Proximal Quasi-Newton Method for Composite Optimization over the Stiefel Manifold

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Abstract

In this paper, we consider the composite optimization problems over the Stiefel manifold. A successful method to solve this class of problems is the proximal gradient method proposed by [Chen et al., SIAM J. Optim., 30 (2020), pp. 210–239]. Motivated by the proximal Newton-type techniques in the Euclidean space, we present a Riemannian proximal quasi-Newton method, named ManPQN, to solve the composite optimization problems. The global convergence of the ManPQN method is proved and iteration complexity for obtaining an ϵ -stationary point is analyzed. Under some mild conditions, we also establish the local linear convergence result of the ManPQN method. Numerical results are encouraging, which shows that the proximal quasi-Newton technique can be used to accelerate the proximal gradient method.

Keywords: Proximal Newton-type method. Stiefel manifold. Quasi-Newton method. Nonmonotone line search. Linear convergence

Mathematics Subject Classification: 90C30

1 Introduction

In this paper, we consider the following composite optimization problem

$$\min_{X} F(X) := f(X) + h(X),$$

$$s.t. \ X^{\top}X = I_{r},$$

$$(1.1)$$

where $f: \mathbb{R}^{n \times r} \to \mathbb{R}$ is a smooth function and $h: \mathbb{R}^{n \times r} \to \mathbb{R}$ is a convex nonsmooth function. The feasible set $\operatorname{St}(n,r) := \{X \in \mathbb{R}^{n \times r} : X^\top X = I_r\}$ is referred to as the Stiefel manifold.

Problem (1.1) has wide applications in many fields such as machine learning, signal processing and numerical linear algebra. For example, when $f(X) = -\operatorname{tr}(X^TA^TAX)$ and $h(X) = \|X\|_1$, (1.1) is just the sparse PCA problem; When $f(X) = \operatorname{tr}(X^TMX)$ and $h(X) = \|X\|_{2,1}$, where M is a given matrix and $\|X\|_{2,1} := \sum_{i=1}^{n} \|X(i,i)\|_{2}$, (1.1) becomes the UFS (unsupervised feature selection) problem, which finds features that represent the distribution of the input data best, both to reduce the dimension of the data and to eliminate the noisy features. For more applications of composite optimization over the Stiefel manifold, we refer the readers to [1, 2, 6].

In the Euclidean setting, we can use the subgradient method to solve the composite optimization problems. In [36], Shor proved the convergence of subgradient method for nonsmooth convex optimization. There are several works which extend subgradient methods from Euclidean space to Riemannian manifolds. Ferreira and Oliveira [9] studied the convergence of subgradient method. Grohs and Hosseini [14] proposed an ε -subgradient method and establish the global converge result. In [15], they proposed an algorithm which combines the subgradient method with the trust-region model.

Another interesting approach is to use the operator splitting method to separate the manifold constraint part and the nonsmooth function part. In the Euclidean space, it is known that the operator splitting method needs more iterations to achieve the same accuracy as the proximal gradient method. Chen et al. [6] showed similar results in numerical experiments for the Riemannian setting.

A popular and efficient method for composite optimization in the Euclidean space is the proximal gradient (PG) method [26]. For a nonsmooth convex function h, the proximal mapping of h is defined by

$$\operatorname{prox}_{h}(x) = \arg\min_{y} \left\{ h(y) + \frac{1}{2} ||y - x||_{2}^{2} \right\}.$$
 (1.2)

To minimize f(x) + h(x), where f is smooth, the PG method takes the step

$$x_{k+1} = \operatorname{prox}_{th}(x_k - t\nabla f(x_k)),$$

where t > 0. It is well known that

$$x_{k+1} = \arg\min_{x} \left\{ \langle \nabla f(x_k), x \rangle + \frac{1}{2t} ||x - x_k||_2^2 + h(x) \right\}.$$
 (1.3)

There are several techniques can be used to accelerate the PG method. Beck and Teboulle [3] use Nesterov's acceleration technique to propose an algorithm, named FISTA, which shows the improved rate $O(1/k^2)$.

Another acceleration technique is the proximal Newton-type method, which is proposed in [11, 20]. Based on (1.2), Lee et al. [20] define the scaled proximal mapping as

$$\operatorname{prox}_{h}^{B}(x) = \arg\min_{y} \left\{ h(y) + \frac{1}{2} (y - x)^{T} B(y - x) \right\}.$$
 (1.4)

where B is a positive definite matrix. The motivation of the proximal Newton-type method is to replace the term $||x - x_k||_2^2/(2t)$ in (1.3) by $(x - x_k)^T B_k(x - x_k)/2$, where B_k is an approximate matrix of $\nabla^2 f(x_k)$. The proximal Newton-type method

takes the step

$$x_{k+1} = \operatorname{prox}_{h}^{B_{k}}(x_{k} - B_{k}^{-1}\nabla f(x_{k}))$$

$$= \arg \min_{x} \left\{ \langle \nabla f(x_{k}), x \rangle + \frac{1}{2}(x - x_{k})^{T} B_{k}(x - x_{k}) + h(x) \right\}.$$
 (1.5)

Superlinear convergence rate of the proximal Newton-type method has been established in [20, 23]. In [25], Nakayama proved the local linear rate of the inexact proximal quasi-Newton method.

Recently, many researchers have extended proximal-type methods to Riemannian manifolds. See [4, 5, 10, 12, 17, 18, 29, 42]. In [12], Gao et al. propose a parallelized proximal linearized augmented Lagrangian algorithm for solving optimization problems over the Stiefel manifold and show its convergence property. Oviedo [29] designs an iterative proximal point algorithm to minimize a continuously differentiable function over the Stiefel manifold, which avoids to construct geodesics and can be proved to converge globally. Zhang et al. [42] extend the smoothing steepest descent method for nonconvex and non-Lipschitz optimization from Euclidean space to Riemannian manifolds. The method can be applied to solve composite optimization problems. In [6], Chen et al. propose a retraction-based proximal gradient method, named ManPG, for composite optimization over the Stiefel manifold. Numerical experiments in [6] show that the performance of ManPG outperforms subgradient-based methods and ADMM-type methods for sparse PCA and CM problems. At the k-th iteration, the ManPG method solves the following subproblem to get a descent direction at X_k :

$$V_{k} = \underset{V \in T_{X_{k}} \mathcal{M}}{\arg \min} \left\{ \langle \operatorname{grad} f(X_{k}), V \rangle + \frac{1}{2} ||V||^{2} + h(X_{k} + V) \right\}.$$
 (1.6)

To accelerate the proximal gradient method, we propose a Riemannian proximal quasi-Newton method (ManPQN) to solve (1.1), which replaces $\frac{1}{2}||V||^2$ in (1.6) by $\frac{1}{2}||V||^2_{\mathcal{B}_k}$, where \mathcal{B}_k is a linear operator on $T_{X_k}\mathcal{M}$ updated by a quasi-Newton strategy. The ManPQN method can be regarded as an extension of the proximal quasi-Newton method from Euclidean space to Riemannian manifolds.

Our main contributions can be summarized as follows. We propose a proximal quasi-Newton method named ManPQN to solve (1.1). Under some mild conditions, we establish the global convergence and local linear convergence results of ManPQN. Since the computational cost of updating \mathcal{B}_k by the quasi-Newton strategy is very large, we use a strategy for updating \mathcal{B}_k , which can reduce the amount of computation significantly. Numerical experiments demonstrate that the proximal quasi-Newton technique can be used to accelerate the ManPG method.

The organization of the paper is shown as follows. In section 2, we introduce some notations and definitions that will be frequently used throughout the paper. In section 3, we propose the ManPQN algorithm in detail. The global convergence of ManPQN is proved and iteration complexity for obtaining an ϵ -stationary point is analyzed in section 4. Under some mild conditions, we also establish the local linear convergence result of the ManPQN method in this section. In section 5, we compare the ManPQN method with ManPG related methods in the numerical experiments. The paper ends with some conclusions and a short discussion on possible future works.

4

2 Notations and Preliminaries

In this section, we introduce some notations and definitions which will be used in the rest of the paper. Throughout this section, \mathcal{M} denotes a general manifold.

Definition 2.1 (Tangent space [2, p.33]) Let $X \in \mathcal{M}$. A tangent vector ξ_X to a manifold \mathcal{M} at X is a mapping from $\mathfrak{F}_X(\mathcal{M})$ to \mathbb{R} such that there exists a smooth curve γ on \mathcal{M} with $\gamma(0) = X$, satisfying

$$\xi_X f = \dot{\gamma}(0) f := \left. \frac{\mathrm{d}(f(\gamma(t)))}{\mathrm{d}t} \right|_{t=0},$$

for all $f \in \mathfrak{F}_X(\mathcal{M})$, where $\mathfrak{F}_X(\mathcal{M})$ denotes the set of smooth real-valued functions defined on a neighborhood of X over the manifold \mathcal{M} . The tangent space to \mathcal{M} at X, denoted by $T_X \mathcal{M}$, is the set of all tangent vectors to \mathcal{M} at X. The tangent bundle $T\mathcal{M} := \bigcup_X T_X \mathcal{M}$ consists of all tangent vectors to \mathcal{M} .

The Riemannian manifold \mathcal{M} is a manifold whose tangent spaces are endowed with a smoothly varying inner product $\langle \xi, \zeta \rangle_X$, where $\xi, \zeta \in \mathcal{T}_X \mathcal{M}$. The norm induced by the Riemannian inner product is denoted by $\|\cdot\|_X$, where $\|\xi\|_X := (\langle \xi, \xi \rangle_X)^{1/2}$. In this work, for the Stiefel manifold $\operatorname{St}(n,r)$, we consider the Riemannian metric defined by $\langle \xi, \zeta \rangle_X := tr(\xi^\top \zeta)$. For simplicity of notation, we write $\|\cdot\|$ instead of $\|\cdot\|_X$ in the rest of the paper.

The tangent space of the Stiefel manifold St(n, r) at X is [2, p.42]

$$T_X St(n,r) = \{ V \mid V^{\top} X + X^{\top} V = 0 \}.$$

The projection operator onto $T_X St(n,r)$ is given by [2, p.48]

$$\operatorname{Proj}_{\mathbf{T}_X \operatorname{St}(n,r)} Z = Z - \frac{1}{2} X (X^{\top} Z + Z^{\top} X).$$
 (2.1)

For a differentiable function $f: \mathcal{M} \to \mathbb{R}$, the derivative of f at $X \in \mathcal{M}$, denoted by $\mathrm{D}f(X)$, is an element of the dual space to $T_X\mathcal{M}$ which satisfies $\mathrm{D}f(X)\xi = \xi f$ for all $\xi \in T_X\mathcal{M}$. The gradient of a smooth function f at X, denoted by $\mathrm{grad}f(X)$ [2, p.46], is defined as the unique element of $\mathrm{T}_X\mathcal{M}$ that satisfies

$$\langle \operatorname{grad} f(X), \xi \rangle = \operatorname{D} f(X)[\xi] \quad \forall \xi \in T_X \mathcal{M}.$$

If \mathcal{M} is an embedded submanifold of an Euclidean space E, then by [2, p.48],

$$\operatorname{grad} f(X) = \operatorname{Proj}_{T_X \mathcal{M}} \nabla f(X),$$
 (2.2)

where $\operatorname{Proj}_{\mathcal{T}_X\mathcal{M}}$ is the projection operator from E onto $\mathcal{T}_X\mathcal{M}$ and $\nabla f(X)$ is the Euclidean gradient of f at X. For any $\xi \in \mathcal{T}_X\mathcal{M}$, from (2.2), it follows that

$$\langle \operatorname{grad} f(X), \xi \rangle = \langle \nabla f(X), \xi \rangle.$$

Next we introduce the definitions of the retraction and the vector transport.

Definition 2.2 (Retraction [2, Definition 4.1.1]) A retraction on a manifold \mathcal{M} is a smooth mapping \mathbf{R} from the tangent bundle $T\mathcal{M}$ onto \mathcal{M} with the following properties. Let \mathbf{R}_X denote the restriction of \mathbf{R} to $\mathbf{T}_X\mathcal{M}$.

- (1) $\mathbf{R}_X(0_X) = X$, where 0_X denotes the zero element of $T_X \mathcal{M}$.
- (2) With the canonical identification $T_{0_X}(T_X\mathcal{M}) \simeq T_X\mathcal{M}$, \mathbf{R}_X satisfies

$$D\mathbf{R}_X(0_X) = \mathbf{id}_{T_YM},\tag{2.3}$$

where $D\mathbf{R}_X(0_X)$ denotes the differential of the retraction \mathbf{R}_X at the zero element $0_X \in T_X \mathcal{M}$ and $\mathbf{id}_{T_X \mathcal{M}}$ denotes the identity mapping on $T_X \mathcal{M}$.

The following properties for a retraction \mathbf{R} will be used in section 4. For a proof, see [22].

Proposition 2.1 ([22]) Suppose \mathcal{M} is a compact embedded submanifold of an Euclidean space E, and \mathbf{R} is a retraction. Then there exists $M_1, M_2 > 0$ such that for all $X \in \mathcal{M}$ and for all $\xi \in T_X \mathcal{M}$,

$$\|\mathbf{R}_X(\xi) - X\| \le M_1 \|\xi\|,\tag{2.4}$$

$$\|\mathbf{R}_X(\xi) - X - \xi\| \le M_2 \|\xi\|^2. \tag{2.5}$$

Next we will consider the transport of a vector from one tangent space $T_X \mathcal{M}$ into another one $T_Y \mathcal{M}$.

Definition 2.3 (Vector Transport [2, Definition 8.1.1]) A vector transport associated with a retraction \mathbf{R} is defined as a continuous function $\mathcal{T}: T\mathcal{M} \times T\mathcal{M} \to T\mathcal{M}, (\eta_X, \xi_X) \mapsto T_{\eta_X}(\xi_X)$, which satisfies the following conditions:

- (i) $\mathcal{T}_{\eta_X}: T_X \mathcal{M} \to T_{\mathbf{R}_X(\eta_X)} \mathcal{M}$ is a linear invertible map,
- (ii) $\mathcal{T}_{0_X}(\xi_X) = \xi_X$.

