

# CDOpt: A Python Package for a Class of Riemannian Optimization

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## Abstract

Optimization over the embedded submanifold defined by constraints  $c(x) = 0$  has attracted much interest over the past few decades due to its wide applications in various areas, including computer vision, signal processing, numerical linear algebra, and deep learning. Plenty of related optimization packages have been developed based on Riemannian optimization approaches, which rely on some basic geometrical materials of Riemannian manifolds, including Riemannian gradients, retractions, vector transports, etc. These geometrical materials can be challenging to determine in general. In fact, existing packages only accommodate a few well-known manifolds whose geometrical materials are easily accessible. For other manifolds which are not contained in these packages, the users have to develop the geometric materials by themselves. In addition, it is not always tractable to adopt the advanced features from various state-of-the-art unconstrained optimization solvers to Riemannian optimization approaches.

We introduce CDOpt (available at <https://cdopt.github.io/> under BSD 3-clause license), a user-friendly Python package for a class of Riemannian optimization. Based on the constraint dissolving approaches, Riemannian optimization problems are transformed into their equivalent unconstrained counterparts in CDOpt. Therefore, solving Riemannian optimization problems through CDOpt directly benefits from various existing solvers and the rich expertise gained over decades for unconstrained optimization. Moreover, all the computations in CDOpt related to any manifold in question are conducted on its constraints expression, hence users can easily define new manifolds in CDOpt without any background on differential geometry. Furthermore, CDOpt extends the neural layers from PyTorch and Flax, thus allows users to train manifold constrained neural networks directly by the solvers for unconstrained optimization. Extensive numerical experiments demonstrate that CDOpt is highly efficient and robust in solving various classes of Riemannian optimization problems.

## 1 Introduction

### 1.1 Problem formulation

In this paper, we consider the following constrained optimization problem

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \text{s.t.} \quad & \mathcal{M} := \{x \in \mathbb{R}^n : c(x) = 0\}, \end{aligned} \tag{OCP}$$

where the objective function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  and constraint mapping  $c : \mathbb{R}^n \rightarrow \mathbb{R}^p$  of OCP satisfy the following assumptions:

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### Assumption 1.1. Blanket assumptions

1.  $f$  is locally Lipschitz continuous in  $\mathbb{R}^n$ ;
2. The transposed Jacobian of  $c$ , denoted as  $J_c(x) \in \mathbb{R}^{n \times p}$ , is locally Lipschitz continuous in  $\mathbb{R}^n$ ;
3. The relaxed constant rank constraint qualification (RCRCQ) [34] holds for any  $x \in \mathcal{M}$ , i.e. there exists a constant  $p' \leq p$  and a neighborhood  $\mathcal{X}$  of  $\mathcal{M}$  such that the rank of  $J_c(x)$  equals to  $p'$  for any  $x \in \mathcal{X}$ .

Since  $c$  is smooth in  $\mathbb{R}^n$ , the feasible region  $\mathcal{M}$  is a closed submanifold embedded in  $\mathbb{R}^n$  [13]. In fact, OCP satisfying Assumption 1.1 covers a great number of practically interesting Riemannian optimization problems [19, 49] arising over the past few decades. These Riemannian optimization problems can be categorized into two different categories. One is the so-called *standard Riemannian optimization problem*, where the function value and derivatives of the objective function are explicitly formulated and affordable to evaluate, hence can be directly provided to optimization packages. These problems include the Kohn-Sham total energy minimization [5], dictionary learning [51], dual principle component pursuit [42, 20], symplectic eigenvalue problems [40], etc. Interested readers may refer to the books [3, 8] and a recent survey paper [19] for more details of these problems.

Another category is referred as *training neural networks with manifold constraints* throughout this paper. Training deep neural networks (DNNs) is usually thought to be challenging both theoretically and practically, where the gradient vanishing and exploding problem is one of the most important reasons [15]. To address this issue, several recent works focus on training DNNs while imposing manifold constraints to the weights of their neural layers, especially on restricting the weights over the Stiefel manifold [4, 6, 24, 30]. As orthogonality can be used to impose energy preservation properties to these DNNs [53], some existing works demonstrate that the orthogonal constraints can stabilize the distribution of activations among neural layers within DNNs and make their optimization more efficient. Moreover, many existing works [6, 24, 44] observe encouraging improvements in the accuracy and robustness of the DNNs with orthogonally constrained weights.

In training neural networks with manifold constraints, the neural network is built by the composition of neural layers, while the objective function is formulated as the expectation of the losses over samples. Therefore, the function value and differentials of the objective function are usually unaffordable to evaluate exactly, and most of the *optimizers* (i.e., solvers for training neural networks) are developed based on stochastic optimization algorithms to reduce the computational costs. Moreover, existing deep-learning frameworks (e.g. PyTorch [37], JAX [10], TensorFlow [1]) provide various advanced features, including GPU/TPU acceleration, automatic differentiation (AD), just-in-time compilation, to further accelerate the training. As a result, training neural networks with manifold constraints requires specialized optimization solvers (i.e., optimizers) to utilize the advanced features of these frameworks, leading to great differences between their optimizers and the solvers for standard Riemannian optimization problems.

## 1.2 Existing approaches and optimization packages

Due to the diffeomorphisms between an Euclidean space and a Riemannian manifold, various *unconstrained optimization approaches* (i.e., approaches for solving unconstrained nonconvex optimization) can be transferred to their corresponding *Riemannian optimization approaches* (i.e., the approaches for Riemannian optimization). In particular, [3] provides several well-recognized frameworks based on geometrical materials from differential geometry, including geodesics, parallel transports and Riemannian differentials.

The geodesics generalize the concept of straight lines to Riemannian manifolds, but are expensive to compute in most cases. To this end, [3] provides the concept of retractions as relaxations to geodesics, which makes them more affordable to compute. Besides, parallel transports are mappings that move tangent vectors along given curves over a Riemannian manifold “parallelly”. Computing parallel transports is essential in computing the linear combinations of two vectors from different tangent spaces. In particular, it is necessary for those approaches that utilize information in the past iterates (e.g., quasi-Newton methods, nonlinear conjugate gradient methods, momentum SGD,

ADAM). For various Riemannian manifolds, computing the parallel transports amounts to solving differential equations, which is generally unaffordable in practice [3]. Therefore, the concept of vector transports is proposed as approximations to parallel transports to alleviate the computational cost in Riemannian optimization approaches. Although retractions and vector transports make the computation more affordable by approximation, how to develop efficient formulations of retractions and vector transports remains challenging.

Almost all the existing Riemannian optimization packages are developed based on the framework proposed by [3]. These packages are either developed for standard Riemannian optimization problems (e.g., Manopt [9], PyManopt [41], ROPTLIB [25]), or specialized for training neural networks with manifold constraints (e.g., Geoopt [27], McTorch [33]). In these packages, the manifold is described by the constraints, together with the geometrical materials from differential geometry, including retractions and their inverses, vector transports, etc. Some packages, including PyManopt, Geoopt and Manopt, even require the exact formulation of exponential mappings and logarithm mappings. Unfortunately, the task to compute these geometrical materials is usually challenging. Although these Riemannian optimization packages provide several predefined manifolds, it is difficult to add in new manifold constraints for users and developers, especially when they are nonexperts in differential geometry.

As manifold constraints are characterized by geometrical materials, Riemannian optimization solvers are developed from unconstrained optimization solvers to adapt to these geometrical materials. To extend an unconstrained optimization solver to its Riemannian versions, the following three steps are indispensable: (i) replace Euclidean differentials with Riemannian differentials; (ii) invoke retractions to keep the feasibility of the iterates; (iii) employ vector transports to move vectors among the tangent spaces of the manifolds. Therefore, to build up new Riemannian optimization approaches by borrowing the advanced features of state-of-the-art unconstrained optimization approaches is challenging in general. Existing Riemannian optimization packages only provide limited Riemannian optimization algorithms. For example, compared with over 30 efficient optimizers from PyTorch and PyTorch-optimizer packages for unconstrained optimization, Geoopt only provides Riemannian Adam and Riemannian SGD, and McTorch is only integrated with Riemannian AdaDelta and Riemannian SGD.

Additionally, the package GeoTorch [30] is developed based on the trivialization approach for training neural networks with manifold constraints by PyTorch. In GeoTorch, the manifold is characterized by a smooth surjective mapping (trivialization mapping)  $\psi : \mathbb{R}^N \rightarrow \mathcal{M}$  for some constant  $N$ . Then GeoTorch transforms OCP into the following unconstrained optimization problem,

$$\min_{u \in \mathbb{R}^N} f(\psi(u)).$$

However, determining the trivialization mapping  $\psi$  is usually as challenging as determining the geometrical materials of  $\mathcal{M}$ . Until now, the formulations of  $\psi$  are only determined for spheres and Stiefel manifolds.

On the other hand, although GeoTorch enables the direct implementation of unconstrained optimization solvers to OCP for spheres and Stiefel manifolds, the expression of trivialization mappings in GeoTorch are usually too complicated to be computed efficiently. As mentioned in [44, 46, 21, 2], computing the mapping  $\psi$  provided in GeoTorch is usually costly, and could become the major computational bottleneck for the optimizers. For example, when  $\mathcal{M}$  is chosen as the Stiefel manifold  $\mathcal{S}_{m,s}$  embedded in  $\mathbb{R}^{m \times s}$ ,  $\psi$  is chosen as the Cayley transform or matrix exponential of an  $n \times n$  skew-symmetric matrix in GeoTorch. Then computing  $\psi$  and its differentials are extremely expensive, leading to its inferior performance when compared with other optimization approaches [44, 2, 21].

### 1.3 Constraint dissolving approaches

To over the aforementioned drawbacks in existing Riemannian optimization approaches, [49] proposes the *constraint dissolving* approaches for OCP, under the assumption that linear independence constraint qualification (LICQ) holds at any feasible point of  $\mathcal{M}$ . Then their proposed constraint dissolving approaches transform OCP into the unconstrained minimization of the following constraint

dissolving function (CDF).

$$h(x) := f(\mathcal{A}(x)) + \frac{\beta}{2} \|c(x)\|^2. \quad (\text{CDF})$$

Here  $\mathcal{A} : \mathbb{R}^n \rightarrow \mathbb{R}^n$  is called the constraint dissolving mapping, which should satisfy the following assumptions:

**Assumption 1.2. Blanket assumptions on  $\mathcal{A}$**

- $\mathcal{A}$  is locally Lipschitz smooth in  $\mathbb{R}^n$ ;
- $\mathcal{A}(x) = x$  holds for any  $x \in \mathcal{M}$ ;
- The Jacobian of  $c(\mathcal{A}(x))$  equals to 0 for any  $x \in \mathcal{M}$ . That is,  $J_{\mathcal{A}}(x)J_c(x) = 0$  holds for any  $x \in \mathcal{M}$ , where  $J_{\mathcal{A}}(x) \in \mathbb{R}^{n \times n}$  denotes the transposed Jacobian of  $\mathcal{A}$  at  $x$ .

When  $f$  is assumed to be locally Lipschitz smooth, [49] proves that OCP and CDF have the same first-order stationary points, second-order stationary points, local minimizers, and Łojasiewicz exponents in a neighborhood of  $\mathcal{M}$ . More importantly, [49] shows that constructing CDF is completely independent of any geometrical material of  $\mathcal{M}$ . Therefore, we can develop various constraint dissolving approaches to solve optimization problems over a broad class of manifolds embedded in  $\mathbb{R}^n$ , without any prior knowledge of their geometrical properties. Interested readers could further refer to [46, 47, 48] for developing constraint dissolving approaches and efficient algorithms for smooth optimization with orthogonality constraints.

For nonsmooth scenarios, [21] extends the constraint dissolving approaches for nonsmooth optimization over the Stiefel manifold, which enables the direct implementation of various existing unconstrained optimizers from PyTorch for training DNNs with orthogonally constrained weights. [22] shows the feasible region of any nonconvex-strongly-convex bilevel optimization problem is a Riemannian manifold, and proposes a novel constraint dissolving approach for these bilevel optimization problems. Moreover, [22] develops a general framework for designing subgradient methods and proves their convergence properties for bilevel optimization problems.

However, [49] establish the equivalence between OCP and CDF when LICQ holds everywhere on  $\mathcal{M}$ , which is a stricter assumption than Assumption 1.1. On the other hand, the penalty parameter  $\beta$  plays an important rule in the exactness of the constraint dissolving function  $h(x)$ . Although [49] suggests a thresholding value for  $\beta$  to guarantee the equivalence between OCP and CDF, such thresholding value may be difficult to estimate. How to practically choose the penalty parameter  $\beta$  for CDF remains unexplored.

## 1.4 Contributions

In this paper, we present a Python package called CDOpt, which is developed based on the constraint dissolving approaches for both standard Riemannian optimization problems and training neural networks with manifold constraints. Different from existing Riemannian optimization packages, CDOpt simultaneously achieves the following goals,

- **Dissolved constraints** : CDOpt transforms Riemannian optimization problems into equivalent unconstrained optimization problems. Therefore, we can utilize various highly efficient solvers for unconstrained optimization, and directly apply them to solve Riemannian optimization problems. Benefiting from the rich expertise gained over the past decades for unconstrained optimization, CDOpt is very efficient and naturally avoids the difficulties in extending the unconstrained optimization solvers to their Riemannian versions.
- **High compatibility**: CDOpt has high compatibility with various existing numerical backends, including NumPy [17], SciPy [43], Autograd [36], PyTorch [37], JAX [10] and Flax [18]. Users can directly apply the advanced features of these packages to accelerate the optimization, including the automatic differentiation, GPU/TPU supports, just-in-time (JIT) compilation, etc.

- **Customized manifolds:** CDOpt dissolves manifold constraints without involving any geometrical material of the manifold in question. Therefore, users can directly define various Riemannian manifolds in CDOpt through their constraint expressions  $c(x)$ .
- **Plug-in neural layers:** CDOpt provides various plug-in neural layers for PyTorch and Flax packages. With minor changes in the standard PyTorch/Flax codes, users can easily build and train neural networks with various manifold constraints based on PyTorch and JAX.

