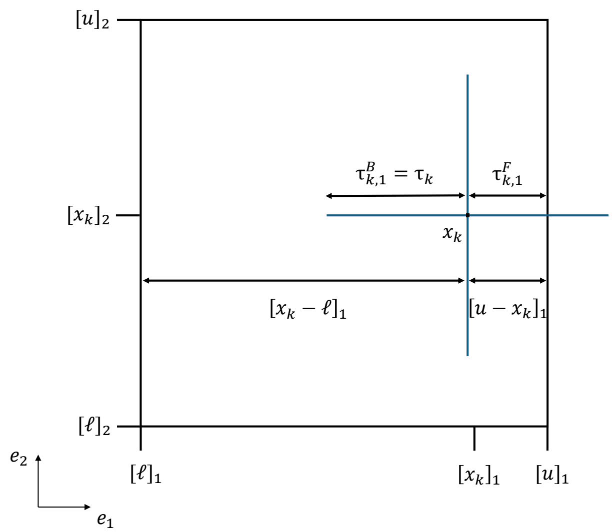

Figure 1: Illustration of Step 1 for unrelaxable bound constraints

Specifically, adapting TRFD-S (Algorithm 1) to handle unrelaxable bound constraints requires only a modification of Step 1; all other steps remain unchanged.

Adaptation of Step 1 in TRFD-S for unrelaxable bound constraints

Step 1. Let

$$\tau^F_{k,i} = \min\{[u - x_k]_i\,, \tau_k\} \quad \text{and} \quad \tau^B_{k,i} = \min\{[x_k - \ell]_i\,, \tau_k\}, \quad i = 1, ..., n.$$

Compute each component of $g_k \in \mathbb{R}^n$ as

$$[g_k]_i = \begin{cases} \frac{f(x_k + \tau^F_{k,i} e_i) - f(x_k)}{\tau^F_{k,i}}, & \text{if } \tau^F_{k,i} \geq \tau^B_{k,i}, \\ \frac{f(x_k) - f(x_k - \tau^B_{k,i} e_i)}{\tau^B_{k,i}}, & \text{otherwise.} \end{cases}$$

Choose a nonzero symmetric matrix $H_k \in \mathbb{R}^{n \times n}$.

Remark 4.1. *By constructing the vector g_k as above, we have that Lemma 2.3 remains true. Moreover, since the update rules of τ_k and Δ_k are unchanged, we have that g_k still satisfies* (7)*. So, we conclude that the worst-case complexity bounds established in Corollaries 3.10 and 3.17 for general nonempty closed convex sets Ω are also true for TRFD-S with unrelaxable bound constraints.*

5 Numerical Experiments

To assess the numerical performance of TRFD-S, we conducted experiments using a MATLAB implementation, comparing it against other derivative-free methods. First, we considered benchmark problems for unconstrained sets and unrelaxable bound constraints. Secondly, we looked at the model fitting of a synthetic Predator-Pray dataset. For unconstrained benchmark problems (see subsection 5.1.1), we compared TRFD-S against NEWUOA [27, 31], DFQRM [19] and an instance of TRFD [16]. For unrelaxable bound constraints benchmark problems (see subsection 5.1.2), TRFD-S was tested with BOBYQA [26, 31], NOMAD [6] and an instance of TRFD. Finally, for the model fitting problem (see subsection 5.2), we compared TRFD-S with BOBYQA.

5.1 Benchmark Problems

For each problem, a budget of 100 simplex gradients was allowed to each solver[1]. In addition, our implementations of TRFD-S were equipped with the stopping criterion $\Delta_k \leq 10^{-13}$. The implementations were compared by using data profiles[2] [24], where a code M is said to solve a problem with some *Tolerance* when it reaches x_M such that

$$f(x_0) - f(x_M) \geq (1 - \mathit{Tolerance})\left(f(x_0) - f(x_{Best})\right),$$

where $f(x_{Best})$ is the lowest function value found among all the methods, and $\mathit{Tolerance} \in (0, 1)$. All experiments were performed with MATLAB (R2023a) on a PC with microprocessor 13-th Gen Intel(R) Core(TM) i5-1345U 1.60 GHz and 32 GB of RAM memory.