Let $Y := \mathbf{R}_X(\eta_X)$, where $\eta_X \in T_X \mathcal{M}$. For ease of notation, we denote

$$\mathcal{T}_{X,Y}(\xi_X) := \mathcal{T}_{n_X}(\xi_X),$$

where $\xi_X \in T_X \mathcal{M}$.

For any $h \in T_X \mathcal{M}$, we use h^{\flat} to denote the linear function on $T_X \mathcal{M}$ induced by

$$h^{\flat} \eta := \langle h, \eta \rangle = \operatorname{tr}(h^T \eta) \quad \forall \eta \in T_X \mathcal{M}.$$

Let $H = [h_1, \ldots, h_m]$, where $h_i \in T_X \mathcal{M}$ for any $i = 1, \ldots, m$. Define $H^{\flat} : T_X \mathcal{M} \to \mathbb{R}^m$ by

$$H^{\flat}\eta = [h_1^{\flat}\eta, \dots, h_m^{\flat}\eta]^T \quad \forall \eta \in T_X \mathcal{M}.$$

Finally, we introduce the definitions of generalized Calrke subdifferential and regular function.

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Definition 2.4 (Generalized Calrke subdifferential [6, 41]) For a locally Lipschitz function ψ on a Riemannian manifold \mathcal{M} , the Riemannian generalized directional derivative of F at $X \in \mathcal{M}$ in the direction $V \in T_X \mathcal{M}$ is defined by

$$\psi^{\circ}(X; V) = \limsup_{Y \to X} \sup_{t \mid 0} \frac{\psi \circ \phi^{-1}(\phi(Y) + tD\phi(X)[V]) - \psi \circ \phi^{-1}(\phi(Y))}{t},$$

where (ϕ, U) is a coordinate chart at X. The generalized Clarke subdifferential of ψ at $X \in \mathcal{M}$, denoted by $\hat{\partial}\psi(X)$, is a subset of $T_X\mathcal{M}$ whose support function is $\psi^{\circ}(X;\cdot)$, defined by

$$\hat{\partial}\psi(X) = \{ \xi \in T_X \mathcal{M} : \langle \xi, V \rangle \le \psi^{\circ}(X; V), \forall V \in T_X \mathcal{M} \}.$$

In the rest of this section, we assume that \mathcal{M} be an embedded submanifold of an Euclidean space E.

Definition 2.5 (Regular function [41]) Let f be a function defined on E. We say that f is regular at $X \in \mathcal{M}$ along $T_X \mathcal{M}$ if

(1) for all $V \in T_X \mathcal{M}$,

$$f'(X; V) = \lim_{t \downarrow 0} \frac{f(X + tV) - f(X)}{t},$$

exists, and

(2) for all $V \in T_X \mathcal{M}$, $f'(X; V) = f^{\circ}(X; V)$.

For a regular nonsmooth function $\psi(X)$, it is proved in [41, Theorem 5.1] that $\hat{\partial}\psi(X) = \operatorname{Proj}_{\mathcal{T}_X\mathcal{M}}(\partial\psi(X))$, where $\partial\psi(X)$ is the Euclidean generalized Clarke sub-differential of ψ at X. Since f is continuously differentiable and h is convex, by [41, Lemma 5.1], the objective function F = f + h is regular. Then the first-order necessary condition of problem (1.1) can be written as

$$0 \in \hat{\partial}F(X^*) = \operatorname{grad}f(X^*) + \operatorname{Proj}_{T_{X^*}\mathcal{M}}(\partial h(X^*)), \tag{2.6}$$

where X^* is a local optimal solution of (1.1).

3 Proximal Quasi-Newton Method

In this section, we propose a proximal quasi-Newton algorithm over the Stiefel manifold, named ManPQN, which takes a proximal quasi-Newton step at each iteration, and uses the nonmonotone line search strategy to determine the stepsize. In the rest of the paper, we use $\mathcal M$ to denote the Stiefel manifold.

3.1 The ManPQN Algorithm

At the current iterate X_k , the ManPQN method solves the following problem to get the descent direction V_k :

$$V_k = \arg\min \langle \nabla f(X_k), V \rangle + \frac{1}{2} ||V||_{\mathcal{B}_k}^2 + h(X_k + V)$$
 (3.1)

s.t.
$$A_k(V) := V^T X_k + X_k^T V = 0,$$
 (3.2)

where \mathcal{B}_k is a symmetric positive definite operator on $T_{X_k}\mathcal{M}$, and $\|V\|_{\mathcal{B}_k}^2 = \langle V, \mathcal{B}_k[V] \rangle$. From (3.2), we know that $V_k \in T_{X_k}\mathcal{M}$.

To guarantee the positive definiteness of \mathcal{B}_k , we use a damped LBFGS strategy to generate \mathcal{B}_k . We leave the details of the updating in the next subsection.

After V_k is obtained, we apply the nonmonotone line search technique to determine the stepsize α_k . The nonmonotone technique was first introduced in [13]. Specifically, α_k is set to be γ^{N_k} , where N_k is the smallest integer such that

$$F(\mathbf{R}_{X_k}(\alpha_k V_k)) \le \max_{\max\{0, k-m\} \le j \le k} F(X_j) - \frac{1}{2} \sigma \alpha_k ||V_k||_{\mathcal{B}_k}^2, \tag{3.3}$$

in which m>0 is an integer, $\sigma,\gamma\in(0,1)$. For simplicity, we use the notation

$$l(k) := \underset{\max\{k-m,0\} \le j \le k}{\arg \max} F(X_j).$$
 (3.4)

Then $F(X_{l(k)}) = \max_{\max\{k-m,0\} \le j \le k} F(X_j)$.

Now we summarize the ManPQN method as follows:

Algorithm 1 Proximal quasi-Newton algorithm with nonmonotone line search to solve problem (1.1)

```
Require: Initial point X_0 \in \mathcal{M}, \gamma, \sigma \in (0, 1), m, p > 0 are integers.
 1: for k = 0, 1, \dots do
         if k \ge 1 then
 2:
              Update \mathcal{B}_k by quasi-Newton strategy;
 3:
         else
 4:
 5:
             Set \mathcal{B}_k = I;
         end if
 6.
         Solve the subproblem (3.1) to get the search direction V_k;
 7:
 8.
         Set initial stepsize \alpha_k = 1;
         while (3.3) is satisfied do
 9:
             \alpha_k = \gamma \alpha_k;
10:
11:
         end while
         Set X_{k+1} = \mathbf{R}_{X_k}(\alpha_k V_k);
12:
13: end for
```

3.2 Damped LBFGS Method

If the operator \mathcal{B}_k in (3.1) is updated by the Riemannian BFGS method, the total amount of computation is very large. It is well known that the Limited memory BFGS method (LBFGS) [28] is more suitable for large scale problems. Comparing with the BFGS method, the LBFGS method only needs the information of the last p steps, where p is the memory size.

To give the Riemannian LBFGS update formula, we introduce some notations first. For $k \geq 0$, let $g_k = \operatorname{grad} f(X_k) \in T_{X_k} \mathcal{M}$ and $\mathcal{T}_{k,k+1} := \mathcal{T}_{X_k,X_{k+1}}$. Define

$$S_k := \mathcal{T}_{k,k+1}(\mathbf{R}_{X_k}^{-1}(X_{k+1})), \ Y_k := g_{k+1} - \mathcal{T}_{k,k+1}(g_k).$$

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Given an initial estimate $\mathcal{B}_{k,0}$ at iteration k and two sequences $\{S_j\}$ and $\{Y_j\}$, $j = k - p, \ldots, k - 1$, the Riemannian LBFGS method updates $\mathcal{B}_{k,i}$ recursively as

$$\mathcal{B}_{k,i} = \widetilde{\mathcal{B}}_{k,i-1} - \frac{\widetilde{\mathcal{B}}_{k,i-1} S_j (\widetilde{\mathcal{B}}_{k,i-1} S_j)^{\flat}}{S_j^{\flat} \widetilde{\mathcal{B}}_{k,i-1} S_j} + \rho_j Y_j Y_j^{\flat},$$

$$j = k - (p - i + 1), \ i = 1, \dots, p,$$
(3.5)

where

$$\widetilde{\mathcal{B}}_{k,i-1} = \mathcal{T}_{j,j+1} \circ \mathcal{B}_{k,i-1} \circ \mathcal{T}_{j,j+1}^{-1} \text{ and } \rho_j = \frac{1}{Y_i^{\flat} S_j}.$$

The output $\mathcal{B}_{k,p}$ is set to be \mathcal{B}_k , the Riemannian LBFGS operator. It is easy to see \mathcal{B}_k is a linear operator on $T_{X_k}\mathcal{M}$.

The inverse of $\mathcal{B}_{k,i}$ is denoted by $\mathcal{H}_{k,i}$, $i = 0, 1, \dots, p$. By the Sherman-Morrison-Woodbury formula [35], we have

$$\mathcal{H}_{k,i} = (\mathbf{id} - \rho_j S_j Y_j^{\flat}) \mathcal{T}_{j,j+1} \mathcal{H}_{k,i-1} \mathcal{T}_{j,j+1}^{-1} (\mathbf{id} - \rho_j Y_j S_j^{\flat}) + \rho_j S_j S_j^{\flat},$$

$$j = k - (p - i + 1), \ i = 1, \dots, p,$$

where **id** denotes the identity map. It is obvious that $\mathcal{H}_k = \mathcal{H}_{k,p}$, where \mathcal{H}_k is the inverse of \mathcal{B}_k .

From (3.5), we know that the update of \mathcal{B}_k is computationally expensive because it involves the calculation of vector transports. Since the Stiefel manifold \mathcal{M} is a submanifold of a $\mathbb{R}^{n \times r}$, we can calculate the Euclidean differences s_k and y_k to replace S_k and Y_k , that is

$$s_k = X_{k+1} - X_k \in \mathbb{R}^{n \times r}, \quad y_k = g_{k+1} - g_k \in \mathbb{R}^{n \times r}.$$

Calculating s_k and y_k is much cheaper than calculating S_k and Y_k . Such a strategy was used in [16, 38].

To reduce the computational cost further, we will use a simple and easily computed \mathbf{B}_k to approximate \mathcal{B}_k . Such a strategy was used in [21, 31] for the Euclidean setting. In the ManPQN method, we solve the following subproblem to get V_k :

$$V_k = \underset{V \in \mathcal{T}_{X_k} \mathcal{M}}{\operatorname{arg \, min}} \left\{ \langle \nabla f(X_k), V \rangle + \frac{1}{2} \operatorname{tr}(V^T \mathbf{B}_k[V]) + h(X_k + V) \right\}, \tag{3.6}$$

where

$$\mathbf{B}_{k}[V] = \operatorname{Proj}_{\mathbf{T}_{X_{k}}\mathcal{M}}((\operatorname{diag}B_{k})(\operatorname{Proj}_{\mathbf{T}_{X_{k}}\mathcal{M}}V)), \tag{3.7}$$

in which $B_k \in \mathbb{R}^{n \times n}$ is a symmetric matrix. By (3.7), we can deduce that

$$\operatorname{tr}(V^T \mathbf{B}_k[V]) = \operatorname{tr}(V^T (\operatorname{diag} B_k) V) \quad \forall V \in \mathbf{T}_{X_k} \mathcal{M}.$$
 (3.8)

To ensure V_k is a descent direction of F at X_k , a sufficient condition is that B_k is a positive definite matrix. To guarantee the positive definitness of B_k , we use the damped technique employed in [32, 37]. Specifically, for $k \geq 0$, define

$$\overline{y}_{k-1} = \beta_{k-1} y_{k-1} + (1 - \beta_{k-1}) H_{k,0}^{-1} s_{k-1}, \tag{3.9}$$

where

$$\beta_{k-1} = \begin{cases} \frac{0.75 \text{tr}(s_{k-1}^T H_{k,0}^{-1} s_{k-1})}{\frac{\text{tr}(s_{k-1}^T H_{k,0}^{-1} s_{k-1}) - \text{tr}(s_{k-1}^T y_{k-1})}{\text{tr}(s_{k-1}^T H_{k,0}^{-1} s_{k-1}) + \text{tr}(s_{k-1}^T y_{k-1})}, \text{ if } \text{tr}(s_{k-1}^T y_{k-1}) < 0.25 \text{tr}(s_{k-1}^T H_{k,0}^{-1} s_{k-1}); \\ 1, \text{ otherwise.} \end{cases}$$

We set $H_{k,0} = (1/\delta)I$ for some $\delta > 0$. Then we can define B_k as follows:

$$\begin{cases}
B_{k} = B_{k,p}, \\
B_{k,i} = B_{k,i-1} - \frac{B_{k,i-1}s_{j}s_{j}^{T}B_{k,i-1}}{\operatorname{tr}(s_{j}^{T}B_{k,i-1}s_{j})} + \frac{\overline{y}_{j}\overline{y}_{j}^{T}}{\operatorname{tr}(s_{j}^{T}\overline{y}_{j})}, \\
j = k - (p - i + 1), i = 1, \dots, p, \\
B_{k,0} = \delta I_{n}.
\end{cases} (3.10)$$

Similar to the proof of [37, Lemma 3.1], we can show that B_k are positive definite matrices for all k. We omit the detail. The inverse of $B_{k,i}$ and B_k are denoted by $H_{k,i}$ and H_k . Thus, it holds that

$$\begin{cases}
H_{k} = H_{k,p}, \\
H_{k,i} = (I - \overline{\rho}_{j} s_{j} \overline{y}_{j}^{T}) H_{k,i-1} (I - \overline{\rho}_{j} \overline{y}_{j} s_{j}^{T}) + \overline{\rho}_{j} s_{j} s_{j}^{T}, \\
j = k - (p - i + 1), \quad i = 1, \dots, p, \\
H_{k,0} = (1/\delta) I_{n},
\end{cases}$$
(3.11)

where $\overline{\rho}_j = 1/\text{tr}(s_j^T \overline{y}_j)$. The following lemma shows that \mathbf{B}_k and its inverse are all bounded operators. In the proof of the lemma, we will use the notation

$$\varrho := \sup_{X \in \mathcal{M}} \|\nabla f(X)\|. \tag{3.12}$$

Since \mathcal{M} is a compact set in $\mathbb{R}^{n\times r}$, it follows that $\varrho < \infty$. We will also use the notations

$$\kappa_1 = \left(\frac{v^{2p} - 1}{v^2 - 1} \cdot \frac{4}{\delta} + \frac{v^{2p}}{\delta}\right)^{-1}, \qquad \kappa_2 = \delta + \frac{4(L + \varrho + \delta)^2}{\delta}p, \tag{3.13}$$

where $v := (4L + 4\rho + 5\delta)/\delta$, and δ is as in (3.10).