Furthermore, we also present improved theoretical analysis on the equivalence between CDF and OCP,

- **Relaxed constraint qualification** We prove the equivalence between OCP and CDF with the RCRCQ condition, which is weaker than the LICQ condition assumed in existing works [46, 49, 21, 22]. Therefore, the constraint dissolving approaches can be applied to the optimization problems over a broader class of embedded Riemannian submanifolds, including the Stiefel manifold with range constraints.
- **Practical scheme for penalty parameter** We propose a practical scheme for computing the penalty parameter  $\beta$  for CDF, which preserves the exactness of CDF. Therefore, one can easily compute an appropriate penalty parameter for CDF in practice and directly apply various of unconstrained optimization approaches with theoretical guarantees.

## 1.5 Organizations

The rest of this paper is organized as follows. Section 2 presents some basic notations, definitions and the constants that are necessary for the theoretical analysis in later parts. We establish the theoretical properties of CDF and propose a practical scheme for choosing the penalty parameter in Section 3. Section 4 illustrates the structure of CDOpt and describe its main modules. In Section 5, we present a brief comparison between CDOpt and other existing python Riemannian optimization packages. Section 4 exhibits several illustrative examples on applying CDOpt to solve standard Riemannian optimization problems and train neural networks with manifold constraints. Some examples on how to use CDOpt to solve Riemannian optimization problems are presented in Section 6. In Section 7, we present preliminary numerical experiments to illustrate that CDOpt enables efficient and direct implementation of various existing unconstrained solvers to solve OCP. We draw a brief conclusion in the last section.

## 2 Notations, definitions and constants

### 2.1 Notations

Let  $\text{range}(A)$  be the subspace spanned by the column vectors of matrix  $A$ , and  $\|\cdot\|$  represents the  $\ell_2$ -norm of a vector or an operator. The notations  $\text{diag}(A)$  and  $\text{Diag}(x)$  stand for the vector formed by the diagonal entries of a matrix  $A$ , and the diagonal matrix with the entries of  $x \in \mathbb{R}^n$  as its diagonal, respectively. We denote the smallest and largest eigenvalues of  $A$  by  $\lambda_{\min}(A)$  and  $\lambda_{\max}(A)$ , respectively. Besides,  $\sigma_s(A)$  refers to the  $s$ -th largest singular value of  $A$  while  $\sigma_{\min}(A)$  refers to the smallest singular value of matrix  $A$ . Furthermore, for any matrix  $A \in \mathbb{R}^{n \times p}$ , the pseudo-inverse of  $A$  is denoted by  $A^\dagger \in \mathbb{R}^{p \times n}$ , which satisfies  $AA^\dagger A = A$ ,  $A^\dagger AA^\dagger = A^\dagger$ , and both  $A^\dagger A$  and  $AA^\dagger$  are symmetric [16].

In this paper, the Riemannian metric for  $\mathcal{M}$  is chosen as the Euclidean metric in  $\mathbb{R}^n$ . For any  $x \in \mathcal{M}$ , we denote the Riemannian gradient of  $f$  at  $x$  as  $\text{grad} f(x)$ , and  $\text{hess} f(x)$  refers to the Riemannian Hessian of  $f$  at  $x$ .

For any  $x \in \mathbb{R}^n$ , we define the projection from  $x \in \mathbb{R}^n$  to  $\mathcal{M}$  as

$$\text{proj}(x, \mathcal{M}) := \arg \min_{y \in \mathcal{M}} \|x - y\|.$$

It is worth mentioning that the optimality condition of the above problem leads to the fact that  $x - w \in \text{range}(J_c(w))$  for any  $w \in \text{proj}(x, \mathcal{M})$ . Furthermore,  $\text{dist}(x, \mathcal{M})$  refers to the distance between  $x$  and  $\mathcal{M}$ , i.e.

$$\text{dist}(x, \mathcal{M}) := \inf_{y \in \mathcal{M}} \|x - y\|.$$

The transposed Jacobian of the mapping  $\mathcal{A}$  is denoted as  $J_{\mathcal{A}}(x) \in \mathbb{R}^{n \times n}$ . Recall the definition of  $J_c(x)$ , and let  $c_i$  and  $\mathcal{A}_i$  be the  $i$ -th coordinate of the mapping  $c$  and  $\mathcal{A}$  respectively, then  $J_c$  and  $J_{\mathcal{A}}$  can be expressed by

$$J_c(x) := \begin{bmatrix} \frac{\partial c_1(x_1)}{\partial x_1} & \dots & \frac{\partial c_p(x_1)}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial c_1(x_n)}{\partial x_n} & \dots & \frac{\partial c_p(x_n)}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{n \times p}, \quad \text{and } J_{\mathcal{A}}(x) := \begin{bmatrix} \frac{\partial \mathcal{A}_1(x_1)}{\partial x_1} & \dots & \frac{\partial \mathcal{A}_n(x_1)}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial \mathcal{A}_1(x_n)}{\partial x_n} & \dots & \frac{\partial \mathcal{A}_n(x_n)}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

Besides,  $\mathcal{D}_{J_{\mathcal{A}}}(x) : d \mapsto \mathcal{D}_{J_{\mathcal{A}}}(x)[d]$  denotes the second-order derivative of the mapping  $\mathcal{A}$ , which can be regarded as a linear mapping from  $\mathbb{R}^n$  to  $\mathbb{R}^{n \times n}$  and satisfies  $\mathcal{D}_{J_{\mathcal{A}}}(x)[d] = \lim_{t \rightarrow 0} \frac{1}{t}(J_{\mathcal{A}}(x + td) - J_{\mathcal{A}}(x)) \in \mathbb{R}^{n \times n}$ . Similarly,  $\mathcal{D}_{J_c}(x)$  refers to the second-order derivative of the mapping  $c$ , which satisfies  $\mathcal{D}_{J_c}(x)[d] = \lim_{t \rightarrow 0} \frac{1}{t}(J_c(x + td) - J_c(x)) \in \mathbb{R}^{n \times p}$ . Additionally, we set

$$\mathcal{A}^k(x) := \underbrace{\mathcal{A}(\mathcal{A}(\dots \mathcal{A}(x) \dots))}_{k \text{ times}},$$

for  $k \geq 1$ , and define  $\mathcal{A}^0(x) := x$ ,  $\mathcal{A}^\infty(x) := \lim_{k \rightarrow +\infty} \mathcal{A}^k(x)$ . Furthermore, we denote  $g(x) := f(\mathcal{A}(x))$  and use  $\nabla f(\mathcal{A}(x))$  to denote  $\nabla f(z)|_{z=\mathcal{A}(x)}$  in the rest of this paper.

## 2.2 Definitions

We first state the first-order optimality condition of OCP as follows.

**Definition 2.1** ([35]). *Given  $x \in \mathbb{R}^n$ , we say  $x$  is a first-order stationary point of OCP if there exists  $\tilde{\lambda} \in \mathbb{R}^p$  that satisfies*

$$\begin{cases} \nabla f(x) - \sum_{i=1}^p \tilde{\lambda}_i \nabla c_i(x) = 0, \\ c(x) = 0. \end{cases} \quad (2.1)$$

For any given  $x \in \mathcal{M}$ , we define  $\lambda(x)$  as

$$\lambda(x) := J_c(x)^\dagger \nabla f(x) \in \arg \min_{\lambda \in \mathbb{R}^p} \|\nabla f(x) - J_c(x)\lambda\|.$$

Then it can be easily verified that

$$\nabla f(x) = J_c(x)\lambda(x), \quad (2.2)$$

whenever  $x$  is a first-order stationary point of OCP.

**Definition 2.2.** *Given  $x \in \mathbb{R}^n$ , we say  $x$  is a second-order stationary point of OCP if  $x$  is a first-order stationary point of OCP and for any  $d \in \mathcal{T}_x$ , it holds that*

$$d^\top \left( \nabla^2 f(x) - \sum_{i=1}^p \lambda_i(x) \nabla^2 c_i(x) \right) d \geq 0. \quad (2.3)$$

As the Riemannian metric on  $\mathcal{M}$  is fixed as the Euclidean metric in  $\mathbb{R}^n$ , the following propositions present the closed-form expressions for the tangent space, normal space, Riemannian gradient  $\text{grad } f(x)$  and Riemannian Hessian  $\text{hess } f(x)$  for any  $x \in \mathcal{M}$ . The proofs of these propositions directly follow [3, 8], and hence is omitted for simplicity.

**Proposition 2.3.** Given  $x \in \mathcal{M}$ , the tangent space of  $\mathcal{M}$  at  $x$  can be expressed as  $\mathcal{T}_x = \{d \in \mathbb{R}^n : d^\top J_c(x) = 0\}$ , while the normal space of  $\mathcal{M}$  at  $x$  can be expressed as  $\mathcal{N}_x = \text{Range}(J_c(x))$ .

**Proposition 2.4.** The Riemannian gradient of  $f$  at  $x$  can be expressed as

$$\text{grad } f(x) = \nabla f(x) - J_c(x)\lambda(x). \quad (2.4)$$

Moreover,  $\text{hess } f(x)$  can be expressed as the following self-adjoint linear transform  $\text{hess } f(x) : \mathcal{T}_x \rightarrow \mathcal{T}_x$  such that

$$d^\top \text{hess } f(x)d = d^\top \left( \nabla^2 f(x) - \sum_{i=1}^p \lambda_i(x) \nabla^2 c_i(x) \right) d, \quad \text{for any } d \in \mathcal{T}_x.$$

Given  $x \in \mathcal{M}$ , the smallest eigenvalue of  $\text{hess } f(x)$  is defined as

$$\lambda_{\min}(\text{hess } f(x)) := \min_{d \in \mathcal{T}_x, \|d\|=1} d^\top \text{hess } f(x)d.$$

Let  $U_x$  be a matrix whose columns forms an orthonormal basis of  $\mathcal{T}_x$ , we define the projected Hessian of OCP at  $x$  as

$$\mathcal{H}(x) := U_x^\top \left( \nabla^2 f(x) - \sum_{i=1}^p \lambda_i(x) \nabla^2 c_i(x) \right) U_x, \quad (2.5)$$

The following proposition characterizes the relationship between  $\mathcal{H}(x)$  and  $\text{hess } f(x)$ .

**Proposition 2.5.** Given any  $x \in \mathcal{M}$ , suppose  $x$  is a first-order stationary point of OCP, then  $\mathcal{H}(x)$  and  $\text{hess } f(x)$  have the same eigenvalues. Moreover,  $\lambda_{\min}(\text{hess } f(x)) = \lambda_{\min}(\mathcal{H}(x))$  and  $x$  is a second-order stationary point of OCP if and only if  $\mathcal{H}(x) \succeq 0$ .

The proof of the above proposition directly follows from the Proposition 2.4 and [3], and hence we omit it for simplicity.

**Definition 2.6.** Given  $x \in \mathbb{R}^n$ , we say  $x$  is a first-order stationary point of CDF if

$$\nabla h(x) = 0. \quad (2.6)$$

Besides, when  $h$  is twice-order differentiable, we say a point  $x \in \mathbb{R}^n$  is a second-order stationary point of  $h$  if  $x$  is a first-order stationary point of  $h$  and satisfies

$$\nabla^2 h(x) \succeq 0. \quad (2.7)$$

### 2.3 Constants

For any given  $x \in \mathcal{M}$ , we define the positive scalar  $\rho_x \leq 1$  as

$$\rho_x := \arg \max_{0 < \rho \leq 1, \mathcal{B}_{x,\rho} \subset \mathcal{X}} \rho \quad \text{s.t.} \quad \inf \left\{ \sigma_{p'}(J_c(y)) : y \in \mathcal{B}_{x,\rho} \right\} \geq \frac{1}{2} \sigma_{p'}(J_c(x)).$$

Based on the definition of  $\rho_x$ , we can define the set  $\Theta_x := \{y \in \mathbb{R}^n : \|y - x\| \leq \rho_x\}$  and define several constants as follows:

- $\sigma_{x,c} := \sigma_{p'}(J_c(x));$
- $M_{x,f} := \sup_{y \in \Theta_x} \|\nabla f(\mathcal{A}(y))\|;$
- $M_{x,c} := \sup_{y \in \Theta_x} \|J_c(y)\|;$
- $M_{x,A} := \sup_{y \in \Theta_x} \|J_{\mathcal{A}}(y)\|;$
- $L_{x,g} := \sup_{y,z \in \Theta_x, y \neq z} \frac{\|\nabla g(y) - \nabla g(z)\|}{\|y - z\|};$

- $L_{x,c} := \sup_{y,z \in \Theta_x, y \neq z} \frac{\|J_c(y) - J_c(z)\|}{\|y - z\|};$
- $L_{x,A} := \sup_{y,z \in \Theta_x, y \neq z} \frac{\|J_A(y) - J_A(z)\|}{\|y - z\|};$
- $L_{x,b} := \sup_{y,z \in \Theta_x, y \neq z} \frac{\|J_A(y)J_c(\mathcal{A}(y)) - J_A(z)J_c(\mathcal{A}(z))\|}{\|y - z\|}.$

Based on these constants, we further set

$$\varepsilon_x := \min \left\{ \frac{\rho_x}{2}, \frac{\sigma_{x,c}}{32L_{x,c}(M_{x,A} + 1)}, \frac{\sigma_{x,c}^2}{8L_{x,b}M_{x,c}} \right\},$$

and define the following sets:

- $\Omega_x := \{y \in \mathbb{R}^n : \|y - x\| \leq \varepsilon_x\};$
- $\bar{\Omega}_x := \left\{ y \in \mathbb{R}^n : \|y - x\| \leq \frac{\sigma_{x,c}\varepsilon_x}{4M_{x,c}(M_{x,A} + 1) + \sigma_{x,c}} \right\};$
- $\Omega := \bigcup_{x \in \mathcal{M}} \Omega_x;$
- $\bar{\Omega} := \bigcup_{x \in \mathcal{M}} \bar{\Omega}_x.$

It is worth mentioning that Assumption 1.1 guarantees that  $\sigma_{x,c} > 0$  for any given  $x \in \mathcal{M}$ , which implies that  $\varepsilon_x > 0$ . On the other hand, we can conclude that  $\bar{\Omega}_x \subset \Omega_x \subset \Theta_x$  holds for any given  $x \in \mathcal{M}$ , and  $\mathcal{M}$  lies in the interior of  $\bar{\Omega}$ .

Finally, the following assumption is needed in analyzing the second-order stationarity of CDF.

**Assumption 2.7. Assumption on twice-order differentiability**

- $f, c$  and  $\mathcal{A}$  are twice differentiable in  $\mathbb{R}^n$ .

