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Conjugate Gradient Methods for Optimization Problems on Symplectic Stiefel Manifold

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***Abstract*— The symplectic Stiefel manifold is a Riemannian manifold that is a generalization of the symplectic group. In this study, we propose novel conjugate gradient methods on the symplectic Stiefel manifold and compare them with the steepest descent method proposed in existing studies through numerical experiments. Although the theoretical basis of the Riemannian conjugate gradient methods has already been established, special treatment is required to address specific manifolds since these methods utilize some mappings, such as a retraction and vector transport, on the manifold. Numerical experiments demonstrate that the proposed method outperforms existing methods and is efficient.**

I. Introduction

When the search space of a constrained optimization problem on the Euclidean space $\mathbb{R}^n$ is a Riemannian manifold M, the problem can be considered an unconstrained optimization problem on M and solved efficiently using optimization methods on M such as the steepest descent, conjugate gradient (CG), and Newton's methods [1], [17]. In recent years, many studies have been conducted on optimization on Riemannian manifolds, particularly problems on matrix manifolds, such as the Stiefel manifold [23], [27] and Grassmann manifold [19], which are essential from a practical point of view since they have many applications in real-world problems. In this study, we discuss optimization on the symplectic Stiefel manifold, which is related to a type of eigenvalue problem of matrices, and propose a novel efficient CG method on this manifold.

We consider optimization problems of the following form:

> *Problem 1:*
>
> $$\begin{aligned} &\text{Minimize} && f(X) \\ &\text{subject to} && X^\top J_{2n} X = J_{2p},\ X \in \mathbb{R}^{2n\times 2p}. \end{aligned}$$

Here, $p \leq n$, $J_{2m} = \begin{bmatrix} 0 & I_m \\ -I_m & 0 \end{bmatrix}$, I_m is the $m \times m$ identity matrix, and f is a smooth objective function defined in $\mathbb{R}^{2n\times 2p}$. In the following, we also denote both J_{2n} and J_{2p} simply by J and denote the identity matrix by I since their size is clear from the context. Optimization problems expressed in this form appear in various fields. For example, the symplectic eigenvalue problem is represented in this form by defining $f(X) := \mathrm{tr}(X^\top AX)$, where $A \in \mathbb{R}^{2n\times 2n}$ is a symmetric positive definite matrix, which can be applied in fields such as quantum mechanics [7].

The feasible region of Problem 1 is the following symplectic Stiefel manifold:

$$\mathrm{Sp}(2p, 2n) := \{X \in \mathbb{R}^{2n\times 2p} \mid X^\top J_{2n} X = J_{2p}\}.$$

Note that when $n = p$, the manifold $\mathrm{Sp}(2n, 2n)$ has the structure of a group and is called the symplectic group. We denote the restriction of the objective function f to $\mathrm{Sp}(2p, 2n)$, that is, $f|_{\mathrm{Sp}(2p,2n)}$, also by f. Thus, Problem 1 can be expressed as follows:

> *Problem 2:*
>
> $$\begin{aligned} &\text{Minimize} && f(X) \\ &\text{subject to} && X \in \mathrm{Sp}(2p, 2n). \end{aligned}$$

For Problem 2, the steepest descent method was proposed [8]. Moreover, two types of retraction on $\mathrm{Sp}(2p, 2n)$ have been proposed in the literature: the quasi-geodesic retraction and Cayley retraction. Later, in [13], [14], a more efficient retraction was proposed, showing numerical and experimental superiority over the Cayley retraction in [8]. For the case $n = p$, Newton's method was proposed in [4] as an optimization method for symplectic groups. However, Newton's method cannot be applied straightforwardly when $n > p$.

In this study, we propose effective CG methods for Problem 2. The Riemannian CG method [1], [15], [18], [20], [28], which is a nonlinear CG method to generate a sequence $\{x_k\}$ on a Riemannian manifold M, updates the search direction η_k at $x_k \in M$ using an algorithm-specific parameter β_k, an appropriate map $\mathscr{T}^{(k)} \colon T_{x_k}M \to T_{x_{k+1}}M$, and a scaling parameter s_k at each iteration number k as $\eta_{k+1} = -\operatorname{grad} f(x_{k+1}) + \beta_{k+1} s_k \mathscr{T}^{(k)}(\eta_k)$. Note that $\eta_0 = -\operatorname{grad} f(x_0)$ at $x_0 \in M$. The CG method is known to converge numerically faster than the steepest descent method. However, it is difficult to implement on a particular manifold compared with the steepest descent method since we need an appropriate map $\mathscr{T}^{(k)}$, whereas the search direction η_k in the steepest descent method is simply taken as $\eta_k = -\operatorname{grad} f(x_k)$ for every k. There is no literature dealing with the Riemannian CG methods on the symplectic Stiefel manifold, and to the best of the authors' knowledge, this study is the first attempt to address them.