Lemma 3.1 Suppose that ∇f is Lipschitz continuous with the Lipschitz constant L. Suppose \mathbf{B}_k and B_k are defined by (3.7) and (3.10) respectively. Denote $\|V\|_{\mathbf{B}_k}^2 :=$ $\operatorname{tr}(V^T \mathbf{B}_k[V])$. Then for all k, we have

$$\kappa_1 ||V||^2 \le ||V||_{\mathbf{B}_k}^2 \le \kappa_2 ||V||^2 \quad \forall V \in \mathbf{T}_{X_k} \mathcal{M}.$$
(3.14)

Proof. To prove (3.14), by (3.8), we only need to show $\lambda_{\max}(B_k) \leq \kappa_2$ and $\lambda_{\max}(H_k) \leq \kappa_1^{-1}$. By (3.9), We have

$$\operatorname{tr}(s_{k-1}^T \bar{y}_{k-1}) = \max\{0.25\delta \|s_{k-1}\|^2, \operatorname{tr}(s_{k-1}^T y_{k-1})\} \ge 0.25\delta \|s_{k-1}\|^2. \tag{3.15}$$

For simplicity, we use the notation $P_k = \operatorname{Proj}_{\mathbf{T}_{X_k}\mathcal{M}}$. From (2.1), it follows that $||P_k - P_{k-1}|| \le ||X_k - X_{k-1}||$, Thus, by (2.2), we have

$$\begin{aligned} \|y_{k-1}\| &= \|P_k \nabla f(X_k) - P_{k-1} \nabla f(X_{k-1})\| \\ &\leq \|P_k \nabla f(X_k) - P_k \nabla f(X_{k-1})\| + \|P_k \nabla f(X_{k-1}) - P_{k-1} \nabla f(X_{k-1})\| \\ &\leq (L+\varrho) \|s_{k-1}\|, \end{aligned}$$

which together with (3.9) implies

$$\|\bar{y}_{k-1}\| \le (L + \rho + \delta)\|s_{k-1}\| \quad \forall k.$$
 (3.16)

By (3.10), (3.15) and (3.16), it holds that

$$\begin{split} \|B_{k,i}\|_{2} &\leq \left\|B_{k,i-1} - \frac{B_{k,i-1}s_{j}s_{j}^{T}B_{k,i-1}}{\operatorname{tr}(s_{j}^{T}B_{k,i-1}s_{j})}\right\|_{2} + \left\|\frac{\overline{y}_{j}\overline{y}_{j}^{T}}{\operatorname{tr}(s_{j}^{T}\overline{y}_{j})}\right\|_{2} \\ &\leq \|B_{k,i-1}\|_{2} + \frac{(L + \varrho + \delta)^{2}\|s_{j}\|^{2}}{0.25\delta\|s_{j}\|^{2}}, \quad j = k - (p - i + 1), i = 1, \dots, p, \end{split}$$

which together with $B_{k,0} = \delta I$ implies $\lambda_{\max}(B_k) \le \kappa_2$.

Recall that $\overline{\rho}_j = 1/\text{tr}(s_j^T \overline{y}_j)$. By (3.16) again, we have $\overline{\rho}_j \|s_j \overline{y}_j^T\| \le 4(L+\varrho+\delta)/\delta$. Thus, by (3.11), (3.15) and (3.16), we have

$$||H_{k,i}||_{2} \leq ||I - \overline{\rho}_{j} s_{j} \overline{y}_{j}^{T}||_{2} \cdot ||H_{k,i-1}||_{2} \cdot ||I - \overline{\rho}_{j} \overline{y}_{j} s_{j}^{T}||_{2} + ||\overline{\rho}_{j} s_{j} s_{j}^{T}||_{2}$$

$$\leq (1 + \overline{\rho}_{j} ||s_{j} \overline{y}_{j}^{T}||_{2})^{2} ||H_{k,i-1}||_{2} + 4/\delta$$

$$\leq (1 + 4(L + \rho + \delta)/\delta)^{2} ||H_{k,i-1}||_{2} + 4/\delta, \quad j = k - (p - i + 1), i = 1, \dots, p.$$

By the above inequality, it is easy to prove $\lambda_{\max}(H_k) \leq \kappa_1^{-1}$ by induction. We omit the detail.

Lemma 3.1 shows that $\{\mathbf{B}_k\}$ are uniformly positive definite if \mathbf{B}_k is generated by (3.7). In the following, we show how to solve the subproblem (3.1). Let Λ be the Lagrange multiplier for the constraint (3.2). Then $\Lambda \in \mathbb{S}^r$, where \mathbb{S}^r denotes the set of symmetric $r \times r$ matrices. The Lagrangian function for (3.1) is

$$\mathcal{L}_{k}(V,\Lambda) = \langle \nabla f(X_{k}), V \rangle + \frac{1}{2} \|V\|_{\mathbf{B}_{k}}^{2} + h(X_{k} + V) - \langle \mathcal{A}_{k}^{*}(\Lambda), V \rangle$$
$$= \langle \nabla f(X_{k}) - \mathcal{A}_{k}^{*}(\Lambda), V \rangle + \frac{1}{2} \operatorname{tr}(V^{T}(\operatorname{diag}B_{k})V) + h(X_{k} + V), (3.17)$$

where \mathcal{A}_k^* denotes the adjoint operator of \mathcal{A}_k . For a fixed Λ , $\mathcal{L}_k(V,\Lambda)$ is a strongly convex function of V since B_k is a positive definite matrix. We use $V(\Lambda)$ to denote the unique minimum of $\min \mathcal{L}_k(V,\Lambda)$. By (1.4) and (3.17), we have

$$V(\Lambda) = \operatorname{prox}_{h}^{\mathbf{B}_{k}} \left(X_{k} - (\operatorname{diag} H_{k})(\nabla f(X_{k}) - \mathcal{A}_{k}^{*}(\Lambda)) \right) - X_{k}$$

$$= \operatorname{prox}_{h}^{\mathbf{B}_{k}} (B(\Lambda)) - X_{k},$$
(3.18)

where $B(\Lambda) := X_k - (\operatorname{diag} H_k)(\nabla f(X_k) - \mathcal{A}_k^*(\Lambda))$ and H_k is the inverse of B_k . Substituting (3.18) into (3.2) yields

$$E(\Lambda) \equiv \mathcal{A}_k(V(\Lambda)) = V(\Lambda)^T X_k + X_k^T V(\Lambda) = 0.$$
(3.19)

Similar to the discussion at [6, p.221], we can prove that $E(\Lambda)$ is a monotone and Lipschitz continuous operator on \mathbb{S}^r . Then the adaptive regularized semismooth Newton (ASSN) method can be used to solve (3.19). We give a brief description in the following.

The vectorization of (3.19) can be written as

$$\operatorname{vec}(E(\Lambda)) = (K_{rr} + I_{r^2})(I_r \otimes X_k^T) \left[\operatorname{prox}_h^{\mathbf{B}_k} (\operatorname{vec}(X_k - (\operatorname{diag} H_k) \nabla f(X_k)) + 2(I_r \otimes ((\operatorname{diag} H_k) X_k)) \operatorname{vec}(\Lambda)) - \operatorname{vec}(X_k) \right],$$

where K_{nr} and K_{rr} are comutation matrices. Define

$$\mathcal{G}(\operatorname{vec}(\Lambda)) := 2(K_{rr} + I_{r^2})(I_r \otimes X_k^T)\mathcal{J}(y)|_{y = \operatorname{vec}(B(\Lambda))}(I_r \otimes ((\operatorname{diag} H_k)X_k)), (3.20)$$

where $\mathcal{J}(y)$ is the generalized Jacobian of $\operatorname{prox}_h^{\mathbf{B}_k}(y)$. Then, we know that $\mathcal{G}(\operatorname{vec}(\Lambda)) \in \partial \operatorname{vec}(E(\operatorname{vec}(\Lambda)))$.

Denote $\overline{\text{vec}}(\Lambda)$ as the vectorization of the lower triangular part of Λ . Then there exists a duplication matrix $U_r \in \mathbb{R}^{r^2 \times \frac{1}{2}r(r+1)}$ such that $\overline{\text{vec}}(\Lambda) = U_r^+ \text{vec}(\Lambda)$, where $U_r^+ = (U_r^T U_r)^{-1} U_r$ is the Moore-Penrose inverse of U_r . By (3.20), the generalized Jacobian of $\overline{\text{vec}}(E(U_r \overline{\text{vec}}(\Lambda)))$ can be written as

$$\mathcal{G}(\overline{\text{vec}}(\Lambda)) = U_r^+ \mathcal{G}(\text{vec}(\Lambda)) U_r$$

= $4U_r^+ (I_r \otimes X_k^T) \mathcal{J}(y)|_{y=\text{vec}(B(\Lambda))} (I_r \otimes ((\text{diag}H_k)X_k)) U_r.$

At the current iterate Λ_l , to get the Newton direction d_l , we can apply the conjugate gradient method to solve the following equation

$$(\mathcal{G}(\overline{\text{vec}}(\Lambda_l)) + \eta I)d = -\overline{\text{vec}}(E(\Lambda_l)), \tag{3.21}$$

where $\eta > 0$ is a regularization parameter. Then, we use the same strategy as that in [40] to obtain the next iterate Λ_{l+1} . For more details, we refer the reader to [6, 40].

4 Convergence Analysis of ManPQN Algorithm

In this section, we study the convergence properties of the ManPQN algorithm. Under mild assumptions, we prove the global convergence of Algorithm 1. We also analyze the local convergence rate of the ManPQN method. It is proved that the iterates of the algorithms converge locally linearly to the nondegenerate local minimum point.

4.1 Global Convergence

First, we give the following assumption which is required in the rest of the paper.

Assumption 4.1 $f: \mathbb{R}^{n \times r} \to \mathbb{R}$ is smooth, and ∇f is Lipschitz continuous with Lipschitz constant $L; h: \mathbb{R}^{n \times r} \to \mathbb{R}$ is a convex but nonsmooth function, and h is Lipschitz continuous with Lipschitz constant L_h .

Given X_k , we denote the objective function of (3.1) by ϕ_k , that is

$$\phi_k(V) := \langle \nabla f(X_k), V \rangle + \frac{1}{2} ||V||_{\mathcal{B}_k}^2 + h(X_k + V),$$
 (4.1)

where \mathcal{B}_k is a linear operator on $\mathbb{R}^{n \times r}$ satisfying $\mathcal{B}_k T_{X_k} \mathcal{M} \subseteq T_{X_k} \mathcal{M}$. In our convergence analysis, the only requirement of \mathcal{B}_k is that it satisfies (3.14), that is, For analysis, the only requirement of \mathcal{B}_k is that it satisfies (3.14), that is, $\kappa_1 \|V\|^2 \leq \|V\|_{\mathcal{B}_k}^2 \leq \kappa_2 \|V\|^2$ for all $V \in T_{X_k} \mathcal{M}$. This and Assumption 4.1 imply that ϕ_k is a convex function on $T_{X_k} \mathcal{M}$.

Since $V_k = \underset{V \in T_{X_k} \mathcal{M}}{\min} \phi_k(V)$, by (2.2), we have

$$0 \in \operatorname{Proj}_{\operatorname{T}_{X_k} \mathcal{M}} \partial \phi_k(V_k) = \operatorname{grad} f(X_k) + \mathcal{B}_k[V_k] + \operatorname{Proj}_{\operatorname{T}_{X_k} \mathcal{M}} \partial h(X_k + V_k). \tag{4.2}$$

If $V_k = 0$, then X_k satisfies (2.6), and therefore is a stationary point of (1.1); If $V_k \neq 0$, the following result shows that V_k is a descent direction of ϕ_k . The proof is similar to that of [6, Lemma 5.1]. We give a proof for completeness.

Lemma 4.1 Suppose Assumption 4.1 holds. For any $\alpha \in [0,1]$, it holds that

$$\phi_k(\alpha V_k) - \phi_k(0) \le \frac{\alpha(\alpha - 2)}{2} \|V_k\|_{\mathcal{B}_k}^2. \tag{4.3}$$

Proof. By (4.2), there exists $\xi \in \partial h(X_k + V_k)$ such that $\operatorname{grad} f(X_k) + \mathcal{B}_k[V_k] +$ $\operatorname{Proj}_{T_{X_k},\mathcal{M}}\xi = 0$. From $\xi + \operatorname{grad} f(X_k) \in \partial \left(\phi_k - \frac{1}{2} \|\cdot\|_{\mathcal{B}_k}^2\right)(V_k)$, it follows that

$$\phi_{k}(0) - \phi_{k}(V_{k}) \geq \langle \operatorname{grad} f(X_{k}) + \xi, -V_{k} \rangle - \frac{1}{2} \|V\|_{\mathcal{B}_{k}}^{2}$$

$$= \langle \operatorname{grad} f(X_{k}) + \operatorname{Proj}_{T_{X_{k}} \mathcal{M}} \xi + \mathcal{B}_{k}[V], -V_{k} \rangle + \frac{1}{2} \|V_{k}\|_{\mathcal{B}_{k}}^{2}$$

$$= \frac{1}{2} \|V_{k}\|_{\mathcal{B}_{k}}^{2}. \tag{4.4}$$

Since h is a convex function, for all $0 \le \alpha \le 1$, we have

$$h(X_k + \alpha V_k) - h(X_k) \le \alpha (h(X_k + V_k) - h(X_k)). \tag{4.5}$$

Combining (4.4) and (4.5) yields

$$\begin{aligned} \phi_{k}(\alpha V_{k}) - \phi_{k}(0) &= \langle \nabla f(X_{k}), \alpha V_{k} \rangle + \frac{1}{2} \|\alpha V_{k}\|_{\mathcal{B}_{k}}^{2} + h(X_{k} + \alpha V_{k}) - h(X_{k}) \\ &\leq \alpha \left(\langle \nabla f(X_{k}), V_{k} \rangle + \frac{\alpha}{2} \|V_{k}\|_{\mathcal{B}_{k}}^{2} + h(X_{k} + V_{k})) - h(X_{k}) \right) \\ &= \alpha (\phi_{k}(V_{k}) - \phi_{k}(0) + \frac{\alpha - 1}{2} \|V_{k}\|_{\mathcal{B}_{k}}^{2}) \\ &\leq \frac{\alpha (\alpha - 2)}{2} \|V_{k}\|_{\mathcal{B}_{k}}^{2}. \end{aligned}$$

The assertion holds.

