ADAPTIVE REGULARIZED NEWTON METHOD FOR RIEMANNIAN OPTIMIZATION
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Abstract. Optimization on Riemannian manifolds widely arises in eigenvalue computation, density functional theory, Bose-Einstein condensates, low rank nearest correlation, image registration, and signal processing, etc. We propose an adaptive regularized Newton method which approximates the original objective function by the second-order Taylor expansion in Euclidean space but keeps the Riemannian manifold constraints. The regularization term in the objective function of the subproblem enables us to establish a Cauchy-point like condition as the standard trust-region method for proving global convergence. The subproblem can be solved inexactly either by first-order methods or a modified Riemannian Newton method. In the later case, it can further take advantage of negative curvature directions. Both global convergence and superlinear local convergence are guaranteed under mild conditions. Extensive computational experiments and comparisons with other state-of-the-art methods indicate that the proposed algorithm is very promising.

Key words. Riemannian optimization, regularization, Newton methods, convergence.

AMS subject classifications. 15A18, 65K10, 65F15, 90C26, 90C30

1. Introduction. We consider minimization problems on a Riemannian manifold of the form:

\[ \min_{x \in \mathcal{M}} f(x), \]

where \( \mathcal{M} \) is a Riemannian submanifold of an Euclidean space \( \mathcal{E} \) and \( f: \mathcal{M} \rightarrow \mathbb{R} \) is a smooth real-valued function on \( \mathcal{M} \). This problem widely exists in eigenvalue decomposition [2], density functional theory [34], Bose-Einstein condensates [37], low rank nearest correlation matrix completion [33], and many other varieties of applications.

Riemannian optimization has been extensively studied over decades of years. Since problem (1.1) can be viewed as a general nonlinear optimization problem with constraints, many standard algorithms [36] can be applied to it directly. These algorithms may not be efficient since they do not utilize the intrinsic structure of the manifold. A first and basic class of manifold optimization methods can be obtained via modifying and transfering the nonlinear programming approaches to the manifold setting. In particular, by performing curvilinear search along the geodesic, Gabay [12], Udrisë et al. [31], Yang [40] and Smith et al. [29] propose globally convergent steepest descent, Newton, quasi-Newton and trust-region methods, respectively. Because the computation of the geodesic may be difficult and expensive, Absil et al. [2, 4] develop a first-order approximation called retraction to the geodesic. The previously mentioned algorithms can be generalized by replacing the geodesic by the retraction and their global and local convergence properties have been analyzed in [1, 2]. Qi [27] and Huang et al. [18, 19] propose an extensive class of quasi-Newton methods for

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Riemannian manifold problems based on retractions and vector transport. In [2], a nonlinear conjugate gradient method for Riemannian manifold problems is presented. Bart [33] and Kressner et al. [22] show that algorithms using the geometry of a manifold can be efficient on a large variety of applications. Boumal et al. [5] establish global convergence rates for optimization methods on manifolds. Moreover, a selection of Riemannian first-order and second-order methods has been implemented in the software package Manopt [7].

Optimization over the Stiefel manifold (i.e., problems with orthogonality constraints) is an important special case of Riemannian optimization. Edelman et al. [11] analyze the geometry of this manifold and propose Newton and conjugate gradient methods along the geodesic. From the perspective of Euclidean constrained optimization, Wen et al. [35] propose a constraint-preserving algorithm on the Stiefel manifold. Jiang et al. [21] further extend their methods and construct a generalized framework. Gao et al. [13] propose a gradient-type and column-wise block coordinate descent algorithm. Lai et al. [24] study a folding-free global conformal mapping for genus-0 surfaces via harmonic energy minimization over multiple spheres. Zhang et al. [42] and Ulbrich et al. [32] present gradient-based algorithms for density functional theory which coincide with optimization problems on the Stiefel manifold. Wen et al. [34] develop an adaptively regularized Newton method which uses a quadratic approximation with exact Euclidean Hessian of the original problem. It often exhibits superlinear or quadratic local convergence rate when the subproblem is solved accurately. This method has also been extended to Bose-Einstein condensates in [37].

In this paper, we extend the regularized Newton method in [34, 37] to general Riemannian optimization problems. Specifically, we approximate problem (1.1) and construct a quadratic subproblem by adding a regularization term to the second-order Taylor expansion of the objective function in Euclidean space. This leads to a class of Euclidean-based model problems that is generally different from classical trust-region-type approaches on Riemannian manifolds [2]. Typically, the resulting subproblems are easier to be solved than the original problem to a certain extent. We show that, whenever the subproblem can be handled efficiently, a fast rate of convergence can be achieved. Since a regularization term is added, global convergence can be ensured by adjusting the regularization parameters appropriately. In fact, convergence can be guaranteed even if the subproblem is only solved inexactly as long as it attains a reduction similar to that of a single gradient descent step. Different from minimizing the subproblem by the gradient-type methods in [34, 37], we develop a modified Newton method using the conjugate gradient method to solve the Newton equation followed by a curvilinear search. In particular, our algorithm detects directions of negative curvature. We combine them with the previous conjugate directions to construct new search directions and update the regularization parameter based on the negative curvature information. Our extensive numerical experiments show that the proposed method is promising and performs comparably well.

We should point out that similar second-order type methods have also been developed for composite convex programs where the objective function is a summation of a smooth function and an $\ell_1$-norm or more general convex term. The subproblem in the proximal Newton method by Lee et al. [25] keeps the $\ell_1$-norm function but approximates the smooth part by its second-order Taylor expansion. A first-order method is then used to solve the resulting proximal subproblem. Byrd et al. [8] essentially consider the same algorithm but propose a specialized active set strategy to solve the quadratic subproblem.

This paper is organized as follows. In Section 2, we review some preliminaries on
Riemannian optimization and present the Riemannian gradient method. The adaptive regularized Newton method is proposed in Section 3 and its convergence properties are analyzed in Section 4. Finally, robustness and efficiency of the proposed algorithms are demonstrated based on several practical examples in Section 5.

1.1. Notation. Let \((M, g)\) be a Riemannian manifold. By \(\mathcal{F}_x(M)\), we denote the set of all real-valued functions \(f\) defined in a neighborhood of \(x\) in \(M\). For a given differentiable function \(f\) and a point \(x \in M\), \(\nabla f(x)\) (\(\nabla^2 f(x)\)) and \(\text{grad} f(x)\) (\(\text{Hess} f(x)\)) denote the Euclidean and Riemannian gradient (Hessian) of \(f\), respectively. Let \(\langle \cdot, \cdot \rangle_{(\|\cdot\|)}\) and \(\langle \cdot, \cdot \rangle_x\) (\(\|\cdot\|_x\)) be the inner product (norm) with Euclidean and Riemannian metric, respectively.

2. Preliminaries on Riemannian optimization. Many concepts of Riemannian optimization can be regarded as generalizations of the theory and algorithms from unconstrained Euclidean optimization to problems on manifolds. A detailed description of the properties of a few commonly used manifold algorithms are given in [2]. Here, we only introduce some necessary definitions briefly.

A \(d\)-dimensional manifold \(M\) is a Hausdorff and second-countable topological space, which is homeomorphic to the \(d\)-dimensional Euclidean space locally via a family of charts. When the transition maps of intersecting charts are smooth, manifold \(M\) is called a smooth manifold. A function \(f\) on \(M\) is said to be \(C^k\) at a point \(x\) if \(f \circ \psi : \psi(U) \subset \mathbb{R}^d \rightarrow \mathbb{R}\) is \(C^k\) in which \(U\) is an open set in \(M\) containing \(x\) and \(\psi\) is the mapping defining the chart. A tangent vector \(\xi_x\) to \(M\) at \(x\) is a mapping such that there exists a curve \(\gamma\) on \(M\) with \(\gamma(0) = x\), satisfying

\[
\xi_xu := \dot{\gamma}(0)u \triangleq \frac{d(u(\gamma(t)))}{dt} \bigg|_{t=0}, \quad \forall \; u \in \mathcal{F}_x(M).
\]

Then, the tangent space \(T_xM\) to \(M\) is defined as the set of all tangent vectors to \(M\) at \(x\). If the manifold \(M\) can be equipped with a smoothly varying inner product \(\langle \cdot, \cdot \rangle_x\) between the tangent vectors of the same tangent space, then \(M\) is called a Riemannian manifold. Here, we will always assume that \(M\) is a Riemannian submanifold of an Euclidean space \(\mathcal{E}\), see, e.g., [2, Section 3.6] for further details. The norm induced by the Riemannian metric is equivalent to the Euclidean norm, i.e., for all \(x \in M\) there exist parameters \(\varpi^m_x, \varpi^M_x > 0\), which depend continuously on \(x\), such that

\[
\varpi^m_x \|\xi\|^2 \leq \|\xi\|^2 \leq \varpi^M_x \|\xi\|^2, \quad \forall \; \xi \in T_xM.
\]

The gradient of a real-valued function \(f\) on the Riemannian manifold is defined as the unique tangent vector satisfying

\[
\langle \text{grad} f(x), \xi \rangle_x = Df(x)[\xi], \quad \forall \; \xi \in T_xM,
\]

where \(Df(x)[\xi] = \xi_x f\) and \(\text{grad} f(x)\) is called the Riemannian gradient of \(f\) at \(x\). The Riemannian Hessian of \(f\) is a linear mapping from \(T_xM\) to \(T_xM\) defined by

\[
\text{Hess} f(x)[\xi] = \bar{\nabla}_\xi \text{grad} f(x), \quad \forall \; \xi \in T_xM,
\]

where \(\bar{\nabla}\) is the Riemannian connection which is a unique symmetric affine connection satisfying the Levi-Civita conditions [1]. We refer to [2] for a more detailed discussion of the Riemannian gradient and Hessian.

First- and second-order optimality conditions for Riemannian optimization problems take a similar form as standard optimality conditions in the Euclidean space. In
particular, let $\mathcal{M}$ be a smooth manifold and let $f : \mathcal{M} \to \mathbb{R}$ be a smooth function on $\mathcal{M}$. Suppose that $x_* \in \mathcal{M}$ is a stationary point of problem (1.1), i.e., it holds $\nabla f(x_*) = 0$. Furthermore, let $\text{Hess} f(x_*)$ be positive definite on $T_{x_*} \mathcal{M}$ (w.r.t. the Riemannian metric), then by [39, Corollary 4.3], $x_*$ is a strict local solution of (1.1). Analogous second order necessary conditions are presented in [39].

### 2.1. Gradient methods on manifold

Curvilinear search methods generalize the concept of backtracking line search and gradient descent to the manifold setting and are based on so-called retractions. A retraction $R$ on $\mathcal{M}$ is a smooth mapping from the tangent bundle $T \mathcal{M} := \bigcup_{x \in \mathcal{M}} T_x \mathcal{M}$ to the manifold $\mathcal{M}$. Moreover, the restriction $R_x$ of $R$ to $T_x \mathcal{M}$ has to satisfy $R_x(0_x) = x$ and $D R_x(0_x) = \text{id}_{T_x \mathcal{M}}$, where $\text{id}_{T_x \mathcal{M}}$ is the identity mapping on $T_x \mathcal{M}$.

Given a retraction $R$, the curvilinear search method computes

$$x_{k+1} = R_x(t_k \eta_k),$$

where $\eta_k \in T_{x_k} \mathcal{M}$ and $t_k$ is a scalar. Similar to Euclidean line search methods, $\eta_k$ is chosen as a descent direction and $t_k$ is a proper step size determined by either exact or inexact curvilinear search conditions. Given $\rho, \varrho, \delta \in (0, 1)$, the monotone and nonmonotone Armijo rules [41] try to find the smallest integer $h$ satisfying

\begin{align}
(2.2) \quad f(R_{x_k}(t_k \eta_k)) & \leq f(x_k) + \rho t_k \langle \nabla f(x_k), \eta_k \rangle_{x_k}, \\
(2.3) \quad f(R_{x_k}(t_k \eta_k)) & \leq C_k + \rho t_k \langle \nabla f(x_k), \eta_k \rangle_{x_k},
\end{align}

respectively, where $t_k = \gamma_k \delta^h$ and $\gamma_k$ is an initial step size. Here, the reference value $C_{k+1}$ is a convex combination of $C_k$ and $f(x_{k+1})$ and is calculated via $C_{k+1} = (\varrho Q_k C_k + f(x_{k+1}))/Q_{k+1}$, where $C_0 = f(x_0), Q_{k+1} = \varrho Q_k + 1$ and $Q_0 = 1$.

It is well known that an initial step size computed by the Barzilai-Borwein (BB) method often speeds up the convergence in Euclidean optimization. Similarly and as in [20], we can consider the following initial step sizes

$$\gamma_k^{(1)} = \frac{\langle s_{k-1}, s_{k-1} \rangle_{x_k}}{\langle s_{k-1}, v_{k-1} \rangle_{x_k}} \quad \text{or} \quad \gamma_k^{(2)} = \frac{|\langle s_{k-1}, v_{k-1} \rangle_{x_k}|}{\langle v_{k-1}, v_{k-1} \rangle_{x_k}},$$

where we can take either

$$s_{k-1} = x_k - x_{k-1}, \quad v_{k-1} = \nabla f(x_k) - \nabla f(x_{k-1}).$$

or

$$s_{k-1} = -t_{k-1} \cdot T_{x_{k-1}} \to x_k (\nabla f(x_{k-1})), \quad v_{k-1} = \nabla f(x_k) + t_{k-1}^{-1} \cdot s_{k-1},$$

and $T_{x_{k-1}} \to x_k : T_{x_{k-1}} \mathcal{M} \to T_x \mathcal{M}$ denotes an appropriate vector transport mapping connecting $x_{k-1}$ and $x_k$; see [2, 20]. The nonmonotone curvilinear search algorithms using the BB step size is outlined in Algorithm 1.

### 2.2. Proximal gradient method

The optimization problem (1.1) can also be solved by the proximal gradient method. At the $k$th iteration, the proximal gradient method linearizes $f(x)$ with a proximal term to obtain the subproblem

\begin{equation}
(2.4) \quad \min_{x \in \mathcal{M}} m_k^T(x) = \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2 \eta_k} \|x - x_k\|^2,
\end{equation}
Algorithm 1: Riemannian Curvilinear Search Method

Input $x_0 \in \mathcal{M}$. Set $k = 0$, $\gamma_{\min} \in [0, 1]$, $\gamma_{\max} \geq 1$, $C_0 = f(x_0)$, $Q_0 = 1$.

while $\|\nabla f(x_k)\| \neq 0$

Compute $\eta_k = -\nabla f(x_k)$.
Calculate $\gamma_k$ according to (2.1) and set $\gamma_k = \max(\gamma_{\min}, \min(\gamma_k, \gamma_{\max}))$.
Then, compute $C_k$, $Q_k$ and find a step size $t_k$ satisfying (2.3).
Set $x_{k+1} \leftarrow R_{x_k}(t_k \eta_k)$.
Set $k \leftarrow k + 1$.

where $\tau_k$ is the proximal step size and the inner products are defined in Euclidean space. It is easy to see that the solution of (2.4), denoted by $x_{k+1}$, is

$$x_{k+1} = \text{P}_{\mathcal{M}}(x_k - \tau_k \nabla f(x_k)) = \arg\min_{x \in \mathcal{M}} \frac{1}{2\tau_k} \|x - x_k + \tau_k \nabla f(x_k)\|^2,$$

where $\text{P}_{\mathcal{M}}(x) := \arg\min\{\|x - y\| : y \in \mathcal{M}\}$ is the projection operator onto $\mathcal{M}$. Notice that $\text{P}_{\mathcal{M}}(x)$ exists if the manifold $\mathcal{M}$ is closed, but it may not be single-valued. If $\mathcal{M}$ is closed and convex, then $\text{P}_{\mathcal{M}} : \mathbb{R}^n \rightarrow \mathcal{M}$ defines a function on $\mathbb{R}^n$, see, e.g., [16]. Furthermore, if $\mathcal{M}$ is a submanifold of class $C^2$ around $x \in \mathcal{M}$, Proposition 5 in [4] implies that $R_x(u) = \text{P}_{\mathcal{M}}(x + u)$ is a retraction at $x$ from $T_x\mathcal{M}$ to $\mathcal{M}$. In this situation, the proximal gradient scheme (2.5) can be seen a special case of Algorithm 1.