### 3 Theoretical Properties

In this section, we present the theoretical analysis on the equivalence between OCP and CDF with the RCRCQ condition. Therefore, we first establish some basic properties of the constraint dissolving mapping  $\mathcal{A}$  in Section 3.1. Based on these theoretical properties of  $\mathcal{A}$ , we propose a practical scheme on choosing the thresholding value for penalty parameter  $\beta$  for CDF, and discuss how to compute thresholding value in practice. Finally, we prove that for any penalty  $\beta$  larger than the proposed thresholding value, OCP and CDF have the same first-order and second-order stationary points in a neighborhood of  $\mathcal{M}$ .

#### 3.1 Theoretical properties of $\mathcal{A}$

In this subsection, we aim to establish the same theoretical results as [49, Section 3.1] under Assumption 1.1, where we only assume RCRCQ holds for every feasible point of OCP. We start with evaluating the relationships among  $\|c(x)\|$ ,  $\|c(\mathcal{A}(x))\|$  and  $\text{dist}(x, \mathcal{M})$  in the following lemmas.

**Lemma 3.1.** *For any given  $x \in \mathcal{M}$ , the following inequalities hold for any  $y \in \Omega_x$ ,*

$$\frac{1}{M_{x,c}} \|c(y)\| \leq \text{dist}(y, \mathcal{M}) \leq \frac{2}{\sigma_{x,c}} \|c(y)\|. \quad (3.1)$$

*Proof.* Let  $z \in \text{proj}(y, \mathcal{M})$ , then from the definition of  $z$  we can conclude that  $\|z - y\| \leq \|y - x\|$ . Thus  $\|z - x\| \leq \|z - y\| + \|y - x\| \leq 2\varepsilon_x \leq \rho_x$ , and hence  $z \in \Theta_x$ . By the mean-value theorem, for any fixed  $v \in \mathbb{R}^p$  there exists a point  $\xi_v \in \mathbb{R}^n$  that is a convex combination of  $y$  and  $z$  such that  $v^\top c(y) = (y - x)^\top J_c(\xi_v)v$ . By the convexity of  $\Theta_x$ ,  $\xi_v \in \Theta_x$  holds for any  $v \in \mathbb{R}^p$ . Therefore, we get

$$\|c(y)\| = \sup_{v \in \mathbb{R}^p, \|v\|=1} v^\top c(y) = \sup_{v \in \mathbb{R}^p, \|v\|=1} (y - x)^\top J_c(\xi_v)v \leq \sup_{v \in \Theta_x} \|J_c(\xi_v)\| \|y - z\| \leq M_{x,c} \text{dist}(y, \mathcal{M}).$$



Moreover, it follows from the definition of  $z$  that  $y - z \in \text{range}(J_c(z))$ . As a result, let  $\tilde{v} = \frac{J_c(z)^\top(y-z)}{\|J_c(z)^\top(y-z)\|}$ , we have

$$\begin{aligned}
\|c(y)\| &= \sup_{v \in \mathbb{R}^p, \|v\|=1} (y-z)^\top J_c(\xi_v) v \geq (y-z)^\top J_c(\xi_{\tilde{v}}) \tilde{v} \\
&= (y-z)^\top J_c(z) \tilde{v} + (y-z)^\top (J_c(z) - J_c(\xi_{\tilde{v}})) \tilde{v} \\
&= \left\| J_c(z)^\top (y-z) \right\| + (y-z)^\top (J_c(z) - J_c(\xi_{\tilde{v}})) \tilde{v} \\
&\geq \left\| J_c(z)^\top (y-z) \right\| - L_{x,c} \|y-z\|^2 \\
&\geq (\sigma_{x,c} - \varepsilon_x L_{x,c}) \text{dist}(y, \mathcal{M}) \geq \frac{\sigma_{x,c}}{2} \text{dist}(y, \mathcal{M}).
\end{aligned}$$

□

**Lemma 3.2.** For any given  $x \in \mathcal{M}$ , it holds that

$$\|\mathcal{A}(y) - y\| \leq \frac{2(M_{x,A} + 1)}{\sigma_{x,c}} \|c(y)\|, \quad \text{for any } y \in \Omega_x. \quad (3.2)$$

*Proof.* For any given  $y \in \Omega_x$ , we choose  $z \in \text{proj}(y, \mathcal{M})$ . Then we can conclude that  $z \in \Theta_x$ . Furthermore, from the Lipschitz continuity of  $\mathcal{A}$  and the fact that  $\mathcal{A}(z) - z = 0$ , it holds that

$$\|\mathcal{A}(y) - y\| = \|(\mathcal{A}(y) - y) - (\mathcal{A}(z) - z)\| \leq (M_{x,A} + 1) \text{dist}(y, \mathcal{M}) \leq \frac{2(M_{x,A} + 1)}{\sigma_{x,c}} \|c(y)\|, \quad (3.3)$$

where the last inequality follows from Lemma 3.1. □

**Lemma 3.3.** For any given  $x \in \mathcal{M}$ , it holds that

$$\|c(\mathcal{A}(y))\| \leq \frac{4L_{x,b}}{\sigma_{x,c}^2} \|c(y)\|^2, \quad \text{for any } y \in \Omega_x. \quad (3.4)$$

*Proof.* For any given  $y \in \Omega_x$ , we choose  $z \in \text{proj}(y, \mathcal{M})$ . It holds that  $z \in \Theta_x$ . By the mean-value theorem, for any  $v \in \mathbb{R}^p$ , there exists  $t_v \in [0, 1]$  and  $\xi_v = t_v y + (1 - t_v)z$  such that

$$v^\top c(\mathcal{A}(y)) = v^\top (J_{\mathcal{A}}(\xi_v) J_c(\mathcal{A}(\xi_v)))^\top (y - z). \quad (3.5)$$

The convexity of  $\Theta_x$  ensures that  $\xi_v \in \Theta_x$  holds for any  $v \in \mathbb{R}^p$ . Therefore, from the definition of  $L_{x,b}$  and  $\Omega_x$ , we get

$$\begin{aligned}
\|c(\mathcal{A}(y))\| &= \sup_{v \in \mathbb{R}^p, \|v\|=1} v^\top c(\mathcal{A}(y)) = \sup_{v \in \mathbb{R}^p, \|v\|=1} v^\top (J_{\mathcal{A}}(\xi_v) J_c(\mathcal{A}(\xi_v)))^\top (y - z) \\
&\leq \sup_{v \in \mathbb{R}^p, \|v\|=1} \left\| (J_{\mathcal{A}}(\xi_v) J_c(\mathcal{A}(\xi_v)))^\top (y - z) \right\| \leq \sup_{v \in \mathbb{R}^p, \|v\|=1} \|J_{\mathcal{A}}(\xi_v) J_c(\mathcal{A}(\xi_v))\| \text{dist}(y, \mathcal{M}) \\
&\leq L_{x,b} \sup_{v \in \mathbb{R}^p, \|v\|=1} \|\xi_v - z\| \text{dist}(y, \mathcal{M}) \leq L_{x,b} \text{dist}(y, \mathcal{M})^2 \leq \frac{4L_{x,b}}{\sigma_{x,c}^2} \|c(y)\|^2,
\end{aligned} \quad (3.6)$$

where the last inequality follows from Lemma 3.1. □

For any given  $x \in \mathcal{M}$  and  $y \in \Omega_x$ , Lemma 3.3 illustrates that the operator  $\mathcal{A}$  can reduce the feasibility violation of  $y$  quadratically when  $y$  is sufficiently close to  $\mathcal{M}$ .

In the rest of this subsection, we present the theoretical property of  $\mathcal{A}^\infty$  and  $J_{\mathcal{A}}$  in Lemma 3.4 - Lemma 3.7, whose proof directly follows the routines in [49, Section 3] and thus is omitted for simplicity.

**Lemma 3.4.** For any given  $x \in \mathcal{M}$  and any  $y \in \bar{\Omega}_x$ ,  $\mathcal{A}^\infty(y)$  exists and  $\mathcal{A}^\infty(y) \in \Omega_x \cap \mathcal{M}$ . Moreover, it holds that

$$\|\mathcal{A}^\infty(y) - y\| \leq \frac{4(M_{x,A} + 1)}{\sigma_{x,c}} \|c(y)\|. \quad (3.7)$$

**Lemma 3.5.** For any given  $x \in \mathcal{M}$ , the inclusion  $J_{\mathcal{A}}(x)^\top d \in \mathcal{T}_x$  holds for any  $d \in \mathbb{R}^n$ . Moreover, when  $d \in \mathcal{T}_x$ , it holds that  $J_{\mathcal{A}}(x)^\top d = d$ .

**Lemma 3.6.** For any given  $x \in \mathcal{M}$ , the equality  $J_{\mathcal{A}}(x)d = 0$  holds if and only if  $d \in \mathcal{N}_x$ .

**Lemma 3.7.** For any given  $x \in \mathcal{M}$ , it holds that  $J_{\mathcal{A}}(x)^2 = J_{\mathcal{A}}(x)$ .

## 3.2 A practical scheme for estimating penalty parameter

In this subsection, we discuss how to practically choose an appropriate penalty parameter for CDF. Let the thresholding value for the penalty parameter  $\beta$  in CDF be defined as the following definition.

**Definition 3.8.** For any given  $x \in \mathcal{M}$ , we set

$$\tilde{\beta}_x := \sup_{y \in \Omega_x} \left\{ \max \left\{ \frac{2(f(\mathcal{A}^2(y)) - f(\mathcal{A}(y))))}{\|c(y)\|^2 - \|c(\mathcal{A}(y))\|^2}, \frac{(\mathcal{A}(y) - y)^\top J_{\mathcal{A}}(y) \nabla f(\mathcal{A}(y))}{(y - \mathcal{A}(y))^\top J_c(y) c(y)}, 0 \right\} \right\}$$

We first show that  $\tilde{\beta}_x < +\infty$  for any  $x \in \mathcal{M}$  in the following proposition.

**Proposition 3.9.** For any  $x \in \mathcal{M}$ , it holds that

$$\tilde{\beta}_x \leq \max \left\{ \frac{64M_{x,f}(M_{x,A} + 1)L_{x,b}}{3\sigma_{x,c}^3}, \frac{4(L_{x,b} + (L_{x,A} + 1))M_{x,A}M_{x,f}}{\sigma_{x,c}^2} \right\}.$$

*Proof.* Firstly, it directly follows [49, Proposition 4.2] that

$$\sup_{y \in \Omega_x} \left\{ \frac{2(f(\mathcal{A}^2(y)) - f(\mathcal{A}(y))))}{\|c(y)\|^2 - \|c(\mathcal{A}(y))\|^2} \right\} \leq \frac{64M_{x,f}(M_{x,A} + 1)L_{x,b}}{3\sigma_{x,c}^3}.$$

Moreover, for any  $x \in \mathcal{M}$  and any  $y \in \Omega_x$ , let  $z \in \text{proj}(y, \mathcal{M})$ , then there exists  $\xi = ty + (1-t)z$  for some  $t \in [0, 1]$  such that

$$\begin{aligned} (y - \mathcal{A}(y))^\top J_c(y) c(y) &= (y - z)(I_n - J_{\mathcal{A}}(\xi)) J_c(y) c(y) \\ &\geq (y - z)^\top J_c(y) c(y) - \left| (y - z)^\top J_{\mathcal{A}}(y) J_c(y) c(y) \right| - L_{x,A} M_{x,c} \|c(y)\| \|y - z\|^2 \\ &\geq \sigma_{x,c} \|y - z\| \|c(y)\| - (L_{x,c} + L_{x,A} M_{x,c} + L_{x,b}) \|y - z\|^2 \|c(y)\| \\ &\geq \frac{\sigma_{x,c}}{2} \|y - z\| \|c(y)\|. \end{aligned}$$

Together with Lemma 3.1, we achieve that

$$(y - \mathcal{A}(y))^\top J_c(y) c(y) \geq \frac{\sigma_{x,c}}{2M_{x,c}} \|c(y)\|^2.$$

Moreover, from the middle-value theorem, it holds that

$$\begin{aligned} & |(y - \mathcal{A}(y))^\top J_{\mathcal{A}}(y) \nabla f(\mathcal{A}(y))| \\ & \leq |(y - z)^\top (I_n - J_{\mathcal{A}}(y)) J_{\mathcal{A}}(y) \nabla f(\mathcal{A}(y))| + (L_{x,A} + 1) M_{x,A} M_{x,f} \|y - z\|^2 \\ & \leq (L_{x,b} + (L_{x,A} + 1) M_{x,A}) M_{x,f} \|y - z\|^2 \\ & \leq \frac{2(L_{x,b} + (L_{x,A} + 1)) M_{x,A} M_{x,f}}{\sigma_{x,c}} \|c(y)\| \|y - z\|. \end{aligned}$$

Therefore, for any  $y \in \Omega_x$ , we obtain

$$\begin{aligned} \frac{(y - \mathcal{A}(y))^\top J_{\mathcal{A}}(y) \nabla f(\mathcal{A}(y))}{(y - \mathcal{A}(y))^\top J_c(y) c(y)} &\leq \frac{\frac{2(L_{x,b} + (L_{x,A} + 1))M_{x,A}M_{x,f}}{\sigma_{x,c}} \|c(y)\| \|y - z\|}{\frac{\sigma_{x,c}}{2} \|c(y)\| \|y - z\|} \\ &\leq \frac{4(L_{x,b} + (L_{x,A} + 1))M_{x,A}M_{x,f}}{\sigma_{x,c}^2}, \end{aligned}$$

hence complete the proof.  $\square$

### 3.3 Results on equivalence

This subsection investigates the relationships between OCP and CDF on their stationary points and local minimizers. We start by presenting the explicit expression for the gradient and Hessian of CDF.

**Proposition 3.10.** *The gradient of  $h$  in CDF can be expressed as*

$$\nabla h(x) = J_{\mathcal{A}}(x) \nabla f(\mathcal{A}(x)) + \beta J_c(x) c(x). \quad (3.8)$$

Furthermore, under Assumption 2.7, the Hessian of  $g(x) := f(\mathcal{A}(x))$  can be expressed as

$$\nabla^2 g(x) = J_{\mathcal{A}}(x) \nabla^2 f(\mathcal{A}(x)) J_{\mathcal{A}}(x)^\top + \mathcal{D}_{J_{\mathcal{A}}}(x) [\nabla f(\mathcal{A}(x))]. \quad (3.9)$$

and the Hessian of  $h(x)$  is

$$\nabla^2 h(x) = \nabla^2 g(x) + \beta \left( J_c(x) J_c(x)^\top + \mathcal{D}_{J_c}(x) [c(x)] \right). \quad (3.10)$$

The proof for Proposition 3.10 is straightforward from the expression of  $h$  in CDF, hence is omitted in this paper.