In the rest of the paper, we use F_k to denote $F(X_k)$. By the definition of l(k)(see (3.4)), we have $F_{l(k)} = \max_{\max\{k-m,0\} \le j \le k} F_j$. We will use the notation

$$\overline{\alpha} := \min\{1, \frac{(2-\sigma)\kappa_1}{2(\varrho M_2 + \frac{1}{2}LM_1^2 + L_h M_2)}\},\tag{4.6}$$

where L and L_h are Lipschitz constants, M_1 , M_2 , σ , ϱ and κ_1 are parameters in (2.4), (2.5), (3.3), (3.12) and (3.13) respectively.

Lemma 4.2 Suppose Assumption 4.1 holds, and \mathcal{B}_k satisfies (3.14). Let α_k be the stepsize of the k-th iteration of Algorithm 1. Then $\alpha_k \geq \gamma \bar{\alpha}$, where $\bar{\alpha}$ is defined by (4.6) and γ is the parameter of Algorithm 1. Moreover,

$$F_{k+1} - F_{l(k)} \le -\frac{1}{2}\sigma\alpha_k \|V_k\|_{\mathcal{B}_k}^2.$$

Proof. Since ∇f is Lipschitz continuous with constant L, for any $\alpha > 0$, we have $f(\mathbf{R}_{X_k}(\alpha V_k))$

$$\leq f(X_k) + \langle \nabla f(X_k), \mathbf{R}_{X_k}(\alpha V_k) - X_k \rangle + \frac{L}{2} \|\mathbf{R}_{X_k}(\alpha V_k) - X_k\|^2
\leq f(X_k) + \langle \nabla f(X_k), \mathbf{R}_{X_k}(\alpha V_k) - (X_k + \alpha V_k) \rangle + \langle \nabla f(X_k), \alpha V_k \rangle + \frac{1}{2} L M_1^2 \|\alpha V_k\|^2,
\leq f(X_k) + \langle \nabla f(X_k), \alpha V_k \rangle + (\varrho M_2 + \frac{1}{2} L M_1^2) \|\alpha V_k\|^2
= f(X_k) + \langle \nabla f(X_k), \alpha V_k \rangle + c_1 \|\alpha V_k\|^2,$$
(4.7)

where $c_1 := \varrho M_2 + \frac{1}{2}LM_1^2$, the second inequality follows from (2.4), and the third inequality follows from (2.5) and (3.12).

By Assumption 4.1 and (2.5), it holds that

$$h(\mathbf{R}_{X_k}(\alpha V_k)) - h(X_k + \alpha V_k) \le L_h \|\mathbf{R}_{X_k}(\alpha V_k) - X_k - \alpha V_k\|$$

$$\le L_h M_2 \|\alpha V_k\|^2. \tag{4.8}$$

Combining (4.7) and (4.8) yields

$$F(\mathbf{R}_{X_{k}}(\alpha V_{k}))$$

$$\leq f(X_{k}) + \langle \nabla f(X_{k}), \alpha V_{k} \rangle + (c_{1} + L_{h}M_{2}) \|\alpha V_{k}\|^{2} + h(X_{k} + \alpha V_{k}) \qquad (4.9)$$

$$= f(X_{k}) + \phi_{k}(\alpha V_{k}) + c_{2} \|\alpha V_{k}\|^{2} - \frac{1}{2} \|\alpha V_{k}\|_{\mathcal{B}_{k}}^{2}$$

$$\leq F_{l(k)} + \phi_{k}(\alpha V_{k}) - \phi_{k}(0) + (c_{2}\kappa_{1}^{-1} - \frac{1}{2}) \|\alpha V_{k}\|_{\mathcal{B}_{k}}^{2}, \qquad (4.10)$$

where $c_2 := c_1 + L_h M_2 = \varrho M_2 + \frac{1}{2} L M_1^2 + L_h M_2$. For any $0 < \alpha \le 1$, by (4.3) and (4.10), we have

$$F(\mathbf{R}_{X_k}(\alpha V_k)) \le F_{l(k)} + (c_2 \kappa_1^{-1} - \alpha^{-1}) \alpha^2 ||V_k||_{\mathcal{B}_k}^2$$

Thus, if $0 < \alpha \leq \overline{\alpha}$, it holds that

$$F(\mathbf{R}_{X_k}(\alpha V_k)) - F_{l(k)} \le (c_2 \kappa_1^{-1} \overline{\alpha} - 1) \alpha \|V_k\|_{\mathcal{B}_k}^2 \le -\frac{1}{2} \sigma \alpha \|V_k\|_{\mathcal{B}_k}^2. \tag{4.11}$$

By steps 8-11 of Algorithm 1, we conclude that $\alpha_k \geq \gamma \overline{\alpha}$. Substituting $\alpha = \alpha_k$ into (4.11) yields

$$F_{k+1} - F_{l(k)} = F(\mathbf{R}_{X_k}(\alpha_k V_k)) - F_{l(k)} \le -\frac{1}{2}\sigma\alpha_k \|V_k\|_{\mathcal{B}_k}^2.$$
 (4.12)

The proof is complete.

Now we are in a position to present the main result of this section, the global convergence of Algorithm 1.

Theorem 4.1 Suppose Assumption 4.1 holds, and \mathcal{B}_k satisfies (3.14). Then all accumulation points of $\{X_k\}$ are stationary points of problem (1.1).

Proof. Let X^* be an accumulation point of sequence $\{X_k\}$. We need to prove that X^* satisfies (2.6). By Lemma 4.2, we have that

$$\begin{split} F_{l(k+1)} &= \max_{0 \leq j \leq \min\{m,k+1\}} F_{k+1-j} \\ &= \max\{F_{k+1}, \max_{0 \leq j \leq \min\{m-1,k\}} F_{k-j}\} \\ &\leq \max\{F_{l(k)} - \frac{1}{2} \sigma \alpha_k \|V_k\|_{\mathcal{B}_k}^2, F_{l(k)}\}, \text{ by}(4.12) \\ &\leq F_{l(k)}, \end{split}$$

which implies that $\{F_{l(k)}\}_k$ is a monotone nonincreasing sequence. Since \mathcal{M} is compact, F_k is bounded below. Thus, there exists a scalar F^* such that

$$\lim_{k \to \infty} F_{l(k)} = F^*. \tag{4.13}$$

By (3.14) and (4.12), we have

$$F_{l(k)} \leq F_{l(l(k)-1)} - \frac{1}{2}\sigma\alpha_{l(k)-1} \|V_{l(k)-1}\|_{\mathcal{B}_{l(k)-1}}^{2}$$

$$\leq F_{l(l(k)-1)} - \frac{1}{2}\sigma\kappa_{1}\alpha_{l(k)-1} \|V_{l(k)-1}\|^{2}.$$

From Lemma 4.2, it follows that $\alpha_k \geq \gamma \overline{\alpha}$ for all k, Thus, we must have

$$\lim_{k \to \infty} V_{l(k)-1} = 0.$$

Combining it with (4.13) yields that

$$\begin{split} \lim_{k\to\infty} F_{l(k)-1} &= \lim_{k\to\infty} F(\mathbf{R}_{X_{l(k)-1}}(\alpha_{l(k)-1}V_{l(k)-1})) \\ &= \lim_{k\to\infty} F(X_{l(k)}) = F^*. \end{split}$$

For all $1 \leq j \leq m$, we can prove by induction that

$$\lim_{k \to \infty} V_{l(k)-j} = 0, \text{ and } \lim_{k \to \infty} F_{l(k)-j} = F^*.$$
(4.14)

The proof is similar to that of [39, Theorem 1], and so we omit it.

For any k, there exists an integer $1 \le j(k) \le m$ such that k = l(k+m) - j(k), which together with (4.14) implies

$$\lim_{k \to \infty} V_k = \lim_{k \to \infty} V_{l(k+m)-j(k)} = 0, \tag{4.15}$$

and

$$\lim_{k \to \infty} F_k = \lim_{k \to \infty} F_{l(k+m)-j(k)} = F^*.$$
 (4.16)

By (4.15) and (4.2), we can deduce that X^* satisfies (2.6), which completes the proof.

In the following, we introduce the definition of an ϵ -stationary point of the problem (1.1).

Definition 4.1 (ϵ -stationary point [6]) Given $\epsilon > 0$ and X_k generated by Algorithm 1, we say that $X_k \in \mathcal{M}$ is an ϵ -stationary point of (1.1) if the solution V_k to (3.1) satisfies $||V_k||_F \leq \epsilon$.

In Algorithm 1, we use $||V_k||_F \le \epsilon$ as our stopping criterion. Similar to [6, Theorem 5.5], we give the iteration complexity analysis of Algorithm 1.

Corollary 4.1 Algorithm 1 will find an ϵ -stationary point in at most $m\lceil 2(F(X_0) - F^*)/(\sigma \kappa_1 \gamma \overline{\alpha} \epsilon^2) \rceil$ iterations, where m, σ , κ_1 , $\overline{\alpha}$ are defined in (3.3), (3.13), (4.6) respectively and F^* is the optimal value of (1.1).

Proof. Similar to the proof of Theorem 3.2 in [7], we can obtain that for $j \geq 0$,

$$F(X_{l((j+1)m)}) - F(X_{l(jm)}) \le \max_{0 \le i \le m-1} \{-\frac{1}{2}\sigma\alpha_{jm+i} \|V_{jm+i}\|_{\mathcal{B}_{jm+i}}^2\}$$

$$\le \max_{0 \le i \le m-1} \{-\frac{1}{2}\sigma\kappa_1\alpha_{jm+i} \|V_{jm+i}\|_F^2\}. \quad (4.17)$$

Given K > 0, suppose that after mK iterations, Algorithm 1 does not terminate, which means that $||V_k||^2_{\mathcal{B}_k} > \kappa_1 \epsilon^2$ for any $0 \le k \le Km - 1$. It follows that

$$F(X_0) - F^* \ge F(X_{l(0)}) - F(X_{l(Km)})$$

$$\ge \sum_{i=0}^{K-1} \min_{0 \le i \le m-1} \{ \frac{1}{2} \sigma \kappa_1 \alpha_{jm+i} ||V_{jm+i}||_F^2 \} > \frac{1}{2} \sigma \kappa_1 \epsilon^2 K \gamma \overline{\alpha},$$

where the second inequality follows from (4.17). Thus, Algorithm 1 will return an ϵ -stationary point in at most $m\lceil 2(F(X_0) - F^*)/(\sigma \kappa_1 \gamma \overline{\alpha} \epsilon^2) \rceil$ iterations.

4.2 Locally Linear Convergence

The objective of this subsection is to show that Algorithm 1 has a local linear convergence rate around the nondegenerate local minimum point. Let $\{X_k\}$ be the sequence of iterates generated by Algorithm 1 and \overline{X}^* be any accumulation point of $\{X_k\}$. By (4.16), we know that

$$F(\overline{X}^*) = F^*, \tag{4.18}$$

where F^* is the scalar in (4.16).

We need the following assumption before presenting our main results.

Assumption 4.2 The function f is twice continuously differentiable. The sequence $\{X_k\}$ has an accumulation point X^* such that

$$\lambda_{\min}(\operatorname{Hess}(f \circ \mathbf{R}_{X^*})(0_{X^*})) \ge \widetilde{\eta},\tag{4.19}$$

where $\widetilde{\eta} > 5L_h M_2$.

The constant M_2 is defined in (2.5). We should point out Assumption 4.2 is not a strong condition. In some typical applications, $h(X) = \mu ||X||_1$. We can see that if

$$\mu < \frac{1}{5M_2} \lambda_{\min}(\operatorname{Hess}(f \circ \mathbf{R}_{X^*})(0_{X^*})),$$

then (4.19) will be satisfied.

Definition 4.2 (ς -strongly convex function [27, Definition 2.1.3]) The function g(x) is said to be a ς -strongly convex function if $g(x) - \frac{1}{2} \varsigma ||x||^2$ is convex, where ς is called the convexity parameter of g.

By the definition, if g(x) is strongly convex with parameter ς , it is easy to prove

$$g(x) - g(x^*) \ge \frac{\varsigma}{2} ||x - x^*||^2 \quad \forall x,$$
 (4.20)

where x^* is the unique minimizer of g. We also use the following property of strongly convex functions. If g is twice continuously differentiable, then

$$\lambda_{\min}(\nabla^2 g(x)) \ge \varsigma$$
, $\forall x \iff g$ is strongly convex with parameter ς . (4.21)

For a proof, see [27].

To establish the main results, we need some preparing results.

Lemma 4.3 Suppose Assumptions 4.1 and 4.2 hold. Let X^* be the accumulation point satisfying (4.19). Then there exists a neighbourhood \mathcal{U}_{X^*} of X^* and $\epsilon > 0$ such that:

- (1) For all $X \in \mathcal{U}_{X^*}$, $f \circ \mathbf{R}_X$ is a convex function on the set $\{\xi \in T_X \mathcal{M} : \|\xi\| < \epsilon\}$.
- (2) For all $X \in \mathcal{U}_{X^*}$,

$$F(X) - F(X^*) \ge \eta \|\mathbf{R}_X^{-1}(X^*)\|^2,$$
 (4.22)

for some $\eta > L_h M_2$.