5.1.1 Unconstrained Problems

Here, we considered smooth unconstrained problems. We tested 134 functions $f : \mathbb{R}^n \to \mathbb{R}$ defined by the OPM collection [20], for which $2 \leq n \leq 110$, and where the initial points x_0 were provided by the collection. The following codes were compared:

- **TRFD-S**: Implementation of TRFD-S, freely available on GitHub[3], with initial parameters: $\epsilon = 10^{-5}$, $\alpha = 0.01$, $\Delta_0 = \max\{1, \tau_0\sqrt{n}\}$, $\Delta_{\max} = \max\{1000, \Delta_0\}$ and $\sigma = \frac{\epsilon}{\sqrt{n}\sqrt{eps}}$, where *eps* is the machine precision, and with the matrix H_k updated according to the safeguarded BFGS rule:

$$H_{k+1} = \begin{cases} H_k + \frac{y_k y_k^T}{s_k^T y_k} - \frac{H_k s_k s_k^T H_k}{s_k^T H_k s_k} & \text{if} \quad |\langle s_k, y_k \rangle| > 0, \\ H_k \quad \text{otherwise}, \end{cases}$$

with $H_0 = I$, $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$. The trust-region subproblem is solved via the method proposed in [2], which is implemented in the function `TRSgep.m` from the MANOPT toolbox, freely available on GitHub[4].

- **NEWUOA**: Implementation of Powell's method [27, 31], freely available on GitHub[5]. The initial

[1] One simplex gradient corresponds to $n + 1$ function evaluations, with n being the number of variables of the problem.

[2] The data profiles were generated using the code `data_profile.m`, freely available at the website `https://www.mcs.anl.gov/~more/dfo/`.

[3] `https://github.com/danadavar/TRFD-S`

[4] `https://github.com/NicolasBoumal/manopt`

[5] `https://github.com/libprima/prima`

parameters were not changed.

- **DFQRM**: Implementation of the quadratic regularization method described in Section 4 of [19].

- **TRFD-2**: Implementation of TRFD [16], with $p = 2$, $m = 1$ and $h(z) = z$, $\forall z \in \mathbb{R}$, freely available on GitHub[6]. The initial threshold is set to $\alpha = 0.01$, while the other parameters follow the same setup as Section 4 in [16].

Data profiles are presented in Figure 2. As we can see, TRFD-S outperforms DFQRM and TRFD-2 for all presented tolerances, while exhibiting a competitive performance with NEWUOA. Notably, TRFD-S achieves better results than NEWUOA for tolerances 10^{-5} and 10^{-7}.