We use the Cayley retraction proposed by [8] as a retraction on $\mathrm{Sp}(2p, 2n)$. When $n = p$, the inverse map of the

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retraction according to [28] is used as the map $\mathscr{T}^{(k)}$. When $n > p$, instead of the inverse retraction, a novel method using the orthogonal projections onto the tangent spaces of $\mathrm{Sp}(2p, 2n)$ is proposed. Numerical experiments with these implementations show that the proposed methods outperform the naive and improved steepest descent methods proposed by [8] in terms of the convergence speed.

The remainder of this paper is organized as follows. Section II reviews the concepts necessary for optimization on $\mathrm{Sp}(2p, 2n)$. Section III provides an overview of the proposed CG algorithm, followed by a discussion of cases $n = p$ and $n > p$. We also discuss how to choose the step length and β_k to enhance the efficacy of the proposed methods. In Section IV, the results of numerical experiments are presented; the CG methods proposed in this paper are demonstrated to be superior to existing methods, such as [8], mainly in terms of performance. Finally, a summary and the conclusions of this study are presented in Section V.

II. Optimization on symplectic Stiefel manifold

In this section, we review the concepts on the symplectic Stiefel manifold $\mathrm{Sp}(2p, 2n)$ necessary for optimization on it.

A. Tangent spaces

Given a point $X \in \mathrm{Sp}(2p, 2n)$, the tangent space $T_X\mathrm{Sp}(2p, 2n)$ at X is expressed in three forms [8], where $\mathrm{Sym}(2n)$ is the set of all symmetric matrices of size $2n \times 2n$:

$$\begin{aligned} & T_X\mathrm{Sp}(2p, 2n) \\ &= \{Z \in \mathbb{R}^{2n\times 2p} \mid Z^\top JX + X^\top JZ = 0\} \\ &= \{XJW + JX_\perp K \mid W \in \mathrm{Sym}(2p), K \in \mathbb{R}^{2(n-p)\times 2p}\} \\ &= \{SJX \mid S \in \mathrm{Sym}(2n)\}. \end{aligned} \tag{1}$$

Here, $X_\perp \in \mathbb{R}^{2n\times 2(n-p)}$ is an orthonormal matrix that spans the orthogonal complement of the subspace spanned by the columns of X, where orthogonality is defined with respect to the standard inner product in $\mathbb{R}^{2n}$. Therefore, such $X_\perp$ is not unique and can be arbitrary in subsequent discussions. In the following, we arbitrarily fix one such $X_\perp$.

B. Retraction

As a retraction on $\mathrm{Sp}(2p, 2n)$, we use the following Cayley retraction R^{cay} [8], which is defined for $X \in \mathrm{Sp}(2p, 2n)$ and $Z \in T_X\mathrm{Sp}(2p, 2n)$, as

$$R_X^{\mathrm{cay}}(Z) := \left(I - \frac{1}{2}S_{X,Z}J\right)^{-1}\left(I + \frac{1}{2}S_{X,Z}J\right)X,$$

where $S_{X,Z} = G_X Z(XJ)^\top + XJ(G_X Z)^\top$ and $G_X = I - \frac{1}{2}XJX^\top J^\top$. See [1] for a general theory of retraction.

C. Riemannian metrics and gradients

A family of smoothly varying inner products on $T_X\mathrm{Sp}(2p, 2n)$, that is, a Riemannian metric, can be defined using the parameter $\rho > 0$ and the matrices W and K used in the representation of tangent spaces in (1) as follows [8]:

$$g_\rho(Z_1, Z_2) := \frac{1}{\rho}\,\mathrm{tr}\left(W_1^\top W_2\right) + \mathrm{tr}\left(K_1^\top K_2\right), \tag{2}$$

where $Z_i = XJW_i + JX_\perp K_i \in T_X\,\mathrm{Sp}(2p, 2n)$ for $i = 1, 2$. Here, the parameter $\rho > 0$ plays a role of weighting $\mathrm{tr}\left(W_1^\top W_2\right)$ for $\mathrm{tr}\left(K_1^\top K_2\right)$. We also denote $g_\rho(Z_1, Z_2)$ as $\langle Z_1, Z_2\rangle$ by omitting the parameter ρ since we do not consider varying ρ in this study, and there is no confusion.

Regarding the Riemannian metric g_ρ in (2), the orthogonal projection onto the tangent spaces of the symplectic Stiefel manifold is given as follows [8]:

Proposition 1: Given $X \in \mathrm{Sp}(2p, 2n)$ the orthogonal projection of $Y \in \mathbb{R}^{2n\times 2p}$ onto $T_X\mathrm{Sp}(2p, 2n)$ with respect to the metric g_ρ is written as $P_X(Y) = S_{X,Y}JX$, where $S_{X,Y} = 2\,\mathrm{sym}(G_X Y(XJ)^\top)$, $G_X = I - \frac{1}{2}XJX^\top J^\top$, $\mathrm{sym}(B) := \frac{1}{2}(B + B^\top)$, and $\mathrm{skew}(B) := \frac{1}{2}(B - B^\top)$ for a square matrix B.