Recently, Duchi [10] propose the so-called Adagrad algorithm to solve online learning and stochastic optimization problems. An interesting feature of Adagrad is that it can choose different step sizes for every variable. Similarly, we can define an updating formula as

$$
\begin{align*}
G_k &= G_{k-1} + \nabla f(x_k) \odot \nabla f(x_k), \\
x_{k+1} &= \text{P}_{\mathcal{M}}(x_k - \eta \nabla f(x_k) \odot \sqrt{G_k + \epsilon}),
\end{align*}
$$

where $\eta, \epsilon > 0$ and the multiplication “$\odot$” and division “$\oslash$” are performed component-wise. Other stochastic approaches in deep learning [14] may be applied as well.

2.3. Convergence of Algorithm 1. In this subsection, we give a convergence proof of Algorithm 1 for the sake of completeness. Our result is a simple generalization of the theory available for monotone line search methods, see, e.g., [2, Section 4.2]. Let us also mention that Iannazzo and Porcelli [20] establish convergence for a similar Riemannian Barzilai-Borwein method using a nonmonotone max-type line search. In the following, the set $\mathcal{L} := \{x \in \mathcal{M} : f(x) \leq f(x_0)\}$ denotes the level set of $f$ at $x_0$. In comparison to [20], our next and first convergence result does not require the level set $\mathcal{L}$ to be compact.

**Theorem 1.** Suppose that $f$ is continuously differentiable on the manifold $\mathcal{M}$. Let $\{x_k\}$ be a sequence generated by Algorithm 1 using the nonmonotone line search (2.3). Then, every accumulation point $x_*$ of the sequence $\{x_k\}$ is a stationary point of problem (1.1), i.e., it holds $\nabla f(x_*) = 0$.

**Proof.** At first, by using $\langle \nabla f(x_k), \eta_k \rangle_{x_k} = -\|\nabla f(x_k)\|^2_{x_k} < 0$ and applying
[41, Lemma 1.1], it follows $f(x_k) \leq C_k$ and $x_k \in \mathcal{L}$ for all $k \in \mathbb{N}$. Next, due to

$$
\lim_{t \to 0} \frac{(f \circ R_{x_k})(t \eta_k) - f(x_k)}{t} - \rho \langle \text{grad } f(x_k), \eta_k \rangle_{x_k}
= \nabla f(R_{x_k}(0))^\top DR_{x_k}(0) \eta_k + \rho \|\text{grad } f(x_k)\|_{x_k}^2 = -(1 - \rho)\|\text{grad } f(x_k)\|_{x_k}^2 < 0,
$$

there always exists a positive step size $t_k \in (0, \gamma_k)$ satisfying the monotone and non-monotone Armijo conditions (2.2) and (2.3), respectively. Now, let $x_k \in \mathcal{M}$ be an arbitrary accumulation point of $\{x_k\}$ and let $\{x_k\}_K$ be a corresponding subsequence that converges to $x_*$. By the definition of $C_{k+1}$ and (2.2), we have

$$
C_{k+1} = \frac{\rho Q_k C_k + f(x_{k+1})}{Q_{k+1}} < \frac{(\rho Q_k + 1) C_k}{Q_{k+1}} = C_k.
$$

Hence, $\{C_k\}$ is monotonically decreasing and converges to some limit $\bar{C} \in \mathbb{R} \cup \{-\infty\}$. Using $f(x_k) \to f(x_*)$ for $K \ni k \to \infty$, we can infer $\bar{C} \in \mathbb{R}$ and thus, we obtain

$$
\infty > C_0 - \bar{C} = \sum_{k=0}^{\infty} C_k - C_{k+1} \geq \sum_{k=0}^{\infty} \frac{\rho t_k\|\text{grad } f(x_k)\|_{x_k}^2}{Q_{k+1}}.
$$

Due to $Q_{k+1} = 1 + \rho Q_k = 1 + \rho + \rho^2 Q_{k-1} = \ldots = \sum_{i=0}^{k} \rho^i < (1 - \rho)^{-1}$, this implies $\{t_k\|\text{grad } f(x_k)\|_{x_k}^2\} \to 0$. Let us now assume $\|\text{grad } f(x_*)\| \neq 0$. In this case, we have $\{t_k\}_K \to 0$ and consequently, by the construction of Algorithm 1, the step size $\delta^{-1} t_k$ does not satisfy (2.3), i.e., it holds

$$
(2.7) \quad \rho (\delta^{-1} t_k)\|\text{grad } f(x_k)\|_{x_k}^2 < f(R_{x_k}(\delta^{-1} t_k \eta_k)) - C_k \leq f(R_{x_k}(\delta^{-1} t_k \eta_k)) - f(x_k)
$$

for all $k \in K$ sufficiently large. Since the sequence $\{\eta_k\}_K$ is bounded, the rest of the proof is now identical to the proof of [2, Theorem 4.3.1]. In particular, applying the mean value theorem in (2.7) and using the continuity of the Riemannian metric, this easily yields a contradiction. We refer to [2] for more details.

Since the iterates generated by Algorithm 1 stay in the level set $\mathcal{L}$ (see again [41]), we can derive a slightly stronger convergence result under an additional compactness assumption.

**Corollary 2.** Let the sequence $\{x_k\}$ be generated by Algorithm 1 and let $f$ be continuously differentiable on $\mathcal{M}$. Suppose that the level set $\mathcal{L}$ is compact. Then, it follows $\lim_{k \to \infty} \|\text{grad } f(x_k)\|_{x_k} = 0$.

**Proof.** The result is a direct consequence of Theorem 1 and of the compactness of $\mathcal{L}$. Let us also refer to [2, Corollary 4.3.2].

**3. An Adaptive Regularized Newton Method.** Gradient-type methods often perform reasonably well but might converge slowly when the generated iterates are close to an optimal solution. Usually, fast local convergence cannot be expected if only the gradient information is used, in particular, for difficult non-quadratic or nonconvex problems. Starting from an initial point $x_0$, the Riemannian trust-region method [1, 2] generates the $k$th subproblem as follows

$$
\begin{align*}
\min_{\xi \in \mathcal{T}_{x_k}, \mathcal{M}} \quad & \bar{m}_k(\xi) := f(x_k) + \langle \text{grad } f(x_k), \xi \rangle_{x_k} + \frac{1}{2} \langle \text{Hess } f(x_k)[\xi], \xi \rangle_{x_k} \\
\text{s.t.} \quad & \langle \xi, \xi \rangle_{x_k} \leq \Delta_k,
\end{align*}
$$

where $\mathcal{M}$ is a suitable manifold and $\mathcal{T}_{x_k}$ is a suitable tangent space at $x_k$. The subproblem (3.1) is solved by a trust-region method, and the step size $\delta$ is chosen to satisfy some descent condition. The trust-region radius $\Delta_k$ is updated at each iteration to ensure convergence.

Theorem 1 can be generalized to this case as well. In particular, if the manifold $\mathcal{M}$ is compact, then the sequence $\{x_k\}$ is bounded and the iterations converge to an optimal solution.
where $\Delta_k$ is the trust-region radius. A common strategy is to apply the truncated preconditioned conjugate gradient method (PCG) to solve (3.1) via the linear system

\begin{equation}
\text{grad} f(x_k) + \text{Hess} f(x_k)[\xi] = 0
\end{equation}

to obtain an approximate (but maybe infeasible) solution $\xi$. The truncated PCG method terminates when either the residual becomes small enough, a negative curvature direction is detected, or the trust-region constraint is violated. Then, a trial point is generated via $z_k = R_{x_k}(\xi_k)$ and the new iterate $x_{k+1}$ is set to $z_k$ if a certain reduction condition is satisfied. Otherwise, the iterate is not updated, i.e., it holds $x_{k+1} := x_k$. Note that (3.2) differs from the KKT condition for (3.1), since no Lagrange multiplier is involved.

In this paper, we develop an adaptively regularized Riemannian Newton scheme as an alternative approach. Specifically, we use a second-order Taylor model to approximate the original objective function in the Euclidean space. Moreover, in order to control the definiteness of the model Hessian, a proximal-type penalization is added. The complete objective function of our subproblem is given by

\begin{equation}
m_k(x) := \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2} \langle H_k(x - x_k), x - x_k \rangle + \frac{\sigma_k}{2} \|x - x_k\|^2,
\end{equation}

where $\nabla f(x_k)$ is the Euclidean gradient and $H_k$ is the Euclidean Hessian of $f$ at $x_k$ or a suitable approximation. The regularization parameter $\sigma_k > 0$ plays a similar role as the trust-region radius $\Delta_k$ in the trust-region subproblem (3.1). A specific choice of $\sigma_k$ will be discussed in subsection 3.2. Our overall idea now is to solve and replace the initial problem (1.1) by a sequence of simpler, quadratic subproblems of the form

\begin{equation}
\min_{x \in \mathcal{M}} m_k(x),
\end{equation}

that maintain the manifold constraints. Note that the regularized subproblem (3.4) always attains a solution whenever the manifold $\mathcal{M}$ is compact.

Similar to the classical approaches [26, 1, 2], we embed this basic methodology in a trust-region framework to monitor the acceptance of trial steps and to control the model precision by adjusting the regularization parameter $\sigma_k$. A detailed description of our method can be found in subsection 3.2. Moreover, comparing (3.4) and (2.4), our approach can also be seen as a hybrid of existing regularized trust-region algorithms [9, 27] and of the proximal Newton scheme [25] used in convex composite optimization.

In general, we do not need to solve the subproblem (3.4) exactly, we only need to find a point $z_k$ that ensures a sufficient reduction of the model function $m_k$. For example, as in the classical trust-region method [26], a fraction of Cauchy decrease condition can be used to guarantee the required model decrease. In this respect, the gradient-type methods introduced in subsection 2.1 can be ideal for solving the regularized Newton subproblems at the early stage of the algorithm when high accuracy is not needed or when a good initial guess is not available. Gradient steps can be also useful when the computational cost of evaluating the Riemannian Hessian is too expensive. When a high accuracy is required, the subproblem (3.4) can be solved more efficiently by a single or multiple Riemannian Newton steps as explained in the next subsection. Together with our specific exploitation of negative curvature information, our approach can be a good alternative to the trust-region-type methods [1, 2].
3.1. Solving the Riemannian Subproblem. We use an inexact method for minimizing the model (3.4) and perform a single (or multiple) Riemannian Newton step based on the associated linear system:

\[(3.5) \quad \text{grad} m_k(x_k) + \text{Hess} m_k(x_k)[\xi] = 0.\]

The system (3.5) is solved approximately with a modified conjugate gradient (CG) method up to a certain accuracy. Since the model Hessian may be indefinite, we terminate the CG method when either the residual becomes small or negative curvature is detected. Then, a new gradient-related direction is constructed based on the conjugated directions and a necessary curvilinear search along this direction is utilized to reach a sufficient reduction of the objective function. The detailed procedure is presented in Algorithm 2.

We next discuss a connection between (3.5) and the classical approach (3.1)–(3.2) in the exact case \(H_k = \nabla^2 f(x_k)\). In fact, the definition of the Riemannian gradient implies

\[\text{grad} m_k(x_k) = P_{x_k}(\nabla m_k(x_k)) = P_{x_k}(\nabla f(x_k)) = \text{grad} f(x_k),\]

where \(P_{x_k}(u) := \arg\min_{v \in T_{x_k}M} \|v - u\|_2\) denotes the orthogonal projection onto \(T_{x_k}M\). Using \(\nabla^2 m_k(x_k) = \nabla^2 f(x_k) + \sigma_k I\) and introducing the so-called Weingarten map \(\mathfrak{W}_x(\cdot, v) : T_xM \to T_xM\) for some \(v \in T^\perp_x M\), it holds

\[\text{Hess} m_k(x_k)[\xi] = P_{x_k}(\nabla^2 m_k(x_k)[\xi]) + \mathfrak{W}_x(x_k, P_{x_k}^\perp(\nabla m_k(x_k)))
\]

\[= \text{Hess} f(x_k)[\xi] + \sigma_k \xi\]

for all \(\xi \in T_{x_k}M\). The Weingarten map \(\mathfrak{W}_x(\cdot, v)\) is a symmetric linear operator that is closely related to the second fundamental form of \(M\). The projection \(P_{x_k}^\perp\) in (3.6) is given explicitly by \(P_{x_k}^\perp = I - P_{x_k}\). For a detailed derivation of the expression (3.6) and further information on the Weingarten map, we refer to [3].

Although the linear systems (3.5) and (3.2) have a similar form, our approach is based on a different model formulation and uses different trial points and reduction ratios. Moreover, inspired by Steihaug’s CG method [30] and by related techniques in trust-region based optimization [15, 2], we implement a specific termination strategy whenever the CG methods encounter small or negative curvature. In particular, we utilize the detected negative curvature information to modify and improve our current search direction.

An overview of the procedure is given in Algorithm 2. The method generates two different output vectors \(s_k\) and \(d_k\), where the vector \(d_k\) represents and transports the negative curvature information. The new search direction \(\xi_k\) is then computed as follows

\[(3.7) \quad \xi_k = \begin{cases} s_k + \tau_k d_k & \text{if } d_k \neq 0, \\ s_k & \text{if } d_k = 0, \end{cases} \text{ with } \tau_k := \frac{\langle d_k, \text{grad} m_k(x_k) \rangle_{x_k}}{\langle d_k, \text{Hess} m_k(x_k)[d_k] \rangle_{x_k}}.\]

In section 4, we will show that \(\xi_k\) is a descent direction. Note that the rescaling factor \(\tau_k\) in (3.7) can be obtained without any additional costs. The choice of \(\tau_k\) is mainly motivated by our numerical experiments, see also (4.3) and [15] for a related variant.

Once the direction \(\xi_k\) is constructed, we carry out a curvilinear search along \(\xi_k\) to generate a trial point \(z_k\), i.e.,

\[(3.8) \quad z_k = R_{x_k}(\alpha_k \xi_k).\]
The step size $\alpha_k = \alpha_0 \delta^k$ is again chosen by the (monotone) Armijo rule such that $h$ is the smallest integer satisfying
\begin{equation}
\sigma_k(R_{x_k}(\alpha_0 \delta^k \xi_k)) \leq \rho \alpha_0 \delta^k \langle \nabla m_k(x_k), \xi_k \rangle_{x_k},
\end{equation}
where $\rho, \delta \in (0,1)$ and $\alpha_0 \in (0,1]$ are given constants.