Proof. (1). Since f is twice continuously differentiable and \mathbf{R} is smooth, $\lambda_{\min}(\operatorname{Hess}(f \circ \mathbf{R}))$ is a continuous function of $T\mathcal{M}$, which together with (4.19) implies that there exists a neighbourhood \mathcal{U}_{X^*} of X^* and $\epsilon > 0$ such that

$$\lambda_{\min}(\operatorname{Hess}(f \circ \mathbf{R}_X)(\xi_X)) > \frac{9}{10}\widetilde{\eta},$$
 (4.23)

for all $X \in \mathcal{U}_{X^*}$ and all $\xi_X \in \{\xi \in T_X \mathcal{M} : ||\xi|| < \epsilon\}$. Thus $f \circ \mathbf{R}_X$ is a convex function on $\{\xi \in T_X \mathcal{M} : ||\xi|| < \epsilon\}$.

(2). By (4.21) and (4.23), we know that $f(\mathbf{R}_{X^*}(\xi))$ is $9\widetilde{\eta}/10$ -strongly convex on \mathcal{D}_{X^*} where $\mathcal{D}_{X^*} := \{\xi \in \mathrm{T}_{X^*}\mathcal{M} : \|\xi\| < \epsilon\}.$

Define $\Gamma: T_{X^*}\mathcal{M} \to \mathbb{R}$ by $\Gamma(\xi) = f(\mathbf{R}_{X^*}(\xi)) + h(X^* + \xi)$. Then Γ is also $9\widetilde{\eta}/10$ -strongly convex on \mathcal{D}_{X^*} . By (2.3), we have

$$\partial\Gamma(0_{X^*}) = \operatorname{Proj}_{\mathbf{T}_{X^*}\mathcal{M}} \left(\operatorname{D}\mathbf{R}_{X^*}(0_{X^*}) \nabla f(X^*) + \partial h(X^*) \right)$$

= $\operatorname{grad} f(X^*) + \operatorname{Proj}_{\mathbf{T}_{X^*}\mathcal{M}} (\partial h(X^*)),$

which together with (2.6) implies $0 \in \partial \Gamma(0_{X^*})$. Thus 0_{X^*} is the unique minimizer of Γ in \mathcal{D}_{X^*} . By (4.20), we have

$$\Gamma(\xi) - F(X^*) = \Gamma(\xi) - \Gamma(0_{X^*}) \ge \frac{9}{20} \tilde{\eta} \|\xi\|^2 \quad \forall \xi \in \mathcal{D}_{X^*}.$$
 (4.24)

Let $\varphi(\xi) = h(\mathbf{R}_{X^*}(\xi)) - h(X^* + \xi)$. From (2.5) and Assumption 4.1, it holds that

$$|\varphi(\xi)| \le L_h M_2 \|\xi\|^2 \quad \forall \xi \in \mathcal{D}_{X^*}. \tag{4.25}$$

By (4.24) and (4.25), we can deduce that

$$F(\mathbf{R}_{X^*}(\xi)) - F(X^*) = f(\mathbf{R}_{X^*}(\xi)) + h(\mathbf{R}_{X^*}(\xi)) - F(X^*)$$
$$= \Gamma(\xi) + \varphi(\xi) - \Gamma(0_{X^*})$$

$$\geq \left(\frac{9}{20}\widetilde{\eta} - L_h M_2\right) \|\xi\|^2. \tag{4.26}$$

Substituting $\xi = \mathbf{R}_{X^*}^{-1}(X)$ into (4.26) yields

$$F(X) - F(X^*) \ge \frac{1}{4} \widetilde{\eta} \| \mathbf{R}_{X^*}^{-1}(X) \|^2.$$
 (4.27)

By [33, Lemma 6], for any $\varepsilon > 0$, there exists a neighbourhood \mathcal{U}_{X^*} of X^* and $\varepsilon' > 0$ such that for all $X \in \mathcal{U}_{X^*}$ and $V, W \in T_X \mathcal{M}$ with $||V||, ||W|| < \varepsilon'$,

$$(1-\varepsilon)\|V-W\| \le \operatorname{dist}(\mathbf{R}_X(V), \mathbf{R}_X(W)) \le (1+\varepsilon)\|V-W\|. \tag{4.28}$$

Assume that \mathcal{U}_{X^*} is small enough such that $\|\mathbf{R}_{X^*}^{-1}(X)\| < \varepsilon'$ and $\|\mathbf{R}_X^{-1}(X^*)\| < \varepsilon'$ for any $X \in \mathcal{U}_{X^*}$. By (4.28), we have

$$(1 - \varepsilon) \|\mathbf{R}_{\mathbf{X}}^{-1}(X^*)\| \le \|X - X^*\| \le (1 + \varepsilon) \|\mathbf{R}_{\mathbf{X}^*}^{-1}(X)\|, \tag{4.29}$$

where the first inequality follows from substituting $V = 0_X$ and $W = \mathbf{R}_X^{-1}(X^*)$ into (4.28), and the second inequality from $V = \mathbf{R}_{X^*}^{-1}(X)$ and $W = 0_{X^*}$ in (4.28). We can choose ε satisfying $\varepsilon < (\sqrt{5} - 2)^2$. By (4.27) and (4.29), we have

$$F(X) - F(X^*) \ge \frac{(1-\varepsilon)^2}{4(1+\varepsilon)^2} \widetilde{\eta} \|\mathbf{R}_X^{-1}(X^*)\|^2 \ge \frac{1}{5} \widetilde{\eta} \|\mathbf{R}_X^{-1}(X^*)\|^2 \quad \forall X \in \mathcal{U}_{X^*},$$

which together with $\tilde{\eta} > 5L_h M_2$ implies (4.22).

Under the condition of Assumption 4.2, from the following result, we know that the sequence $\{X_k\}$ has only one accumulation point X^* , which is of course the limit of $\{X_k\}$.

Theorem 4.2 Suppose Assumptions 4.1 and 4.2 hold, and X^* is the accumulation point satisfying (4.19). Then, X_k converges to X^* .

Proof. Let \mathcal{U}_{X^*} be the neighbourhood of X^* as in Lemma 4.3. Define $\overline{\mathcal{U}}_{X^*} := \{\mathbf{R}_{X^*}(\xi) : \xi \in \mathcal{U}_{X^*}\}$. By (4.22), X^* is the unique minimizer of F in $\overline{\mathcal{U}}_{X^*}$, which together with (4.18) implies that X^* is an isolated accumulation point of $\{X_k\}$. Since $V_k \to 0$ by (4.15), we have

$$||X_{k+1} - X_k|| = ||\mathbf{R}_{X_k}(\alpha_k V_k) - X_k|| \le M_1 \alpha_k ||V_k|| \to 0.$$

By [24, Lemma (4.10)], we can obtain that $X_k \to X^*$.

From Lemma 4.2, we know that the stepsize α_k satisfies $\gamma \overline{\alpha} < \alpha_k \le 1$ for all $k \ge 0$, where $\overline{\alpha}$ is defined in (4.6). We will use this fact to prove the local linear convergence of Algorithm 1. Our proof is based on a technique used in [19, Theorem 3.4].

Theorem 4.3 Suppose Assumptions 4.1 and 4.2 hold, X^* is the accumulation point satisfying (4.19), and \mathcal{B}_k satisfies (3.14). Then there exists an integer K, $\mu > 0$ and $\tau \in (0,1)$ such that

$$F(X_k) - F(X^*) \le \mu \tau^{k-K} (F(X_{l(K)}) - F(X^*)), \text{ for all } k > K.$$
 (4.30)

Proof. Let \mathcal{U}_{X^*} be the neighbourhood of X^* and $\epsilon > 0$ be the constant such that all statements of Lemma 4.3 hold. By Theorem 4.2, there exists an integer K > 0 such that $X_k \in \mathcal{U}_{X^*}$ for all $k \geq K$. From $X_k \to X^*$, it follows that $\|\mathbf{R}_{X_k}^{-1}(X^*)\| \to 0$. Without loss of generality, assume that $\|\mathbf{R}_{X_k}^{-1}(X^*)\| < \epsilon$ for all $k \geq K$.

We separate our proof into three parts.

Part (1). By (4.9), we have

$$F_{k+1} \le f(X_k) + \langle \nabla f(X_k), \alpha_k V_k \rangle + c_2 \|\alpha_k V_k\|^2 + h(X_k + \alpha_k V_k),$$
 (4.31)

where $c_2 := \varrho M_2 + \frac{1}{2}LM_1^2 + L_h M_2$. Since h is convex and $\alpha_k \in (0,1]$, it holds that $h(X_k + \alpha_k V_k) \leq \alpha_k h(X_k + V_k) + (1 - \alpha_k)h(X_k)$.

Combining it with (4.31) yields

$$F_{k+1} \le (1 - \alpha_k)F_k + \alpha_k(f(X_k) + \phi_k(V_k)) + (c_2 - \frac{\kappa_1}{2\alpha_k})\|\alpha_k V_k\|^2.$$
 (4.32)

From Lemma 4.3, we know that $f \circ \mathbf{R}_X$ is convex on the set $\{V \in T_X \mathcal{M} : ||V|| < \epsilon\}$. For $V \in T_X \mathcal{M}$, it holds that $\operatorname{grad}(f \circ \mathbf{R}_X)(0_X) = \operatorname{Proj}_{T_X \mathcal{M}} \nabla f(X)$. If $||V|| < \epsilon$, then

$$f(\mathbf{R}_X(V)) - f(X) \ge \langle \nabla f(X), V \rangle.$$
 (4.33)

By the definition of ϕ_k (see (4.1)) and $V_k = \arg\min_{V \in T_X, \mathcal{M}} \phi_k(V)$, we have

$$f(X_k) + \phi_k(V_k) = \min_{V \in T_{X_k} \mathcal{M}} \{ f(X_k) + \langle \nabla f(X_k), V \rangle + \frac{1}{2} ||V||_{\mathcal{B}_k}^2 + h(X_k + V) \}.$$

By combining it with (4.33), for all $k \geq K$ and $\theta \in [0, 1]$, we have

$$f(X_k) + \phi_k(V_k)$$

$$\leq \min_{V \in T_{X_{k}} \mathcal{M}, \|V\| < \epsilon} \{ f(\mathbf{R}_{X_{k}}(V)) + \frac{1}{2} \|V\|_{\mathcal{B}_{k}}^{2} + h(X_{k} + V) \}
\leq \theta f(X^{*}) + (1 - \theta) F_{k} + \frac{1}{2} \theta^{2} \kappa_{2} \|\mathbf{R}_{X_{k}}^{-1}(X^{*})\|^{2} + \theta h(X_{k} + \mathbf{R}_{X_{k}}^{-1}(X^{*}))
\leq \theta f(X^{*}) + (1 - \theta) F_{k} + \frac{1}{2} \theta^{2} \kappa_{2} \|\mathbf{R}_{X_{k}}^{-1}(X^{*})\|^{2} + \theta h(X^{*}) + \theta L_{h} M_{2} \|\mathbf{R}_{X_{k}}^{-1}(X^{*})\|^{2}
\leq \theta F(X^{*}) + (1 - \theta) F_{k} + (\frac{1}{2} \theta^{2} \kappa_{2} + \theta L_{h} M_{2}) \|\mathbf{R}_{X_{k}}^{-1}(X^{*})\|^{2}.$$
(4.34)

Denote $\Upsilon := (\frac{1}{2}\theta^2\kappa_2 + \theta L_h M_2) \|\mathbf{R}_{X_k}^{-1}(X^*)\|^2$. From (4.34) and (4.32), it follows that F_{k+1}

$$\leq (1 - \alpha_k) F_k + \alpha_k \left(\theta F(X^*) + (1 - \theta) F_k + \Upsilon \right) + (c_2 - \frac{\kappa_1}{2\alpha_k}) \|\alpha_k V_k\|^2$$

$$\leq F_{l(k)} + \alpha_k \left(\theta (F(X^*) - F_{l(k)}) + \Upsilon \right) + c_2 \|\alpha_k V_k\|^2. \tag{4.35}$$

By (4.22), it holds that

$$F_{l(k)} - F(X^*) \ge F_k - F(X^*) \ge \eta \|\mathbf{R}_{X_k}^{-1}(X^*)\|^2.$$
 (4.36)

Since $\alpha_k \leq 1$, by (4.36) and (4.35), we can deduce that

$$F_{k+1} \le F_{l(k)} + \left(F_{l(k)} - F(X^*)\right) \left(\frac{1}{2n}\kappa_2\theta^2 - \left(1 - \frac{1}{n}L_hM_2\right)\theta\right) + c_2\|V_k\|^2. \tag{4.37}$$

Part (2). Now we prove that there exists a $\nu \in (0,1)$ such that for all k > K,

$$F_{k+1} - F(X^*) \le \nu(F_{l(k)} - F(X^*)).$$
 (4.38)

Let ω be a positive real number such that

$$\omega < \min\{\frac{2}{\sigma\gamma\overline{\alpha}}, \frac{\kappa_2}{2\eta c_2}, \frac{(\eta - L_h M_2)^2}{2\eta\kappa_2 c_2}\}.$$

Next, we consider two cases of the value of $||V_k||^2$.

(i)
$$||V_k||^2 \ge \omega(F_{l(k)} - F(X^*))$$
. By (4.12), we have

$$\frac{2}{\sigma\gamma\alpha}(F_{l(k)} - F_{k+1}) \ge \frac{2}{\sigma\alpha_k}(F_{l(k)} - F_{k+1}) \ge ||V_k||^2 \ge \omega(F_{l(k)} - F(X^*)).$$

Thus

$$F_{k+1} - F(X^*) \le (1 - \frac{\sigma \gamma \bar{\alpha} \omega}{2})(F_{l(k)} - F(X^*)),$$

which implies (4.38).