Note that the expression of $P_X(Y)$ does not depend on ρ. Using the orthogonal projection, from the general theory of Riemannian geometry [1], we can compute the Riemannian gradient of a function on $\mathrm{Sp}(2p, 2n)$ as follows [8]:

Proposition 2: Assume that $\mathrm{Sp}(2p, 2n)$ is endowed with the Riemannian metric (2). Let $\bar{f}$ and $\nabla\bar{f}$ be a smooth extension of a smooth function $f\colon \mathrm{Sp}(2p, 2n) \to \mathbb{R}$ to $\mathbb{R}^{2n\times 2p}$ and its Euclidean gradient, respectively. Then, the Riemannian gradient of f satisfies $\mathrm{grad}_\rho f(X) = S_X JX$ at $X \in \mathrm{Sp}(2p, 2n)$, where $S_X = 2\,\mathrm{sym}(H_X\nabla\bar{f}(X)(XJ)^\top)$ with $H_X = \frac{\rho}{2}XX^\top + JX_\perp X_\perp^\top J^\top$.

III. CG methods on symplectic Stiefel manifold

In this section, we provide an outline and implementation details of our proposed CG method on the symplectic Stiefel manifolds.

First, we briefly review basic CG methods in Euclidean spaces. The CG method in the Euclidean space $\mathbb{R}^n$ is a descent method that generates a sequence $\{x_k\}$ by iterating $x_{k+1} = x_k + t_k\eta_k$ with the search direction η_k and step length $t_k > 0$, where $\eta_0 = -\nabla f(x_0)$ and η_k for $k \geq 1$ is updated as $\eta_{k+1} = -\nabla f(x_{k+1}) + \beta_{k+1}\eta_k$. The sequence $\{x_k\}$ obtained in this manner is guaranteed to have a global convergence property with appropriate assumptions, step lengths, and β_k [18]. Its convergence is generally known to be numerically faster than that of the steepest descent method. Various formulas for computing the parameter β_k in the above updating formula for η_k have been proposed. See [9] for a review of Euclidean CG methods.

A. CG methods on general Riemannian manifold

In the CG method on a Riemannian manifold M, the situation differs from that in Euclidean spaces since we have $-\,\mathrm{grad}\,f(x_{k+1}) \in T_{x_{k+1}}M$ and $\eta_k \in T_{x_k}M$. Therefore, a map $\mathscr{T}^{(k)}\colon T_{x_k}M \to T_{x_{k+1}}M$ is required to add them together. The update formula for the search direction is defined using the map $\mathscr{T}^{(k)}$ as

$$\eta_{k+1} := -\,\mathrm{grad}\,f(x_{k+1}) + \beta_{k+1}s_k\mathscr{T}^{(k)}(\eta_k),$$

where $s_k > 0$ is a parameter that scales the norm of the obtained tangent vector and guarantees convergence, which is defined as $s_k := \min\{1, \|\eta_k\|_{x_k}/\|\mathscr{T}^{(k)}(\eta_k)\|_{x_{k+1}}\} > 0$, where $\|\cdot\|_x$ with $x \in M$ is the induced norm in T_xM by the Riemannian metric. Then, $\|s_k \mathscr{T}^{(k)}(\eta_k)\|_{x_{k+1}} \leq \|\eta_k\|_{x_k}$ holds for each $k \geq 0$. This inequality is crucial for guaranteeing convergence.

B. Proposed algorithms

In this subsection, we first outline the proposed CG method on the symplectic Stiefel manifold and then describe how to determine the step length and β_k in the algorithm.

The proposed algorithm is outlined in Algorithm 1. The

Algorithm 1 CG method on symplectic Stiefel manifold

Input: Objective function f on $\mathrm{Sp}(2p, 2n)$, retraction R, map $\mathscr{T}^{(k)}$, initial point $X_0 \in \mathrm{Sp}(2p, 2n)$, $\epsilon > 0$, and positive integer maxItr.

Output: Sequence $\{X_k\}$ on $\mathrm{Sp}(2p, 2n)$.