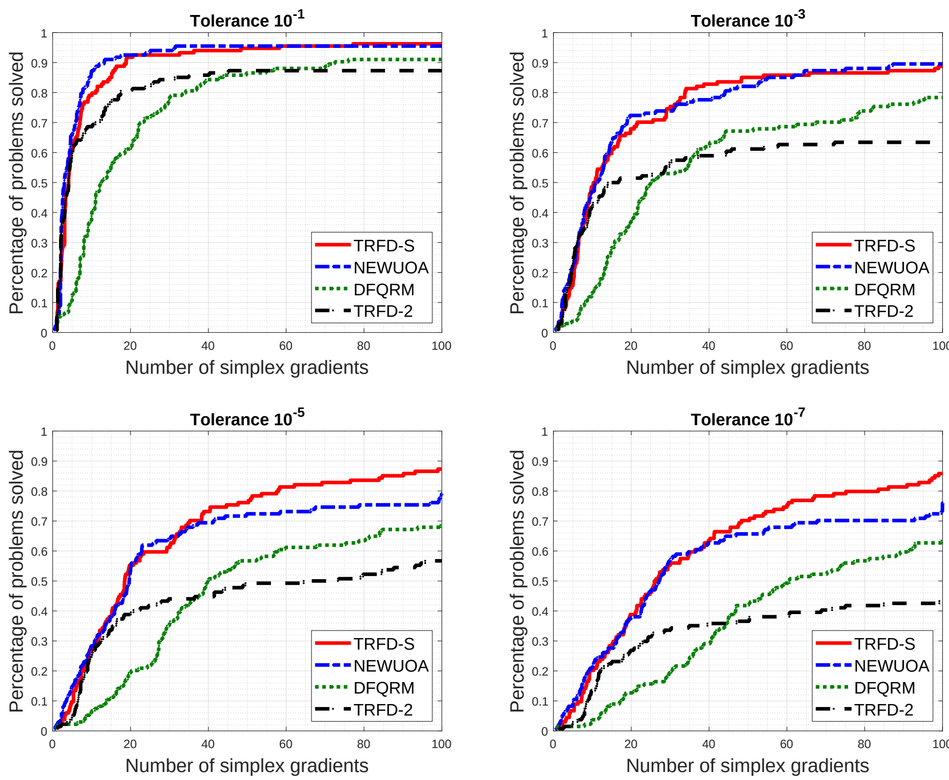

Figure 2: Data profiles for smooth unconstrained problems

5.1.2 Unrelaxable Bound Constraints Problems

Here, we considered smooth problems of the form

$$\min_{x \in \Omega} f(x) \equiv \|F(x)\|_2^2 \,,$$

where Ω is defined by the unrelaxable bounds $\ell_i = 0.1$ and $u_i = 20$, for $i = 1, ..., n$, as set in Section 5 of [21]. We tested 53 functions $F : \mathbb{R}^n \to \mathbb{R}^m$ defined by the Moré-Wild collection [24], for which $2 \leq n \leq 12$ and $2 \leq m \leq 65$, and where the initial points x_0 were provided by the collection. In the case where x_0 violated the bound constraints, an orthogonal projection was applied to Ω. With this

[6] `https://github.com/danadavar/TRFD`

setting, the following codes were compared:

- **TRFD-S**: Implementation of TRFD-S, freely available on GitHub[7], with the same update rule for H_k and with the same initial parameters as in subsection 5.1.1. The inner solver used for solving the trust-region subproblem was FISTA [9] with Dykstra's algorithm [15, 10] for projection to the set Ω. The same parameters and stopping criteria were used than those described in Section 5 of [21], except for the stopping criterion on Dykstra's algorithm, which we set to 10^{-8}.

- **BOBYQA**: Implementation of Powell's method [26, 31]. The initial parameters were unchanged, while the option `honour_x0` was set to *true* to force the method not to move the position of the initial point.

- **NOMAD**: Implementation of the version 4 of NOMAD, proposed in [6]. The initial parameters were not changed.

- **TRFD-Inf**: Implementation of TRFD [16], freely available on GitHub[8], with $p = +\infty$, $m = 1$ and $h(z) = z$, $\forall z \in \mathbb{R}$. The threshold is the same as in subsection 5.1.1, namely, $\alpha = 0.01$, while the other parameters follow the same setup as in Section 4 of [16].

Data profiles are shown in Figure 3. As shown, TRFD-S outperforms NOMAD and TRFD-Inf, while exhibiting a performance comparable to BOBYQA. In particular, TRFD-S achieves better results than BOBYQA when the tolerance is set to 10^{-7}.