### 3.2. The Algorithmic Framework.
We now present our regularized Newton framework starting from a feasible initial point $x_0$ and a regularization parameter $\sigma_0$. As described in the last section, the algorithm first computes a trial point $z_k$ to approximately solve the regularized subproblem (3.4). In order to decide whether $z_k$ should be accepted as the next iterate and whether the regularization parameter $\sigma_k$ should be updated or not, we calculate the ratio between the actual reduction of the objective function $f(x)$ and the predicted reduction:
\begin{equation}
(3.10) \quad \rho_k = \frac{f(z_k) - f(x_k)}{m_k(z_k)}.
\end{equation}
If $\rho_k \geq \eta_1 > 0$, then the iteration is successful and we set $x_{k+1} = z_k$; otherwise, the iteration is not successful and we set $x_{k+1} = x_k$, i.e., we have
\begin{equation}
(3.11) \quad x_{k+1} = \begin{cases} z_k, & \text{if } \rho_k \geq \eta_1, \\ x_k, & \text{otherwise.} \end{cases}
\end{equation}

The regularization parameter $\sigma_{k+1}$ is updated as follows
\begin{equation}
(3.12) \quad \sigma_{k+1} \in \begin{cases} (0, \gamma_0 \sigma_k) & \text{if } \rho_k \geq \eta_2, \\ \{\gamma_0 \sigma_k, \gamma_1 \sigma_k\} & \text{if } \eta_1 \leq \rho_k < \eta_2, \\ \{\gamma_1 \sigma_k, \gamma_2 \sigma_k\} & \text{otherwise,} \end{cases}
\end{equation}
where $0 < \eta_1 \leq \eta_2 < 1$ and $0 < \gamma_0 < 1 < \gamma_1 \leq \gamma_2$. These parameters determine how aggressively the regularization parameter is adjusted when an iteration is successful or unsuccessful. The complete regularized Newton method to solve (1.1) is summarized in Algorithm 3.
Algorithm 3: An Adaptive Regularized Newton Method

\begin{algorithm}
\begin{algorithmic}
\STATE Choose a feasible initial point \(x_0 \in \mathcal{M}\) and an initial regularization parameter \(\sigma_0 > 0\). Choose \(0 < \eta_1 \leq \eta_2 < 1\), \(0 < \gamma_0 < 1 < \gamma_1 \leq \gamma_2\). Set \(k := 0\).
\WHILE {stopping conditions not met}
\STATE Compute a new trial point \(z_k\) according to (3.8) and (3.9).
\STATE Compute the ratio \(\rho_k\) via (3.10).
\STATE Update \(x_{k+1}\) from the trial point \(z_k\) based on (3.11).
\STATE Update \(\sigma_k\) according to (3.12).
\STATE \(k \leftarrow k + 1\).
\ENDWHILE
\end{algorithmic}
\end{algorithm}

4. Convergence Analysis. We now analyze the convergence of Algorithm 3 based on the model (3.4). Let us note that the analysis can be similarly extended to the algorithm using cubically regularized subproblems as well. In the following, we summarize and present our main assumptions.

Assumption 3. Let \(\{x_k\}\) be generated by Algorithm 3. We assume:
\begin{enumerate}
\item[(A.1)] The gradient \(\nabla f\) is Lipschitz continuous on the convex hull of the manifold \(\mathcal{M}\) denoted by \(\text{conv}(\mathcal{M})\), i.e., there exists \(L_f > 0\) such that
\[
\|\nabla f(x) - \nabla f(y)\| \leq L_f\|x - y\|, \quad \forall \ x, y \in \text{conv}(\mathcal{M}).
\]
\item[(A.2)] There exists \(\kappa_g > 0\) such that \(\|\nabla f(x_k)\| \leq \kappa_g\) for all \(k \in \mathbb{N}\).
\item[(A.3)] There exists \(\kappa_H > 0\) such that \(\|H_k\| \leq \kappa_H\) for all \(k \in \mathbb{N}\).
\item[(A.4)] The Euclidean and the Riemannian Hessian are bounded, i.e., there exist \(\kappa_F\) and \(\kappa_R \geq 1\) such that
\[
\|\nabla^2 f(x_k)\| \leq \kappa_F \quad \text{and} \quad \|\Hess_f(x_k)\| \leq \kappa_R, \quad \forall \ k \in \mathbb{N}.
\]
\item[(A.5)] Let \(\omega^M_{x_k}, \omega^L_{x_k}\) be given as in (2.1). Then, suppose there exists \(\overline{\omega} > 0\), \(\overline{\omega} \geq 1\) such that \(\overline{\omega} \leq \omega_{x_k}^m\) and \(\omega_{x_k}^M \leq \overline{\omega}\) for all \(k \in \mathbb{N}\).
\end{enumerate}

Remark 4. Suppose that the level set \(\mathcal{L}\) is compact. Then, by construction of Algorithm 3, we have \(f(x_{k+1}) = f(x_k) + \rho_k m_k(z_k) \leq f(x_k)\) if iteration \(k\) is successful. Due to (3.11), it follows \(x_k \in \mathcal{L}\) for all \(k\) and the sequence \(\{x_k\}\) must be bounded. Hence, in this case, the assumptions (A.2) and (A.4) hold automatically. Furthermore, since the parameters \(\omega_{x_k}^m, \omega_{x_k}^L, k \in \mathbb{N}\), depend continuously on \(x_k\), assumption (A.5) is also satisfied.

Remark 5. The bounds in Assumption 3 can also be used to derive a bound for \(\Hess m_k(x_k)\). In fact, under the conditions (A.3)–(A.5) and by (3.6), we have
\[
\langle \xi, \Hess m_k(x_k)[\xi]\rangle_{x_k} = \langle \xi, \Hess f(x_k)[\xi] + P_{x_k}((H_k - \nabla^2 f(x_k))[\xi])\rangle_{x_k} + \sigma_k \|\xi\|^2_{x_k} \\
\leq \left(\kappa_R + (\omega^L_{x_k})^\frac{1}{2}(\omega^m_{x_k})^{-\frac{1}{2}}(\kappa_H + \kappa_F) + \sigma_k\right)\|\xi\|^2_{x_k}
\]
where we used the linearity and nonexpansiveness of the operator \(P_{x_k}\). In the following, we set \(\kappa^M_{x_k} := \kappa_R + (\omega^L_{x_k})^\frac{1}{2}(\omega^m_{x_k})^{-\frac{1}{2}}(\kappa_H + \kappa_F)\).

4.1. Analysis of the Inner Subproblem. At first, we briefly discuss several useful properties of the modified CG method.

Lemma 6. Let the sequences \(\{p_i\}_{i=0}^\ell, \{r_i\}_{i=0}^\ell, \{\eta_i\}_{i=0}^\ell\), and the direction \(\xi_k\) be generated by Algorithm 2. Then, we have:
(i) For all \( j = 1, \ldots, \ell \), it holds \( p_j \in T_{x_k} \mathcal{M} \),

(4.1) \[ \langle p_j, \text{Hess} m_k(x_k)p_i \rangle_{x_k} = 0, \quad \text{and} \quad \langle r_j, r_i \rangle_{x_k} = 0, \quad \forall \ i = 0, \ldots, j - 1. \]

(ii) The sequence \( \{ \tilde{m}_k(\eta_i) \} \) is strictly decreasing and it holds \( \tilde{m}_k(\xi_k) < \tilde{m}_k(\eta_k) \).

(iii) The sequence \( \{ \| \eta_i \|_{x_k} \} \) is strictly increasing and it holds \( \| \xi_k \|_{x_k} \geq \| \eta_i \|_{x_k} \).

Proof. Except for step S2, Algorithm 2 coincides with the standard CG method applied to the quadratic problem min\( \xi \) \( \tilde{m}_k(\xi) \). Since \( \text{Hess} m_k(x_k) \) is a linear operator from \( T_{x_k} \mathcal{M} \) to \( T_{x_k} \mathcal{M} \), all iterates generated by Algorithm 2 will stay in the tangent space \( T_{x_k} \mathcal{M} \). Furthermore, since the Riemannian Hessian is symmetric with respect to the metric \( \langle \cdot, \cdot \rangle_{x_k} \), Proposition 5.5.3, part (i) and (ii) essentially follow from the properties of the CG method in Euclidean space. We refer to [26, Section 5.1] for further details. If \( d_k \neq 0 \), the estimate \( \tilde{m}_k(\xi_k) \leq \tilde{m}_k(\eta_i) \) follows from (4.1) and \( \pi_\ell < 0 \). The first claim in (iii) is proven in [26, Theorem 7.3]; To verify \( \| \xi_k \|_{x_k} \geq \| \eta_i \|_{x_k} \), we first show

(4.2) \[ \| r_i \|_{x_k}^2 = -\langle \text{grad} m_k(x_k), p_i \rangle_{x_k}, \quad \forall \ i = 0, \ldots, \ell - 1 \]

by induction. For \( i = 0 \), (4.2) is obviously satisfied by definition of \( r_0 \) and \( p_0 \). Now, let us suppose that (4.2) holds for \( i = \ell - 1 \). Then, by (4.1) we have

\[
-\langle \text{grad} m_k(x_k), p_\ell \rangle_{x_k} = \langle r_0, r_\ell - \beta_\ell p_{\ell-1} \rangle_{x_k} = -\frac{\| r_\ell \|_{x_k}^2}{\| r_{\ell-1} \|_{x_k}^2} \langle r_0, p_{\ell-1} \rangle_{x_k} = \| r_\ell \|_{x_k}^2.
\]

Thus, if \( d_k \neq 0 \), this implies

(4.3) \[ \xi_k = \eta_\ell + \tau_\ell d_k = \sum_{i=0}^{\ell-1} \alpha_i p_i - \frac{\| r_\ell \|_{x_k}^2}{\pi_\ell} p_\ell = \sum_{i=0}^{\ell} |\alpha_i| p_i. \]

Consequently, since \( \xi_k \) and \( \eta_\ell \) coincide in the case \( d_k = 0 \), the estimate \( \| \xi_k \|_{x_k} \geq \| \eta_i \|_{x_k} \) again follows from [26, Theorem 7.3] (and from the special structure of \( \xi_k \)).

We now prove that the direction \( \xi_k \) is a descent direction.

Lemma 7. Let \( \{ \alpha_i \}, \{ \pi_i \}, \{ p_i \}, \) and \( \{ \eta_i \} \) be generated by Algorithm 2 and suppose that the conditions (A.3)–(A.4) are satisfied. Then, the direction \( \xi_k \) – given in (3.7) – is a descent direction and it holds

(4.4) \[ \frac{\langle \text{grad} m_k(x_k), \xi_k \rangle_{x_k}}{\| \text{grad} m_k(x_k) \|_{x_k} \| \xi_k \|_{x_k}} \leq -\min \left\{ \frac{\epsilon}{2}, 1 \right\} \frac{1}{n(M_{\mathcal{M}} + 1)} =: -\lambda_k. \]

Proof. We first analyze the case where Algorithm 2 detects a small or negative curvature and terminates in step S2. In this situation, we have

\[ \xi_k = s_k + \tau_k d_k = \begin{cases} -\text{grad} m_k(x_k) & \text{if } \ell = 0 \text{ and } |\pi_\ell| \leq \epsilon \| p_\ell \|_{x_k}^2, \\ \eta_\ell & \text{if } \ell > 0 \text{ and } |\pi_\ell| \leq \epsilon \| p_\ell \|_{x_k}^2, \\ \eta_\ell + \tau_k p_\ell & \text{if } \ell > 0 \text{ and } \pi_\ell < -\epsilon \| p_\ell \|_{x_k}^2 \end{cases} \]

with \( \tau_k = \pi_\ell^{-1} \langle \text{grad} m_k(x_k), p_\ell \rangle_{x_k} \). We note that condition (4.4) is obviously satisfied with \( \lambda_k := 1 \) in the case \( \ell = 0 \). Next, let us consider the case \( \ell > 0 \) and \( \pi_\ell < -\epsilon \| p_\ell \|_{x_k}^2 \). Due to (4.2), we have

\[
\langle \text{grad} m_k(x_k), \eta_\ell \rangle_{x_k} = \sum_{i=0}^{\ell-1} \alpha_i \langle \text{grad} m_k(x_k), p_i \rangle_{x_k} = -\sum_{i=0}^{\ell-1} \frac{\langle \text{grad} m_k(x_k), p_i \rangle_{x_k}^2}{\pi_i}.
\]
and thus
\[
\langle \nabla m_k(x_k), \xi_k \rangle_{x_k} = - \sum_{i=0}^{\ell} \frac{\langle \nabla m_k(x_k), p_i \rangle_{x_k}^2}{|\pi_i|} \leq - \frac{\|p_0\|^2}{\pi_0} \leq - \frac{\|\nabla m_k(x_k)\|_{x_k}^2}{\kappa_{x_k}^M + \sigma_k},
\]
where we used the conditions (A.3)–(A.4), Remark 5, and \(\pi_i > 0, i = 0, \ldots, \ell - 1\). By construction of the algorithm, it holds \(|\pi_i| = \pi_i > \epsilon\|p_i\|_{x_k}^2\) for all \(i = 0, \ldots, \ell - 1\) and \(|\pi_\ell| = -\pi_\ell > \epsilon\|p_\ell\|^2_{x_k}\). Hence, we obtain
\[
\|\xi_k\|_{x_k} \leq \sum_{j=0}^{\ell} \frac{|\langle \nabla m_k(x_k), p_i \rangle_{x_k}|}{|\pi_i|} \cdot \|p_i\|_{x_k} \leq (\ell + 1)\|\nabla m_k(x_k)\|_{x_k} \cdot \max_{i} \frac{\|p_i\|^2_{x_k}}{|\pi_i|} \leq \frac{n}{\epsilon} \|\nabla m_k(x_k)\|_{x_k}.
\]
Moreover, if \(\sigma_k \geq \kappa_{x_k}^M + 2\), then we have \(\|\pi_i\|_{x_k}^{-2} \geq \sigma_k - \kappa_{x_k}^M > 0\) and the last estimate becomes \(\|\xi_k\|_{x_k} \leq \frac{n}{\epsilon} (\sigma_k - \kappa_{x_k}^M)^{-1} \|\nabla m_k(x_k)\|_{x_k}\). Combining these results, we now get
\[
\frac{\langle \nabla m_k(x_k), \xi_k \rangle_{x_k}}{\|\nabla m_k(x_k)\|_{x_k} \cdot \|\xi_k\|_{x_k}} \leq - \frac{\epsilon}{\kappa_{x_k}^M + 1}.
\]
Due to the special structure of \(\xi_k\) (see again (4.3)), the same estimates can also be used and derived in the remaining cases. This finishes the proof.

In the next lemma, we prove that the descent property of \(\xi_k\) can be carried over to the Euclidean model \(m_k\) using the smooth retraction \(R\) and that a sufficient reduction of the objective function \(m_k\) in the sense of (3.9) can be ensured.

**Lemma 8.** Suppose that the assumptions (A.2)–(A.4) are satisfied. Let \(\rho \in (0, 1)\) be arbitrary and set \(z_k(t) := R_{x_k}(t\xi_k)\). Then, we have
\[
m_k(z_k(t)) \leq \rho t \langle \nabla m_k(x_k), \xi_k \rangle_{x_k}, \quad \forall t \in [0, \zeta_k],
\]
where
\[
\zeta_k := \min \left\{ \left( \frac{\chi}{M x_k} \right)^{-1}, 1 \right\} \min \left\{ \frac{1}{\|\xi_k\|_{x_k}}, \frac{2(1 - \rho)\lambda_k}{\kappa_2 \kappa_1^2 + \kappa_2^2 (\kappa_H + \sigma_k)} \right\} \|\nabla f(x_k)\|_{x_k}
\]
and \(\kappa_1, \kappa_2, \chi\) are constants that do not depend on \(x_k\).