$\eta_0 \leftarrow -\operatorname{grad} f(X_0)$.
$k \leftarrow 0$.
while $\|\operatorname{grad} f(X_k)\| > \epsilon$ and $k < \mathrm{maxItr}$ **do**
  Choose a step length t_k.
  $X_{k+1} \leftarrow R_{X_k}(t_k \eta_k)$.
  Compute $\mathscr{T}^{(k)}(\eta_k)$.
  Compute $s_k := \min\left\{1, \frac{\|\eta_k\|_{X_k}}{\|\mathscr{T}^{(k)}(\eta_k)\|_{X_{k+1}}}\right\}$ and β_{k+1}.
  $\eta_{k+1} \leftarrow -\operatorname{grad} f(X_{k+1}) + \beta_{k+1} s_k \mathscr{T}^{(k)}(\eta_k)$.
  $k \leftarrow k+1$.
end while
return X_k.

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step length t_k in the algorithm is computed, e.g., such that the following Armijo condition is satisfied in each iteration:

$$f(R_{X_k}(t_k \eta_k)) \leq f(X_k) + \alpha t_k \langle \operatorname{grad} f(X_k), \eta_k \rangle_{X_k}. \quad (3)$$

Note that α is a positive constant, which was set to 10^{-4} in our numerical experiments. In fact, to theoretically guarantee the global convergence property, the Riemannian CG methods usually require step lengths to satisfy the Wolfe conditions or related conditions, such as the strong or generalized Wolfe conditions [18]. However, in practice, step lengths satisfying the Armijo condition (3), which is weaker than the Wolfe conditions, are also used since they are easily implemented and computed.

The search for a step length t_k satisfying the above conditions is performed based on a backtracking strategy, that is, we set

$$t_k = 10^{-i_k} \gamma_k, \quad (4)$$

where $i_k \in \{0, 1, 2, \cdots\}$ is the smallest integer for which $t_k = 10^{-i_k}\gamma_k$ satisfies (3). For the initial trial step length γ_k in (4), we used $\gamma_k = \frac{2(f(X_{k+1}) - f(X_k))}{\langle \operatorname{grad} f(X_k), -\eta_k \rangle_{X_k}}$, whose Euclidean counterpart is discussed in [12].

Furthermore, for β_k, we used the following $\beta_k^{\text{R-DY}}$ [16], [18], [28]:

$$\beta_k^{\text{R-DY}} = \frac{\|g_{k+1}\|^2_{X_{k+1}}}{\langle g_{k+1}, s_k \mathscr{T}^{(k)}(\eta_k) \rangle_{X_{k+1}} - \langle g_k, \eta_k \rangle_{X_k}},$$

where $g_k := \operatorname{grad} f(X_k)$. This $\beta_k^{\text{R-DY}}$ is a generalization of the Euclidean version of β_k^{DY} proposed in [6].

Note that the denominators of the formulas for γ_k and $\beta_k^{\text{R-DY}}$ are always positive under some mild assumptions given in Proposition 6.3 in [18].

C. Case of symplectic group

If $\mathrm{Sp}(2p, 2n)$ is the symplectic group, that is, if $n = p$, we use a strategy that uses the inverse map of a retraction as $\mathscr{T}^{(k)}(\eta_k)$, whose general theory is discussed in [28]. Specifically, using the Cayley retraction $R = R^{\text{cay}}$, we update X_k as $X_{k+1} = R^{\text{cay}}_{X_k}(t_k \eta_k)$ and define $\mathscr{T}^{(k)}(\eta_k)$ in Algorithm 1 as $\mathscr{T}^{(k)}(\eta_k) = -t_k^{-1}(R^{\text{cay}}_{X_{k+1}})^{-1}(X_k)$. For this $\mathscr{T}^{(k)}(\eta_k)$ and appropriately chosen t_k and β_k, the general theory in [28] guarantees the global convergence of the resultant CG method on $\mathrm{Sp}(2p, 2n)$.

The Cayley retraction $R^{\text{cay}}_X(Z)$ is, as mentioned above, defined as follows:

$$R^{\text{cay}}_X(Z) := \left(I - \frac{1}{2} S_{X,Z} J\right)^{-1} \left(I + \frac{1}{2} S_{X,Z} J\right) X, \quad (5)$$

where $S_{X,Z} = G_X Z (XJ)^\top + XJ\,(G_X Z)^\top$ and $G_X = I - \frac{1}{2} X J X^\top J^\top$. Hence, letting $\tilde{Z} := (R^{\text{cay}}_{X_{k+1}})^{-1}(X_k)$, we have

$$X_k = \left(I - \frac{1}{2} S_{X_{k+1},\tilde{Z}} J\right)^{-1} \left(I + \frac{1}{2} S_{X_{k+1},\tilde{Z}} J\right) X_{k+1},$$

that is,

$$\left(I - \frac{1}{2} S_{X_{k+1},\tilde{Z}} J\right) X_k = \left(I + \frac{1}{2} S_{X_{k+1},\tilde{Z}} J\right) X_{k+1}.$$

It follows that

$$2(X_k - X_{k+1}) = S_{X_{k+1},\tilde{Z}} J (X_k + X_{k+1}). \quad (6)$$

Therefore, if we know that $X_k + X_{k+1}$ is regular, noting that $J^{-1} = -J$ holds, $S_{X_{k+1},\tilde{Z}}$ can be calculated as

$$S_{X_{k+1},\tilde{Z}} = -2(X_k - X_{k+1})(X_k + X_{k+1})^{-1} J. \quad (7)$$

Furthermore, it follows from $\tilde{Z} \in T_{X_{k+1}} \mathrm{Sp}(2p, 2n)$ and [8, Corollary 4.4] that $\tilde{Z} = S_{X_{k+1},\tilde{Z}} J X_{k+1}$.