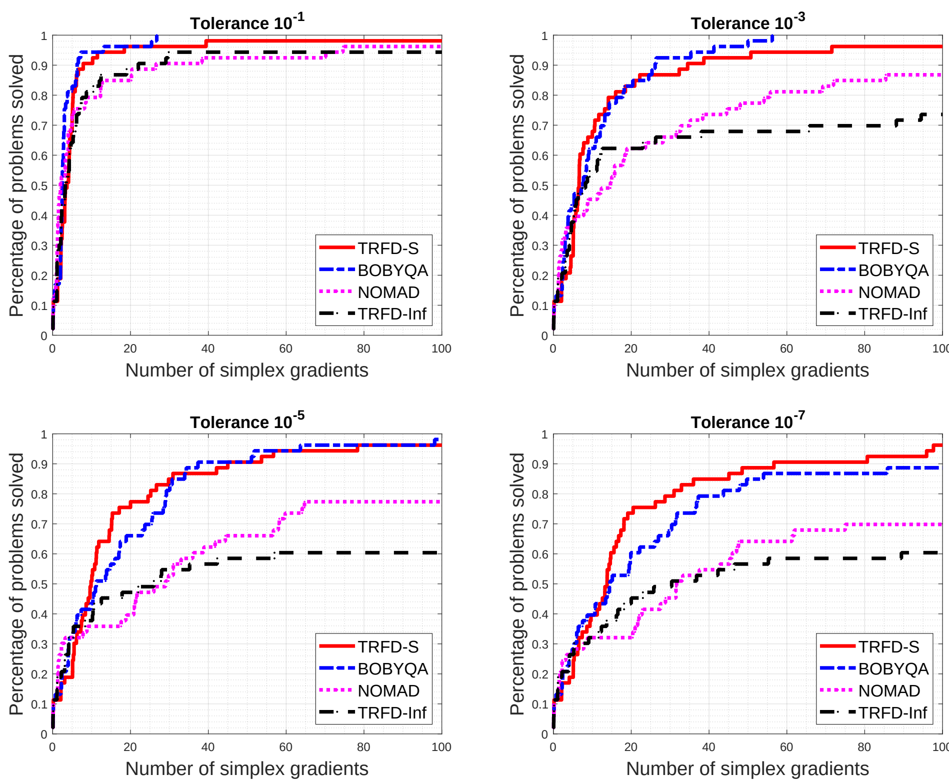

Figure 3: Data profiles for smooth unrelaxable bound constraints problems

[7] `https://github.com/danadavar/TRFD-S`

[8] `https://github.com/danadavar/TRFD`

5.2 Calibration of an ODE Model

Parameter calibration in differential equation models plays a central role in describing physical, biological, and engineering processes. Although gradient-based optimization methods provide an efficient framework for this task, their practical use is often limited by the complexity of implementing adjoint equations or automatic differentiation techniques. Consequently, many practitioners still favor derivative-free methods for their ease of application (see, e.g., [3, 4, 7, 8, 23, 30]). In this section, we compare the performance of TRFD-S and BOBYQA in calibrating the parameters of the Rosenzweig–MacArthur extension of the Lotka–Volterra Predator-Prey model [28, 29]:

$$\begin{aligned} \frac{d\,Y(t)}{dt} &= \zeta\, Y(t)\left(1 - \frac{Y(t)}{\theta}\right) - \lambda\, \frac{Y(t)\,Z(t)}{\mu + Y(t)}, \\ \frac{d\,Z(t)}{dt} &= \nu\, \frac{Y(t)\,Z(t)}{\mu + Y(t)} - \xi\, Z(t), \end{aligned} \tag{61}$$

where $Y(t)$ and $Z(t)$ are the Preys and Predators densities, respectively. Using the initial conditions $Y(0) = 400$ and $Z(0) = 20$, we generated a synthetic dataset based on the solutions of the system (61), which depend on the vector of parameters $x = [\zeta, \theta, \lambda, \mu, \nu, \xi]^T$. The solutions of the system (61) are denoted by $Y(t; x)$ and $Z(t; x)$.

We begin by selecting a ground-truth parameter vector $x^* = [0.723, 447, 2.88, 21.9, 5.54, 4.99]^T$. Using this reference set of parameters, we numerically solved the system with the MATLAB function `ode45` to obtain the solutions at a discrete set of time points $\{t_i = 0.5i\}_{i=0}^{70}$, yielding the trajectories $\{Y(t_i; x^*)\}_{i=0}^{70}$ and $\{Z(t_i; x^*)\}_{i=0}^{70}$. To simulate observational noise, we perturbed the exact solutions with additive Gaussian noise. Specifically, we defined the synthetic observations as:

$$\tilde{Y}_i = Y(t_i; x^*) + 10\varepsilon_i, \quad \tilde{Z}_i = Z(t_i; x^*) + 10\varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, 1),$$

for $i = 0, \ldots, 70$. The resulting datasets $\{(t_i, \tilde{Y}_i)\}_{i=0}^{70}$ and $\{(t_i, \tilde{Z}_i)\}_{i=0}^{70}$ served as the testbed for calibrating x. Thus, given both datasets, by denoting $\bar{Y}$ and $\bar{Z}$ as the mean values of the Preys and Predators populations, respectively, we defined the least-square error as:

$$f(x) \equiv \frac{1}{\bar{Y}^2} \sum_{i=0}^{70} \left(Y(t_i; x) - \tilde{Y}_i\right)^2 + \frac{1}{\bar{Z}^2} \sum_{i=0}^{70} \left(Z(t_i; x) - \tilde{Z}_i\right)^2.$$