(ii) $||V_k||^2 < \omega(F_{l(k)} - F(X^*))$. Combining it with (4.37) yields

$$F_{k+1} \le F_{l(k)} + (F_{l(k)} - F(X^*))(\frac{1}{2n}\kappa_2\theta^2 - (1 - \frac{1}{n}L_hM_2)\theta + c_2\omega).$$

Denote $r_{k+1} := F_{k+1} - F(X^*)$. Then, we have

$$r_{k+1} \le \left[1 + \frac{1}{2\eta}\kappa_2\theta^2 - \left(1 - \frac{1}{\eta}L_hM_2\right)\theta + c_2\omega\right] \cdot r_{l(k)}.$$
 (4.39)

Define $q(\theta) := 1 + \frac{1}{2\eta} \kappa_2 \theta^2 - (1 - \frac{1}{\eta} L_h M_2) \theta + c_2 \omega$. Let $\theta_{\min} := \underset{0 \le \theta \le 1}{\arg\min} q(\theta)$. Then

$$\theta_{\min} = \min\{1, (\eta - L_h M_2)/\kappa_2\}.$$

Consider the following two cases:

(a) If $\theta_{\min} = 1$, then

$$\frac{1}{2\eta}\kappa_2 \le \frac{1}{2}(1 - \frac{1}{\eta}L_h M_2),$$

which together with $\omega < \kappa_2/(2\eta c_2)$ implies

$$q(\theta_{\min}) = 1 + \left[\frac{1}{2\eta}\kappa_2 - \left(1 - \frac{1}{\eta}L_h M_2\right)\right] + c_2 \omega$$

$$\leq 1 - \frac{1}{2\eta}\kappa_2 + c_2 \omega < 1.$$

(b) Otherwise, $\theta_{\min} = (\eta - L_h M_2)/\kappa_2 < 1$. By $\omega < (\eta - L_h M_2)^2/(2\eta\kappa_2 c_2)$, we have

$$q(\theta_{\min}) = 1 + \left(-\frac{1}{2n\kappa_2}(\eta - L_h M_2)^2 + c_2\omega\right) < 1.$$

In either case (a) or (b), substituting θ_{\min} into (4.39), we can see that (4.38) holds.

Part (3). For any k > K, there exists an integer $i \ge 1$ such that $(i-1)m < k - K \le im$ where m is the memory size parameter of the nonmonotone line search in (3.3). By using (4.38) recursively, we have

$$r_k \le r_{l(k)} \le \nu r_{l(l(k)-1)} \le \nu r_{l(k-m)} \le \dots$$

 $\le \nu^{i-1} r_{l(k-(i-1)m)} \le \nu^{i-1} r_{l(K)} \le \nu^{(k-K)/m-1} r_{l(K)}.$

Then (4.30) follows from the above inequality by taking

$$\mu := \frac{1}{\nu}, \ \tau := \nu^{1/m}.$$

The proof is complete.

Corollary 4.2 Suppose the same assumptions hold as in Theorem 4.3. Then there exists an integer K and a constant $C_K > 0$ such that

$$||X_k - X^*|| \le C_K \sqrt{\tau}^k$$
, for all $k > K$, (4.40)

where $\tau \in (0,1)$ is as in Theorem 4.3.

Proof. By (2.4), (4.27) and (4.30), for any $k \geq K$, we have

$$||X_k - X^*|| \le M_1 ||\mathbf{R}_{X^*}^{-1}(X_k)||$$

$$\le 2M_1 \left(\frac{1}{\tilde{\eta}}(F_k - F^*)\right)^{1/2}$$

$$\le 2M_1 \left(\frac{1}{\tilde{\eta}}\mu\tau^{-K}(F_{l(K)} - F^*)\right)^{1/2}\sqrt{\tau}^k.$$

Taking $C_K := 2M_1 \left(\mu \tau^{-K} (F_{l(K)} - F^*)/\widetilde{\eta}\right)^{1/2}$ in the above inequality yields (4.40).

Remark 1 The constant τ in (4.40) only depends on f and h, while K and C_K depend on more factors. Different initial point X_0 and stepsize α_k may lead to different K and C_K .

5 Numerical Experiments

In this section, we report our numerical experiments comparing our method with Riemannian proximal gradient methods, including ManPG and ManPG-Ada in [6], and NLS-ManPG which equips ManPG with the nonmonotone line search strategy. Our objective is to show the efficiency of the proximal quasi-Newton method for composite optimization problems over the Stiefel Manifold.

Our test problems include the compressed modes (CM) problem, sparse principle component analysis (Sparse PCA), and the joint diagonalization problem with a regularization term. All of these experiments were conducted in MATLAB R2018b on a PC using Windows 10 (64bit) system with Intel Core i5 CPU (2.3GHz) and 8GB memory.

For the stopping criterion, we terminate our algorithm when $||V_k||^2 \leq 10^{-8} nr$, where $V_k \in \mathbb{R}^{n \times r}$ is defined by (3.6), or the algorithm reaches the maximum iteration number 30000. For other parameters, the maximum iteration number of the inner loop is set to be 100. In the implementation of ManPQN, we set m = 10 and p = 5 (for m and p, see (3.3) and (3.11)). The parameters used in ManPG, ManPG-Ada and NLS-ManPG are set to be the default values in [6]. For all the problems, we use the singular value decomposition (SVD) as the retraction mapping in ManPQN, ManPG, ManPG-Ada and NLS-ManPG.

We report the numerical results obtained by solving randomly generated instances. Specifically, we randomly generate 50 instances and record the averaged numerical performance of these instances. Numerical results are shown in several figures and tables. In each figure, \mathbf{CPU} denotes the CPU time in seconds, \mathbf{Iter} represents the number of iterations, $\mathbf{Sparsity}$ denotes the percentage of zeros in the local minimum X^* . In each table, the total number of line search steps and the averaged iteration number of the adaptive regularized semismooth Newton (ASSN) method are reported.

5.1 CM Problem

The compressed modes (CM) problem aims to find sparse solutions of systems of equations in physics, including the Schrödinger equation in quantum mechanics. The

¹Our MATLAB code is available at https://github.com/QinsiWang2022/ManPQN.

CM problem can be written as

$$\min_{X \in \mathcal{M}} tr(X^T H X) + \mu ||X||_1, \tag{5.1}$$

where H is the discretized Schrödinger operator. For details of the CM problem, the reader is referred to [30].

We can observe from Figures 1-3 and Tables 1-3 that the ManPQN method outperforms ManPG, ManPG-Ada and NLS-ManPG, which demonstrates the efficiency of the quasi-Newton strategy used in ManPQN. ManPQN requires less computational time and less iterations than ManPG related methods, especially when n and r are large. From these results, we can see that the quasi-Newton technique can accelerate the proximal gradient method for composite optimization problems over the Stiefel manifold. ManPG related methods can achieve a solution with slightly better sparsity than ManPQN. The reason for this is that we use an approximate quasi-Newton strategy in our method (see (3.6) and (3.7)).

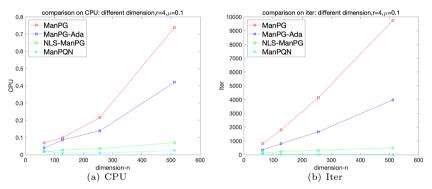


Fig. 1 Comparison on CM problem, different $n=\{64,128,256,512\}$ with r=4 and $\mu=0.1$.

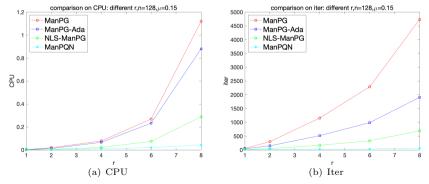


Fig. 2 Comparison on CM problem, different $r = \{1, 2, 4, 6, 8\}$ with n = 128 and $\mu = 0.15$.

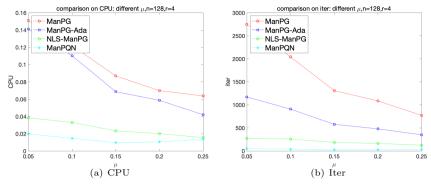


Fig. 3 Comparison on CM problem, different $\mu = \{0.05, 0.10, 0.15, 0.20, 0.25\}$ with n = 128 and r = 4.

Table 1 Comparison on CM problem, different $n = \{64, 128, 256, 512\}$ with r = 4 and $\mu = 0.1$.

| n = 64 | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
|-----------|---------|----------|----------|----------|---------------|-----------|
| ManPG | 800.74 | 1.424 | 0.82 | 0.0685 | 130.18 | 0.97 |
| ManPG-Ada | 347.80 | 1.424 | 0.82 | 0.0396 | 130.72 | 1.26 |
| NLS-ManPG | 128.74 | 1.424 | 0.82 | 0.0170 | 0.16 | 1.57 |
| ManPQN | 56.32 | 1.432 | 0.80 | 0.0213 | 116.20 | 5.91 |
| n = 128 | | | | | | |
| ManPG | 1808.54 | 1.885 | 0.83 | 0.0985 | 86.98 | 0.53 |
| ManPG-Ada | 801.16 | 1.885 | 0.83 | 0.0857 | 566.30 | 1.07 |
| NLS-ManPG | 235.20 | 1.885 | 0.83 | 0.0277 | 10.12 | 1.47 |
| ManPQN | 22.52 | 1.890 | 0.81 | 0.0088 | 18.76 | 4.44 |
| n = 256 | | | | | | |
| ManPG | 4141.94 | 2.489 | 0.85 | 0.2162 | 72.14 | 0.45 |
| ManPG-Ada | 1662.62 | 2.489 | 0.85 | 0.1388 | 1161.84 | 0.62 |
| NLS-ManPG | 317.06 | 2.489 | 0.85 | 0.0354 | 19.06 | 1.33 |
| ManPQN | 17.60 | 2.497 | 0.84 | 0.0101 | 19.00 | 4.33 |
| n = 512 | | | | | | |
| ManPG | 9755.60 | 3.286 | 0.87 | 0.7385 | 50.66 | 0.16 |
| ManPG-Ada | 3983.06 | 3.286 | 0.87 | 0.4208 | 2623.98 | 0.25 |
| NLS-ManPG | 501.92 | 3.286 | 0.87 | 0.0704 | 25.06 | 0.92 |
| ManPQN | 16.54 | 3.293 | 0.86 | 0.0250 | 15.58 | 3.28 |

The total number of line-search steps and the averaged iteration number of the ASSN method are shown in Tables 1-3. ManPQN and NLS-ManPG need less line-search steps than the other methods since they use the nonmonotone line search technique. From Tables 1-3, we can see that the ASSN method in ManPQN needs more iterations than that of the other three methods. The reason for this is that

the matrix $\operatorname{diag} H_k$ is involved in $\mathcal{G}(\overline{\operatorname{vec}}(\Lambda_l))$ and therefore the condition number of $\mathcal{G}(\overline{\operatorname{vec}}(\Lambda_l))$ becomes larger (see (3.20) and (3.21)).

Table 2 Comparison on CM problem, different $r = \{1, 2, 4, 6, 8\}$ with n = 128 and $\mu = 0.15$.

| r = 1 | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
|-----------|---------|----------|----------|----------|---------------|-----------|
| ManPG | 54.12 | 0.6513 | 0.87 | 0.0034 | 0.00 | 0.93 |
| ManPG-Ada | 42.20 | 0.6513 | 0.87 | 0.0027 | 0.00 | 1.04 |
| NLS-ManPG | 16.94 | 0.6513 | 0.87 | 0.0015 | 0.08 | 1.12 |
| ManPQN | 12.78 | 0.6603 | 0.86 | 0.0039 | 4.94 | 2.29 |
| r = 2 | | | | | | |
| ManPG | 298.62 | 1.302 | 0.86 | 0.0190 | 15.04 | 0.91 |
| ManPG-Ada | 147.52 | 1.302 | 0.86 | 0.0120 | 94.92 | 1.06 |
| NLS-ManPG | 49.04 | 1.302 | 0.86 | 0.0048 | 1.46 | 1.24 |
| ManPQN | 16.58 | 1.303 | 0.86 | 0.0047 | 5.24 | 2.71 |
| r=4 | | | | | | |
| ManPG | 1156.72 | 2.605 | 0.86 | 0.0775 | 95.56 | 0.82 |
| ManPG-Ada | 516.68 | 2.605 | 0.86 | 0.0659 | 371.62 | 1.25 |
| NLS-ManPG | 167.60 | 2.605 | 0.86 | 0.0210 | 5.56 | 1.65 |
| ManPQN | 26.26 | 2.610 | 0.85 | 0.0104 | 16.86 | 4.33 |
| r = 6 | | | | | | |
| ManPG | 2287.98 | 3.909 | 0.85 | 0.2688 | 163.14 | 0.60 |
| ManPG-Ada | 987.78 | 3.909 | 0.85 | 0.2330 | 709.94 | 1.57 |
| NLS-ManPG | 329.22 | 3.909 | 0.85 | 0.0742 | 8.98 | 1.79 |
| ManPQN | 34.08 | 3.920 | 0.84 | 0.0197 | 29.38 | 4.32 |
| r = 8 | | | | | | |
| ManPG | 4727.60 | 5.214 | 0.84 | 1.1193 | 220.42 | 1.24 |
| ManPG-Ada | 1905.44 | 5.214 | 0.84 | 0.8793 | 1265.02 | 2.82 |
| NLS-ManPG | 692.14 | 5.214 | 0.84 | 0.2878 | 15.86 | 2.87 |
| ManPQN | 56.56 | 5.248 | 0.82 | 0.0437 | 51.76 | 5.96 |

5.2 Sparse PCA

The sparse PCA model can be formulated as

$$\min_{X \in \mathcal{M}} -tr(X^T A^T A X) + \mu ||X||_1, \tag{5.2}$$

where $A \in \mathbb{R}^{m \times n}$. We apply ManPQN and ManPG related algorithms to (5.2) and compare their performance. The matrix A^TA is generated by the following two ways. In Section 5.2.1, A is generated by normal distribution. In Section 5.2.2, the matrix A^TA is chosen from real symmetric positive definite matrices in "UF Sparse Matrix Collection" [8].