The Cayley retraction itself is not globally defined [8, Proposition 5.4]. However, in fact, when X_{k+1} is computed as $X_{k+1} = R^{\text{cay}}_{X_k}(t_k \eta_k)$, the inverse retraction $R^{-1}_{X_{k+1}}$ is globally defined. This is guaranteed by the fact that $X_k + X_{k+1}$ is always invertible, as proved in the following proposition.

Proposition 3: Let $n = p$, $X \in \mathrm{Sp}(2p, 2n)$, and $Z \in T_X \mathrm{Sp}(2p, 2n)$. Assume that $X_+ := R^{\text{cay}}_X(Z)$ is defined. Then, the matrix $X + X_+ \in \mathbb{R}^{2n \times 2n}$ is invertible.

Proof: Letting $G := I - \frac{1}{2} X J X^\top J$ and $S := GZ(XJ)^\top + XJ(GZ)^\top$, it follows from (5) that $X_+ = (I - \frac{1}{2}SJ)^{-1}(I + \frac{1}{2}SJ)X$, where we note that $I - \frac{1}{2}SJ$ is invertible since we assume that $X_+ = R^{\text{cay}}_X(Z)$ is defined. Therefore, we have

$$\begin{aligned} X + X_+ &= X + \left(I - \frac{1}{2}SJ\right)^{-1}\left(I + \frac{1}{2}SJ\right)X \\ &= \left(I - \frac{1}{2}SJ\right)^{-1}\left(\left(I - \frac{1}{2}SJ\right) + \left(I + \frac{1}{2}SJ\right)\right)X \\ &= 2\left(I - \frac{1}{2}SJ\right)^{-1} X. \end{aligned}$$

Here, from $X^\top JX = J$, we have $\det(X)^2 = 1$, which means that X is invertible. Hence, $X + X_+$ is invertible because, specifically, we have

$$(X + X_+)^{-1} = \frac{1}{2}X^{-1}\left(I - \frac{1}{2}SJ\right).$$

■

Therefore, for $n = p$, the proposed method implements the CG algorithm by defining the search direction as follows: We calculate $S := -2(X_k - X_{k+1})(X_k + X_{k+1})^{-1}J$ and define $\mathscr{T}^{(k)}(\eta_k)$ as $\mathscr{T}^{(k)}(\eta_k) := (R^{\text{cay}}_{X_{k+1}})^{-1}(X_k) = SJX_{k+1}$ to update the search direction in Algorithm 1.

D. Case of general symplectic Stiefel manifold

If $n > p$, there are several $S_{X_{k+1},\tilde{Z}}$ such that (6) is satisfied. To use the inverse retraction strategy, it is necessary to find $S_{X_{k+1},\tilde{Z}}$ such that $S_{X_{k+1},\tilde{Z}}JX_{k+1} \in T_{X_{k+1}}\operatorname{Sp}(2p, 2n)$. In other words, it is necessary to find $S_{X_{k+1},\tilde{Z}}$ such that it is a symmetric matrix from [8, Proposition 3.3 (3.8c)]. However, this is challenging to find.

Therefore, we do not use the inverse retraction in this case; instead, we use the orthogonal projection onto $T_{X_{k+1}}M$ in Proposition 1 as $\mathscr{T}^{(k)}(\eta_k) = S_{X_{k+1},\eta_k}JX_{k+1}$, where $S_{X_{k+1},\eta_k} = G_{X_{k+1}}\eta_k(X_{k+1}J)^\top + X_{k+1}J\left(G_{X_{k+1}}\eta_k\right)^\top$ and $G_{X_{k+1}} = I - \frac{1}{2}X_{k+1}JX_{k+1}^\top J^\top$. In other words, in the case of $n > p$, we implement the CG method using the above $\mathscr{T}^{(k)}(\eta_k)$ to define the search direction at every step. The orthogonal projection-based Riemannian CG methods are not always guaranteed to converge globally. This is because the projection-based map $\mathscr{T}^{(k)}$ is not known to satisfy the condition that $\mathscr{T}^{(k)}$ is sufficiently close to the differentiated retraction $\mathrm{D}R_{X_k}(t_k\eta_k)$, which causes the CG method to converge globally. See Assumption 4.2 in [18] for more details. However, in our numerical experiments in the next section, this method is effective in minimizing the objective function compared with existing optimization methods on the symplectic Stiefel manifold. In fact, some examples in which the orthogonal projection-based Riemannian CG methods are guaranteed to converge globally are discussed in [18] such as methods on the sphere and Grassmann manifold. Clarifying whether the proposed method on the general symplectic Stiefel manifold always globally converges is left for future work.