**Proof.** Let us set \(\phi(t) := m_k(R_{x_k}(t\xi_k))\). Then, since \(M\) is an embedded submanifold and using the properties of the retraction \(R_{x_k}\), it follows
\[
m_k(R_{x_k}(t\xi_k)) = \phi(0) + t \phi'(0) + \int_0^t \phi'(s) - \phi'(0) \, ds
\]
\[
= t \langle \nabla f(x_k), \xi_k \rangle + \int_0^t \langle \nabla f(x_k), (D_{x_k} (s\xi_k) - \text{id})[\xi_k] \rangle + \langle (R_{x_k} (s\xi_k) - x_k), (H_k + \sigma_k I)[D_{x_k} (s\xi_k)] \rangle \, ds,
\]
where \(\text{id} \equiv \text{id}_{T_x M}\) denotes the identity mapping on \(T_x M\). As in [6, Section B], we define the compact set \(K_\chi := \{ \xi \in T_x M : \|\xi\| \leq \chi \}\). The smoothness of \(R\) now implies
\[
\|R_{x_k}(\xi) - x_k\| \leq \int_0^1 \|D_{x_k} (s\xi)\|_\xi \, ds \leq \max_{y \in K_\chi} \|D_{R_y}\| \|\xi\|
\]
and

\[(4.8) \quad \|DR_{x_k}(\xi) - \text{id}\| \leq \int_0^1 \|D^2R_{x_k}(s\xi)\| \, ds \leq \max_{y \in K_\chi} \|D^2R(y)\| \|\xi\| \]

for all $\xi \in K_\chi$. Setting $\kappa_1 := \max_{y \in K_\chi} \|DR(y)\|$ and $\kappa_2 := \max_{y \in K_\chi} \|D^2R(y)\|$ and using the assumptions (A.2)–(A.3), this yields

\[m_k(R_{x_k}(t\xi_k)) \leq t \langle \nabla f(x_k), \xi_k \rangle + \int_0^t (\kappa_2\kappa_g + \kappa_1^2(\kappa_H + \sigma_k))s\|\xi_k\|^2 \, ds \]

\[= t \langle \text{grad} f(x_k), \xi_k \rangle + \frac{1}{2}(\kappa_2\kappa_g + \kappa_1^2(\kappa_H + \sigma_k))t^2\|\xi_k\|^2. \]

if $t\|\xi_k\| \leq \chi$. Thus, by Lemma 7 and setting $\kappa := \kappa_2\kappa_g + \kappa_1^2(\kappa_H + \sigma_k)$, we obtain

\[m_k(R_{x_k}(t\xi_k)) - \rho t \langle \text{grad} m(x_k), \xi_k \rangle_{x_k} \]

\[\leq -(1 - \rho)\lambda_k t\|\text{grad} f(x_k)\|_{x_k}\|\xi_k\|_{x_k} + \frac{1}{2}\kappa \kappa_g^M t^2\|\xi_k\|_{x_k}^2. \]

\[\leq \left[\frac{1}{2}\kappa \kappa_g^M t - (1 - \rho)\lambda_k \frac{\|\text{grad} f(x_k)\|_{x_k}}{\|\xi_k\|_{x_k}}\right] t\|\xi_k\|_{x_k}^2 \]

if $t\|\xi_k\| \leq \chi$. Finally, using the last estimate, (2.1), and $(\kappa_g^M)^{-\frac{1}{2}} \leq \max\{\kappa_g^M, 1\}$, this establishes (4.5) and (4.6).

\section*{4.2. Global Convergence.} In this section, based on the techniques used in [9], we present global convergence properties of the adaptive regularized Newton method. We first investigate the relationship between the reduction ratio $\rho_k$ defined in (3.10), the regularization parameter $\sigma_k$, and the gradient norm $\|\text{grad} f(x_k)\|_{x_k}$. Under the assumption $\|\text{grad} f(x_k)\|_{x_k} \geq \tau > 0$, we then derive an upper bound for $\sigma_k$ and show that the iterations will be successful, (i.e., $\rho_k \geq \eta_1$), whenever $\sigma_k$ exceeds this bound.

In Theorem 13 we combine our observations and establish convergence of our method.

The next lemma shows that the distance between $z_k$ and $x_k$ is bounded by some value related to the regularization parameter $\sigma_k$.

\textbf{Lemma 9.} Suppose that the assumptions (A.2)–(A.3) hold and that $z_k$ satisfies the Armijo condition (3.9). Then, it holds

\[\|z_k - x_k\| \leq \frac{2\kappa_g}{\sigma_k - \kappa_H}, \]

whenever $\sigma_k > \kappa_H$.

\textit{Proof.} By Lemma 7 we have $m_k(z_k) \leq 0$. Thus, it follows

\[\langle \nabla f(x_k), z_k - x_k \rangle + \frac{1}{2} (z_k - x_k, H_k[z_k - x_k]) + \frac{\sigma_k}{2} \|z_k - x_k\|^2 \leq 0. \]

If $\sigma_k \geq \kappa_H$, then the term $\|z_k - x_k\|$ can be bounded by

\[-\|\nabla f(x_k)\| \|z_k - x_k\| - \frac{1}{2}\kappa_H \|z_k - x_k\|^2 + \frac{1}{2}\sigma_k \|z_k - x_k\|^2 \leq 0, \]

and hence,

\[\|z_k - x_k\| \leq \frac{2\|\nabla f(x_k)\|}{\sigma_k - \kappa_H} \leq \frac{2\kappa_g}{\sigma_k - \kappa_H}. \]
When the regularization parameter is sufficiently large, our model defines a good approximation of the initial problem \((1.1)\). In this case, a successful iteration and sufficient reduction of the objective function can be ensured.

**Lemma 10.** Suppose that the conditions \((A.1)–(A.4)\) hold and that \(z_k\) satisfies the Armijo condition \((3.9)\). Furthermore, let us assume \(g_k \coloneqq \|\nabla f(x_k)\|_{x_k} \neq 0\) and

\[
\sigma_k \geq \max \left\{ \kappa_{Mx_k}^2, \kappa_H + \vartheta_k \max \left\{ \frac{1}{\sqrt{\chi}}, \frac{A_k^k \vartheta_k}{g_k} \right\} \right\}, \quad \vartheta_k \coloneqq \sqrt{\frac{A_k^k \max\{\varpi_M^M, 1\}}{(1 - \eta_2)g_k}}
\]

where \(\kappa \coloneqq \kappa_2 \kappa_\eta + 2 \kappa_2^2 \kappa_H, A_1^k \coloneqq 2 \kappa_2^2 \alpha_0 (\rho \lambda_k \delta)^{-1} (L_f + \kappa_H), A_2^k \coloneqq ((1 - \rho) \lambda_k)^{-1} \kappa, \) and \(A_3^k \coloneqq ((1 - \rho) \lambda_k)^{-1} \kappa_2^2.\) Then, iteration \(k\) is very successful, i.e., it holds \(\rho_k \geq \eta_2\) and \(\sigma_{k+1} \leq \gamma_0 \sigma_k.\)

**Proof.** Using the Lipschitz continuity of \(\nabla f\) and \((A.3)\), it follows

\[
f(z_k) - f(x_k) - m_k(z_k) = \langle \nabla f(x_k + \tau(z_k - x_k)) - \nabla f(x_k), z_k - x_k \rangle
\]

\[
- \frac{1}{2} (H_k[z_k - x_k], z_k - x_k) - \frac{\sigma_k^2}{2} \|z_k - x_k\|^2
\]

\[
\leq \frac{1}{2} (L_f + \kappa_H) \|z_k - x_k\|^2,
\]

for some \(\tau \in (0, 1)\). Applying Lemma 8, Lemma 9, and the Armijo condition \((3.9)\), we now obtain

\[
1 - \rho_k = \frac{f(z_k) - f(x_k) - m_k(z_k)}{-m_k(z_k)} \leq \frac{(L_f + \kappa_H) \|z_k - x_k\|^2}{2 \rho \lambda_k \alpha_k \|\nabla f(x_k)\|_{x_k} \|\xi_k\|_{x_k}}
\]

\[
\leq \frac{2(L_f + \kappa_H) \kappa_2^2}{\rho \lambda_k \alpha_0^{-1} \delta} \max\{\varpi_M^M, 1\} \max \left\{ \frac{1}{\chi}, \frac{\kappa_2 \kappa_\eta + \kappa_2^2 (\sigma_k + \kappa_H)}{2(1 - \rho) \lambda_k g_k} \right\}
\]

\[
\leq \frac{A_1^k \max\{\varpi_M^M, 1\}}{(\sigma_k - \kappa_H)^2 g_k} \max \left\{ \frac{1}{\chi}, \frac{\kappa_2 \kappa_\eta + \kappa_2^2 (\sigma_k + \kappa_H)}{(1 - \rho) \lambda_k g_k} \right\}
\]

\[
= \frac{A_1^k \max\{\varpi_M^M, 1\}}{(\sigma_k - \kappa_H)^2 g_k} \max \left\{ \frac{1}{\chi}, \frac{A_2^k}{g_k} \frac{A_3^k}{(\sigma_k - \kappa_H)} \right\}
\]

\[
\leq 1 - \eta_2.
\]

The above inequality shows \(\rho_k \geq \eta_2\). Finally, step S4 of Algorithm 3 implies \(\sigma_{k+1} \leq \gamma_0 \sigma_k,\) as desired.

We next prove that the regularization parameters can be bounded.

**Lemma 11.** Suppose that the assumptions \((A.1)–(A.5)\) are satisfied and there exists \(\tau > 0\) such that \(\|\nabla f(x_k)\|_{x_k} \geq \tau\) for all \(k \in \mathbb{N}\). Then, the sequence \(\{\sigma_k\}\) is bounded, i.e., there exists \(L_\tau \geq 0\) such that

\[(4.9)\]

\[
\sigma_k \leq L_\tau, \quad \forall k \in \mathbb{N}.
\]

**Proof.** At first, using the bounds in \((A.5)\), it holds \(\kappa_{Mx_k}^2 \leq \kappa_H + (\varpi M)^{-\frac{1}{2}} (\kappa_H + \kappa_F) =: \kappa_M.\) Hence, it follows \(\lambda_k \geq \min \left\{ \frac{1}{\varpi M}, 1 \right\} (n(\kappa_M + 1))^{-1} =: \lambda\) and similarly,

\[
A_1^k \leq (2 \kappa_2^2 \alpha_0 (L_f + \kappa_H)) (\rho \delta \lambda)^{-1} =: A_1, \quad A_2^k \leq (1 - \rho) \lambda^{-1} =: A_2.
\]
and $A_k^3 \leq \kappa^2_1((1 - \rho)\bar{\lambda})^{-1} =: A_3$. We now define

$$\kappa_{\tau} := \max \left\{ \tilde{\kappa}_M, \kappa_H + \vartheta_{\tau} \max \left\{ \frac{1}{\sqrt{\chi}}, \frac{\sqrt{A_3}}{\sqrt{\tau}}, A_3 \vartheta_{\tau} \right\} \right\}, \quad \vartheta_{\tau} := \sqrt{\frac{A_1}{\sqrt{1 - \eta_2}}}. $$

Let us assume that the bound $\sigma_k \geq \kappa_{\tau}$ holds for some $k \geq 0$. Then, Lemma 10 implies that iteration $k$ is very successful with $\sigma_{k+1} \leq \sigma_k$. Consequently, when $\sigma_0 \leq \gamma_2 \kappa_{\tau}$, we have $\sigma_k \leq \gamma_2 \kappa_{\tau}$, $k \geq 0$, where the factor $\gamma_2$ is introduced to cover the case that $\sigma_k$ is less than $\kappa_{\tau}$ and iteration $k$ is not very successful. Setting $L_{\tau} := \max \{\sigma_0, \gamma_2 \kappa_{\tau}\}$, we obtain (4.9).

Based on the results in [9], [2, Section 7] and similar to [27], we now show global convergence of our adaptive regularized Newton method. We first analyze the behavior of Algorithm 3 under the assumption that only finitely many successful iterations are performed.

**Lemma 12.** Suppose that the assumption (A.1)–(A.5) are satisfied and there are only finitely many successful iterations. Then, it holds $x_k = x_*$ for all sufficiently large $k$ and $\text{grad} f(x_k) = 0$.

**Proof.** Let the last successful iteration be indexed by $\ell$, then, due to the construction of Algorithm 3, it holds $x_{\ell+1} = x_k = x_*$, for all $k \geq \ell + 1$. Since all iterations $k \geq \ell + 1$ are unsuccessful, the regularization parameter $\sigma_k$ tends to infinity as $k \to \infty$. If $\|\text{grad} f(x_{\ell+1})\|_{x_{\ell+1}} > 0$, then we have $\|\text{grad} f(x_k)\|_{x_k} = \|\text{grad} f(x_{\ell+1})\|_{x_{\ell+1}} > 0$ for all $k \geq \ell + 1$, and Lemma 11 implies that $\sigma_k$ is bounded above, $k \geq \ell + 1$. This contradiction completes the proof.

The following theorem generalizes [9, Theorem 2.5] and represents our main convergence result in this section.

**Theorem 13.** Suppose that the assumptions (A.1)–(A.5) hold and let $\{f(x_k)\}$ be bounded from below. Then, either

$$\text{grad} f(x_\ell) = 0 \quad \text{for some} \quad \ell \geq 0 \quad \text{or} \quad \liminf_{k \to \infty} \|\text{grad} f(x_k)\|_{x_k} = 0. $$

**Proof.** Due to Lemma 12, we only have to consider the case when infinitely many successful iterations occur. Let us assume that there exists $\tau > 0$ such that

(4.10) $$\|\text{grad} f(x_k)\|_{x_k} \geq \tau, \quad \forall k \geq 0$$

and let $k \in \mathcal{S}$ with $\mathcal{S} := \{k \in \mathbb{N} : \text{iteration } k \text{ is successful or very successful} \}$ be given. As in the proof of Lemma 11 there exists $\bar{\lambda}$ such that $\lambda_k \geq \bar{\lambda}$ for all $k \in \mathbb{N}$. Now, Lemma 8 and Lemma 11 imply

$$f(x_k) - f(z_k) \geq \eta_1 \cdot (-m_k(z_k)) \geq \eta_1 \rho \bar{\lambda} \alpha_0^{-1} \delta \xi_k \cdot \|\text{grad} f(x_k)\|_{x_k} \|\xi_k\|_{x_k} \geq \eta_1 \rho \bar{\lambda} \delta (\alpha_0 \vartheta_{\tau})^{-1} \cdot \min \left\{ \chi, \frac{2(1 - \rho)\bar{\lambda}}{\kappa + \kappa^2_1(L_{\tau} - \kappa_H)} \right\} =: \delta_{\tau}. $$

Summing up over all iterates yields

(4.11) $$f(x_0) - f(x_{k+1}) = \sum_{j=0, j \in \mathcal{S}}^{k} f(x_j) - f(x_{j+1}) \geq |\mathcal{S} \cap \{1,...,k\}| \cdot \delta_{\tau}. $$
Since $S$ is not finite, we have $|S \cap \{1, \ldots, k\}| \to \infty$ as $k \to \infty$. Consequently, inequality (4.11) implies $\lim_{k \to \infty} f(x_k) - f(x_{k+1}) = \infty$ which is contradiction to the lower boundedness of $\{f(x_k)\}$. Hence, assumption (4.10) must be false and $\{\|\nabla f(x_k)\|_{x_k}\}$ has a subsequence that converges to zero.