**Proposition 3.11.** *For any  $x \in \mathcal{M}$ , then  $x$  is a first-order stationary point of OCP if and only if  $x$  is a first-order stationary point of CDF.*

*Proof.* For any first-order stationary point,  $x \in \mathcal{M}$  of OCP, it follows from the equality (2.2) that

$$\nabla h(x) = J_{\mathcal{A}}(x) \nabla f(x) + \beta J_c(x) c(x) = J_{\mathcal{A}}(x) J_c(x) \lambda(x) = 0,$$

which implies that  $x$  is a first-order stationary point of CDF.

On the other hand, for any  $x \in \mathcal{M}$  that is a first-order stationary point of CDF, it holds that

$$J_{\mathcal{A}}(x) \nabla f(x) = 0,$$

which results in the inclusion  $\nabla f(x) \in \mathcal{N}_x = \text{range}(J_c(x))$  from Lemma 3.6. By Definition 2.1, we conclude that  $x$  is a first-order stationary point of OCP.  $\square$

**Theorem 3.12.** *For any given  $x \in \mathcal{M}$ , suppose  $\beta > \tilde{\beta}_x$ , then any first-order stationary point of CDF in  $\Omega_x$  is a first-order stationary point of OCP.*

*Proof.* For any  $y \in \Omega_x$  that is a first-order stationary point of CDF, it holds from Proposition 3.10 that

$$0 = (y - \mathcal{A}(y))^\top \nabla h(y) = (y - \mathcal{A}(y))^\top J_{\mathcal{A}}(y) \nabla f(\mathcal{A}(y)) + \beta (y - \mathcal{A}(y))^\top J_c(y) c(y). \quad (3.11)$$

Moreover, for any  $y \in \Omega_x$ , it holds that

$$\begin{aligned} \|(J_{\mathcal{A}}(y) - I_n) J_c(y) c(y)\| &\geq \|J_c(y) c(y)\| - \|J_{\mathcal{A}}(y) J_c(y) c(y)\| \\ &\geq \frac{\sigma_{x,c}}{2} \|c(y)\| - \|J_{\mathcal{A}}(y) J_c(y)\| \|c(y)\| \geq \frac{\sigma_{x,c}}{2} \|c(y)\| - L_{x,b} \text{dist}(y, \mathcal{M}) \|c(y)\| \\ &\geq \frac{\sigma_{x,c}}{2} \|c(y)\| - L_{x,b} \varepsilon_x \|c(y)\| \geq \frac{\sigma_{x,c}}{4} \|c(y)\|. \end{aligned}$$

Therefore, from Definition 3.8, it holds that

$$\begin{aligned}
0 &= \|(J_{\mathcal{A}}(y) - I_n)\nabla h(y)\| \\
&= \|(J_{\mathcal{A}}(y) - I_n)J_{\mathcal{A}}(y)\nabla f(\mathcal{A}(y)) + \beta(J_{\mathcal{A}}(y) - I_n)J_c(y)c(y)\| \\
&\geq \beta\|(J_{\mathcal{A}}(y) - I_n)J_c(y)c(y)\| - \|(J_{\mathcal{A}}(y) - I_n)J_{\mathcal{A}}(y)\nabla f(\mathcal{A}(y))\| \\
&\geq (\beta - \tilde{\beta}_x)\|(J_{\mathcal{A}}(y) - I_n)J_c(y)c(y)\| \\
&\geq (\beta - \tilde{\beta}_x)\frac{\sigma_{x,c}}{4}\|c(y)\|,
\end{aligned} \tag{3.12}$$

which illustrates that  $\|c(y)\| = 0$  and thus  $y \in \mathcal{M}$ . Together with Proposition 3.11, we conclude that  $y$  is a first-order stationary point of OCP, and complete the proof.  $\square$

**Theorem 3.13.** *Suppose Assumption 2.7 holds. Any second-order stationary point of OCP is a second-order stationary point of CDF. On the other hand, for any given  $x \in \mathcal{M}$ , if  $\beta \geq \tilde{\beta}_x$  and  $y \in \Omega_x$  is a second-order stationary point of CDF, then  $y$  is a second-order stationary point of OCP.*

*Proof.* We prove this proposition by contradiction. Suppose  $x$  is a second-order stationary point of OCP but is not a second-order stationary point for CDF. Then there exists a constant  $\tau > 0$  and a sequence  $\{y_i\} \subset \bar{\Omega}_x$  such that  $\{y_i\} \rightarrow x$  and  $h(y_i) < h(x) - \tau\|y_i - x\|^2$  holds for any  $i \geq 1$ .

From the inequality

$$\beta \geq 2 \cdot \sup_{y \in \Omega_x} \left\{ \max \left\{ -\frac{f(\mathcal{A}(y)) - f(\mathcal{A}^2(y))}{\|c(\mathcal{A}(y))\|^2 - \|c(y)\|^2}, 0 \right\} \right\},$$

it is easy to verify that the following inequality holds for any  $y \in \Omega_x$ ,

$$h(\mathcal{A}(y)) = f(\mathcal{A}^2(y)) + \frac{\beta}{2}\|c(\mathcal{A}(y))\|^2 \leq f(\mathcal{A}(y)) + \frac{\beta}{2}\|c(y)\|^2 = h(y). \tag{3.13}$$

Therefore, together with (3.13), we can conclude that for any  $y \in \bar{\Omega}_x$ , it holds that

$$f(\mathcal{A}^\infty(y)) = h(\mathcal{A}^\infty(y)) \leq h(\mathcal{A}(y)) \leq h(y) - \tau\|y_i - x\|^2. \tag{3.14}$$

Furthermore, notice that

$$\|\mathcal{A}^\infty(y_i) - y_i\| \leq \frac{4(M_{x,A} + 1)}{\sigma_{x,c}}\|c(y_i)\|, \tag{3.15}$$

then it holds that

$$\begin{aligned}
\|\mathcal{A}^\infty(y_i) - x\| &\leq \frac{4(M_{x,A} + 1)}{\sigma_{x,c}}\|c(y_i)\| + \|y_i - x\| \\
&\leq \frac{4(M_{x,A} + 1)L_{x,c}}{\sigma_{x,c}}\text{dist}(y_i, \mathcal{M}) + \|y_i - x\| \\
&\leq \left( \frac{4(M_{x,A} + 1)L_{x,c}}{\sigma_{x,c}} + 1 \right) \|y_i - x\|.
\end{aligned} \tag{3.16}$$

Therefore, from (3.14) and (3.16), it holds that  $\{\mathcal{A}^\infty(y_i)\} \rightarrow x$  and for any  $i \geq 1$ ,

$$f(\mathcal{A}^\infty(y_i)) \leq f(x) - \frac{\tau}{\left( \frac{4(M_{x,A} + 1)L_{x,c}}{\sigma_{x,c}} + 1 \right)^2} \|\mathcal{A}^\infty(y_i) - x\|^2,$$

which contradicts the fact that  $x$  is a second-order stationary point of OCP as illustrated in [3, Proposition 5.5.5]. Therefore, from the contradiction, we can conclude that  $x$  is a second-order stationary for CDF and complete the proof.  $\square$

**Remark 3.14.** As illustrated in Proposition 3.9,  $\tilde{\beta}_x$  is well-defined for any given  $x \in \mathcal{M}$ . Moreover, the theoretical results in this subsection illustrate that for any  $x \in \mathcal{M}$ , choosing  $\beta > \tilde{\beta}_x$  can guarantee that OCP and CDF have the same first-order and second-order stationary points in  $\Omega_x$ . Therefore, we suggest the following procedures for choosing the penalty parameter for CDF. We first choose a reference point  $\tilde{x} \in \mathcal{M}$  and randomly sample  $N_\beta$  points  $\{x_1^{ref}, \dots, x_{N_\beta}^{ref}\} \in \mathcal{B}(\tilde{x}, \delta_\beta) := \{x \in \mathbb{R}^n : \|x - \tilde{x}\| \leq \delta_\beta\}$ . Then we compute an estimated value for  $\beta$  as follows:

$$\tilde{\beta}^* = \theta_\beta \cdot \max_{1 \leq i \leq N_\beta} \left\{ \max \left\{ \frac{2(f(\mathcal{A}^2(x_i^{ref})) - f(\mathcal{A}(x_i^{ref})))}{\|c(x_i^{ref})\|^2 - \|c(\mathcal{A}(x_i^{ref}))\|^2 + \varepsilon_\beta}, \frac{(\mathcal{A}(x_i^{ref}) - x_i^{ref})^\top J_{\mathcal{A}}(x_i^{ref}) \nabla f(\mathcal{A}(x_i^{ref}))}{|(x_i^{ref} - \mathcal{A}(x_i^{ref}))^\top J_c(x_i^{ref}) c(x_i^{ref})| + \varepsilon_\beta}, 0 \right\} \right\}. \quad (3.17)$$

Here  $\delta_\beta > 0$ ,  $\varepsilon_\beta \geq 0$  and  $\theta_\beta \geq 1$  are some prefixed hyper-parameters.

## 4 Software Description

In this section, we give a brief overview on the structure of CDOpt. The idea behind the design for CDOpt is to guarantee the ease-of-use features for various types of users, including the users from optimization communities for solving standard Riemannian optimization problems over commonly used manifolds, the users from machine learning communities who wish to train neural networks with manifold constraints, and developers who aim to develop new manifolds and introduce more advanced features for CDOpt. As illustrated in Figure 1, we organize the CDOpt package into the following three parts:

- The manifold classes;
- The problem classes;
- The neural layers.

These three parts are mutually separated, hence it is easy to add new manifolds, and new neural layers in CDOpt with maximum code reuse for developers.

### 4.1 The manifold classes

The module “manifold” in CDOpt describes the manifold constraints by the following essential components for describing the corresponding constraint dissolving mapping,

- The expression of constraints  $c(x)$ ,  $J_c(x)$  and the Hessian-vector product of  $\|c(x)\|^2$ ;
- The expression of  $\mathcal{A}(x)$ ,  $J_{\mathcal{A}}(x)$  and the second-order differential of  $\mathcal{A}(x)$ ;
- The rules to compute  $h(x)$ ,  $\nabla h(x)$ , and  $\nabla^2 f(x)$  from  $f$ ,  $\mathcal{A}$ ,  $c$  and their derivatives.

All the manifolds in CDOpt are available as derived classes from the base class named `basic_manifold`, which is available in the `manifold` module of CDOpt. Note that all the essential components in these manifold classes can be expressed by  $c(x)$ ,  $\mathcal{A}(x)$  and their differentials. Therefore, if some of these materials are not provided in the derived classes of the `basic_manifold`, all the essential materials can be automatically calculated based on the selected automatic differentiation (AD) packages from the supported numerical backends. In particular, if only the expression of  $c(x)$  is provided in the derived class of `basic_manifold`, the constraint dissolving mapping is automatically chosen as

$$\mathcal{A}_c(x) = x - J_c(x)(J_c(x)^\top J_c(x) + \sigma I_p)^{-1} c(x). \quad (4.1)$$

Here  $J_c(x) \in \mathbb{R}^{n \times p}$  denotes the transpose of the Jacobian of  $c$  at  $x$ , which is also computed by the selected AD packages if it is not provided. As a result, users only need to provide the expression of the manifold constraints  $c(x)$  and its corresponding numerical backends for defining new manifold constraints though `basic_manifold` from the `manifold` module in CDOpt.

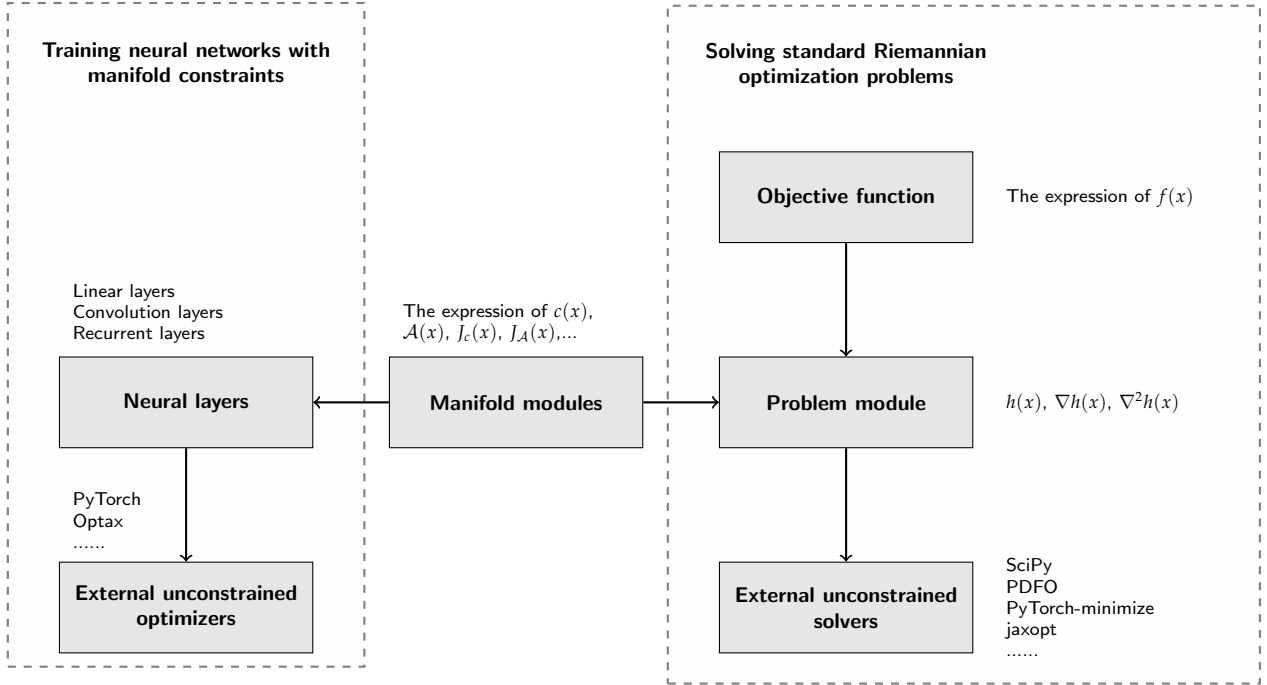


Figure 1: The sketch of the structure of CDOpt.