We note that the projection-based CG method discussed here can be also applied to the case of $n = p$. However, in that case, the CG method based on the inverse retraction is theoretically superior since global convergence can be guaranteed under some assumptions, as discussed in the previous subsection.

IV. Numerical experiments

In this section, we present the results of numerical experiments in which Algorithm 1 is applied. We choose the symplectic eigenvalue problem as our target problem, which is one of the problems used in the numerical experiments in a previous work [8]. In addition, we prepared instances for cases $n = p$ and $n > p$ and performed a CG search, each using the appropriate technique described in the previous section. The runtime environment was MATLAB2021b, Mac Pro (processor: 3 GHz 8-core Intel Xeon E5, memory: 32 GB). The code for the proposed method was written by modifying that for [8] provided in `https://github.com/opt-gaobin/spopt`.

A. Symplectic eigenvalue problem

Any positive definite symmetric matrix $A \in \mathbb{R}^{2n\times 2n}$ can be diagonalized by a symplectic matrix $X \in \operatorname{Sp}(2n, 2n)$, as described in [25]. Specifically, for every symmetric positive definite matrix $A \in \mathbb{R}^{2n\times 2n}$, there exists $X \in \operatorname{Sp}(2n, 2n)$ such that

$$X^\top AX = \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix},$$

where $D = \operatorname{diag}(d_1, d_2, \ldots, d_n)$ and $0 < d_1 \leq \cdots \leq d_n$. These $d_1, d_2, \ldots, d_n$ are called symplectic eigenvalues, and finding X and D is called the symplectic eigenvalue problem. We note that the term "symplectic eigenvalue problem" is sometimes used with a different meaning, e.g., in [3]. This is noted in detail in [22], which is an arXiv version of [21].

In this situation, from the smallest to the pth symplectic eigenvalues can be obtained by solving the following optimization problem on $\operatorname{Sp}(2p, 2n)$:

Problem 3:

$$\begin{aligned} &\text{Minimize} && f(X) := \operatorname{tr}(X^\top AX) \\ &\text{subject to} && X \in \operatorname{Sp}(2p, 2n). \end{aligned}$$

A smooth extension of $f\colon \operatorname{Sp}(2p, 2n) \to \mathbb{R}$ to the entire space $\mathbb{R}^{2n\times 2p}$ is $\bar{f}(X) = \operatorname{tr}\left(X^\top AX\right)$ and its Euclidean gradient is $\nabla\bar{f}(X) = 2AX$. Therefore, the Riemannian gradient can be computed as in Proposition 2.

The details and results of our numerical experiments on the above problem are as follows. We set parameter $\rho = 0.5$ for the Riemannian metric g_ρ. The parameters of the termination conditions in Algorithm 1 were set as $\epsilon = 10^{-5}$ and $\mathrm{maxItr} = 2000$, and n and p were set as $(n, p) = (80, 80), (80, 40)$. Matrix $A \in \mathbb{R}^{2n\times 2n}$ was randomly generated as a positive definite symmetric matrix by the following procedure, based on previous studies [8], using the parameter $\lambda \geq 1$ to control the condition number. 1) Let $\Lambda \in \mathbb{R}^{2n\times 2n}$ be a diagonal matrix such that $\Lambda_{ii} = \lambda^{1-i}$, $i = 1, 2, \ldots, 2n$; 2) Matrix $Q \in \mathbb{R}^{2n\times 2n}$ is an orthogonal matrix obtained by the QR decomposition of a random matrix in MATLAB as `Q = qr(randn(2*n, 2*n));` 3) Matrix A is generated by $A = Q\Lambda Q^\top$. Note that parameter λ was set to $\lambda = 1.04$ in this experiment. Here, the diagonal elements of Λ are the eigenvalues of A in terms of the standard eigenvalue problem. In addition, the initial point $X_0 \in \operatorname{Sp}(2p, 2n)$ was randomly constructed in the same manner as for the code in `https://github.com/opt-gaobin/spopt`. Specifically, we constructed $\tilde{W} \in \mathbb{R}^{2p\times 2p}$ each of whose element follows the standard normal distribution and computed $W := \tilde{W}^\top\tilde{W} + 0.1I$.

