Rieoptax: Riemannian Optimization in JAX

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Abstract

We present Rieoptax, an open source Python library for Riemannian optimization in JAX. We show that many differential geometric primitives, such as Riemannian exponential and logarithm maps, are usually faster in Rieoptax than existing frameworks in Python, both on CPU and GPU. We support various range of basic and advanced stochastic optimization solvers like Riemannian stochastic gradient, stochastic variance reduction, and adaptive gradient methods. A distinguishing feature of the proposed toolbox is that we also support differentially private optimization on Riemannian manifolds.

1. Introduction

Riemannian geometry is a generalization of the Euclidean geometry [49, 66] and includes several nonlinear spaces such as positive definite matrices [18, 92], Grassmann manifold [5, 15, 33], Stiefel manifold [5, 25, 33], kendall shape spaces [59, 60, 71], hyperbolic spaces [94, 95], and special Euclidean and orthogonal group [38, 87], to name a few. Optimization with manifold based constraints has become increasingly popular and has been employed in various applications such as low rank matrix completion [21], learning taxonomy embeddings [76, 77], neural networks [53–55, 75, 81], optimal transport [9, 26, 46, 73, 88], shape analysis [52, 90], and topological dimension reduction [56], among others. In addition, privacy preserving machine learning [29, 31] has become crucial in real applications, which has been generalized to manifold-valued problems very recently [44, 82, 96]. Nevertheless, such feature is absent in existing Riemannian optimization libraries.

In this work, we introduce Rieoptax (**Rie**mannian **Opt**imization in **Jax**), an open source Python library for Riemannian optimization in JAX [23, 37]. The proposed library is mainly driven by the needs of efficient implementation of manifold-valued operations and optimization solvers, readily compatible with GPU and even TPU processors as well as the needs of privacy-supported Riemannian optimization. To the best of our knowledge, Rieoptax is the first library to provide privacy guarantees within the Riemannian optimization framework.

1.1. Background on Riemannian optimization, privacy, and JAX

Riemannian Optimization. Riemannian Optimization [5, 20] considers the following problem

$$\min_{w \in \mathcal{M}} f(w) \tag{1}$$

where $f : \mathcal{M} \to \mathbb{R}$, and $\mathcal{M}$ denotes a Riemannian manifold. Instead of considering (1) as a constrained problem, Riemannian optimization [5, 20] views it as an unconstrained problem on the manifold space. Riemannian (stochastic) gradient descent [19, 98] generalizes the Euclidean

gradient descent with intrinsic updates on manifold, i.e., $w_{t+1} = \mathrm{Exp}_{w_t}(-\eta_t \operatorname{grad} f(w_t))$, where $\operatorname{grad} f(w_t)$ is the Riemannian (stochastic) gradient, $\mathrm{Exp}_w(\cdot)$ is the Riemannian exponential map at w and η_t is the step size. Recent years have witnessed significant advancements for Riemannian optimization where more advanced solvers are generalized from the Euclidean space to Riemannian manifolds. These include variance reduction methods [42, 43, 57, 85, 100, 101], adaptive gradient methods [14, 58], accelerated gradient methods [7, 8, 45, 68, 99], quasi-Newton methods [51, 80], zeroth-order methods [67] and second order methods, such as trust region methods [4] and cubic regularized Newton's methods [6].

Differential privacy on Riemannian Manifolds. Differential privacy (DP) provides a rigorous treatment for data privacy by precisely quantifying the deviation in the model's output distribution under modification of a small number of data points [29–32]. Provable guarantees of DP coupled with properties like immunity to arbitrary post-processing and graceful composability have made it a de-facto standard of privacy with steadfast adoption in the real applications [3, 10, 28, 34, 74].

Recently, there is a surge of interest on differential privacy over Riemannian manifolds, which has been explored in the context of Fréchet mean computation [82, 96] and, more generally, empirical risk minimization problems where the parameters are constrained to lie on a Riemannian manifold [44].

JAX and its ecosystem. JAX [23, 37] is recently introduced machine learning framework which support automatic differentiation capabilities [13] via `grad()`. Further some of the distinguishing features of JAX are just-in-time (JIT) compilation using the accelerated linear algebra (XLA) compiler [41] via `jit()`, automatic vectorization (batch-level parallelism) support with `vmap()`, and strong support for parallel computation via `pmap()`. All the above transformations can be composed arbitrarily because JAX follows the functional programming paradigm and implements these as pure functions.

Given that JAX has so many interesting features, its ecosystem has been constantly expanding in the last couple of years. Examples include neural network modules (Flax [48], Haiku [50], Equinox [62], Jraph [39], Equivariant-MLP [35]), reinforcement learning agents (Rlax [12]), Euclidean optimization algorithms (Optax [12]), federated learning (Fedjax [83]), optimal transport toolboxes (Ott [27]), sampling algorithms (Blackjax [64]), differential equation solvers (Diffrax [61]), rigid body simulators (Brax [36]), differentiable physics (Jax-md [86]).