CDOpt supports various numerical backends, where the type of the variables, APIs for build-in functions, and AD packages differ among different numerical backends. As a result, CDOpt provides some derived classes from `basic_manifold`: `basic_manifold_np`, `basic_manifold_torch` and `basic_manifold_jax`. In these derived classes, only the expression of  $c(x)$  is required in defining a manifold, and their numerical backends are fixed as NumPy + Autograd, PyTorch and JAX, respectively. Then various specific manifolds, with different numerical backends, are developed by inheriting `basic_manifold_np`, `basic_manifold_torch` or `basic_manifold_jax`. Listing 1 illustrates how to define the Riemannian manifold  $\{X \in \mathbb{R}^{m \times s} : X^\top X T = I_s\}$  in CDOpt only by the expression of the constraints  $X^\top X T - I_s = 0$ .

---

```

class customized_manifold(basic_manifold_np):
    def __init__(self, var_shape, T):
        m, s = *var_shape
        self.T = T
        self.Is = np.eye(s)
        super().__init__('customized_manifold', (m, s), (s, s))

    def C(self, X):
        return (X.T @ X) @ self.T - self.Is

```

---

Listing 1: Define customized Riemannian manifold in CDOpt

Furthermore, CDOpt provides various predefined manifolds, where the essential components are prefixed manually to achieve the best computational efficiency. Table 1 illustrates these predefined manifolds in CDOpt.

## 4.2 Problem class

The `problem` class in CDOpt describes the Riemannian optimization problem OCP by the manifold class for the constraints  $c(x)$ , the objective function  $f(x)$  and its derivatives. As shown in Listing 2,

Name	$\mathcal{M}$	Predefined manifolds with different backends
Euclidean space	$\mathbb{R}^n$	eudliean_np eudliean_torch eudliean_jax
Sphere	$\{x \in \mathbb{R}^n : \ x\  = 1\}$	sphere_np sphere_torch sphere_jax
Oblique manifold	$\{X \in \mathbb{R}^{m \times s} : \text{Diag}(XX^\top) = I_m\}$	oblique_np oblique_torch oblique_jax
Stiefel manifold	$\{X \in \mathbb{R}^{m \times s} : X^\top X = I_p\}$	stiefel_np stiefel_torch stiefel_jax
Grassmann manifold	$\{X \in \mathbb{R}^{m \times s} : X^\top X = I_p\}$	stiefel_np stiefel_torch stiefel_jax
Generalized Stiefel manifold	$\{X \in \mathbb{R}^{m \times s} : X^\top B X = I_p\}, B \succeq 0$	generalized_stiefel_np generalized_stiefel_torch generalized_stiefel_jax
Hyperbolic manifold	$\{X \in \mathbb{R}^{m \times s} : X^\top B X = I_p\}, B$ is indefinite	hyperbolic_np hyperbolic_torch hyperbolic_jax
Symplectic Stiefel manifold	$\{X \in \mathbb{R}^{2m \times 2s} : X^\top Q_m X = Q_s\}, Q_m := \begin{bmatrix} 0_{m \times m} & I_m \\ -I_m & 0_{m \times m} \end{bmatrix}$	symp_stiefel_np symp_stiefel_torch symp_stiefel_jax
Complex sphere	$\{x \in \mathbb{C}^n : \ x\  = 1\}$	complex_sphere_np complex_sphere_torch complex_sphere_jax
Complex oblique manifold	$\{X \in \mathbb{C}^{m \times s} : \text{Diag}(XX^H) = I_m\}$	complex_oblique_np complex_oblique_torch complex_oblique_jax
Complex Stiefel manifold	$\{X \in \mathbb{C}^{m \times s} : X^H X = I_s\}$	complex_stiefel_np complex_stiefel_torch complex_stiefel_jax
Product manifold	$\mathcal{M}_1 \times \mathcal{M}_2 \times \dots$	product_manifold

Table 1: Predefined manifold in CDOpt.

CDOpt allows users to describe the optimization problem only from the expression of the objective function and the instantiated manifold.

---

```
manifold = stiefel_torch( (100,10) )
prob = cdopt.core.problem(manifold, obj_fun, beta = 'auto')
```

---

Listing 2: Describe Riemannian optimization problem in CDOpt

When instantiating the `problem` class, the argument `obj_fun` should be a callable object, and the argument `manifold` should be the instantiation of the `manifold` class in CDOpt. Other materials for optimization, including the gradient and Hessian of the objective function  $f$ , are optional in the instantiation of `problem` class. If these materials are not provided, the `problem` class automatically computes them by the chosen numerical backends behind the interface.

Furthermore, if the penalty parameter  $\beta$  in CDF is not provided in the instantiation of the `problem` class, CDOpt can automatically estimate an appropriate value of  $\beta$ . When the argument `beta` is set as `'auto'`, CDOpt randomly chooses the penalty parameter by the scheme presented in Remark 3.14, where the reference point  $\tilde{x} \in \mathcal{M}$  from the `Init_point` method of the `manifold` class, and the default values for the hyperparameters are chosen as  $N_\beta = 100$ ,  $\delta_\beta = 0.01$ ,  $\varepsilon_\beta = 10^{-14}$  and  $\theta_\beta = 2$ . Users can set their customized hyperparameters via the argument `autobeta_args`.

After instantiation, the `problem` class provides the constraint dissolving function CDF and its derivatives as callable objects. In the attributes of the `problem` class, `cdf_obj`, `cdf_grad` and `cdf_hvp` are callable objects that return the function value, gradient and Hessian-vector product of the constraint dissolving function, respectively. Their input arguments and outputs are of the same type as the selected numerical backend of the problem. Moreover, to adapt the optimizers that are developed based on NumPy and SciPy, the `problem` class provides the attributes `cdf_obj_vec_np`, `cdf_grad_vec_np` and `cdf_hvp_vec_np`, where their inputs and outputs are all NumPy 1D array. Based on the provided attributes from the `problem` class, users can directly apply the unconstrained optimization solvers from various existing packages, such as SciPy, PDFO, PyTorch-minimize and jaxopt.

### 4.3 Neural layers

PyTorch and Flax are powerful frameworks for training neural networks, where neural networks are built by neural layers from `torch.nn` or `flax.linen` modules. For those users that aim to train neural networks with manifold constraints, CDOpt provides various predefined neural layers in its `cdopt.nn` and `cdopt.linen` modules for PyTorch and Flax, respectively. These predefined layers in CDOpt preserve the same APIs as the layers from PyTorch and Flax, hence users can plug these layers into the neural networks with minimal modification to the standard PyTorch or Flax codes.

The neural layers from `cdopt.nn` module are the derived classes of the `module` class from `torch.nn`, hence can be integrated with any neural network built from the neural layers from `torch.nn`. Therefore, users can build neural networks by mixing the layers from both `cdopt.nn` and `torch.nn`. In the instantiation of the neural layers from `cdopt.nn`, users can set the manifold constraints by the `manifold_class` argument and choose the penalty parameter  $\beta$  by the `penalty_param` argument. When instantiated, the neural layers in the `cdopt.nn` module first call its `__init__` method to instantiate the manifold according to the `manifold_class` argument and generate the initial weights on the manifold. After instantiation, the neural layers provide the attributes `manifold` and `quad_penalty` to access the instantiated manifolds and the value of  $\|c(x)\|^2$ , respectively. Moreover, for any neural network that is built from the neural layers from `cdopt.nn` and `torch.nn`, we can call the function `get_quad_penalty()` from `cdopt.nn` to compute the sum of all the quadratic penalty terms of its neural layers from `cdopt.nn`.

Currently, CDOpt implements the following neural layers for PyTorch in the `cdopt.nn` module,

- `Linear`, `Bilinear`, `LazyLinear`;
- `Conv1d`, `Conv2d`, `Conv3d`, `ConvTranspose1d`, `ConvTranspose2d`, `ConvTranspose3d`;
- `RNN`, `LSTM`, `GRU`, `RNNCell`, `LSTMCell`, `GRUCell`.

Listing 3 presents a simple example, where we build a two-layer neural network by the layers from CDOpt.nn and PyTorch.nn.

---

```
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv = Conv2d_cdopt(1, 6, 5,
                                manifold_class=stiefel_torch, penalty_param = 0.05)
        self.fc = nn.Linear(84, 10)

    def forward(self, x):
        x = F.max_pool2d(F.relu(self.conv(x)), (2, 2))
        x = self.fc(x)
        x = F.log_softmax(x, dim=1)
        return x
```

---

Listing 3: Building a two-layer neural network with manifold constraints in PyTorch by predefined neural layers from `cdopt.nn`.

Furthermore, for those neural layers that are not available from `cdopt.nn`, CDOpt provides a simple way to add manifold constraints to the parameters of these neural layers. Through the function `set_constraint_dissolving` from `cdopt.nn.utils.set_constraints`, users can set the manifold constraints to the neural layers by just providing the neural layers, the name of target parameters, and the manifold class. Listing 4 presents a simple example on how to set the manifold constraints for the weights in a two-layer neural network.

---

```
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv = nn.Conv2d(1, 6, 5)
```

---



```

self.fc = nn.Linear(84, 10)
set_constraint_dissolving(self.conv, 'weight',
                          manifold_class=stiefel_torch, penalty_param = 0.05)

def forward(self, x):
    x = F.max_pool2d(F.relu(self.conv(x)), (2, 2))
    x = self.fc(x)
    x = F.log_softmax(x, dim=1)
    return x

```

Listing 4: Building a two-layer neural network with manifold constraints in PyTorch by the function `set_constraint_dissolving` from `cdopt.nn.utils.set_constraints`.

For Flax, CDOpt implements the following neural layers for training neural networks,

- Dense, DenseGeneral;
- Conv, ConvTranspose.

It is worth mentioning that the neural layers in Flax are designed in a different way from those in PyTorch.nn. In Flax, the neural layers are separated from their weights and behave as functions that map the inputs and weights to their outputs by the `__call__` method. As a result, although the neural layers from `linen` module can be called by the same arguments as those from `Flax.linen`, the quadratic penalty term  $\|c(x)\|^2$  is returned by the `__call__` method. Listing 5 illustrates how to build a neural network by the neural layers from `CDOpt.linen` and `Flax.linen`.

```

class model(flax.linen.Module):
    @flax.linen.compact
    def __call__(self, x):
        x, quad_penalty = cdopt.linen.Conv_cdopt(features=32, kernel_size=(3, 3),
                                                manifold_class = stiefel_jax)(x)
        x = flax.linen.relu(x)
        x = flax.linen.avg_pool(x, window_shape=(2, 2), strides=(2, 2))
        x = flax.linen.Dense(features=10)(x)
        return x, quad_penalty

```

Listing 5: Building a two-layer neural network with manifold constraints in Flax by predefined neural layers from `cdopt.linen`

## 4.4 Optimization through CDOpt

In CDOpt, the Riemannian optimization problem OCP is transformed into the unconstrained minimization of the constraint dissolving function CDF. Therefore, various existing unconstrained optimization solvers can be directly applied to solve OCP through minimizing CDF. CDOpt only requires the following steps for solving the optimization problem through the `problem` class,

1. Define the objective function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ ;
2. Instantiation of the manifold  $\mathcal{M} = \{x \in \mathbb{R}^n : c(x) = 0\}$ ;
3. Describe the optimization problem through `problem` class;
4. Call an external solver to minimize the constraint dissolving function.

As far as we tested, CDOpt supports the following solvers from SciPy, PDFO [38], PyTorch-minimize [14], and jaxopt [7],

- SciPy: CG, BFGS, Newton-CG, L-BFGS-B, TNC, trust-ncg, and trust-krylov;

- PyTorch-minimize: CG, L-BFGS, trust-ncg, and trust-krylov;
- jaxopt: GradientDescent, LBFGS, NonlinearCG, and its interface for `scipy.optimize.minimize`;
- PDFO: newuoa, bobyqa, lincoa.

On the other hand, CDOpt provides simple approaches to build and train neural networks that invoke manifold constraints. To impose manifold constraints to the weights of a neural layer, users only need the following two steps,

1. Replace that neural layer by its corresponding neural layers from `cdopt.nn` and `cdopt.linen`;
2. Add the quadratic penalty terms to the loss function in the training process.

Then various unconstrained optimizers (i.e. solvers for training neural networks) can be directly applied to train the modified neural network. Currently, CDOpt is tested to successfully support the following optimizers,

- All the optimizers from PyTorch and PyTorch-optimizer;
- All the optimizers from Optax.

## 5 Comparison with Existing Packages

In this section, we present a brief comparison between CDOpt and existing Python Riemannian optimization packages, including PyManopt, Geoopt, McTorch and GeoTorch. The major difference between CDOpt and these existing packages is how the OCP is treated. Developed from constraint dissolving approaches, CDOpt transfers OCP into the unconstrained minimization of CDF, where the construction of CDF avoids the need of geometrical materials from differential geometry.

CDOpt only requires  $c(x)$ ,  $\mathcal{A}(x)$  and their derivatives to describe the Riemannian manifold, hence it provides great convenience in defining Riemannian manifolds. As demonstrated in [49], it is usually easy to design the constraint dissolving mapping  $\mathcal{A}$  for  $\mathcal{M}$  since the constraint dissolving mappings only need to satisfy Assumption 1.2. When only  $c(x)$  is provided, we can choose the constraint dissolving mapping as in (4.1) with appropriate  $\alpha \geq 0$ . Due to the great convenience in describing the manifolds, CDOpt provides a wider range of pre-defined manifold classes than existing Riemannian optimization packages. Moreover, CDOpt enables users to define new manifolds only from the expression of the constraints, hence defining a new manifold in CDOpt is significantly easier than the existing Riemannian optimization packages. A detailed comparison of the supported manifolds and essential materials for new manifolds is presented in Table 2.

As CDOpt transforms OCP into the unconstrained minimization of the constraint dissolving function, CDOpt can directly and efficiently utilize existing unconstrained optimization solvers without modifying them to adapt the geometrical material. Currently, CDOpt is compatible with various existing unconstrained optimization solvers. For the optimization problem defined by the `problem` class, CDOpt can directly call all the solvers provided by SciPy, PyTorch-minimize, PDFO, jaxopt and various other unconstrained optimization packages. For training neural networks, CDOpt is compatible to the optimizers from PyTorch, PyTorch-optimizer, Optax, and various open-sourced optimizers. However, most existing Riemannian optimization packages have to develop specialized solvers to utilize the geometrical materials. Therefore, their supported solvers are relatively limited. Detailed comparisons are presented in Table 3.