Subsequently, letting $W =: \begin{bmatrix} W_1 \\ W_2 \end{bmatrix}$ with $W_1, W_2 \in \mathbb{R}^{p \times 2p}$, we computed $E := \exp\left(\begin{bmatrix} W_2 \\ -W_1 \end{bmatrix}\right) \in \mathbb{R}^{2p \times 2p}$, where exp is the matrix exponential function. Finally, letting $E =: \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}$ with $E_1, E_2 \in \mathbb{R}^{p \times 2p}$, we computed $X_0 := \begin{bmatrix} E_1 \\ 0 \\ E_2 \\ 0 \end{bmatrix}$, where the size of the zero matrix 0 is $(n-p) \times 2p$.

Under the above conditions, the following three methods were compared: SD (steepest descent method); SD-nBB (improved steepest descent method); CG (conjugate gradient method (proposed method)).

The SD method is a simple steepest descent method, in which the search direction is $\eta_k = -\operatorname{grad} f(X_k)$ at X_k. We set the method for determining the step length in this method as in Section III-B.

The SD-nBB method is an improved steepest descent method proposed in a previous study [8]. This method searches for an appropriate step length using the backtracking formula (3) in the same manner as our proposed method but has two different features for determining the step length. The first feature is "nonmonotone line search" [26], which concerns the conditions for updating the step length. This method was extended to the Stiefel manifold [24] and to general Riemannian manifolds [10, section 3.3], [11] . In the nonmonotone line search, the step length at every step k is determined to satisfy the following condition:

$$f\left(R_{X_k}\left(t_k \eta_k\right)\right) \leq c_k + \alpha t_k \left\langle \operatorname{grad} f\left(X_k\right), \eta_k \right\rangle_{X_k}, \tag{8}$$

where $\alpha \in (0,1)$ is a parameter, $q_0 = 1$ and $c_0 = f(X_0)$, and q_k and c_k for $k \geq 1$ are defined as $q_k = \tau q_{k-1} + 1$ and $c_k = \frac{\tau q_{k-1}}{q_k} c_{k-1} + \frac{1}{q_k} f\left(X_k\right)$ with a parameter $\tau \in [0,1]$. Note that the nonmonotone condition (8) reduces to the standard Armijo condition (3) when $\tau = 0$. In the experiments, we set $\tau = 0.85$. The second feature is the "Barzilai–Borwein (BB) method" [2], which concerns the choice of the initial trial step length γ_k in (4). This method was extended to general Riemannian manifolds in [11], and a method called "alternating BB strategy," which is a further improvement on the BB method in terms of speed, was proposed in [5]. In nSD-BB, the alternating BB strategy was used to determine γ_k. First, γ_k^{BB1} and γ_k^{BB2} were defined as follows:

$$\gamma_k^{\mathrm{BB1}} := \frac{\langle S_{k-1}, S_{k-1} \rangle}{|\langle S_{k-1}, Y_{k-1} \rangle|}, \quad \gamma_k^{\mathrm{BB2}} := \frac{|\langle S_{k-1}, Y_{k-1} \rangle|}{\langle Y_{k-1}, Y_{k-1} \rangle}, \tag{9}$$

where $S_{k-1} = X_k - X_{k-1}$ and $Y_{k-1} = \operatorname{grad}_\rho f\left(X_k\right) - \operatorname{grad}_\rho f\left(X_{k-1}\right)$. Using this γ_k^{BB1} and γ_k^{BB2}, the initial trial step length γ_k in (4) is chosen as $\gamma_k = \gamma_k^{\mathrm{BB1}}$ if k is odd and $\gamma_k = \gamma_k^{\mathrm{BB2}}$ if k is even. Note that the inner product in (9) is the Euclidean inner product $\langle \cdot, \cdot \rangle$ instead of g_ρ because it was confirmed in [8] that this would accelerate the speed of the algorithm of the steepest descent method.

The CG method is the proposed method. When we considered the implementation of this method, we attempted to use methods with the nonmonotone line search and BB strategies to search for step lengths. However, in this method, they did not accelerate the speed of convergence, but rather worsened it. Therefore, we did not use them and implemented the backtracking line search method in Section III-B as an alternative method for the step length search.

The numerical results for $n = p = 80$ and $(n,p) = (80,40)$ are shown in Figures 1 and 2. The vertical axis represents the norm of the gradient, and the horizontal axis represents the number of iterations. In both cases $n = p$ and $n > p$, the proposed CG method converges faster than the SD and nSD-BB methods. Moreover, the norm of the gradient decreases almost monotonically and steadily in the proposed method compared with the nSD-BB case, where the norm of the gradient oscillates by increasing and decreasing rapidly.