We set the initial point $x_0 = [0.6, 400, 1, 10, 3, 2]$, the unrelaxable bounds

$$\ell = [0.001, 0.001, 0.001, 0.001, 0.001, 0.001]^T \quad \text{and} \quad u = [5, 1000, 10, 500, 10, 5]^T.$$

A budget of 350 evaluations (corresponding to 50 simplex gradients) was given to TRFD-S and BOBYQA. Moreover, the initial parameters of both methods were the same as in subsection 5.1.2.

On the left-hand side of Figure 4, we see the evolution of the lowest function value found with respect to the number of function evaluations that were executed. In addition, the right-hand side of Figure 4 provides the resulting Predator-Prey models after 350 evaluations. As we can see, within the given function evaluation budget, TRFD-S identified a parameter vector that outperforms the one found by BOBYQA, as reflected in the superior quality of the corresponding fits.

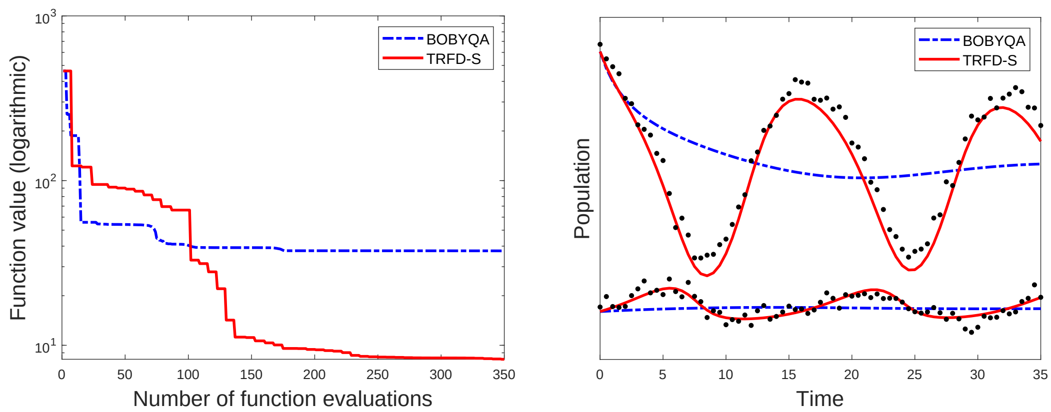

Figure 4: Model Fitting on a Synthetic Predator–Prey Dataset

6 Conclusion

This work presented TRFD-S, a derivative-free trust-region method based on finite-difference gradient approximations designed for smooth convexly constrained optimization problems. TRFD-S relies on second-order models, which are assumed to produce at least a Cauchy decrease. Moreover, the method does not require the computation of the approximate stationarity measure $\eta_{\Delta_{\max}}(x_k)$. In this setting, worst-case evaluation complexity bounds were established. Specifically, for nonconvex problems, it was shown that TRFD-S requires at most $\mathcal{O}\left(n\left(\frac{L}{\sigma}\epsilon\right)^{-2}\right)$ function evaluations to reach an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate stationary point of $f(\cdot)$ in Ω, while a bound of $\mathcal{O}\left(n\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)$ was proved for convex problems to find an $\left(\frac{L}{\sigma}\epsilon\right)$-approximate minimizer of $f(\cdot)$ in Ω. Also, a bound of $\mathcal{O}\left(n\log\left(\left(\frac{L}{\sigma}\epsilon\right)^{-1}\right)\right)$ was obtained when $\Omega=\mathbb{R}^n$ for Polyak-Lojasiewicz functions. In addition, a simple adaptation of the method was proposed for problems with unrelaxable bound constraints. Numerical results were also presented, illustrating the efficiency of TRFD-S on smooth problems with respect to TRFD [16], DFQRM [19] and NOMAD [6], and its competitve behaviour with NEWUOA [27, 31] and BOBYQA [26, 31].

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