Table 3 Comparison on CM problem, different $\mu = \{0.05, 0.10, 0.15, 0.20, 0.25\}$ with n = 128 and r = 4.

| $\mu = 0.05$ | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
|--------------|---------|----------|----------|----------|---------------|-----------|
| ManPG | 2751.68 | 1.083 | 0.76 | 0.1511 | 57.08 | 0.28 |
| ManPG-Ada | 1173.30 | 1.083 | 0.76 | 0.1413 | 710.14 | 0.85 |
| NLS-ManPG | 276.12 | 1.083 | 0.76 | 0.0383 | 14.76 | 1.37 |
| ManPQN | 53.78 | 1.111 | 0.73 | 0.0197 | 92.40 | 5.35 |
| $\mu = 0.10$ | | | | | | |
| ManPG | 2041.74 | 1.885 | 0.83 | 0.1221 | 79.06 | 0.52 |
| ManPG-Ada | 909.02 | 1.885 | 0.83 | 0.1103 | 703.42 | 1.10 |
| NLS-ManPG | 259.48 | 1.885 | 0.83 | 0.0332 | 11.30 | 1.47 |
| ManPQN | 42.04 | 1.902 | 0.81 | 0.0147 | 37.10 | 4.27 |
| $\mu = 0.15$ | | | | | | |
| ManPG | 1312.30 | 2.605 | 0.86 | 0.0869 | 130.72 | 0.77 |
| ManPG-Ada | 580.08 | 2.605 | 0.86 | 0.0687 | 424.32 | 1.28 |
| NLS-ManPG | 185.76 | 2.605 | 0.86 | 0.0233 | 5.74 | 1.63 |
| ManPQN | 27.54 | 2.610 | 0.85 | 0.0097 | 18.36 | 4.15 |
| $\mu = 0.20$ | | | | | | |
| ManPG | 1087.28 | 3.278 | 0.88 | 0.0699 | 90.14 | 0.88 |
| ManPG-Ada | 481.32 | 3.278 | 0.88 | 0.0587 | 365.34 | 1.35 |
| NLS-ManPG | 164.26 | 3.278 | 0.88 | 0.0201 | 3.88 | 1.80 |
| ManPQN | 28.12 | 3.280 | 0.87 | 0.0106 | 23.40 | 4.91 |
| $\mu = 0.25$ | | | | | | |
| ManPG | 773.86 | 3.916 | 0.89 | 0.0638 | 86.08 | 0.55 |
| ManPG-Ada | 352.60 | 3.916 | 0.89 | 0.0420 | 211.18 | 1.00 |
| NLS-ManPG | 126.10 | 3.916 | 0.89 | 0.0155 | 1.70 | 1.22 |
| ManPQN | 36.24 | 3.920 | 0.88 | 0.0135 | 21.82 | 3.34 |

5.2.1 Random generated sparse PCA problem

From Figures 4-6 and Tables 4-6, we can see that ManPQN shows better performance than ManPG, ManPG-Ada and NLS-ManPG in terms of CPU time and iteration number, especially when n and r are large. In some cases, ManPG related methods can achieve a solution, the sparsity of which is a little better than that of Man-PQN. Taking CPU time, the total number of line search steps and the averaged SSN iteration number in Tables 4-6 into account, we can deduce that the quasi-Newton strategy can have a significant effect on accelerating our method.

Next, we investigate the convergence of $F(X_k)$ generated by ManPQN, ManPG and ManPG-Ada. We select six cases with different n and r, and plot numerical results of these three algorithms in Figures 7-9. We can see that when X_k is close to X^* , $F(X_k)$ converges to $F(X^*)$ approximately at a linear rate, which matches our theoretical results in Theorem 4.3.

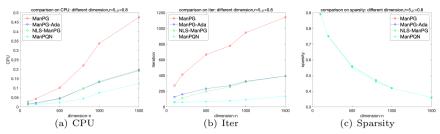


Fig. 4 Comparison on Sparse PCA problem, different $n = \{100, 200, 500, 800, 1000, 1500\}$ with r = 5 and $\mu = 0.8$.

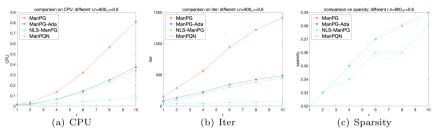


Fig. 5 Comparison on Sparse PCA problem, different $r = \{1, 2, 4, 8, 10\}$ with n = 800 and $\mu = 0.6$.

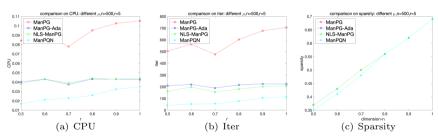


Fig. 6 Comparison on Sparse PCA problem, different $\mu = \{0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ with n = 500 and r = 5.

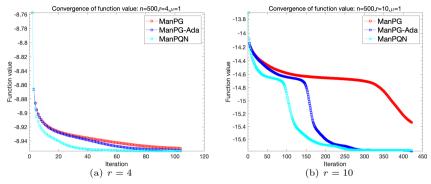


Fig. 7 Convergence of function value on Sparse PCA problem with $n = 500, \mu = 1.0$.

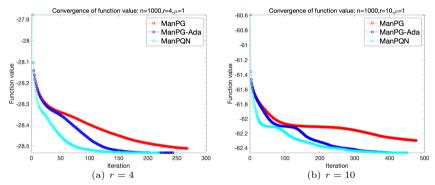


Fig. 8 Convergence of function value on Sparse PCA problem with $n = 1000, \mu = 1.0$.

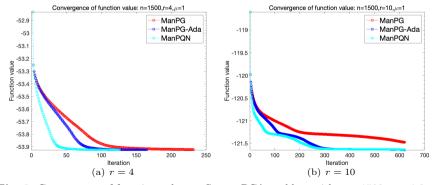


Fig. 9 Convergence of function value on Sparse PCA problem with $n = 1500, \mu = 1.0$.

Table 4 Comparison on Sparse PCA problem, different $n = \{100, 200, 500, 800, 1000, 1500\}$ with r = 5 and $\mu = 0.8$.

| n = 100 | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
|------------|---------|----------|----------|----------|---------------|-----------|
| ManPG | 271.02 | -2.285 | 0.89 | 0.0267 | 1.86 | 1.20 |
| ManPG-Ada | 126.40 | -2.285 | 0.89 | 0.0158 | 0.38 | 1.49 |
| NLS-ManPG | 60.96 | -2.285 | 0.89 | 0.0125 | 0.00 | 2.34 |
| ManPQN | 57.64 | -2.274 | 0.89 | 0.0193 | 23.94 | 2.68 |
| n = 200 | | | | | | |
| ManPG | 412.32 | -5.449 | 0.75 | 0.0434 | 1.94 | 1.07 |
| ManPG-Ada | 160.38 | -5.449 | 0.75 | 0.0212 | 7.22 | 1.33 |
| NLS-ManPG | 112.48 | -5.449 | 0.75 | 0.0180 | 0.00 | 1.50 |
| ManPQN | 58.72 | -5.428 | 0.75 | 0.0138 | 37.92 | 2.03 |
| n = 500 | | | | | | |
| ManPG | 667.08 | -20.30 | 0.56 | 0.1017 | 0.00 | 1.02 |
| ManPG-Ada | 232.50 | -20.30 | 0.56 | 0.0451 | 48.86 | 1.22 |
| NLS-ManPG | 199.50 | -20.30 | 0.56 | 0.0432 | 0.00 | 1.38 |
| ManPQN | 66.34 | -20.21 | 0.55 | 0.0226 | 41.76 | 1.96 |
| n = 800 | | | | | | |
| ManPG | 778.82 | -39.16 | 0.47 | 0.2204 | 0.00 | 1.02 |
| ManPG-Ada | 272.06 | -39.16 | 0.47 | 0.0979 | 70.66 | 1.19 |
| NLS-ManPG | 251.44 | -39.16 | 0.47 | 0.0978 | 0.00 | 1.30 |
| ManPQN | 77.32 | -39.07 | 0.46 | 0.0439 | 50.14 | 1.95 |
| n = 1000 | | | | | | |
| ManPG | 947.26 | -53.23 | 0.42 | 0.3370 | 0.00 | 1.01 |
| ManPG-Ada | 325.62 | -53.23 | 0.42 | 0.1323 | 102.98 | 1.17 |
| NLS-ManPG | 320.90 | -53.23 | 0.42 | 0.1354 | 0.00 | 1.24 |
| ManPQN | 92.50 | -53.17 | 0.42 | 0.0754 | 68.24 | 1.92 |
| n = 1500 | | | | | | |
| ManPG | 1142.60 | -89.60 | 0.36 | 0.4757 | 19.04 | 1.01 |
| ManPG-Ada | 394.10 | -89.60 | 0.36 | 0.1929 | 150.80 | 1.12 |
| NLS-ManPG | 393.40 | -89.60 | 0.36 | 0.1981 | 0.00 | 1.20 |
| ManPQN | 137.94 | -89.50 | 0.36 | 0.1238 | 171.00 | 1.87 |
| ſ <u>-</u> | | | | | | |

5.2.2 Sparse PCA problem from "UF Sparse Matrix Collection"

To further evaluate the performance of ManPQN and ManPG related algorithms, we apply them to (5.2), where $A \in \mathbb{R}^{m \times n}$ is chosen from real matrices in [8]. We choose four matrices named "lpi_klein1", "bcsstk22", "lp_fit1d" and "fidap003" whose dimensions are $(m,n)=(54,108),\ (m,n)=(138,138),\ (m,n)=(24,1049)$ and (m,n)=(1821,1821) respectively. We set $r=4,\ \mu=0.2$. Experiments are repeated for 50 times with different random initial point. The numerical results are given in Table 7.

Table 5 Comparison on Sparse PCA problem, different $r = \{1, 2, 4, 8, 10\}$ with n = 800 and $\mu = 0.6$.

| r = 1 | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
|-----------|---------|----------|----------|----------|---------------|-----------|
| ManPG | 149.56 | -12.21 | 0.32 | 0.0163 | 0.00 | 0.78 |
| ManPG-Ada | 87.18 | -12.21 | 0.32 | 0.0117 | 2.00 | 0.93 |
| NLS-ManPG | 55.10 | -12.21 | 0.33 | 0.0109 | 0.00 | 1.03 |
| ManPQN | 35.16 | -12.21 | 0.32 | 0.0134 | 34.04 | 1.26 |
| r = 2 | | | | | | |
| ManPG | 286.48 | -24.01 | 0.33 | 0.0352 | 93.48 | 0.99 |
| ManPG-Ada | 133.80 | -24.01 | 0.33 | 0.0185 | 14.92 | 1.06 |
| NLS-ManPG | 96.58 | -24.01 | 0.33 | 0.0166 | 0.02 | 1.11 |
| ManPQN | 42.04 | -23.98 | 0.33 | 0.0160 | 39.32 | 1.63 |
| r = 4 | | | | | | |
| ManPG | 564.46 | -45.83 | 0.35 | 0.1357 | 4.52 | 1.02 |
| ManPG-Ada | 225.32 | -45.83 | 0.35 | 0.0647 | 56.36 | 1.07 |
| NLS-ManPG | 198.54 | -45.83 | 0.35 | 0.0652 | 0.00 | 1.16 |
| ManPQN | 44.10 | -45.77 | 0.34 | 0.0260 | 31.94 | 1.83 |
| r = 6 | | | | | | |
| ManPG | 941.32 | -66.18 | 0.37 | 0.3209 | 0.00 | 1.01 |
| ManPG-Ada | 345.08 | -66.18 | 0.37 | 0.1451 | 120.30 | 1.19 |
| NLS-ManPG | 304.30 | -66.18 | 0.37 | 0.1285 | 0.00 | 1.28 |
| ManPQN | 59.18 | -66.03 | 0.36 | 0.0448 | 39.76 | 1.96 |
| r = 8 | | | | | | |
| ManPG | 1219.04 | -85.57 | 0.38 | 0.5664 | 0.00 | 1.01 |
| ManPG-Ada | 425.80 | -85.57 | 0.38 | 0.2508 | 171.44 | 1.32 |
| NLS-ManPG | 385.58 | -85.57 | 0.38 | 0.2298 | 0.00 | 1.37 |
| ManPQN | 65.56 | -85.39 | 0.36 | 0.0594 | 40.82 | 2.01 |
| r = 10 | | | | | | |
| ManPG | 1412.26 | -103.59 | 0.39 | 0.8113 | 0.00 | 1.02 |
| ManPG-Ada | 486.46 | -103.59 | 0.39 | 0.3737 | 206.70 | 1.44 |
| NLS-ManPG | 447.34 | -103.59 | 0.39 | 0.3418 | 0.00 | 1.41 |
| ManPQN | 68.52 | -103.40 | 0.38 | 0.0799 | 42.38 | 2.10 |

Since A^TA generated by these four matrices are ill-conditioned, all algorithms need more iteration numbers and CPU time to converge. In Table 7, we can observe that ManPQN and NLS-ManPG show much better performance than ManPG and ManPG-Ada in terms of iteration numbers and CPU time. Only for matrix "lpi_klein1", ManPQN needs slightly more CPU time than NLS-ManPG. For the other three matrices, ManPQN outperforms NLS-ManPG.