Furthermore, as all of the existing Riemannian optimization packages require geometrical materials or specialized solvers, their supported numerical backends are also relatively limited. For example, although PyManopt supports PyTorch, Autograd and Tensorflow in its AD modules, its manifold module and solver module only support Numpy as the numerical backend. Additionally, the packages GeoTorch, Geoopt and McTorch are only developed based on PyTorch. As a comparison, CDOpt supports various of numerical backends in its modules, including the Numpy, PyTorch, JAX, etc. We present a detailed comparison in Table 4.

	CDopt	Pymanopt	Geoopt	McTorch	GeoTorch
Euclidean space	✓	✓	✓	✓	✓
Sphere	✓	✓	✓	✓	✓
Oblique manifold	✓	✓	×	×	×
Stiefel manifold	✓	✓	✓	✓	✓
Grassmann manifold	✓	✓	✓	✓	✓
Generalized Stiefel manifold	✓	×	×	×	×
Hyperbolic manifold	✓	×	×	×	×
Symplectic Stiefel manifold	✓	×	×	×	×
Complex sphere	✓	✓	×	×	×
Complex oblique manifold	✓	×	×	×	×
Complex Stiefel manifold	✓	×	×	×	×
Product manifold	✓	✓	✓	×	✓
Defining new manifolds	The expression of $c(x)$	Exponential and logarithmic maps, retraction, vector transport, egrad2rgrad, ehess2rhess, inner product, distance, norm	Exponential and logarithmic maps, retraction, vector transport, egrad2rgrad, ehess2rhess, inner product, distance, norm	Exponential and logarithmic maps, retraction, vector transport, egrad2rgrad, ehess2rhess, inner product, distance, norm	The explicit formation of a projection from $\mathbb{R}^N$ onto $\mathcal{M}$ for some $N > 0$ .

Table 2: Comparison of the compared packages in terms of manifold and necessary materials for defining a new manifold.

	CDopt	Pymanopt	Geoopt	McTorch	GeoTorch
Derivate-free solvers	NEWUOA, BOBYQA, LINCOA from PDFO	N.A.	N.A.	N.A.	N.A.
First-order solvers	Conjugate gradient, BFGS, limit-memory BFGS from SciPy, PyTorch-minimize and jaxopt	Riemannian conjugate gradient, Riemannian steepest descent, Riemannian line-search.	N.A.	N.A.	N.A.
Second-order solvers	Newton-CG, truncated Newton, trust-region with Krylov subsolver, trust-region Newton-CG from SciPy and PyTorch-minimize	Riemannian trust-region	N.A.	N.A.	N.A.
Training in PyTorch	All the optimizers from PyTorch.optim and PyTorch-optimizer	N.A.	Riemannian Adam, Riemannian line-search, Riemannian SGD	Riemannian Adam, Riemannian SGD	All the optimizers from PyTorch.optim and PyTorch-optimizer
Training in JAX	All the optimizers from Optax	N.A.	N.A.	N.A.	N.A.

Table 3: Comparison on available solvers in general optimization (the optimization tasks defined by derivatives of the objective functions and manifolds), and training neural network via PyTorch.

	CDopt	Pymanopt	Geoopt	McTorch	GeoTorch
Automatic differentiation	Autograd, PyTorch, JAX	Autograd, PyTorch, TensorFlow, Theano	PyTorch	PyTorch	PyTorch
Manifold	NumPy, SciPy, PyTorch, JAX	NumPy, SciPy	PyTorch	PyTorch	PyTorch
Optimization	SciPy, PyTorch, JAX, Optax	NumPy	PyTorch	PyTorch	PyTorch

Table 4: Comparison of the supported backends in different components of the compared packages.

## 6 Examples

In this section, we briefly introduce the features of CDOpt through several illustrative examples. Interested readers can refer to [https://cdopt.github.io/md\\_files/examples.html](https://cdopt.github.io/md_files/examples.html) for more examples on applying CDOpt to solve Riemannian optimization problems.

### 6.1 Orthogonal dictionary learning

CDOpt is easy-to-use when it is employed to solve standard Riemannian optimization problems through its `problem` class. CDOpt integrates various numerical backends such as Autograd, PyTorch and JAX. Various important features of these packages, including AD packages, GPU supports and JIT compilation, are performed behind CDOpt's `problem` and `manifold` modules. Therefore, users are only required to provide small amount of set-up codes for solving Riemannian optimization problems through CDOpt.

We briefly demonstrate the easy-to-use features of CDOpt by a simple example on orthogonal dictionary learning (ODL). Given data  $\{y_i\}_{i=1,\dots,m}$  generated by  $y_i = Qz_i$ , where  $Q$  is a fixed unknown orthogonal matrix and each  $z_i$  follows an i.i.d. Bernoulli-Gaussian distribution with parameter  $\theta \in (0, 1)$ . ODL aims to recover the matrix  $Z = [z_1, \dots, z_m] \in \mathbb{R}^{m \times n}$  and the orthogonal matrix  $Q \in \mathbb{R}^{n \times n}$  from the given data  $Y = [y_1, \dots, y_m]^T \in \mathbb{R}^{m \times n}$ .

Based on the  $\ell_4$ -norm maximization model proposed in [20, 51], we consider the following optimization problem over the Stiefel manifold:

$$\begin{aligned} \min_{X=[x_1, \dots, x_n] \in \mathbb{R}^{n \times n}} f(X) &:= - \sum_{1 \leq i \leq m, 1 \leq j \leq n} (y_i^\top x_j)^4 \\ \text{s. t. } X^T X &= I_n. \end{aligned} \tag{6.1}$$

The following script demonstrates how to solve (6.1) through CDOpt and JAX:

```
import numpy as np
import scipy as sp
import jax
import jax.numpy as jnp
import cdopt
from cdopt.manifold_jax import stiefel_jax

# Generating the data
n = 30
m = 10*n**2
theta = 0.3

# Set jax device and data type
device = jax.devices('gpu')[0]

Q, R = np.linalg.qr(np.random.randn(n,n))
Y = jax.device_put(jnp.array(
    ((np.random.rand(m,n)) * (np.random.rand(m,n) <= theta)) @ Q), device)

# Define objective function and Stiefel manifold
def obj_fun(X):
    return -jnp.sum(jnp.matmul(Y, X) **4 )

M = stiefel_jax((n,n), device= device)

# Describe the optimization problem and set the penalty parameter \beta.
problem_test = cdopt.core.problem(M, obj_fun, beta = 'auto')
```

```

# The vectorized function value, gradient and Hessian-vector product
# of the constraint dissolving function.
cdf_fun_np = problem_test.cdf_fun_vec_np
cdf_grad_np = problem_test.cdf_grad_vec_np
cdf_hvp_np = problem_test.cdf_hvp_vec_np

## Apply limit memory BFGS solver from scipy.minimize
from scipy.optimize import fmin_bfgs, fmin_cg, fmin_l_bfgs_b, fmin_ncg

# optimize by L-BFGS method
out_msg = sp.optimize.minimize(cdf_fun_np, problem_test.Xinit_vec_np,
                              method='L-BFGS-B', jac = cdf_grad_np)

```

---

## 6.2 Training neural network with orthogonal weight normalization

In this subsection, we present a simple example on training VGG19 [39] with orthogonally constrained convolutional kernels. The following script further demonstrates that neural networks with manifold constraints can be easily defined and trained through CDOpt. Since all the neural layers from `cdopt.nn` has the same APIs as those from `torch.nn`, modifying a neural network to involve manifold constraints through CDOpt is simple and requires minimum modifications to the standard PyTorch codes.

---

```

import torch
import torch.nn as nn
import torch.optim as optim
import torch.nn.functional as F

import torchvision
import torchvision.transforms as transforms

import cdopt
from cdopt.nn import Conv2d_cdopt, get_quad_penalty
from cdopt.manifold_torch import stiefel_torch

cfg_vgg19 = [64, 64, 'M', 128, 128, 'M', 256, 256, 256, 256, 'M',
            512, 512, 512, 512, 'M', 512, 512, 512, 512, 'M']

class VGG(nn.Module):
    def __init__(self):
        super(VGG, self).__init__()
        self.features= self._make_layers(cfg_vgg19)
        self.classifier = nn.Sequential(
            nn.Linear(512 * 7 * 7, 4096),
            nn.ReLU(inplace=True),
            nn.Dropout(0.5),
            nn.Linear(4096, 4096),
            nn.ReLU(inplace=True),
            nn.Dropout(0.5),
            nn.Linear(4096, 10),
        )
        self.avgpool = nn.AdaptiveAvgPool2d(7)

```

```

def forward(self, x):
    out = self.features(x)
    out = self.avgpool(out)
    out = out.reshape(out.size(0), -1)
    out = self.classifier(out)
    return out

def _make_layers(self, cfg):
    layers = []
    in_channels = 3
    for x in cfg:
        if x == 'M':
            layers += [nn.MaxPool2d(kernel_size=2, stride=2)]
        else:
            local_block = [Conv2d_cdopt(in_channels, x, kernel_size=3,
                padding=1, manifold_class=stiefel_torch, penalty_param = 0.05),
                nn.BatchNorm2d(x), nn.ReLU(inplace=True)]
            layers += local_block
            in_channels = x
    layers += [nn.AvgPool2d(kernel_size=1, stride=1)]
    return nn.Sequential(*layers)

def train(model, device, train_loader, optimizer, epoch):
    model.train()
    for batch_idx, (data, target) in enumerate(train_loader):
        data, target = data.to(device), target.to(device)
        optimizer.zero_grad()
        output = model(data)
        # Add quadratic penalty terms to the loss function.
        loss = F.nll_loss(output, target) + get_quad_penalty(model)
        loss.backward()
        optimizer.step()

device = torch.device("cuda")
model = VGG().to(device)
optimizer = optim.Adam(model.parameters(), lr= 1e-3)
transform=transforms.Compose([ transforms.ToTensor(), ])
trainset = torchvision.datasets.CIFAR10(
    root='./data', train=True, download=True, transform=transform)
train_loader = torch.utils.data.DataLoader(trainset, batch_size=128,
    shuffle=True, pin_memory=True)

for epoch in range(100):
    train(model, device, train_loader, optimizer, epoch)

```

---

## 7 Numerical Experiments

In this section, we test the performance of CDOpt on several important applications of OCP. All the experiments are performed on Ubuntu 20.02 platform with Intel Xeon 6342 and NVIDIA GeForce RTX 3090. Moreover, we run all these numerical experiments in Python 3.8.10 with NumPy 1.23, SciPy 1.8.1, PyTorch 1.9.0, CUDA 11.4 and JAX 0.3.14.

## 7.1 Nearest correlation matrix

In this subsection, we test the numerical performance of CDOpt on optimization problems defined by its problem interface. Moreover, we compare CDOpt with the state-of-the-art Riemannian optimization package PyManopt (version 2.0.0), where the Riemannian optimization problems must be defined through its problem interface.

Our test example is the problem of finding the nearest low-rank correlation matrix (NCM) to a given matrix  $G \in \mathbb{R}^{n \times p}$ , which can be reshaped as an optimization problem over the oblique manifold

$$\begin{aligned} \min_{X \in \mathbb{R}^{n \times p}} \quad & f(X) = \frac{1}{2} \left\| H \circ (XX^\top - G) \right\|_F^2 \\ \text{s.t.} \quad & \text{Diag}(XX^\top) = I_n, \end{aligned} \tag{7.1}$$

where  $H \in \mathbb{R}^{n \times n}$  is a nonnegative weight matrix. For all the numerical experiments in this subsection, we generate the matrix  $\hat{G}$  from the gene expression data provided in [31]. Then the matrix  $G$  is generated by perturbing  $\hat{G}$  by  $G = (1 - \theta)\hat{G} + \theta E$ , where  $\theta \geq 0$  is a prefixed parameter, and  $E \in \mathbb{R}^{n \times n}$  is a randomly generated matrix with all of its diagonal entry equals to 1. The weight matrix  $H$  in (7.1) is chosen as a symmetric matrix whose entries are uniformly distributed in  $[0, 1]$ .

We set the penalty parameter  $\beta$  for CDF by setting `beta = 'auto'` in the instantiation of the `problem` class in CDOpt. We choose the L-BFGS, CG and trust-region solvers from SciPy to test the numerical performance of CDOpt. For comparison, we choose the Riemannian CG solver and Riemannian trust-region solver from PyManopt since L-BFGS is not available in PyManopt. For CDOpt, we stop these solvers when the maximum number of iterations exceeds 10000 or the norm of the gradient its corresponding constraint dissolving function is less than  $10^{-5}$ . For the solvers from PyManopt, we stop these solvers once the norm of its Riemannian gradient is smaller than  $10^{-5}$ , or the maximum number of iterations exceeds 10000. All the other parameters are fixed as their default values. Additionally, all the solvers starts from the same initial point, which is randomly generated on the oblique manifold in each test instance.

Furthermore, we fix the numerical backends as the PyTorch package in both CDOpt and PyManopt. We only provide the expression of the objective function in all the test instances, thus the gradient and the Hessian of  $f$  are automatically computed by the AD packages from the PyTorch backends in CDOpt or PyManopt.

Table 5 and Table 6 report the numerical results on the comparison of CDOpt and PyManopt. From these tables, we can observe that CDOpt outperforms PyManopt in almost all the numerical experiments. Although CDOpt needs to reshape the variables in each iteration, applying the conjugate gradient method and trust-region method from SciPy package shows superior performance over their Riemannian versions from PyManopt. Moreover, benefited from the highly efficient L-BFGS solver that is programmed by FORTRAN and wrapped by SciPy package, CDOpt gains significant advantages against the Riemannian solvers from PyManopt. Furthermore, through its PyTorch backend, CDOpt can be greatly accelerated by computing the objective function and manifold structures on GPU.