**Remark 14.** As in subsection 2.3, it is possible to obtain a slightly stronger result and establish convergence of the full sequence $\|\nabla f(x_k)\|_{x_k} \to 0$ as $k \to \infty$. However, this requires additional assumptions on the retraction and on the Lipschitz continuity of the Riemannian gradient. We refer to [27, Corollary 4.2.1] for a related discussion and result.

### 4.3. Local Convergence

In this part, we analyze the local convergence properties of Algorithm 3. Because our inner solver is a regularized Newton method, the local superlinear convergence can be established using similar techniques as in the standard trust-region method [36]. Following [2, Proposition 7.4.5], we first present an assumption on the boundedness of the second-order covariant derivatives $D dt d dt R_{x}(t\xi)$.

**Assumption 15.** Suppose that there exists $\beta_R, \delta_R > 0$ such that
\[
\left\| \frac{d}{dt} \frac{d}{dt} R_{x}(t\xi) \right\|_{x} \leq \beta_R
\]
for all $x \in M$, all $\xi \in T_xM$ with $\|\xi\|_{x} = 1$ and all $t < \delta_R$.

We refer to [2, Chapter 5] for a detailed discussion of covariant derivatives. Let us note that Assumption 15 is satisfied whenever the manifold $M$ is compact, see, e.g., [2, Corollary 7.4.6]. We now present our main assumptions that are necessary to prove fast local convergence of Algorithm 3. Let us emphasize that our assumptions are similar to the ones used in other Riemannian optimization frameworks.

**Assumption 16.** Let $\{x_k\}$ be generated by Algorithm 3. We assume:

(B.1) The sequence $\{x_k\}$ converges to $x_*$.
(B.2) The Euclidean Hessian $\nabla^2 f$ is continuous on $\text{conv}(M)$.
(B.3) The Riemannian Hessian $\text{Hess} f$ is positive definite at $x_*$ and the constant $\epsilon$ in Algorithm 2 is set to zero.
(B.4) The matrices $H_k, k \in \mathbb{N},$ satisfy the following Dennis-Moré condition:
\[
\frac{\|(H_k - \nabla^2 f(x_k))[z_k - x_k]\|}{\|z_k - x_k\|} \to 0, \quad \text{whenever} \quad \|\nabla f(x_k)\|_{x_k} \to 0,
\]
(B.5) $H_k$ is a good approximation of the Euclidean Hessian $\nabla^2 f$, i.e., it holds
\[
\|H_k - \nabla^2 f(x_k)\| \to 0, \quad \text{whenever} \quad \|\nabla f(x_k)\|_{x_k} \to 0.
\]

In the following lemma and inspired by [9, Theorem 4.3] and [27, Theorem 4.2.2], we show that the iterations generated by Algorithm 3 are eventually very successful. Due to (3.12), this also implies that the sequence of regularization parameters $\{\sigma_k\}$ converges to zero as $k \to \infty$.

**Lemma 17.** Let the conditions (A.3) and (B.1)-(B.4) be satisfied. Then, all iterations are eventually very successful.

**Proof.** First, Theorem 13 implies that $x_*$ is stationary point of problem (1.1), i.e., we have $\nabla f(x_k) \to \nabla f(x_*) = 0$ as $k \to \infty$. Moreover, since $\{x_k\}$ converges to
Lemma 7

It follows that we can now derive a more refined bound for the step size. Using the continuity of the Riemannian Hessian and (B.3) we have

\[ \|z_k - x_k\| \leq \kappa_1 \alpha_k \|\xi_k\| \leq \min\{\varepsilon^{-1}, 1\} n \cdot \|\nabla f(x_k)\|_{x_k} \rightarrow 0, \quad k \to \infty. \]

Hence, we have \(\|\xi_k\| \leq \chi\) for all \(k\) sufficiently large and thus, from (4.7) it follows

\[ \|z_k - x_k\| \leq \kappa_1 \alpha_k \|\xi_k\| \leq \min\{\varepsilon^{-1}, 1\} \sqrt{\omega} \cdot \|\nabla f(x_k)\|_{x_k}. \]

Similar to [6, Section B] and by combining (4.7)–(4.8), we obtain

\[ \|z_k - x_k - \alpha_k \xi_k\| = \|R_{z_k}(\alpha_k \xi_k) - x_k - \alpha_k \xi_k\| \leq \frac{\sqrt{\omega} \kappa_2}{2} \alpha_k^2 \|\xi_k\|_{x_k}^2 \]

for all \(k\) sufficiently large. Using the continuity of the Riemannian Hessian and (B.3) there exists \(\nu > 0\) such that \(\langle \xi, \text{Hess} f(x_k)(\xi)\rangle_{x_k} \geq \nu \|\xi\|_{x_k}^2\) for all \(\xi \in T_{x_k}M\) and \(k \in \mathbb{N}\) sufficiently large. Setting \(m_k^F(x) := m_k(x) - \frac{\rho}{2} \|x - x_k\|^2\), this implies

\[ \langle \xi_k, \text{Hess} m_k^F(x_k)(\xi_k)\rangle_{x_k} \geq (\nu + \sigma_k) \|\xi_k\|_{x_k}^2 - \|\xi_k, (\text{Hess} m_k^F(x_k) - \text{Hess} f(x_k))(\xi_k)\|_{x_k}. \]

Due to (3.6), we have \(\text{Hess} m_k^F(x_k) - \text{Hess} f(x_k))(\xi_k) = \mathcal{P}_{x_k}((H_k - \nabla^2 f(x_k))(\xi_k))\) and thus, it holds

\[ \langle \xi_k, (\text{Hess} m_k^F(x_k) - \text{Hess} f(x_k))(\xi_k)\rangle_{x_k} \leq c_1 \|H_k - \nabla^2 f(x_k)(z_k - x_k)\| \|z_k - x_k\| + c_2 \|z_k - x_k - \alpha_k \xi_k\| \]

where \(c_1, c_2 > 0\) are suitable constants that only depend on \(\omega, \overline{\omega}, \kappa_H\) and \(\kappa_F\). By (B.4), (4.13), and (4.14), the last term converges to zero as \(k \to \infty\). Consequently, we can infer \(\langle \xi_k, \text{Hess} m_k(x_k)(\xi_k)\rangle_{x_k} \geq \frac{\nu + \sigma_k}{2} \|\xi_k\|_{x_k}^2\) for all \(k\) sufficiently large. This also implies that Algorithm 2 does not stop in iteration \(i = 0\). Hence, applying Lemma 6 (ii), we obtain

\[ \langle \nabla m_k(x_k), \xi_k\rangle_{x_k} \leq \tilde{m}_k(\eta_1) - f(x_k) - \frac{1}{2} \|\xi_k, \text{Hess} m_k(x_k)(\xi_k)\|_{x_k} \]

\[ \leq -\frac{1}{2} \left(\frac{\|g_k\|_{x_k}^2}{\|g_k, \text{Hess} m_k(x_k)(g_k)\|_{x_k}} + \frac{\nu + \sigma_k}{2} \|\xi_k\|_{x_k}^2\right) \leq -\frac{\nu + \sigma_k}{4} \|\xi_k\|_{x_k}^2, \]

where \(g_k := \nabla f(x_k)\). Using this estimate in the proof of Lemma 8, we can now derive a more refined bound for the step size \(\alpha_k\). In particular, it holds

\[ m_k(R_{x_k}(t \xi_k)) \leq -\frac{\rho \nu \delta t}{4}\|\xi_k\|_{x_k}^2, \quad \forall t \in [0, \tilde{t}], \text{ with } \tilde{t} := \frac{1 - \rho}{2\sqrt{\omega}} \min \left\{ \frac{\nu}{\kappa_2 \kappa_g + \kappa^2 \kappa_H}, \frac{1}{\kappa^2} \right\} \]

and thus, we have

\[ -m_k(z_k) \geq \frac{\rho \nu \delta \tilde{t}}{4\alpha_0} \|\xi_k\|_{x_k}^2 \geq \frac{\rho \nu \delta \tilde{t}}{4\alpha_0 \kappa_1 \sqrt{\omega}} \|z_k - x_k\|^2 \]

for all \(k\) sufficiently large. Next, applying a second order Taylor expansion, it follows

\[ f(z_k) - f(x_k) - m_k(z_k) \leq \frac{1}{2} \langle (\nabla^2 f(x_k) - H_k)(z_k - x_k), z_k - x_k \rangle, \]

where...
for some suitable $\delta_k \in [0,1]$ and $x_k^\delta := x_k + \delta_k(z_k-x_k)$. Using the continuity of $\nabla^2 f$, (B.4), and the bound (4.16), we finally obtain

$$1 - \rho_k \leq \frac{1}{2\delta} \left[ \frac{\left\| (\nabla^2 f(x_k) - H_k)(z_k-x_k) \right\|}{\| z_k-x_k \|} + \left\| \nabla^2 f(x_k^\delta) - \nabla^2 f(x_k) \right\| \right] \to 0,$$

as $k \to \infty$. This finishes the proof. 

Next, we establish superlinear convergence of the proposed method. In comparison to Lemma 17, we need a stronger assumption on the matrices $H_k$ to guarantee that the CG method eventually only uses the natural stopping criterion in step S4. In the following, let $f_x := f \circ R_x$ denote the pullback of $f$ through $R_x$ at $x$ and let $0_x$ be the zero element of $T_x \mathcal{M}$.

**Theorem 18.** Suppose that Assumption 15 and the conditions (B.1)–(B.3) and (B.5) are satisfied and let $\alpha_0 = 1$ and $\rho \in (0, \frac{1}{2})$. Then, the sequence $\{x_k\}$ converges $q$-superlinearly to $x_*$.

**Proof.** For convenience, we again set $g_k := \nabla f(x_k)$. We further note that the conditions (B.1) and (B.5) imply (A.2)–(A.5). Due to Assumption 15 and applying [5, Proposition 19], the following bound holds for any smooth function $h$ on $\mathcal{M}$

$$\| \nabla h(x) - \nabla h(0_x) \|_x \leq \beta_R \| \nabla h(x) \|_x,$$

where the operator norm is induced by the Riemannian metric on $T_x \mathcal{M}$. Similar to the proof of Lemma 17 and using (B.3), (B.5), and the uniform estimate

$$\| \langle \xi, (\nabla f(x_k) - \nabla f(0_x))\rangle \|_{x_k, x_k} \leq c \| H_k - \nabla^2 f(x_k) \| \| \xi \|_{x_k}^2,$$

for $\xi \in T_x \mathcal{M}$ and for some constant $c > 0$, we can infer that $\nabla m_k(x_k)$ is positive definite for all $k$ sufficiently large. Thus, the structure of Algorithm 2 now implies

$$\| g_k + \nabla m_k(x_k)\xi_k \|_{x_k} \leq \| g_k \|_{x_k}^\theta, \quad \theta > 1.$$

Also, by Lemma 17, we have $\sigma_k \to 0$ as $k \to \infty$. Hence, there exists $\sigma$ such that $\sigma_k \leq \sigma$ for all $k \in \mathbb{N}$. We next show that the full step size $\alpha_k = 1$ satisfies the Armijo condition (3.9) whenever $k$ is sufficiently large. First, by Lemma 6 (ii) and Remark 5, we have

$$\| g_k \|_{x_k}^2 \geq \| g_k \|_{x_k} \geq \frac{\| g_k \|_{x_k}^2}{\| g_k \|_{x_k} + \frac{\| g_k \|_{x_k}}{\kappa M + \sigma}} \geq \frac{\| g_k \|_{x_k}}{\kappa M + \sigma},$$

where $\kappa M$ is defined in Lemma 11. Let $m^P_k := [\tilde{m_k}]_{x_k} = m_k \circ R_{x_k}$ denote the pullback of the model function $m_k$. Combining (4.17), (4.19), and (4.20), it holds

$$\| g_k + \nabla m^P_k(0_{x_k})\xi_k \|_{x_k} \leq \| (\nabla m^P_k(0_{x_k}) - \nabla m_k(x_k))\xi_k \|_{x_k} + \| g_k + \nabla m_k(x_k)\xi_k \|_{x_k} \leq \| g_k + \nabla m_k(x_k)\xi_k \|_{x_k} \leq \beta_R \| g_k \|_{x_k} + \| g_k \|_{x_k} \leq (\beta_R \| g_k \|_{x_k} + \kappa M + \sigma)\| g_k \|_{x_k} \| \xi_k \|_{x_k} \leq \| g_k \|_{x_k} \| \xi_k \|_{x_k},$$

Similar to [28, Proposition 5] and applying a second order Taylor expansion, it holds

$$m^P_k(\xi_k) - m^P_k(0_{x_k}) - \frac{1}{2} \langle g_k, \xi_k \rangle_{x_k} = \frac{1}{2} \langle g_k + \nabla m^P_k(\delta_k\xi_k)\xi_k, \xi_k \rangle_{x_k} \leq \| C_k(g_k) + \| \nabla m^P_k(\delta_k\xi_k) - \nabla m^P_k(0_{x_k}) \|_{x_k} \| \xi_k \|_{x_k}^2 = o(\| \xi_k \|_{x_k}^2),$$

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where $\delta_k \in [0, 1]$ is a suitable constant and we used the last estimate, $C_k(g_k) \to 0$, and the continuity of the Hessian $H_k^P$. Therefore, due to $\rho < 0.5$ and $\alpha_0 = 1$, the full step size $\alpha_0 = 1$ is chosen in (3.8) if $k$ is sufficiently large and we have $x_{k+1} = R_{x_k}(\xi_k)$. The remaining part of the proof now essentially follows [2, Theorem 7.4.11] and [27, Section 4.2.2]. In particular, calculating a first order Taylor expansion of the pullback gradient $\nabla f_{x_k}$ and using $\nabla f_{x_k}(0_{x_k}) = g_k$, the continuity of the pullback Hessian $\nabla f_{x_k}$, (4.19), (4.17), (4.18), (B.5), $\sigma_k \to 0$, and (4.12), we obtain

\[
\|\nabla f_{x_k}(\xi_k)\|_{x_k} \leq \|\nabla f_{x_{k+1}}\|_{x_{k+1}} + \|g_k + \text{Hess } m_k(x_k)[\xi_k]\|_{x_k} + \|H_k - \text{Hess } f(x_k)+ \frac{\beta}{x_k}\|_{x_k},
\]

for some $\beta > 0$. Moreover, since the Hessian $\text{Hess } f(x_k)$ is positive definite, [2, Lemma 7.4.8], this implies

\[
\text{dist}(x_{k+1}, x_k) \to 0, \quad \text{as} \quad k \to \infty,
\]

as $k \to \infty$. (Here, $\text{dist}(\cdot, \cdot)$ denotes the Riemannian geodesic distance, see [2]).

5. Numerical Results. In this section, we test a variety of examples to illustrate the efficiency of our adaptively regularized Newton method (ARN). We mainly compare Algorithm 3 with the Riemannian gradient method using the BB step size for initialization (GBB) and the Riemannian trust region method (RTR) Manopt. All codes are written in MATLAB. Note that Huang et al. [17] implement a C-language version of RTR to further accelerate the method. The efficiency of ARNT can also be improved in a similar way. All experiments were performed on a workstation with Intel Xenon E5-2680 v3 processors at 2.50GHz×12 and 128GB memory running CentOS 6.8 and MATLAB R2015b.