1.2. Rieoptax

We believe the proposed framework for Riemannian optimization in JAX is a timely contribution, bringing several benefits of JAX and new features (such as privacy support) to the manifold optimization community, which are discussed below.

- *Automatic and efficient vectorization with* `vmap()`: functions that are written for inputs of size 1 can be converted to functions that take batch of inputs by wrapping it with `vmap()`. For example, the function `def dist(point_a, point_b)` for computing distance between a single `point_a` and a single `point_b` can be converted to function that computes distance between a batch of `point_a` and/or a batch `point_b` by wrapping `dist` with `vmap()` without modifying the `dist()` function. This is useful in many cases, e.g., Fréchet mean computation $\min_{w\in\mathcal{M}} \left\{\frac{1}{n}\sum_{i=1}^n f_i(w) := \frac{1}{n}\sum_{i=1}^n \mathrm{dist}^2(w, z_i)\right\}$. Furthermore, vectorization with `vmap()` is usually faster or on par with manual vectorization [23].

- *Per-example gradient clipping* : A key process in differentially private optimization is per-example gradient clipping $\frac{1}{n}\sum_{i=1}^{n}\text{clip}_\tau(\text{grad} f_i(w))$, where clip_τ ensures norm is atmost τ. Here, the order of operations is important: the gradients are first clipped and then averaged. Popular libraries including Autograd [69], Pytorch [78] and Tensorflow [1] are heavily optimized to directly compute the mean gradient $\frac{1}{n}\sum_{i=1}^{n}\text{grad} f_i(w)$ and hence do not expose per-example gradients i.e., $\text{grad} f_i(w)$. Hence, one has to resort to ad-hoc techniques [40, 65, 84] or come up with algorithmic modifications [24] which inherently have speed versus performance trade-off. JAX, however, offers native support for handling such scenarios and JAX-based differentially private Euclidean optimization methods have been shown to be much faster than their non-JAX counterparts [91]. We observe that JAX offer similar benefits for differentially private Riemannian optimization as well.

- *Single Source Multiple Devices (SSMD) Paradigm* : JAX follows SSMD paradigm, and hence code written for CPU can be run on GPU/TPU without any modification.

Rieoptax is made available at `https://anonymous.4open.science/r/Rieoptax/` for review and will be made public.

2. Implementation Overview

The package currently implements several commonly used geometries, optimization algorithms and differentially private mechanisms on manifolds. More geometries and advanced solvers will be added in the future.

2.1. Geometries

Geometry module contains manifolds equipped with Riemannian metrics. Each Geometry contains Riemannian inner product `inp()`, and induced norm `norm()`, Riemannian exponential `exp()` and logarithm maps `log()`, induced Riemannian distance `dist()`, parallel transport `pt()`, and transformation from Euclidean gradient to Riemannian gradient `egrad_to_rgrad()`.

Manifolds include symmetric positive definite (SPD) matrices $\text{SPD}(m) := \{\mathbf{X} \in \mathbb{R}^{m\times m} : \mathbf{X} = \mathbf{X}^\top, \mathbf{X} \succ 0\}$, hyperbolic space, Grassmann manifold $\mathcal{G}(m,r) := \{[\mathbf{X}] : \mathbf{X} \in \mathbb{R}^{m\times r}, \mathbf{X}^\top\mathbf{X} = \mathbf{I}\}$ where $[\mathbf{X}] := \{\mathbf{X}\mathbf{O} : O \in O(r)\}$, $O(r)$ denotes the orthogonal group and hypersphere $\mathcal{S}(d) := \{\mathbf{x} \in \mathbb{R}^d : \mathbf{x}^\top\mathbf{x} = 1\}$. We use $T_x\mathcal{M}$ to represent the tangent space at x and $\langle u, v\rangle_x$ to represent the Riemannian inner product. For more detailed treatment on these geometries, we refer to [5, 20, 95].

- `rieoptax.geometry.spd.SPDAffineInvariant` : SPD matrices with the affine-invariant metric [79]: $\text{SPD}(m)$ with $\langle \mathbf{U}, \mathbf{V}\rangle_{\mathbf{X}} = \text{tr}(\mathbf{X}^{-1}\mathbf{U}\mathbf{X}^{-1}\mathbf{V})$ for $\mathbf{U}, \mathbf{V} \in T_{\mathbf{X}}\text{SPD}(m)$.