## 7.2 Nonlinear eigenvalue problem

In this subsection, we test the numerical performance of the compared packages on solving the following smooth optimization problem over the Stiefel manifold:

$$\begin{aligned} \min_{X \in \mathbb{R}^{n \times p}} \quad & f(X) = \frac{1}{2} \text{tr} \left( X^\top L X \right) + \frac{\alpha}{4} \rho(X)^\top L^\dagger \rho(X) \\ \text{s. t.} \quad & X^\top X = I_p, \end{aligned} \tag{7.2}$$

where  $\rho(X) := \text{diag}(XX^\top)$ ,  $L$  is a tridiagonal matrix with 2 as its diagonal entries and  $-1$  as its subdiagonal and superdiagonal entries. Moreover,  $L^\dagger$  refers to the pseudo-inverse of  $L$ . Problem (7.2), arisen from electronic structure calculation, has become standard testing problems for investigating the convergence of self-consistent field methods due to its simplicity [32].

		CPU					GPU				
		fval	iter	stat	feas	time	fval	iter	stat	feas	time
$p = 10$	cdopt-lbfgs	2.31e+03	171	9.13e-06	4.39e-15	2.02	2.31e+03	167	9.14e-06	4.25e-15	0.43
	cdopt-cg	2.31e+03	197	9.12e-06	6.17e-15	2.25	2.31e+03	206	8.88e-06	8.55e-15	0.56
	cdopt-tr	2.31e+03	48	5.20e-08	4.32e-15	9.62	2.31e+03	47	9.15e-06	4.46e-15	0.94
	pymanopt-rcg	2.31e+03	319	6.17e-06	4.85e-15	1.02	2.31e+03	336	9.44e-06	5.19e-15	0.83
	pymanopt-rtr	2.31e+03	26	3.61e-07	5.59e-15	2.62	2.31e+03	26	3.12e-07	5.36e-15	0.85
$p = 20$	cdopt-lbfgs	7.66e+02	222	7.65e-06	3.98e-15	1.40	7.66e+02	215	9.44e-06	3.98e-15	0.67
	cdopt-cg	7.66e+02	277	8.71e-06	8.21e-15	11.03	7.66e+02	254	9.81e-06	7.16e-15	2.39
	cdopt-tr	7.66e+02	32	5.21e-08	4.43e-15	22.97	7.66e+02	30	3.04e-06	3.58e-15	4.30
	pymanopt-rcg	7.66e+02	336	9.32e-06	5.45e-15	7.69	7.66e+02	371	9.22e-06	5.45e-15	2.60
	pymanopt-rtr	7.66e+02	29	1.66e-06	5.78e-15	26.17	7.66e+02	29	1.69e-06	5.74e-15	6.60
$p = 30$	cdopt-lbfgs	4.26e+02	290	8.78e-06	3.95e-15	1.78	4.26e+02	304	8.16e-06	3.83e-15	1.23
	cdopt-cg	4.26e+02	426	9.95e-06	6.75e-14	19.89	4.26e+02	441	9.27e-06	4.66e-15	4.10
	cdopt-tr	4.26e+02	50	1.01e-06	4.72e-15	63.57	4.26e+02	50	9.86e-07	4.21e-15	9.02
	pymanopt-rcg	4.26e+02	592	7.29e-06	5.05e-15	23.34	4.26e+02	688	8.71e-06	5.42e-15	5.52
	pymanopt-rtr	4.26e+02	31	1.24e-10	6.41e-15	42.44	4.26e+02	31	1.24e-10	6.41e-15	14.63
$p = 50$	cdopt-lbfgs	2.34e+02	431	6.89e-06	6.06e-15	4.45	2.34e+02	457	9.52e-06	2.63e-15	2.15
	cdopt-cg	2.34e+02	964	9.95e-06	5.91e-15	54.29	2.34e+02	897	9.89e-06	4.10e-15	8.42
	cdopt-tr	2.34e+02	49	5.75e-06	5.58e-15	89.73	2.34e+02	61	6.11e-06	4.71e-15	15.69
	pymanopt-rcg	2.34e+02	1176	8.21e-06	5.58e-15	60.86	2.34e+02	1153	7.42e-06	5.82e-15	13.78
	pymanopt-rtr	2.34e+02	48	1.10e-06	5.19e-15	94.00	2.34e+02	48	9.77e-07	5.50e-15	37.29
$p = 100$	cdopt-lbfgs	1.48e+02	842	9.89e-06	2.52e-15	16.12	1.48e+02	844	8.79e-06	7.28e-15	9.35
	cdopt-cg	1.48e+02	2382	8.70e-06	4.10e-15	160.89	1.48e+02	1977	9.71e-06	3.10e-15	25.22
	cdopt-tr	1.48e+02	74	3.51e-08	4.69e-15	348.92	1.48e+02	73	8.55e-06	4.64e-15	45.60
	pymanopt-rcg	1.48e+02	3099	9.94e-06	5.83e-15	154.28	1.48e+02	2510	9.72e-06	5.56e-15	39.50
	pymanopt-rtr	1.48e+02	69	2.03e-07	5.54e-15	462.75	1.48e+02	70	2.06e-06	5.52e-15	342.79
$p = 200$	cdopt-lbfgs	1.30e+02	654	7.47e-06	5.71e-12	13.64	1.30e+02	621	8.57e-06	1.50e-11	10.78
	cdopt-cg	1.30e+02	1271	9.43e-06	8.03e-15	123.24	1.30e+02	1369	9.77e-06	1.22e-13	25.37
	cdopt-tr	1.30e+02	54	3.93e-06	5.49e-15	317.65	1.30e+02	53	6.24e-08	4.14e-15	80.65
	pymanopt-rcg	1.30e+02	1812	9.04e-06	4.75e-15	142.61	1.30e+02	1862	9.20e-06	4.51e-15	50.33
	pymanopt-rtr	1.30e+02	39	2.69e-08	5.07e-15	723.92	1.30e+02	41	2.82e-08	4.82e-15	497.99

Table 5: Nearest correlation matrix problem on the ER dataset.

		CPU					GPU				
		fval	iter	stat	feas	time	fval	iter	stat	feas	time
$p = 10$	cdopt-lbfgs	1.93e+03	218	9.89e-06	4.36e-15	0.87	1.93e+03	215	7.06e-06	3.23e-15	0.50
	cdopt-cg	1.93e+03	282	9.95e-06	5.20e-14	0.97	1.93e+03	268	5.98e-06	7.25e-15	0.93
	cdopt-tr	1.93e+03	42	7.63e-07	4.21e-15	2.59	1.93e+03	43	3.27e-07	3.58e-15	0.65
	pymanopt-rcg	1.93e+03	355	5.87e-06	4.57e-15	1.38	1.93e+03	311	7.59e-06	5.11e-15	0.61
	pymanopt-rtr	1.93e+03	36	1.11e-06	4.87e-15	2.34	1.93e+03	36	8.47e-07	5.23e-15	2.16
$p = 20$	cdopt-lbfgs	6.56e+02	263	9.48e-06	4.41e-15	1.05	6.56e+02	273	6.46e-06	3.50e-15	0.81
	cdopt-cg	6.56e+02	505	8.00e-06	3.89e-15	22.50	6.56e+02	518	9.10e-06	3.99e-14	3.40
	cdopt-tr	6.56e+02	64	1.18e-07	4.40e-15	39.30	6.56e+02	57	3.14e-06	3.21e-15	3.93
	pymanopt-rcg	6.56e+02	624	8.71e-06	5.18e-15	18.97	6.56e+02	673	8.69e-06	4.99e-15	4.98
	pymanopt-rtr	6.56e+02	39	1.26e-06	5.44e-15	33.07	6.56e+02	39	1.27e-06	5.37e-15	11.58
$p = 30$	cdopt-lbfgs	3.57e+02	324	8.52e-06	1.21e-13	1.94	3.57e+02	346	9.20e-06	2.55e-15	1.29
	cdopt-cg	3.57e+02	655	8.77e-06	5.84e-13	19.48	3.57e+02	551	7.45e-06	2.70e-15	4.50
	cdopt-tr	3.57e+02	61	7.79e-07	4.18e-15	58.39	3.57e+02	61	4.39e-08	3.54e-15	7.86
	pymanopt-rcg	3.57e+02	748	9.49e-06	5.09e-15	24.28	3.57e+02	630	9.29e-06	5.12e-15	4.91
	pymanopt-rtr	3.57e+02	41	4.42e-07	5.51e-15	43.80	3.57e+02	41	4.41e-07	5.63e-15	16.59
$p = 50$	cdopt-lbfgs	1.80e+02	395	9.67e-06	5.25e-15	4.48	1.80e+02	397	1.00e-05	2.29e-15	1.97
	cdopt-cg	1.80e+02	708	7.93e-06	8.26e-15	30.87	1.80e+02	686	7.06e-06	6.78e-15	6.83
	cdopt-tr	1.80e+02	49	3.82e-08	3.81e-15	58.41	1.80e+02	49	4.19e-08	3.83e-15	10.59
	pymanopt-rcg	1.80e+02	930	7.85e-06	5.39e-15	41.42	1.80e+02	911	9.05e-06	5.36e-15	10.58
	pymanopt-rtr	1.80e+02	43	6.63e-06	6.54e-15	43.10	1.80e+02	43	6.38e-06	6.32e-15	19.71
$p = 100$	cdopt-lbfgs	1.03e+02	780	9.65e-06	9.31e-13	8.37	1.03e+02	783	9.06e-06	1.93e-12	5.60
	cdopt-cg	1.03e+02	1528	8.91e-06	3.55e-14	93.18	1.03e+02	1697	8.69e-06	2.55e-15	18.14
	cdopt-tr	1.03e+02	91	5.79e-08	4.50e-15	366.87	1.03e+02	87	2.83e-06	3.89e-15	59.59
	pymanopt-rcg	1.03e+02	4274	9.67e-06	5.14e-15	201.31	1.03e+02	4303	9.97e-06	5.44e-15	59.23
	pymanopt-rtr	1.03e+02	64	2.68e-08	5.36e-15	462.41	1.03e+02	65	3.71e-07	5.18e-15	205.38
$p = 200$	cdopt-lbfgs	8.84e+01	469	9.85e-06	1.81e-14	9.83	8.84e+01	493	8.98e-06	1.88e-14	8.76
	cdopt-cg	8.84e+01	718	9.46e-06	9.23e-15	60.17	8.84e+01	846	7.81e-06	7.23e-15	14.96
	cdopt-tr	8.84e+01	50	9.08e-06	1.73e-14	168.31	8.84e+01	50	1.24e-06	3.69e-15	44.07
	pymanopt-rcg	8.84e+01	1345	9.79e-06	4.32e-15	84.23	8.84e+01	1475	9.86e-06	4.67e-15	37.50
	pymanopt-rtr	8.84e+01	38	6.44e-07	4.42e-15	509.31	8.84e+01	38	6.62e-07	4.42e-15	282.04

Table 6: Nearest correlation matrix problem on the Lymph dataset.



In all the numerical experiments of this subsection, we provide the expression of the function value, the gradient and the Hessian-vector product, and set the numerical backends for CDOpt and PyManopt as Numpy. We choose the L-BFGS, CG and trust-region solvers from SciPy to test the numerical performance of CDOpt. For comparison, we choose the Riemannian CG solver and Riemannian trust-region solver from PyManopt since L-BFGS is not available in PyManopt. All the hyperparameters of these solvers are fixed by the same settings in Section 7.1. Furthermore, following the techniques in [46], we first randomly generate a reference point  $\tilde{X} \in \mathcal{S}_{n,p}$ , and generate the initial point  $X_{init}$  as the eigenvectors that corresponds to the largest  $p$  eigenvalues of  $L + \alpha \cdot \text{Diag}(L^\dagger \rho(\tilde{X}))$ .

Table 7 presents the results of the numerical results on the comparison of CDOpt and PyManopt. From Table 7 we can observe that CDOpt achieves same function values and comparable iterations as PyManopt in all the numerical instances. Moreover, CDOpt shows comparable performance in the aspect of CPU time for large-scale problems, especially when  $p$  is large.

		$n = 1000$					$n = 3000$				
		fval	iter	stat	feas	time	fval	iter	stat	feas	time
$p = 10$	cdopt-lbfgs	3.57e+01	90	8.34e-06	1.73e-13	0.19	3.57e+01	107	8.53e-06	1.21e-13	2.24
	cdopt-cg	3.57e+01	95	8.26e-06	6.29e-13	0.13	3.57e+01	105	8.54e-06	4.03e-13	1.30
	cdopt-tr	3.57e+01	19	2.74e-06	1.81e-15	0.14	3.57e+01	18	8.34e-07	6.50e-16	1.93
	pymanopt-rcg	3.57e+01	81	9.28e-06	1.25e-15	0.18	3.57e+01	101	9.25e-06	1.18e-15	1.29
	pymanopt-rtr	3.57e+01	13	2.84e-06	1.11e-15	0.85	3.57e+01	8	8.37e-09	8.94e-16	10.50
$p = 20$	cdopt-lbfgs	2.11e+02	141	8.10e-06	3.27e-12	1.78	2.03e+02	168	5.54e-06	1.41e+00	9.90
	cdopt-cg	2.11e+02	145	6.70e-06	4.39e-13	1.27	2.11e+02	172	6.50e-06	6.03e-13	4.10
	cdopt-tr	2.11e+02	19	1.75e-07	1.27e-15	3.20	2.11e+02	16	3.97e-06	8.98e-15	4.11
	pymanopt-rcg	2.11e+02	143	9.40e-06	1.84e-15	1.61	2.11e+02	172	9.75e-06	1.08e-15	3.92
	pymanopt-rtr	2.11e+02	13	1.42e-06	1.61e-15	2.00	2.11e+02	11	6.80e-07	1.52e-15	17.27
$p = 30$	cdopt-lbfgs	6.48e+02	213	9.49e-06	9.35e-12	12.21	6.48e+02	221	9.01e-06	9.43e-14	12.12
	cdopt-cg	6.48e+02	255	8.45e-06	4.41e-12	6.94	6.48e+02	299	9.91e-06	4.56e-14	8.27
	cdopt-tr	6.48e+02	22	1.07e-06	1.58e-15	8.71	6.48e+02	26	2.70e-07	1.35e-15	16.72
	pymanopt-rcg	6.48e+02	378	1.30e-05	2.31e-15	10.96	6.48e+02	362	1.16e-05	1.77e-15	11.35
	pymanopt-rtr	6.48e+02	13	6.75e-07	2.27e-15	5.55	6.48e+02	9	3.77e-08	2.26e-15	26.53
$p = 50$	cdopt-lbfgs	2.81e+03	375	9.41e-06	1.27e-13	16.20	2.81e+03	396	8.83e-06	9.67e-14	45.26
	cdopt-cg	2.81e+03	543	9.32e-06	9.06e-15	11.74	2.81e+03	490	7.58e-06	3.02e-14	19.80
	cdopt-tr	2.81e+03	34	5.44e-07	1.39e-15	22.98	2.81e+03	33	3.89e-06	1.87e-15	31.61
	pymanopt-rcg	2.81e+03	617	1.04e-04	2.58e-15	22.63	2.81e+03	477	7.32e-05	2.93e-15	23.54
	pymanopt-rtr	2.81e+03	13	3.04e-06	2.77e-15	9.60	2.81e+03	10	2.96e-06	3.93e-15	31.37
$p = 100$	cdopt-lbfgs	2.16e+04	725	1.51e-05	1.66e-14	51.89	2.16e+04	712	1.67e-05	7.87e-15	162.50
	cdopt-cg	2.16e+04	997	1.64e-05	4.44e-14	37.33	2.16e+04	1020	1.31e-05	4.20e-15	96.03
	cdopt-tr	2.16e+04	46	1.32e-07	2.07e-15	71.53	2.16e+04	49	1.30e-07	2.40e-15	158.14
	pymanopt-rcg	2.16e+04	975	4.72e-04	4.12e-15	48.78	2.16e+04	966	3.26e-04	3.46e-15	117.73
	pymanopt-rtr	2.16e+04	16	2.22e-08	5.27e-15	62.38	2.16e+04	12	6.06e-10	5.48e-15	158.45

Table 7: Nonlinear eigenvalue problem.