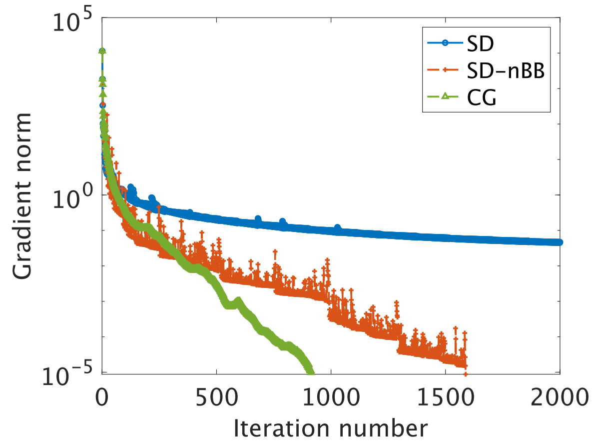

Fig. 1. Convergence history ($n = p = 80$)

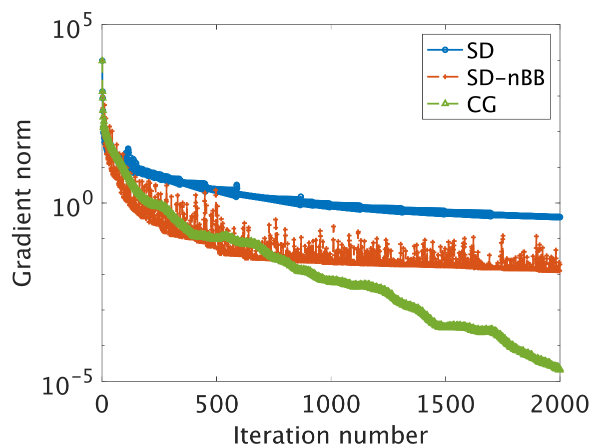

Fig. 2. Convergence history ($n = 80$ and $p = 40$)

In the following, we focus on problems with matrices larger than those considered above to measure and compare the execution times. For ease of measurement, the termination condition was changed to $\epsilon = 10^{-4}$ and $\mathrm{maxItr} = 30000$. We performed experiments for problem sizes $n = p = 120$ and $(n,p) = (120, 60)$. The other conditions were identical to those used in the previous experiment. Tables I and II list the results of the experiments. As the entries in each table indicate, Time refers to the time required to stop the algorithm, and Itr. and $\|\operatorname{grad} f\|$ denote k and

$\|\operatorname{grad} f(X_k)\|_{X_k}$ at the end of the algorithm, respectively. First, as can be observed from the Itr. and $\|\operatorname{grad} f\|$ entries in Tables I and II, the SD method did not reach the $\|\operatorname{grad} f\|$ termination condition for either $n = p = 120$ or $(n, p) = (120, 60)$, whereas the nSD-BB and CG methods reached the $\|\operatorname{grad} f\|$ termination condition. Next, in the case of $n = p = 120$, the CG method terminated in fewer steps than the nSD-BB method, but the CG method required more execution time. This could be because of the time required for solving a system of linear equations to compute (7). On the other hand, when $(n, p) = (120, 60)$, the CG method is superior in terms of both the number of steps and execution time. In the case $(n, p) = (120, 60)$, the number of steps required for convergence increased significantly in the nSD-BB method, whereas convergence was achieved with a relatively small number of steps in the CG method. This confirms the usefulness of the proposed method using orthogonal projection compared with previous methods.

TABLE I

EXECUTION TIMES ($n = p = 120$)

method	Time (s)	Itr.	$\|\operatorname{grad} f\|$
SD	215.6	30000	2.58×10^{-3}
nSD-BB	15.5	2166	1.00×10^{-4}
CG	17.4	1435	9.69×10^{-5}

TABLE II

EXECUTION TIMES ($n = 120$ AND $p = 60$)

method	Time (s)	Itr.	$\|\operatorname{grad} f\|$
SD	162.0	30000	4.64×10^{-2}
nSD-BB	136.7	24554	9.71×10^{-5}
CG	46.1	5011	9.80×10^{-5}

V. CONCLUSION

In this study, we proposed CG methods on the symplectic Stiefel manifolds $\mathrm{Sp}(2p, 2n)$ and derived specific formulas for implementation that are valid for the cases $n = p$ and $n > p$. Their usefulness compared to existing methods, such as the steepest descent method, was demonstrated by numerical experiments on the symplectic eigenvalue problem.

For the case $n = p$, we applied CG methods based on the inverse map of the Cayley retraction on the symplectic Stiefel manifold (symplectic group), and the specific computational formulas in the algorithm were derived. We proved that, when we compute X_{k+1} from X_k by the Cayley retraction $R^{\mathrm{cay}}_{X_k}$, the inverse retraction $(R^{\mathrm{cay}}_{X_{k+1}})^{-1}$ is globally defined. For the case $n > p$, we proposed a CG method using orthogonal projection from a new point of view.

It was demonstrated that the proposed methods for both cases $n = p$ and $n > p$ are superior to the existing methods in terms of convergence speed for the symplectic eigenvalue problem.

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