- `rieoptax.geometry.spd.SPDLogEuclidean` : SPD matrices with the log-Euclidean metric [11]: $\text{SPD}(m)$ with $\langle \mathbf{U}, \mathbf{V}\rangle_{\mathbf{X}} = \text{tr}\big(\text{D}_{\mathbf{U}}\text{logm}(\mathbf{X})\text{D}_{\mathbf{V}}\text{logm}(\mathbf{X})\big)$ where $\text{D}_{\mathbf{U}}\text{logm}(\mathbf{X})$ is the directional derivative of matrix logarithm at $\mathbf{X}$ along $\mathbf{U}$.

- `rieoptax.geometry.hyperbolic.PoincareBall` : Poincare-ball model of Hyperbolic space with Poincare metric [95], i.e., $\mathbb{D}(d) := \{\mathbf{x} \in \mathbb{R}^d : \mathbf{x}^\top\mathbf{x} < 1\}$ with $\langle \mathbf{u}, \mathbf{v}\rangle_{\mathbf{x}} = 4\mathbf{u}^\top\mathbf{v}/(1-\mathbf{x}^\top\mathbf{x})^2$ for $\mathbf{u}, \mathbf{v} \in T_{\mathbf{x}}\mathbb{D}(d)$.

- `rieoptax.geometry.hyperbolic.LorentzHyperboloid` Lorentz Hyperboloid model of Hyperbolic space [95], i.e., $\mathbb{H}(d) = \{\mathbf{x} \in \mathbb{R}^d : \langle \mathbf{x}, \mathbf{x} \rangle_{\mathcal{L}} = -1\}$ with $\langle \mathbf{u}, \mathbf{v} \rangle_{\mathbf{x}} = \langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{L}}$ for $\mathbf{u}, \mathbf{v} \in T_{\mathbf{x}}\mathbb{H}(d)$, where $\langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{L}} := -u_0 v_0 + u_1 v_1 + \cdots u_{d-1} v_{d-1}$.
- `rieoptax.geometry.grassmann.GrassmannCanonicalMetric` : Grassmann manifold with the canonical metric [33], i.e., $\mathcal{G}(m, r)$ with $\langle \mathbf{U}, \mathbf{V} \rangle_{\mathbf{X}} = \mathrm{tr}\big(\mathbf{U}^T \mathbf{V}\big)$ for $\mathbf{U}, \mathbf{V} \in T_{\mathbf{X}}\mathcal{G}(m, r)$.
- `rieoptax.geometry.hypersphere.HypersphereCanonicalMetric` : Hypersphere manifold which canonical metric [5, 20], i.e., $\mathcal{S}(d)$ with $\langle \mathbf{u}, \mathbf{v} \rangle_{\mathbf{x}} = \mathbf{u}^\top \mathbf{v}$ for $\mathbf{u}, \mathbf{v} \in T_{\mathbf{x}}\mathcal{S}(d)$.

2.2. Optimizers

Optimizers module contains Riemannian optimization algorithms.

- `riepotax.optimizers.first_order.rsgd` : Riemannian stochastic gradient descent [19].
- `riepotax.optimizers.first_order.rsvrg` : Riemannian stochastic variance reduced gradient descent [100].
- `riepotax.optimizers.first_order.rsrg` : Riemannian stochastic recursive gradient descent [57].
- `riepotax.optimizers.first_order.rasa` : Riemannian adaptive stochastic gradient algorithm [58].
- `riepotax.optimizers.zeroth_order.zo_rgd` : Zeroth-order Riemannian gradient descent [67].

2.3. Mechanism

Mechanism module contains differential private mechanisms on Riemannian manifolds.

- `rieoptax.mechanism.output_perturbation.RieLaplaceMechanism` : Implements Riemannian Laplace mechanism [82] which is used for privatizing Fréchet mean computation.
- `rieoptax.mechanism.output_perturbation.LogEuclideanMechanism`: Implements log-Euclidean mechanism [96] which is used for differentially private Fréchet mean on SPD matrices with log-Euclidean metric.
- `rieoptax.mechanism.gradient_perturbation.DPRGDMechanism`: Implements noise calibration for Differentially private Riemannian gradient descent [44] based on moments accountant [2] in autodp library [97].
- `rieoptax.mechanism.gradient_perturbation.DPRSGDMechanism` : Implements noise calibration for Differentially private Riemannian stochastic gradient descent [44] based on moments accountant [2] in autodp library [97].