### 7.3 Training orthogonally constrained neural network

In this subsection, we test the numerical performance of CDOpt on training orthogonally constrained deep neural networks (DNNs). Moreover, we compare the numerical performance of CDOpt with existing Riemannian optimization packages GeoTorch and McTorch. It is worth mentioning that although Geoopt is designed for training neural networks, it is not easy to be used in practice. When applied to training neural networks, Geoopt requires the users to write the layers themselves from PyTorch.nn modules, including designing the `__init__()` function that specifies the constrained manifold, the `forward()` function that involves geometrical materials, and the `reset_parameters()` function that reset the parameters to generate a feasible point for training. Therefore, we compare CDOpt only with GeoTorch and McTorch.

Our first test example is to train a modified LeNet [29] for classification on the EMNIST-bymerge dataset [11], which is a set of handwritten character digits derived from the NIST Special Database 19 and converted to a  $28 \times 28$  pixel image format and dataset structure that directly matches the MNIST dataset. The EMNIST-bymerge dataset has 697932 training samples and 116323 test samples in 47 classes. As illustrated in Figure 2(a), the network has 3 convolution layers and 3 fully-connected layers, and we impose the orthogonal constraints on the weight matrix of the first fully-connected layer. Moreover, we also choose to train VGG19 [39] for classification on the CIFAR-10 dataset [28]. CIFAR-10 dataset has 50000 training samples and 10000 test samples that are divided into 10 classes.

The VGG19 network contains 16 convolution layers and 3 fully-connected layers as illustrated in Figure 2(b). Furthermore, we train Densenet121 [23] for classification on the CIFAR-100 dataset [28], which has 100 classes in total, with 500 training images and 100 testing images in each class. Similar to LeNet, we impose the orthogonal constraints on the weight matrix of the first fully-connected layer of VGG19 and Densenet.

In training these orthogonally constrained neural networks by CDOpt, we choose the PyTorch build-in unconstrained optimizers SGD and Adam, together with the AdaMod, Lookahead and Ranger from the PyTorch-optimizer packages. Developed from the trivialization approaches, GeoTorch is also compatible to existing unconstrained optimizers, hence we try to apply SGD, Adam, AdaMod, Lookahead, and Ranger to train these orthogonally constrained networks through GeoTorch. However, among all the aforementioned solvers, only Riemannian SGD is provided in McTorch package. Therefore, we only use the Riemannian SGD from the McTorch package to train these networks.

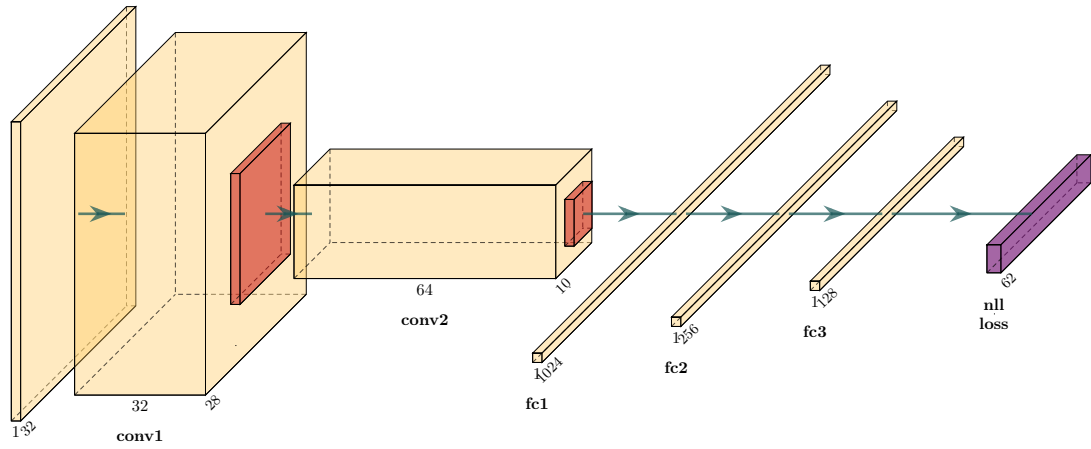
In training the modified LeNet, the batchsize is set as 64, the total number of epochs is set as 30, and the learning rate is set as 0.02 for SGD with momentum parameter as 0.9, 0.001 for Adam [26] and AdaMod [12], 0.3 for Ranger [45] and 0.01 for the base optimizer Yogi [50] in Lookahead [52] optimizer. For training VGG19 and Densenet121, the batchsize is fixed as 256, the total number of epochs is set as 300, while the learning rate is set as 0.01 for SGD (with momentum parameter as 0.9),  $3 \times 10^{-4}$  for Adam, AdaMod and DiffGrad, and 0.3 for Ranger and 0.01 for the base optimizer Yogi in Lookahead optimizer. Moreover, we choose the learning rate decrease strategy for all these optimizers and decrease the learning rate by multiply a factor after every epoch. Such factor is set as 0.9 in training LeNet, and 0.99 in training VGG. Furthermore, when applying CDOpt in training these networks, the penalty parameter  $\beta$  in the constraint dissolving approaches is fixed as 0.01 for all the test instances.

Table 8 exhibits the results of the numerical experiments. Compared with GeoTorch, CDOpt achieves similar accuracy and is compatible with various of unconstrained optimizers from PyTorch and PyTorch-optimizer. However, as computing the matrix exponential function and matrix inverse are expensive on GPU, GeoTorch takes significantly longer CPU time and costs more memory than CDOpt.

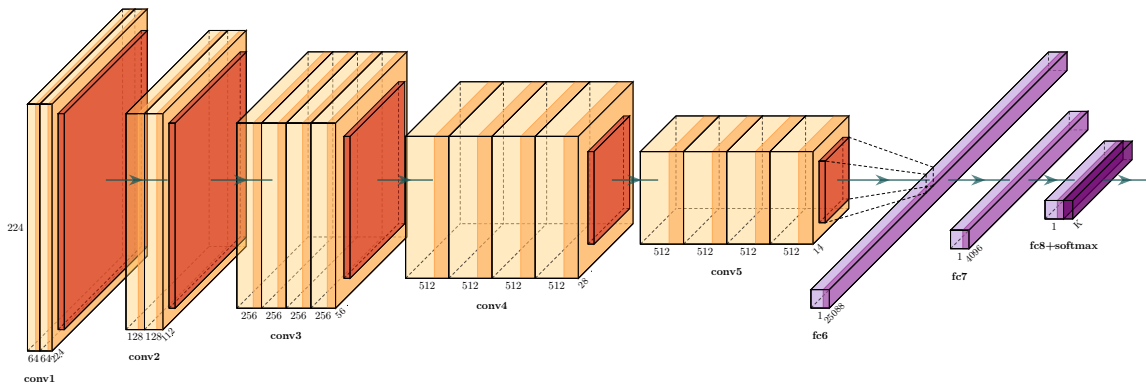
Furthermore, CDOpt achieves similar accuracy as McTorch. However, training manifold constrained neural networks by CDOpt only requires matrix-matrix multiplication, while the optimizers in McTorch involve computing the retractions in each iteration by singular value decomposition. Therefore, running unconstrained SGD by CDOpt is slightly faster than running the Riemannian SGD by McTorch. Moreover, in the presence of difficulties in developing efficient Riemannian solvers, existing PyTorch-based Riemannian solvers are limited. For example, McTorch only provides Riemannian SGD and Riemannian AdaGrad. In contrast, training manifold constrained neural networks by CDOpt is highly adaptive to various existing unconstrained solvers.

		LeNet + EMNIST-byclass			VGG 19 + CIFAR-10			Densenet121 + CIFAR-100		
		acc	feas	time/epoch	acc	feas	time/epoch	acc	feas	time/epoch
SGD	CDOpt	91.07	2.91e-03	68.77	92.81	4.56e-03	54.14	77.08	4.87e-03	52.46
	GeoTorch	91.04	4.25e-03	292.55		out of memory		77.05	4.22e-03	58.03
	McTorch	91.05	3.52e-03	89.41	92.70	5.15e-03	74.75	76.98	4.96e-03	53.31
Adam	CDOpt	91.02	5.39e-03	69.71	92.70	7.75e-03	57.89	76.72	1.85e-03	54.72
	GeoTorch	91.05	4.22e-03	294.83		out of memory		76.75	4.21e-03	60.21
	McTorch		not implemented			not implemented			not implemented	
AdaMod	CDOpt	91.06	3.81e-03	82.53	92.58	4.38e-03	58.78	76.66	1.19e-03	55.81
	GeoTorch	91.05	4.32e-03	319.62		out of memory		76.70	4.35e-03	59.23
	McTorch		not implemented			not implemented			not implemented	
Ranger	CDOpt	91.11	3.37e-03	76.16	92.76	6.29e-03	57.93	76.74	2.07e-03	54.00
	GeoTorch	90.96	4.25e-03	298.07		out of memory		76.79	4.28e-03	59.01
	McTorch		not implemented			not implemented			not implemented	
Lookahead	CDOpt	91.07	3.71e-03	83.15	92.97	4.69e-03	59.66	76.83	3.52e-03	55.75
	GeoTorch	91.01	4.25e-03	295.93		out of memory		76.81	4.20e-03	59.52
	McTorch		not implemented			not implemented			not implemented	

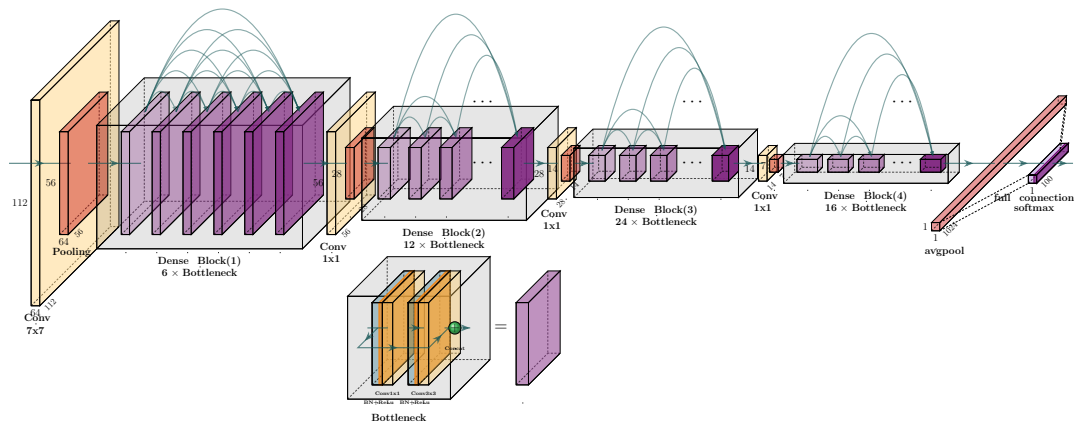
Table 8: Numerical results on orthogonally constrained deep neural networks.



(a) LeNet



(b) VGG19



(c) Densnet121

Figure 2: The structure of the tested neural networks.

## 8 Conclusion

In this paper, we consider how to practically implement constraint dissolving approaches to solve Riemannian optimization problem OCP. We first analyze the equivalence between OCP and CDF under RCRCQ conditions, which is weaker than the assumptions in [49]. Moreover we propose a practical scheme for setting the thresholding value for the penalty parameter  $\beta$  in CDF. We prove that with any penalty parameter  $\beta$  greater than the suggested thresholding value, CDF and OCP have same first-order stationary points, second-order stationary point and local minimums in a neighborhood of  $\mathcal{M}$ . Therefore, we can easily choose a penalty parameter  $\beta$  that guarantees the equivalence between OCP and CDF in practice.

Furthermore, we introduce the Python manifold optimization library package CDOpt, which enables the users to directly employ various existing unconstrained optimization solvers for manifold optimization through the constraint dissolving approaches. CDOpt has user-friendly interfaces and supports various important features from its supported numerical backends, such as the GPU/TPU supports, automatic differentiation, distributed training, JIT compilation, etc. Moreover, CDOpt only requires the expression of  $c(x)$  in defining a new manifold. Therefore, users can enjoy great convenience in defining and solving a wide range of manifold constrained optimization problems, without any knowledge of the geometrical materials in differential geometry. Furthermore, CDOpt provides various predefined neural layers for PyTorch and Flax, which enables the users to build and train the manifold constrained neural networks only with minor modification to the standard PyTorch/JAX codes. Extensive numerical experiments further demonstrate the high efficiency and superior performance of CDOpt when compared with existing Riemannian optimization packages.

CDOpt is still under active development, and some of the future work include adding supports for other numerical backends (e.g., TensorFlow, MindSpore, PaddlePaddle), and integrate CDOpt with more optimization frameworks, such as horovod and Apex for distributed training, FATE for federated learning, and BoTorch for Bayesian optimization.

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