Table 6 Comparison on Sparse PCA problem, different $\mu = \{0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ with n = 500 and r = 5.

| $\mu = 0.5$ | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
|-------------|--------|----------|----------|----------|---------------|-----------|
| ManPG | 504.12 | -39.41 | 0.37 | 0.0843 | 0.00 | 1.02 |
| ManPG-Ada | 209.14 | -39.41 | 0.37 | 0.0401 | 43.44 | 1.13 |
| NLS-ManPG | 160.62 | -39.41 | 0.37 | 0.0381 | 0.00 | 1.27 |
| ManPQN | 41.24 | -39.34 | 0.35 | 0.0168 | 26.60 | 1.87 |
| $\mu = 0.6$ | | | | | | |
| ManPG | 563.02 | -32.69 | 0.43 | 0.0912 | 0.00 | 1.02 |
| ManPG-Ada | 219.42 | -32.69 | 0.43 | 0.0431 | 49.30 | 1.15 |
| NLS-ManPG | 198.58 | -32.69 | 0.43 | 0.0431 | 0.00 | 1.25 |
| ManPQN | 53.16 | -32.63 | 0.41 | 0.0212 | 33.72 | 1.90 |
| $\mu = 0.7$ | | | | | | |
| ManPG | 475.74 | -26.30 | 0.50 | 0.0779 | 0.00 | 1.02 |
| ManPG-Ada | 189.52 | -26.30 | 0.50 | 0.0375 | 25.36 | 1.14 |
| NLS-ManPG | 154.96 | -26.30 | 0.50 | 0.0391 | 0.00 | 1.28 |
| ManPQN | 55.26 | -26.26 | 0.48 | 0.0229 | 34.32 | 1.96 |
| $\mu = 0.8$ | | | | | | |
| ManPG | 602.94 | -20.36 | 0.56 | 0.0952 | 1.40 | 1.02 |
| ManPG-Ada | 216.12 | -20.36 | 0.56 | 0.0433 | 39.86 | 1.24 |
| NLS-ManPG | 180.76 | -20.36 | 0.56 | 0.0438 | 0.00 | 1.40 |
| ManPQN | 77.40 | -20.32 | 0.56 | 0.0259 | 53.34 | 1.96 |
| $\mu = 0.9$ | | | | | | |
| ManPG | 677.48 | -14.63 | 0.62 | 0.1026 | 0.14 | 1.03 |
| ManPG-Ada | 224.90 | -14.63 | 0.62 | 0.0432 | 38.54 | 1.27 |
| NLS-ManPG | 201.88 | -14.63 | 0.62 | 0.0431 | 0.00 | 1.41 |
| ManPQN | 104.62 | -14.59 | 0.62 | 0.0324 | 69.30 | 1.96 |
| $\mu = 1.0$ | | | | | | |
| ManPG | 706.12 | -9.525 | 0.69 | 0.1053 | 0.28 | 1.04 |
| ManPG-Ada | 225.10 | -9.525 | 0.69 | 0.0426 | 32.26 | 1.30 |
| NLS-ManPG | 209.84 | -9.525 | 0.69 | 0.0440 | 0.02 | 1.39 |
| ManPQN | 116.16 | -9.485 | 0.69 | 0.0351 | 109.80 | 1.93 |

5.3 Joint Diagonalization Problem with a Regularization Term

The joint diagonalization problem with a regularization term on the Stiefel manifold [34] can be written in the following formulation:

$$\min_{X \in \mathcal{M}} - \sum_{l=1}^{N} \| \operatorname{diag}(X^{T} A_{l} X) \|_{F}^{2} + \mu \| X \|_{1}, \tag{5.3}$$

where $A_1, A_2, \dots, A_N \in \mathbb{R}^{n \times n}$ are N real symmetric matrices.

| "lpi_klein1" | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
|--------------|----------|----------|----------|----------|---------------|-----------|
| ManPG | 2252.00 | -38.77 | 0.94 | 0.1684 | 0.00 | 1.01 |
| ManPG-Ada | 919.00 | -38.77 | 0.94 | 0.0840 | 533.00 | 1.10 |
| NLS-ManPG | 223.00 | -38.77 | 0.94 | 0.0305 | 170.00 | 1.74 |
| ManPQN | 137.00 | -38.76 | 0.93 | 0.0318 | 58.00 | 1.27 |
| "bcsstk20" | Iter | $F(X^*)$ | sparsity | CPU time | # line-search | SSN iters |
| ManPG | 11276.00 | -4823.74 | 0.82 | 0.8836 | 157.06 | 1.00 |
| ManPG-Ada | 4685.58 | -4823.74 | 0.82 | 0.4489 | 2985.08 | 1.11 |
| NLS-ManPG | 830.22 | -4823.74 | 0.82 | 0.1073 | 833.80 | 1.59 |
| ManPQN | 137.18 | -4823.71 | 0.80 | 0.0322 | 0.00 | 1.00 |
| "lp_fit1d" | | | | | | |
| ManPG | 9596.26 | -2480.94 | 0.08 | 2.9966 | 0.00 | 1.45 |
| ManPG-Ada | 4182.68 | -2480.94 | 0.08 | 1.7876 | 2488.80 | 1.97 |
| NLS-ManPG | 1024.54 | -2480.94 | 0.08 | 0.5133 | 850.58 | 2.31 |
| ManPQN | 210.16 | -2480.64 | 0.05 | 0.1115 | 7.22 | 2.17 |
| "fidap003" | | | | | | |
| ManPG | 4986.52 | -6764.09 | 0.89 | 2.1449 | 0.00 | 1.06 |
| ManPG-Ada | 2169.84 | -6764.09 | 0.89 | 1.1988 | 1249.16 | 1.19 |
| NLS-ManPG | 478.88 | -6764.09 | 0.89 | 0.4152 | 449.62 | 1.93 |
| ManPQN | 95.58 | -6764.08 | 0.87 | 0.1705 | 1.14 | 3.07 |

Table 7 Comparison on Sparse PCA problem with different matrices from [8].

Let $f(X) := -\sum_{l=1}^{N} \|\operatorname{diag}(X^T A_l X)\|_F^2$. We can deduce that the Euclidean gradient of f is

$$\nabla f(X) = -4 \sum_{l=1}^{N} A_l X \operatorname{diag}(X^T A_l X),$$

and the Riemannian gradient of f is

$$\operatorname{grad} f(X) = -4 \sum_{l=1}^{N} (A_l X \operatorname{diag}(X^T A_l X) - X \operatorname{sym}(X^T A_l X \operatorname{diag}(X^T A_l X))),$$

where $\operatorname{sym}(Y) := (Y^T + Y)/2$.

For numerical experiments of (5.3), we generate N randomly chosen $n \times n$ diagonal matrices $\Lambda_1, \Lambda_2, \ldots, \Lambda_N$ and a randomly chosen $n \times n$ orthogonal matrix P. Then, let A_1, A_2, \ldots, A_N be computed by $A_i = P^T \Lambda_i P$ for $i = 1, 2, \ldots, N$. We set N = 5 in the following experiments.

The numerical results of each algorithm are displayed in Figures 10-12 and Tables 8-10. Since all the algorithms need large number of line search steps, we report the average iteration numbers of line search in Tables 8-10. Figures 10-12 show that ManPQN needs much less iterations and time than ManPG and ManPG-Ada. In most cases, ManPQN outperforms NLS-ManPG in terms of CPU time, especially when n and r are large.

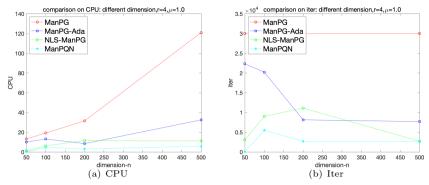


Fig. 10 Comparison on problem (5.3), different $n = \{50, 100, 200, 500\}$ with r = 4 and $\mu = 1.0$.

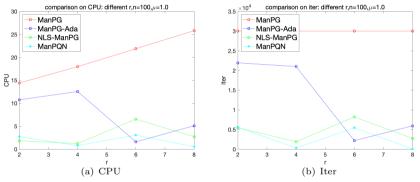


Fig. 11 Comparison on problem (5.3), different $r = \{2, 4, 6, 8\}$ with n = 100 and $\mu = 1.0$.

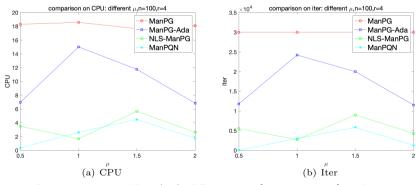


Fig. 12 Comparison on problem (5.3), different $\mu = \{0.5, 1.0, 1.5, 2.0\}$ with n = 100 and r = 4.

Table 8 Comparison on problem (5.3), different $n = \{50, 100, 200, 500\}$ with r = 4 and $\mu = 1.0$.

| n = 50 | Iter | $F(X^*)$ | CPU time | line-search | SSN iters |
|-----------|----------|----------|----------|-------------|-----------|
| ManPG | 30001.00 | -72.804 | 13.3257 | 13.99 | 1.00 |
| ManPG-Ada | 22335.45 | -72.784 | 10.1168 | 13.98 | 1.01 |
| NLS-ManPG | 3073.09 | -72.821 | 1.2158 | 12.09 | 2.91 |
| ManPQN | 68.82 | -72.825 | 0.3008 | 9.48 | 12.54 |
| n = 100 | | | | | |
| ManPG | 30001.00 | -126.85 | 19.2554 | 13.99 | 1.01 |
| ManPG-Ada | 20215.64 | -126.85 | 13.1823 | 13.98 | 1.68 |
| NLS-ManPG | 9032.55 | -126.87 | 6.2430 | 13.97 | 4.04 |
| ManPQN | 5509.45 | -126.81 | 4.6449 | 12.73 | 14.62 |
| n = 200 | | | | | |
| ManPG | 30001.00 | -148.11 | 31.5747 | 13.99 | 1.00 |
| ManPG-Ada | 8143.82 | -148.11 | 8.5102 | 13.97 | 2.44 |
| NLS-ManPG | 11119.36 | -148.11 | 11.6534 | 13.9 | 3.22 |
| ManPQN | 2730.18 | -148.17 | 3.1700 | 13.5 | 13.32 |
| n = 500 | | | | | |
| ManPG | 30001.00 | -222.75 | 120.9160 | 13.99 | 1.00 |
| ManPG-Ada | 7709.36 | -222.77 | 32.5464 | 13.98 | 3.50 |
| NLS-ManPG | 2736.82 | -222.79 | 11.1977 | 13.95 | 4.70 |
| ManPQN | 2729.18 | -222.93 | 5.7707 | 5.54 | 22.69 |

6 Conclusion and Future Work

In this paper, we present a proximal quasi-Newton algorithm, named ManPQN, for the composite optimization problem (1.1) over the Stiefel manifold. The ManPQN method finds the descent direction V_k by solving a subproblem, which is formed by replacing the term $\|V\|^2/2t$ in the subproblem of ManPG by $\frac{1}{2}\|V\|_{\mathcal{B}_k}^2$, where \mathcal{B}_k is a symmetric linear operator on $T_{X_k}\mathcal{M}$. We also use several techniques to accelerate the speed of the ManPQN algorithm. The most important technique is that we use the linear operator \mathbf{B}_k , defined by (3.7), to approximate the linear operator \mathcal{B}_k . To guarantee the positive definiteness of \mathbf{B}_k , a damped LBFGS method is used to update \mathbf{B}_k . Moreover, we use a nonmonotone line search technique to improve the performance of the ManPQN method. Numerical results demonstrate that the ManPQN method is an effective method. Under some mild conditions, we establish the global convergence of ManPQN. If the Hessian operator of the objective function is positive definite at the local minimum, the local linear convergence of ManPQN is also proved.

The main cost of the ManPQN lies in the step of solving the subproblem (3.1). Stimulated by the work in [6], we use the adaptive semismooth Newton (ASSN) method to get the solution of (3.1). But the total cost of the ASSN method is excessive for large n and r. How to reduce the computational cost of the ASSN method will be one of the topics of our future work. We will also investigate other techniques to accelerate the ManPG method. This is another topic of our future work.

| r = 2 | Iter | $F(X^*)$ | CPU time | line-search | SSN iters |
|-----------|----------|----------|----------|-------------|-----------|
| ManPG | 30001.00 | -69.79 | 14.4263 | 13.99 | 0.92 |
| ManPG-Ada | 21941.64 | -69.79 | 10.7613 | 13.98 | 1.22 |
| NLS-ManPG | 5474.55 | -69.80 | 1.8400 | 8.81 | 3.24 |
| ManPQN | 5580.91 | -69.80 | 2.7605 | 8.73 | 16.92 |
| r = 4 | | | | | |
| ManPG | 30001.00 | -119.37 | 17.9799 | 13.99 | 1.00 |
| ManPG-Ada | 21010.00 | -119.38 | 12.5684 | 13.98 | 1.80 |
| NLS-ManPG | 1909.36 | -119.39 | 1.2302 | 12.56 | 4.35 |
| ManPQN | 310.09 | -119.42 | 0.8054 | 12.44 | 18.71 |
| r=6 | | | | | |
| ManPG | 30001.00 | -122.92 | 21.8858 | 13.99 | 1.00 |
| ManPG-Ada | 2190.82 | -122.92 | 1.6054 | 13.98 | 1.47 |
| NLS-ManPG | 8198.64 | -122.91 | 6.5546 | 13.95 | 4.10 |
| ManPQN | 5456.36 | -123.00 | 3.0761 | 5.89 | 10.95 |
| r = 8 | | | | | |
| ManPG | 30001.00 | -142.23 | 25.8129 | 13.99 | 1.00 |
| ManPG-Ada | 5973.36 | -142.29 | 5.1177 | 13.97 | 2.67 |
| NLS-ManPG | 2747.73 | -142.30 | 2.7289 | 13.94 | 5.02 |
| ManPQN | 70.00 | -142.54 | 0.5549 | 9.25 | 17.60 |

Table 9 Comparison on problem (5.3), different $r = \{2, 4, 6, 8\}$ with n = 100 and $\mu = 1.0$.

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Table 10 Comparison on problem (5.3), different $\mu = \{0.5, 1.0, 1.5, 2.0\}$ with n = 100 and r = 4.

| $\mu = 0.5$ | Iter | $F(X^*)$ | CPU time | line-search | SSN iters |
|-------------|----------|----------|----------|-------------|-----------|
| ManPG | 30001.00 | -134.85 | 18.3098 | 13.99 | 1.00 |
| ManPG-Ada | 11813.55 | -134.86 | 6.9803 | 13.96 | 1.84 |
| NLS-ManPG | 5509.45 | -134.86 | 3.5001 | 13.92 | 3.74 |
| ManPQN | 74.27 | -134.87 | 0.3515 | 8.62 | 13.36 |
| $\mu = 1.0$ | | | | | |
| ManPG | 30001.00 | -129.57 | 18.5839 | 13.99 | 0.98 |
| ManPG-Ada | 24221.09 | -129.57 | 15.0166 | 13.99 | 1.24 |
| NLS-ManPG | 2745.73 | -129.59 | 1.6866 | 13.90 | 3.84 |
| ManPQN | 3003.18 | -129.58 | 2.6224 | 13.76 | 12.40 |
| $\mu = 1.5$ | | | | | |
| ManPG | 30001.00 | -112.51 | 17.6801 | 13.99 | 1.00 |
| ManPG-Ada | 19994.13 | -112.51 | 11.7601 | 13.98 | 1.11 |
| NLS-ManPG | 9018.80 | -112.51 | 5.6677 | 13.88 | 3.62 |
| ManPQN | 5854.17 | -112.53 | 4.4855 | 13.5 | 12.66 |
| $\mu = 2.0$ | | | | | |
| ManPG | 30001.00 | -76.63 | 18.0976 | 13.99 | 1.10 |
| ManPG-Ada | 11534.86 | -76.64 | 6.8606 | 13.98 | 1.35 |
| NLS-ManPG | 4306.00 | -76.65 | 2.6373 | 13.91 | 4.01 |
| ManPQN | 1292.71 | -76.71 | 1.7506 | 12.65 | 16.84 |

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