The default values of the GBB parameters are set to $\rho = 10^{-4}, \delta = 0.2$, and $\varphi = 0.85$. We have extensively tuned the stopping criterion of the truncated CG method implemented in RTR and found that adding a rule $\|r_{j+1}\| \leq \min\{0.1, 0.1\|r_0\|\}$ often improve the performance of RTR. All other default settings of RTR were used. For ARNT, we set $\eta_1 = 0.01, \eta_2 = 0.9, \gamma_0 = 0.2, \gamma_1 = 1, \gamma_2 = 10$, and $\sigma_k = \hat{\sigma}_k\|\nabla f(x_k)\|$, where $\hat{\sigma}_k$ is updated by (3.12) with $\hat{\sigma}_0 = 10$. The parameters in Algorithm 2 are chosen as follows: $\rho = 10^{-4}, \omega = 0.2, \theta = 1$, and $T = 0.1$. Furthermore, when an estimation of the absolute value of the negative curvature, denoted by $\sigma_{est}$, is available at the $k$-th subproblem (see step S2 in Algorithm 2), we calculate

\[
\sigma_{k+1}^{\text{new}} = \max\{\sigma_{k+1}, \sigma_{est} + \gamma\},
\]

with some small $\gamma \geq 0$. Then, the parameter $\sigma_{k+1}$ is reset to $\sigma_{k+1}^{\text{new}}$. This change does not affect our convergence results. For fair comparisons, all algorithms are stopped
Table 1

| $p$ | GBB | AdaGBB | ARNT | RTR |
|-----|-----|--------|------|-----|
|     | $n$ |        |      |     |
| 5   | 207 | 3.5e-7 | 1.2  | 227 | 8.8e-7 | 1.2 |
| 10  | 173 | 8.7e-7 | 0.5  | 215 | 9.6e-7 | 0.5 |
| 20  | 293 | 5.3e-7 | 0.9  | 352 | 6.3e-7 | 1.1 |
| 50  | 2622| 1.0e-6 | 9.4  | 1306| 8.6e-7 | 5.8 |
| 100 | 3286| 9.0e-7 | 13.6 | 10000| 3.4e-6| 62.5|
| 200 | 10000| 2.8e-5| 82.1 | 10000| 2.1e-4| 46.7|

when the norm of the Riemannian gradient is less than $10^{-6}$ unless a different tolerance is specified. The algorithms also terminate if a maximum number of iterations is reached. We use a maximum number of $10^4$ iteration in GBB and 500 in ARNT and RTR. In the implementation of ARNT and RTR, the GBB method is used to obtain a better initial point. Here, GBB is run with stopping criterion $\|\text{grad} f(x_k)\| \leq 10^{-3}$ and a maximum of 2000 iterations. The maximum number of inner iterations in ARNT is chosen adaptively depending on the norm of the Riemannian gradient.

In the subsequent tables, the column “its” represents the total number of iterations in GBB, while the two numbers of the column “its” in ARNT and RTR are the number of outer iterations and the average numbers of inner iterations. The columns “f”, “nrmG” and “time” denote the final objective value, the final norm of the Riemannian gradient, and the CPU time that the algorithms spent to reach the stopping criterions, respectively.

5.1. Low Rank Nearest Correlation Matrix Estimation. Given a symmetric matrix $C$ and a nonnegative symmetric weight matrix $H$, the low rank nearest correlation matrix problem is given as

$$\min_{X \in \mathbb{R}^{n \times n}} \frac{1}{2} \| H \odot (X - C) \|_F^2, \quad \text{s.t.} \quad X_{ii} = 1, \quad \text{rank}(X) \leq p, \quad X \succeq 0,$$

for all $i = 1, \ldots, n$ and for $p \leq n$. By expressing $X = V^TV$ with $V = [V_1, \ldots, V_n] \in \mathbb{R}^{p \times n}$, problem (5.1) can be converted into:

$$\min_{V \in \mathbb{R}^{p \times n}} \frac{1}{2} \| H \odot (V^TV - C) \|_F^2, \quad \text{s.t.} \quad \|V_i\|_2 = 1, \quad i = 1, \ldots, n.$$

In this subsection, we also use a version of the Adagrad method (2.6) in our numerical comparison. It is dubbed as AdaGBB because its setting is similar to GBB. We select a few typical test problems as follows.
Table 2
Numerical results of Ex. 3 on low rank nearest correlation estimation

| p  | GBB   | AdaGBB | ARNT  | RTR   |
|----|-------|--------|-------|-------|
|    | its nrmG time | its nrmG time | its nrmG time | its nrmG time |
| 5  | 10000 1.7e+02 196.5 | 4178 6.9e-7 41.3 | 260( 8) 9.4e-7 38.1 | 500( 12) 8.8e-2 78.4 |
| 10 | 10000 5.0e-4 207.4 | 4973 8.2e-7 103.8 | 347(12) 8.4e-7 58.9 | 500( 17) 9.3e-2 102.5 |
| 20 | 10000 3.5e-4 198.3 | 5089 7.1e-7 86.6 | 237( 8) 9.0e-7 38.1 | 500( 22) 9.7e-2 125.0 |
| 50 | 10000 9.1e-5 288.1 | 3675 1.0e-6 86.6 | 34( 8) 9.0e-7 58.9 | 63( 82) 7.7e-7 80.2 |
| 100| 10000 8.6e-4 224.2 | 10000 2.5e-6 258.0 | 26( 8) 7.1e-7 38.1 | 19( 42) 7.1e-7 120.4 |
| 150| 10000 3.5e-2 124.2 | 10000 4.5e-5 241.7 | 35( 13) 3.0e-7 76.1 | 18( 68) 9.0e-7 173.2 |
| 200| 10000 3.5e-2 153.7 | 10000 7.2e-5 245.3 | 37(130) 5.5e-7 78.4 | 16( 75) 8.3e-7 162.0 |

Ex. 1. Let \( n = 500 \) and let \( C_{ij} = 0.5 + e^{-0.05|i-j|} \) for \( i, j = 1, \ldots, n \). The weight matrix \( H \) is either 1 or a random matrix whose entries are mostly uniformly distributed in \([0, 10]\) except that 200 entries are distributed in \([0.01, 100]\).

Ex. 2. The matrix \( C \) is obtained from the real gene correlation matrices such as Lymph, ER, Hereditarybc and Leukemia. The weight matrix \( H \) is either 1 or a random matrix whose entries are set as in Ex. 1.

Ex. 3. Let \( n = 943 \). The matrix \( C \) is based on 100,000 ratings for 1682 movies by 943 users from the Movielens data sets. The weight matrix \( H \) is provided by T. Fushiki at Institute of Statistical Mathematics, Japan. The detailed numerical results are reported in Tables 1-4. For Ex. 1, all methods perform well if \( p \) is small. For the cases with \( H \neq 1 \), ARNT is the best when \( p = 50 \) and \( p = 100 \) while all of them fail when \( p = 150 \) and \( p = 200 \). For Ex. 2, GBB may not converge when \( p \) is large, and ARNT is efficient whenever \( p \) is small or large. In particular, ARNT is better than RTR on ER and Leukemia with \( H \neq 1 \) and RTR may fail on a few instances. For Ex. 3, we can see that GBB and RTR fail to converge when \( p \) is small, while ARNT and AdaGBB still work. In fact, we observe negative curvatures of the Hessian at many iterations of ARNT and the strategy (3.7) indeed helps the convergence.

5.2. Simple Nonlinear Eigenvalue Problems. A simplified model problem for density functional theory is given by

\[
\min_{X \in \mathbb{R}^{n \times k}} \frac{1}{2} \text{tr}(X^\top LX) + \frac{\alpha}{4} \rho(X)^\top L^1(\rho(X)), \quad \text{s.t.} \quad X^\top X = I_k,
\]

where \( L \in \mathbb{R}^{n \times n} \) is a symmetric matrix and \( \rho(X) \) is a vector whose components are the diagonal elements of \( XX^\top \).

In this numerical experiment, \( L \) is set to a tridiagonal matrix whose main diagonal elements are 2 and the secondary diagonal elements are -1. A series of experiments using different values of \( n, k \) and \( \alpha \) are conducted. Specifically, in the first case, we fix \( p = 50, \alpha = 1 \), and try different \( n \) ranging from 2000 to 50000. Then, we set \( n = 10000, \alpha = 1 \) and vary \( p \) from 20 to 100. At last, the performance on different values for \( \alpha \) is also compared. The detailed numerical results are reported in Tables 5, 6 and 7, respectively. In Table 5, we can see that ARNT is most efficient, while the performance of RTR sometimes is not stable. Similar results are shown in Table 6. In Table 7, ARNT is better than RTR, especially for large \( \alpha \). We also observe that GBB often performs comparable to ARNT in CPU time in this example.

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Numerical results of Ex. 2 on low rank nearest correlation estimation

|     | GBB | AdaGBB | ARNT | RTR |
|-----|-----|--------|------|-----|
| p   |     | its nrmG time | its nrmG time | its nrmG time | its nrmG time |
|     |     | H = 1 (Lymph, n = 587) |
| 5   | 252 | 7.3e-7 1.8 | 335 | 3.2e-7 1.3 | 19(14) | 5.3e-7 1.9 | 35( 9) | 3.2e-7 2.3 |
| 10  | 242 | 9.0e-7 1.0 | 309 | 9.7e-7 1.2 | 15(16) | 2.7e-7 1.1 | 28(16) | 1.5e-7 1.9 |
| 20  | 372 | 9.6e-7 1.9 | 402 | 9.4e-7 1.8 | 17(21) | 8.0e-7 1.9 | 12(21) | 3.6e-7 1.4 |
| 50  | 756 | 7.1e-7 4.1 | 979 | 9.8e-7 4.9 | 18(30) | 5.2e-7 3.0 | 20(26) | 1.9e-7 2.8 |
| 100 | 161 | 8.9e-7 10.3 | 2473 | 9.7e-7 14.3 | 33(54) | 1.9e-7 10.0 | 28(42) | 8.7e-7 6.3 |
| 150 | 10000 | 1.8e-6 73.2 | 10000 | 5.5e-6 62.8 | 44( 99) | 5.6e-7 11.2 | 31( 40) | 4.5e-7 8.0 |
| 200 | 50000 | 7.0e-6 79.5 | 10000 | 1.2e-5 69.8 | 25( 44) | 8.9e-7 8.9 | 28( 44) | 5.2e-7 8.7 |
|     |     | H ≠ 1 (Lymph, n = 692) |
| 5   | 1691 | 9.2e-7 14.1 | 723 | 6.8e-7 5.2 | 72( 24) | 2.0e-7 6.4 | 500( 18) | 2.8e-3 43.6 |
| 10  | 1774 | 9.8e-7 13.2 | 742 | 8.4e-7 4.1 | 34( 31) | 6.8e-7 5.3 | 500( 25) | 9.0e-5 65.9 |
| 20  | 2260 | 8.0e-7 19.5 | 836 | 1.0e-6 4.8 | 101( 43) | 8.0e-7 16.8 | 500( 36) | 9.6e-3 93.3 |
| 50  | 6408 | 9.7e-7 47.2 | 2784 | 9.7e-7 14.5 | 83( 83) | 5.5e-7 29.6 | 114( 81) | 3.5e-7 48.3 |
| 100 | 8695 | 9.7e-7 67.6 | 4897 | 9.9e-7 26.9 | 26( 109) | 2.6e-7 15.5 | 32( 108) | 2.5e-7 18.3 |
| 150 | 10000 | 2.2e-3 69.8 | 10000 | 4.0e-3 60.0 | 47(108) | 7.2e-7 34.4 | 46( 99) | 7.5e-7 30.2 |
| 200 | 10000 | 5.0e-3 84.2 | 10000 | 2.3e-3 72.9 | 71(110) | 5.2e-7 60.2 | 58( 129) | 5.9e-7 57.1 |

5.3. Kohn-Sham Total Energy Minimization. Using a suitable discretization scheme, we can formulate a finite dimensional approximation to the continuous KS minimization problem [34] as

\[
\min_{X \in \mathbb{C}^{n \times p}} f(X) \quad \text{s.t.} \quad X^* X = I,
\]

where \( f(X) := \frac{1}{2} \text{tr}(X^* L X) + \frac{1}{2} \text{tr}(X^* V_{\text{ion}} X) + \frac{1}{2} \sum_i \sum_l |x_i l\omega_l|^2 + \frac{1}{2} \rho L^1 + \frac{1}{2} \epsilon_{xc}(\rho) \), \( X = [x_1, \cdots, x_p] \in \mathbb{C}^{n \times p} \), \( \rho(X) := \text{diag}(X X^*) \), \( L \) is a finite dimensional Laplacian operator, \( V_{\text{ion}} \) corresponds to the ionic pseudopotentials, \( w_l \) represents a discretized pseudopotential reference projection function and \( \epsilon_{xc} \) is related to the exchange correlation energy.
### Table 4
Numerical results of Ex. 2 on low rank nearest correlation estimation (continued)

| p    | GBB | AdaGBB | ARNT | RTR |
|------|-----|--------|------|-----|
|      | its | nrmG time | its | nrmG time | its | nrmG time | its | nrmG time |
|      |     |         |     |          |     |          |     |          |
| $H = 1$ (Hereditarybc, $n = 1869$) |
| 5    | 156 | 7.9e-7 4.6 | 189 | 4.0e-8 3.9 | 11(14) | 9.8e-7 8.9 | 13(7) | 1.5e-7 6.2 |
| 10   | 157 | 8.8e-7 3.5 | 220 | 9.3e-7 6.5 | 3(10) | 9.8e-8 5.6 | 3(10) | 9.7e-8 5.6 |
| 20   | 299 | 6.3e-7 7.0 | 304 | 1.9e-7 9.6 | 17(23) | 4.5e-7 18.6 | 18(25) | 4.7e-7 16.8 |
| 50   | 10000 | 9.7e-5 254.3 | 10000 | 7.5e-5 266.5 | 32(15) | 8.5e-7 23.2 | 33(18) | 8.8e-7 23.5 |
| 100  | 10000 | 1.7e-5 294.3 | 10000 | 6.6e-5 369.1 | 33(14) | 5.2e-7 24.8 | 33(17) | 4.5e-7 25.9 |
| 150  | 10000 | 5.3e-5 345.3 | 10000 | 1.1e-4 352.4 | 34(19) | 7.5e-7 27.1 | 34(16) | 6.4e-7 29.5 |
| 200  | 10000 | 2.7e-5 372.3 | 10000 | 3.7e-5 342.1 | 35(15) | 5.9e-7 34.1 | 36(20) | 6.7e-7 35.2 |
|      |     |         |     |          |     |          |     |          |
| $H \neq 1$ (Hereditarybc, $n = 1869$) |
| 5    | 256 | 6.6e-7 6.2 | 238 | 9.3e-7 6.3 | 12(15) | 6.6e-7 9.9 | 52(15) | 4.8e-7 28.5 |
| 10   | 196 | 7.8e-7 5.3 | 242 | 9.6e-7 7.3 | 8(17) | 7.1e-7 7.8 | 7(17) | 5.6e-7 7.2 |
| 20   | 361 | 9.9e-7 12.0 | 315 | 9.6e-7 10.6 | 7(19) | 1.2e-7 11.7 | 6(18) | 6.8e-7 10.8 |
| 50   | 10000 | 1.2e-3 303.5 | 10000 | 1.9e-3 317.7 | 39(23) | 9.9e-8 38.8 | 38(30) | 3.7e-7 43.4 |
| 100  | 10000 | 1.3e-3 352.9 | 10000 | 2.2e-3 338.9 | 34(22) | 8.4e-7 38.0 | 39(29) | 5.3e-7 49.2 |
| 150  | 10000 | 2.4e-3 386.3 | 10000 | 4.1e-3 389.9 | 38(24) | 5.6e-7 45.6 | 41(31) | 4.9e-7 60.0 |
| 200  | 10000 | 1.8e-3 410.0 | 10000 | 7.3e-4 359.1 | 35(24) | 7.7e-7 52.6 | 41(30) | 7.3e-7 63.1 |
|      |     |         |     |          |     |          |     |          |
| $H = 1$ (Leukemia, $n = 1255$) |
| 5    | 272 | 8.9e-7 4.2 | 261 | 4.8e-7 2.9 | 15(16) | 4.0e-7 5.6 | 23(9) | 4.0e-7 5.2 |
| 10   | 540 | 9.6e-7 12.5 | 453 | 8.2e-7 5.7 | 23(20) | 5.6e-7 8.4 | 48(21) | 6.8e-7 13.8 |
| 20   | 1064 | 9.6e-7 23.0 | 1602 | 1.0e-6 26.2 | 34(31) | 4.1e-7 14.8 | 131(25) | 1.5e-7 39.4 |
| 50   | 1917 | 8.5e-7 32.9 | 2535 | 4.0e-7 35.8 | 33(49) | 2.6e-7 26.0 | 28(42) | 1.6e-7 17.4 |
| 100  | 10000 | 4.1e-3 169.4 | 10000 | 2.4e-3 156.9 | 35(27) | 9.6e-7 19.5 | 35(28) | 5.6e-7 18.0 |
| 150  | 10000 | 3.1e-3 194.8 | 10000 | 9.2e-5 184.4 | 40(25) | 4.8e-7 24.4 | 36(27) | 9.5e-7 20.0 |
| 200  | 10000 | 3.2e-5 232.1 | 10000 | 3.9e-4 200.1 | 37(25) | 5.0e-7 24.8 | 36(27) | 4.6e-7 22.5 |
|      |     |         |     |          |     |          |     |          |
| $H \neq 1$ (Leukemia, $n = 1255$) |
| 5    | 1404 | 5.9e-7 55.0 | 762 | 5.5e-7 13.3 | 44(20) | 3.8e-7 16.3 | 500(16) | 3.7e-3 137.7 |
| 10   | 680 | 9.7e-7 21.8 | 608 | 8.9e-7 13.0 | 23(22) | 9.5e-7 11.2 | 500(20) | 2.1e-3 169.5 |
| 20   | 2461 | 9.4e-7 77.1 | 2250 | 9.3e-7 51.6 | 59(32) | 9.5e-7 31.0 | 500(34) | 3.5e-4 289.0 |
| 50   | 3354 | 9.7e-7 82.0 | 1790 | 7.8e-7 47.1 | 33(86) | 4.8e-7 48.2 | 58(74) | 1.2e-7 79.2 |
| 100  | 10000 | 1.8e-2 170.5 | 10000 | 1.8e-3 158.6 | 36(51) | 7.7e-7 37.5 | 44(53) | 4.9e-7 48.7 |
| 150  | 10000 | 3.4e-3 194.9 | 10000 | 2.1e-3 197.8 | 43(52) | 4.8e-7 48.2 | 51(52) | 4.8e-7 57.1 |
| 200  | 10000 | 3.9e-3 216.5 | 10000 | 4.3e-2 205.8 | 46(50) | 4.6e-7 55.9 | 50(52) | 6.5e-7 65.4 |

Our experiments are based on the KSSOLV package [38]. As in [34], we use the Wirtinger calculus [23] to compute the complex gradient and Hessian of the function $f$. Let us also note that the Lipschitz continuity required in Assumption (A.1) may not be satisfied for all types of exchange correlations. However, for the correlation that is defined by the Perdew-Zunger formula and used in this example, Lipschitz continuity was established in [32, Lemma 3.3]. In addition to GBB and RTR, we further compare ARNT with the self-consistent field (SCF) iteration and the regularized trust-region method TRQH in [34]. In the implementation of TRQH, RTR and ARNT, we use the same initial point obtained by GBB. Note that TRQH essentially coincides with ARNT except that the subproblem (3.4) is solved by GBB.
Table 5
Numerical results on nonlinear eigenspace with fixed \((p, \alpha) = (30, 1000)\).

| \(n\) | GBB its nrmG time | ARNT its nrmG time | RTR its nrmG time |
|------|-------------------|--------------------|-------------------|
| 2000 | 1204.1e-6 4.9     | 52(21) 4.1e-7 6.8  | 251(24) 7.9e-7 19.0 |
| 3000 | 1481.12e-7 11.0   | 19(18) 8.5e-7 4.1  | 60(23) 8.8e-7 7.3  |
| 5000 | 1111.7e-7 11.6    | 38(22) 9.4e-7 10.7 | 141(24) 7.8e-7 23.2 |
| 8000 | 1389 9.9e-7 17.7  | 33(19) 4.4e-7 14.4 | 132(24) 8.9e-7 34.2 |
| 10000| 1757 1.0e-6 41.4  | 48(23) 7.6e-7 24.4 | 57(26) 7.9e-7 25.1 |

Table 6
Numerical results on nonlinear eigenspace with fixed \((n, \alpha) = (5000, 1000)\).

| \(p\) | GBB its nrmG time | ARNT its nrmG time | RTR its nrmG time |
|------|-------------------|--------------------|-------------------|
| 10   | 341 5.9e-7 1.7    | 4(10) 4.5e-7 0.4  | 3(10) 4.4e-7 0.3  |
| 20   | 610 8.0e-7 3.2    | 5(15) 3.5e-7 1.9  | 3(16) 3.3e-7 1.7  |
| 30   | 1111 7.0e-7 9.4   | 38(22) 4.9e-7 8.7 | 141(24) 7.8e-7 19.6 |
| 50   | 3627 9.4e-7 62.1  | 46(26) 7.6e-7 31.9 | 500(37) 1.5e-3 175.9 |

A summary of the computational results is given in Table 8. All algorithms reach the same objective function value when the gradient norm criterion is satisfied. ARNT and RTR take a small number of outer iterations to converge and often exhibit a fast convergence rate. In particular, ARNT tends to be more efficient than other algorithms on “graphene30” and “qdot”. It can be even faster than SCF when SCF works well. ARNT also outperforms TRQH. This shows that the accuracy of solving the subproblem (3.4) is indeed important.

5.4. Bose-Einstein Condensates (BEC). The total energy in BEC is defined as

\[
E(\psi) = \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \psi(x)|^2 + V(x)|\psi(x)|^2 + \frac{\beta}{2} |\psi(x)|^4 - \Omega \bar{\psi}(x)L_z(x) \right] dx,
\]

where \(x \in \mathbb{R}^d\) is the spatial coordinate vector, \(\bar{\psi}\) denotes the complex conjugate of \(\psi\), \(L_z = -i(x\partial_y - y\partial_x)\), \(V(x)\) is an external trapping potential, and \(\beta, \Omega\) are given constants. Using a suitable discretization, e.g., such as finite differences or the sine pseudospectral and Fourier pseudospectral (FP) method, we can reformulate the BEC problem as follows

\[
\min_{x \in \mathbb{C}^M} f(x) := \frac{1}{2} x^* Ax + \frac{\beta}{2} \sum_{j=1}^{M} |x_j|^4, \quad \text{s.t.} \quad \|x\|_2 = 1,
\]

where \(M \in \mathbb{N}\), \(\beta\) is a given real constant, and \(A \in \mathbb{C}^{M \times M}\) is a Hermitian matrix.

In this numerical experiment, we again use the Wirtinger calculus to calculate the complex gradient and Hessian of the objective function. We stop GBB, ARNT, RTR, and TRQH (the Newton method in [37]) when the gradient norm is less than \(10^{-4}\) or the maximum number of iterations is reached. For TRQH, the stopping criterion

\[
\|x^{k+1} - x^k\|_\infty \leq \epsilon_x
\]

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Table 7

Numerical results on nonlinear eigenspace with fixed \((n, p) = (8000, 30)\).

|   | GBB | ARNT | RTR |
|---|-----|------|-----|
| \(\alpha\) | its nrmG time | its nrmG time | its nrmG time |
| 1  | 194 6.8e-7 2.4 | 3(28) 8.3e-7 1.9 | 3(28) 6.0e-7 1.7 |
| 10 | 299 3.7e-7 3.7 | 3(36) 4.5e-7 2.3 | 3(36) 3.6e-7 2.0 |
| 100 | 572 9.1e-7 7.3 | 3(26) 5.2e-7 5.0 | 3(26) 5.2e-7 4.8 |
| 1000 | 1389 9.9e-7 18.2 | 33(19) 4.4e-7 13.1 | 132(24) 8.9e-7 33.1 |

is added for some small constant \(\epsilon_x\) since TRQH often does not converge under the gradient norm criterion. We take \(d = 2\) and test two different potential functions

\[ V_1(x, y) = \frac{1}{2} x^2 + \frac{1}{2} y^2, \quad \text{and} \quad V_2(x, y) = -0.1(x^2 + y^2) + 0.3((x^2 + y^2)/2)^2. \]

The BEC problem is discretized by FP on the bounded domain \((-16, 16)^3\) with \(\beta = 500, 1000\) and different values of \(\Omega\) ranging from 0 to 0.95. Under the same settings as in \cite{37}, we use the mesh refinement procedure with the coarse meshes \((2^4+1) \times (2^4+1), (2^5+1) \times (2^5+1), \ldots, (2^{18}+1) \times (2^{18}+1)\) to gradually obtain an initial solution point on the finest mesh \((2^{18}+1) \times (2^{18}+1)\). For a fair comparison, all algorithms are tested with mesh refinement and start from the same initial point on the coarsest mesh with \(\phi(x, y) = \frac{(1-\Omega)^2}{\|1-\Omega\phi_1(x,y)+\Omega\phi_2(x,y)\|^2} \|1-\Omega\phi_1(x,y)+\Omega\phi_2(x,y)\|\) and \(\phi_1(x, y) = \frac{1}{\sqrt{\pi}} e^{-(x^2+y^2)/2}, \phi_2(x, y) = x+iy e^{-(x^2+y^2)/2}/\sqrt{\pi}\).

A summary of the results is presented in the Tables 9–10 for the potential functions \(V_1\) and \(V_2\), respectively. The parameter \(\epsilon_x\) for TRQH is set to \(10^{-8}\) and \(10^{-7}\) in these two cases. The tables show that GBB does not converge within 10000 steps in several cases. TRQH usually performs worse than ARNT in terms of accuracy and time except in the cases \(\beta = 1000\) with \(\Omega = 0.95\) in Table 9 where ARNT finds a point with a smaller objective function value. ARNT performs not worse than RTR in most experiments.

5.5. Low-Rank Matrix Completion. Given a partially observed matrix \(A \in \mathbb{R}^{m \times n}\), we want to find the lowest-rank matrix to fit \(A\) on the known elements. This problem can be formulated as follows:

\[
\min_{X \in \mathbb{R}^{m \times n}} f(X) := \frac{1}{2} \|P_{\Omega}(X) - A\|_F^2 \quad \text{s.t.} \quad X \in \{X \in \mathbb{R}^{m \times n} : \operatorname{rank}(X) = k\}
\]

where \(P_{\Omega} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^{m \times n}\), \(P_{\Omega}(X)_{i,j} := X_{i,j}\) if \((i, j) \in \Omega\) and \(P_{\Omega}(X)_{i,j} := 0\) if \((i, j) \notin \Omega\), is the projection onto \(\Omega\) and \(\Omega\) is a subset of \(\{1, \ldots, m\} \times \{1, \ldots, n\}\). More details can be found in \cite{33}.

Similar to \cite{33}, we construct random numerical examples as follows. We first take two Gaussian random matrices \(A_L, A_R \in \mathbb{R}^{n \times k}\), then uniformly sample the index set \(\Omega\) for a given cardinality and set the matrix \(A := P_{\Omega}(A_L A_R^\top)\). Since the degrees of freedom in a nonsymmetric matrix of rank \(k\) is given \(k(2n - k)\), we define the ratio \(\sigma_S = (k(2n - k))^{-1}\). In this example, we only penalize \(x - x_k\) on the known set \(\Omega\) in the implementation of ARNT to reduce the computational costs. (I.e., the penalization term in the subproblem (3.3) is set to \(\sigma_k\|P_{\Omega}(x - x_k)\|^2\)). In the Tables 11, 12 and 13, we can see that ARNT and RTR perform better than GBB regardless whether the dimension \(n\) and rank \(k\) are large or small. We often observe that ARNT tends to outperform RTR when negative curvature is encountered.
| solver | f its nrmG time | f its nrmG time |
|--------|----------------|----------------|
|        | alanine        | al             |
| SCF    | -6.1162e+01   | 14 3.9e-7 25.0 | -1.5784e+01 101 4.5e-2 146.9 |
| OptM   | -6.1162e+01   | 80 7.1e-7 25.5 | -1.5804e+01 1461 9.9e-7 391.1 |
| TRQH   | -6.1162e+01 6 (16) 6.5e-7 39.7 | -1.5804e+01 39(16) 9.6e-7 411.9 |
| ARNT   | -6.1162e+01 3 (9) 3.9e-7 24.4 | -1.5804e+01 113 3.5e-7 196.4 |
| RTR    | -6.1162e+01 3 (9) 4.1e-7 24.3 | -1.5804e+01 108 9.9e-8 188.9 |
|        | benzene        | c12h26         |
| SCF    | -3.7226e+01   | 13 4.0e-7 14.3 | -8.1536e+01 13 9.1e-7 30.2 |
| OptM   | -3.7226e+01   | 68 5.1e-7 13.4 | -8.1536e+01 89 8.8e-7 34.1 |
| TRQH   | -3.7226e+01 6 (12) 9.3e-7 19.2 | -8.1536e+01 7(12) 9.7e-7 50.0 |
| ARNT   | -3.7226e+01 3 (10) 9.2e-8 13.3 | -8.1536e+01 3(13) 6.4e-7 29.5 |
| RTR    | -3.7226e+01 3 (10) 8.1e-8 13.6 | -8.1536e+01 3(13) 5.2e-7 29.5 |
|        | c2h6           | co2            |
| SCF    | -1.4420e+01   | 10 6.8e-7 2.5  | -3.5124e+01 10 3.1e-7 2.6 |
| OptM   | -1.4420e+01   | 59 9.1e-7 2.6  | -3.5124e+01 59 5.2e-7 2.6 |
| TRQH   | -1.4420e+01 6 (12) 8.7e-7 4.0 | -3.5124e+01 6(12) 3.7e-7 3.9 |
| ARNT   | -1.4420e+01 3 (8) 4.7e-7 2.5 | -3.5124e+01 3(9) 3.1e-7 2.5 |
| RTR    | -1.4420e+01 3 (7) 3.9e-7 2.7 | -3.5124e+01 3(10) 2.5e-7 2.7 |
|        | ctube661       | graphene16     |
| SCF    | -1.3464e+02   | 16 3.1e-7 88.5 | -9.4028e+01 101 5.8e-4 160.0 |
| OptM   | -1.3464e+02   | 101 7.2e-7 93.0 | -9.4046e+01 187 8.5e-7 40.8 |
| TRQH   | -1.3464e+02 6 (19) 3.2e-7 138.5 | -9.4046e+01 8(19) 9.5e-7 70.3 |
| ARNT   | -1.3464e+02 3 (11) 4.9e-7 78.3 | -9.4046e+01 3(19) 8.6e-7 40.3 |
| RTR    | -1.3464e+02 3 (11) 4.2e-7 78.2 | -9.4046e+01 3(19) 7.3e-7 40.7 |
|        | graphene30     | h2o            |
| SCF    | -1.7358e+02   | 101 2.2e-3 860.6 | -1.6441e+01 9 1.4e-7 1.8 |
| OptM   | -1.7360e+02   | 378 6.5e-7 517.0 | -1.6441e+01 58 8.9e-7 2.0 |
| TRQH   | -1.7360e+02 12 (38) 8.6e-7 783.9 | -1.6441e+01 5(38) 8.4e-7 2.9 |
| ARNT   | -1.7360e+02 4 (33) 2.5e-7 446.8 | -1.6441e+01 3(11) 3.9e-7 1.8 |
| RTR    | -1.7360e+02 100(4) 2.3e-5 828.8 | -1.6441e+01 3(11) 3.1e-7 2.1 |
|        | hnc           | nic            |
| SCF    | -2.8635e+01   | 12 3.5e-7 3.3  | -2.3544e+01 10 7.2e-7 1.2 |
| OptM   | -2.8635e+01   | 131 9.7e-7 5.6  | -2.3544e+01 63 9.9e-7 1.1 |
| TRQH   | -2.8635e+01 7 (21) 9.5e-7 6.9 | -2.3544e+01 8(21) 9.3e-7 2.3 |
| ARNT   | -2.8635e+01 3 (15) 7.5e-7 3.7 | -2.3544e+01 3(8) 4.4e-7 1.0 |
| RTR    | -2.8635e+01 3 (16) 7.7e-7 4.5 | -2.3544e+01 3(8) 4.6e-7 1.3 |
|        | ptnio          | qdot           |
| SCF    | -2.2679e+02   | 66 7.7e-7 146.2 | 2.7702e+01 101 3.4e-2 22.3 |
| OptM   | -2.2679e+02   | 495 5.3e-7 145.6 | 2.7695e+01 2000 3.3e-6 70.8 |
| TRQH   | -2.2679e+02 23 (39) 9.3e-7 286.0 | 2.7695e+01 91(39) 9.9e-7 115.8 |
| ARNT   | -2.2679e+02 4 (52) 6.9e-7 132.4 | 2.7695e+01 27(65) 7.1e-7 64.5 |
| RTR    | -2.2679e+02 4 (46) 8.5e-7 122.5 | 2.7695e+01 37(68) 4.0e-7 83.3 |
Table 9  
Numerical results on BEC with the potential function $V_1(x,y)$

| solver | $f$  | its | nrmG | time | $f$  | its | nrmG | time |
|--------|------|-----|------|------|------|-----|------|------|
|        | $\beta = 500$ |       |      |      | $\beta = 1000$ |       |      |      |
| OptM   | 8.5118 | 58  | 6.6e-5 | 1.4  | 11.9718 | 76  | 4.6e-5 | 3.0  |
| TRQH   | 8.5118 | 4(17)| 1.5e-4 | 2.0  | 17.6436 | 352 | 4.6e-4 | 33.6 |
| ARNT   | 8.5118 | 3(24)| 1.2e-5 | 1.5  | 11.9718 | 76  | 4.6e-5 | 3.0  |
| RTR    | 8.5118 | 3(25)| 1.3e-5 | 1.5  | 11.9718 | 76  | 4.6e-5 | 3.0  |
| $\Omega = 0.00$ |       |      |      |      | $\Omega = 0.00$ |       |      |      |
| OptM   | 8.0246 | 276 | 9.0e-5 | 32.3 | 6.9731  | 1000| 1.0e-4 | 1.0e-4 |
| TRQH   | 8.0246 | 5(53)| 2.0e-4 | 60.7 | 6.9731  | 1000| 1.0e-4 | 1.0e-4 |
| ARNT   | 8.0197 | 3(62)| 6.5e-5 | 21.3 | 6.9731  | 1000| 1.0e-4 | 1.0e-4 |
| RTR    | 8.0246 | 11(113)| 1.0e-4 | 56.5 | 6.9731  | 1000| 1.0e-4 | 1.0e-4 |
| $\Omega = 0.25$ |       |      |      |      | $\Omega = 0.25$ |       |      |      |
| OptM   | 6.9731 | 340 | 1.0e-4 | 56.3 | 6.1016  | 386 | 1.0e-4 | 65.2 |
| TRQH   | 6.9731 | 7(55)| 2.0e-4 | 61.6 | 6.1016  | 386 | 1.0e-4 | 65.2 |
| ARNT   | 6.9731 | 10(99)| 8.7e-5 | 44.4 | 6.1016  | 386 | 1.0e-4 | 65.2 |
| RTR    | 6.9731 | 99(118)| 9.3e-5 | 234.2| 6.1016  | 386 | 1.0e-4 | 65.2 |
| $\Omega = 0.50$ |       |      |      |      | $\Omega = 0.50$ |       |      |      |
| OptM   | 4.7784 | 10000| 1.2e-3 | 243.6| 3.7419  | 10000| 1.2e-3 | 243.6|
| TRQH   | 4.7784 | 277(176)| 2.0e-4 | 1090.9| 3.7419  | 10000| 1.2e-3 | 243.6|
| ARNT   | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| RTR    | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| $\Omega = 0.70$ |       |      |      |      | $\Omega = 0.70$ |       |      |      |
| OptM   | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| TRQH   | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| ARNT   | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| RTR    | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| $\Omega = 0.90$ |       |      |      |      | $\Omega = 0.90$ |       |      |      |
| OptM   | 4.7784 | 10000| 1.2e-3 | 243.6| 3.7419  | 10000| 1.2e-3 | 243.6|
| TRQH   | 4.7784 | 277(176)| 2.0e-4 | 1090.9| 3.7419  | 10000| 1.2e-3 | 243.6|
| ARNT   | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| RTR    | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| $\Omega = 0.95$ |       |      |      |      | $\Omega = 0.95$ |       |      |      |
| OptM   | 4.7784 | 10000| 1.2e-3 | 243.6| 3.7419  | 10000| 1.2e-3 | 243.6|
| TRQH   | 4.7784 | 277(176)| 2.0e-4 | 1090.9| 3.7419  | 10000| 1.2e-3 | 243.6|
| ARNT   | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|
| RTR    | 4.7777 | 147(132)| 9.6e-5 | 413.3| 3.7419  | 10000| 1.2e-3 | 243.6|

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Table 10

Numerical results on BEC with the potential function $V_2(x, y)$

| solver | $f$  | its | nrmG time | $f$  | its | nrmG time |
|--------|-----|-----|-----------|-----|-----|-----------|
|        | $\beta = 500$ |        |           | $\beta = 1000$ |       |
| OptM   | 9.3849 | 108 | 7.6e-5 | 2.8 | 9.3849 | 118 | 7.4e-5 | 5.6 |
| TRQH   | 9.3849 | 4(21) | 1.9e-4 | 2.6 | 9.3849 | 5(17) | 1.5e-4 | 5.8 |
| ARNT   | 9.3849 | 3(25) | 5.5e-5 | 1.7 | 9.3849 | 3(26) | 4.6e-5 | 3.6 |
| RTR    | 9.3849 | 3(27) | 5.5e-5 | 1.8 | 9.3849 | 3(27) | 5.6e-5 | 3.7 |
| OptM   | 9.2053 | 142 | 9.2e-5 | 30.2 | 9.1053 | 132 | 9.8e-5 | 25.3 |
| TRQH   | 9.2053 | 5(23) | 1.4e-4 | 24.4 | 9.1053 | 5(20) | 1.5e-4 | 20.4 |
| ARNT   | 9.2053 | 3(27) | 8.4e-5 | 19.5 | 9.1053 | 3(28) | 7.5e-5 | 11.5 |
| RTR    | 9.2053 | 3(29) | 8.3e-5 | 20.2 | 9.1053 | 3(30) | 8.5e-5 | 19.5 |
| OptM   | 8.8307 | 264 | 8.3e-5 | 26.0 | 8.4819 | 374 | 8.2e-5 | 46.9 |
| TRQH   | 8.8307 | 5(47) | 1.8e-4 | 24.0 | 8.4819 | 5(64) | 2.0e-4 | 38.7 |
| ARNT   | 8.8307 | 5(95) | 3.8e-5 | 26.0 | 8.4819 | 3(76) | 8.8e-5 | 30.2 |
| RTR    | 8.8307 | 3(87) | 7.6e-5 | 47.2 | 8.4819 | 3(94) | 7.4e-5 | 26.4 |
| OptM   | 8.0659 | 426 | 1.0e-4 | 75.2 | 7.7455 | 9508 | 9.9e-5 | 244.4 |
| TRQH   | 8.0659 | 5(94) | 1.4e-4 | 124.1 | 7.7455 | 21(155) | 2.0e-4 | 254.8 |
| ARNT   | 8.0659 | 3(99) | 9.0e-5 | 56.4 | 7.7455 | 30(192) | 8.8e-5 | 171.7 |
| RTR    | 8.0659 | 3(108) | 7.6e-5 | 107.6 | 7.7455 | 20(270) | 9.7e-5 | 257.4 |
| OptM   | 14.9351 | 158 | 9.0e-5 | 5.1 | 14.9351 | 113 | 9.5e-5 | 9.2 |
| TRQH   | 14.9351 | 5(22) | 2.0e-4 | 3.1 | 14.9667 | 32(160) | 2.0e-4 | 133.1 |
| ARNT   | 14.9351 | 3(33) | 6.6e-5 | 2.1 | 14.9667 | 41(131) | 7.4e-5 | 105.2 |
| RTR    | 14.9351 | 3(33) | 6.1e-5 | 2.0 | 14.9667 | 37(137) | 7.9e-5 | 118.5 |
| OptM   | 14.7167 | 1261 | 9.9e-5 | 68.6 | 14.4704 | 1128 | 1.0e-4 | 38.6 |
| TRQH   | 14.7167 | 11(123) | 2.0e-4 | 73.3 | 14.6167 | 13(65) | 1.5e-4 | 58.1 |
| ARNT   | 14.7167 | 17(127) | 8.0e-5 | 66.8 | 14.6167 | 7(112) | 7.0e-5 | 43.6 |
| RTR    | 14.7167 | 13(136) | 7.3e-5 | 72.2 | 14.6167 | 3(33) | 6.2e-5 | 42.2 |
| OptM   | 14.2813 | 719 | 1.0e-4 | 47.8 | 13.8647 | 4382 | 1.0e-4 | 118.3 |
| TRQH   | 14.5167 | 7(31) | 1.9e-4 | 41.5 | 13.6368 | 42(169) | 2.0e-4 | 283.4 |
| ARNT   | 14.5167 | 5(104) | 9.9e-5 | 38.2 | 13.6561 | 39(138) | 5.5e-5 | 133.5 |
| RTR    | 14.5167 | 3(33) | 9.3e-5 | 33.2 | 13.6561 | 29(153) | 9.6e-5 | 144.9 |
| OptM   | 13.3733 | 5004 | 1.0e-4 | 166.9 | 12.8180 | 10000 | 3.2e-3 | 270.8 |
| TRQH   | 13.3733 | 6(108) | 1.9e-4 | 117.3 | 12.8048 | 423(143) | 1.8e-4 | 1153.7 |
| ARNT   | 13.3733 | 8(166) | 3.9e-5 | 68.1 | 12.8180 | 53(167) | 6.8e-5 | 191.8 |
| RTR    | 13.3733 | 12(199) | 4.1e-5 | 93.5 | 12.8180 | 66(250) | 9.8e-5 | 339.9 |
Table 11
Numerical results on low rank matrix completion with the fixed $k = 10, r_S = 0.8$ but different $n$.

| $n$ | GBB | ARNT | RTR |
|-----|-----|------|-----|
|     | its nrmG time | its nrmG time | its nrmG time |
| 1000 | 603 5.1e-7 12.5 | 6(84) 3.4e-7 7.7 | 8(91) 6.6e-7 8.2 |
| 2000 | 570 9.2e-7 43.9 | 5(72) 8.9e-7 23.6 | 8(86) 6.2e-7 28.2 |
| 4000 | 671 9.7e-7 179.8 | 6(82) 4.6e-7 94.8 | 9(85) 2.0e-7 104.8 |
| 8000 | 666 9.8e-7 694.2 | 5(104) 5.2e-7 320.1 | 8(130) 5.4e-7 394.5 |

Table 12
Numerical results on low rank matrix completion with fixed $n = 4000, r_S = 0.95$ but different $k$.

| $k$ | GBB | ARNT | RTR |
|-----|-----|------|-----|
|     | its nrmG time | its nrmG time | its nrmG time |
| 10  | 5252 1.0e-6 1415.9 | 13(133) 7.4e-7 392.1 | 12(236) 4.4e-7 438.2 |
| 20  | 2126 1.0e-6 600.8 | 7(125) 3.9e-7 269.5 | 9(195) 2.3e-7 315.9 |
| 30  | 1488 1.0e-6 438.8 | 6(132) 3.1e-7 255.2 | 9(214) 2.6e-7 329.9 |
| 40  | 1010 9.3e-7 311.4 | 5(103) 1.1e-7 220.5 | 5(103) 1.1e-7 219.4 |
| 50  | 1494 7.9e-7 477.1 | 4(103) 1.5e-7 273.8 | 4(103) 1.6e-7 272.5 |
| 60  | 1398 9.9e-7 480.4 | 4(110) 5.7e-7 313.3 | 4(114) 5.7e-7 315.2 |

6. Conclusions. In this paper, we propose a regularized Newton method for optimization problems on Riemannian manifolds. We use a second-order approximation of the objective function in the Euclidean space to form a sequence of quadratic subproblems while keeping the manifold constraints. A modified Newton method is then developed and analyzed to solve the resulting subproblems. Based on a Steihaug-type CG method, we construct a specific search direction that can use negative curvature information of the Riemannian Hessian. We show that our method enjoys favorable convergence properties and converges with a locally superlinear rate. Numerical experiments are performed on the nearest correlation matrix estimation, Kohn-Sham total energy minimization, BEC, and low-rank matrix completion problems. The comparisons illustrate that our proposed method is promising. In particular, it can often reach a certain level of accuracy faster than other state-of-the-art algorithms. Our algorithm performs comparable to the Riemannian trust-region (RTR) method and usually achieves a better convergence rate once negative curvature is encountered. We should point out that our proposed algorithm can be further improved if a more specialized and efficient solver for the inner subproblem is available.

Acknowledgements. We would like to thank Bo Jiang for the helpful discussion on optimization with orthogonality constraints.

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Table 13
Numerical results on low rank matrix completion with fixed $n = 8000$, $k = 10$ but different $r_S$.

| $r_S$ | GBB | ARNT | RTR |
|------|-----|------|-----|
| 0.1  | 86  | 3.7e-7 | 88.1 |
| 0.2  | 89  | 8.6e-7 | 93.9 |
| 0.3  | 117 | 9.5e-7 | 119.7 |
| 0.5  | 173 | 8.5e-7 | 178.8 |
| 0.8  | 666 | 9.8e-7 | 700.2 |

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