3. Benchmarking Rieoptax

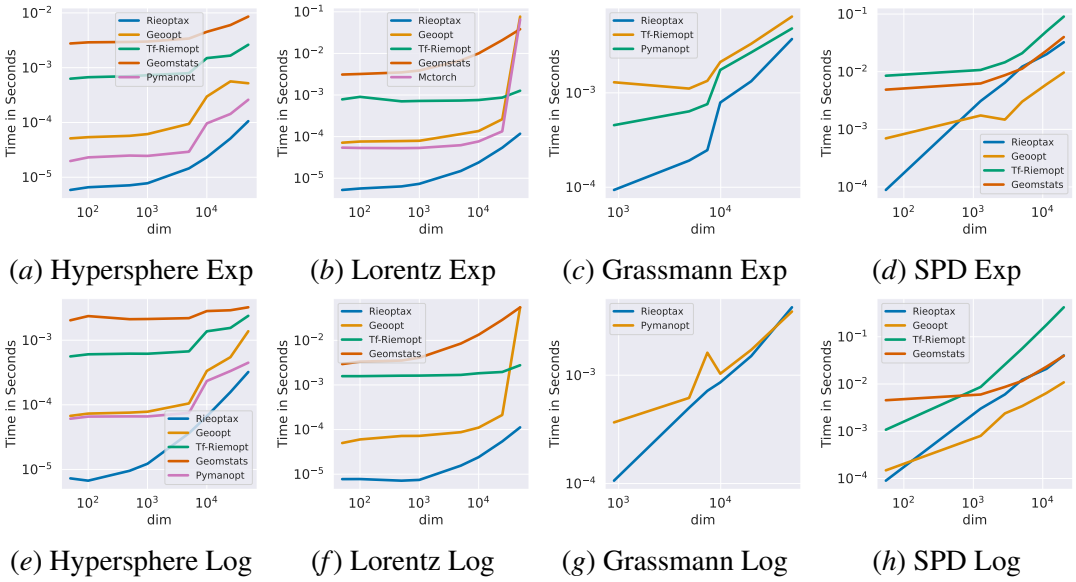
In this section, we benchmark the proposed Rieoptax against existing Riemannian optimization libraries in Python. These include Pytorch [78] based Mctorch [70] and Geoopt [63], Tensorflow [89] based Tensorflow-Riemopt (Tf-Riemopt) [89], Numpy [47] based Pymanopt [93], and Tensorflow based Geomstats [72]. While Geomstats supports Numpy, Pytorch, and Tensorflow as backend, currently only Tensorflow backend provides support for both CPU and GPU. Other non-Python based libraries include Manopt [22] in Matlab and Manopt.jl [16] in Julia [17]. We benchmark the Riemannian exponential (Exp) and logarithm (Log) maps with the proposed Rieoptax against the aforementioned Python libraries whenever available with `64bitfloat` precision. For CPU benchmarking we use Processor AMD EPYC 7B1 with 2 cores and 16GB RAM. For GPU benchmarking, we use CUDA version 11.4 on 16GB Tesla P100.

- **Hypersphere canonical metric:** Hypersphere $\mathcal{S}(d)$ is supported in Geoopt, Tf-Riemopt, Geomstats, and Pyamanopt. On GPU however, Geomstats raises an error. we benchmark for dimensions $d \in \{50, 100, 500, 1000, 5000, 10000, 25000, 50000\}$.
- **Loretnz hyperboloid model:** Loretnz hyperboloid model $\mathbb{H}(d)$ is supported in Geoopt, Tf-Riemopt, Geomstats, and Mctorch. While Riemannian exponential map is available in Mctorch, it does not implement the logarithm map. We benchmark for dimensions $d \in \{50, 100, 500, 1000, 5000, 10000, 25000, 50000\}$.
- **Grassmann with canonical metric** : Grassmann manifold $\mathcal{G}(m, r)$ with canonical metric is supported in Tf-Riemopt, Pymanopt, Geomstats. However, we notice that the logarithm map in Tf-Riemopt is incorrectly implemented and Geomstats represents Grassmann in projector matrix $\mathbf{X}\mathbf{X}^\top \in \mathbb{R}^{m\times m}$ instead of $\mathbf{X} \in \mathbb{R}^{m\times r}$, which is prohibitively expensive. We thus exclude these two libraries from benchmarking. We benchmark for matrix size $(m, r) \in \{(100, 10), (500, 10), (750, 10), (1000, 10), (2000, 10), (5000, 10)\}$.
- **SPD with affine invariant metric** : SPD manifold $\mathrm{SPD}(m)$ with affine invariant metric is supported in Geoopt, Tf-Riemopt, Geomstats. We benchmark for matrix size $m \in \{10, 50, 75, 100, 150, 200\}$.

Figures 1 and 2 present the timing results with CPU- and GPU-based computations, respectively. Overall, we observe that Rieoptax offers significant time improvement, especially on GPU. For SPDAffineInvariant Case, Rieoptax is slightly slower than Geoopt because `eigh` which provides eigen decomposition is slightly slower in JAX compared to Pytorch. Given that JAX is a relatively new framework, we believe it will be faster even in this case in the near future.

4. Conclusion and future roadmap

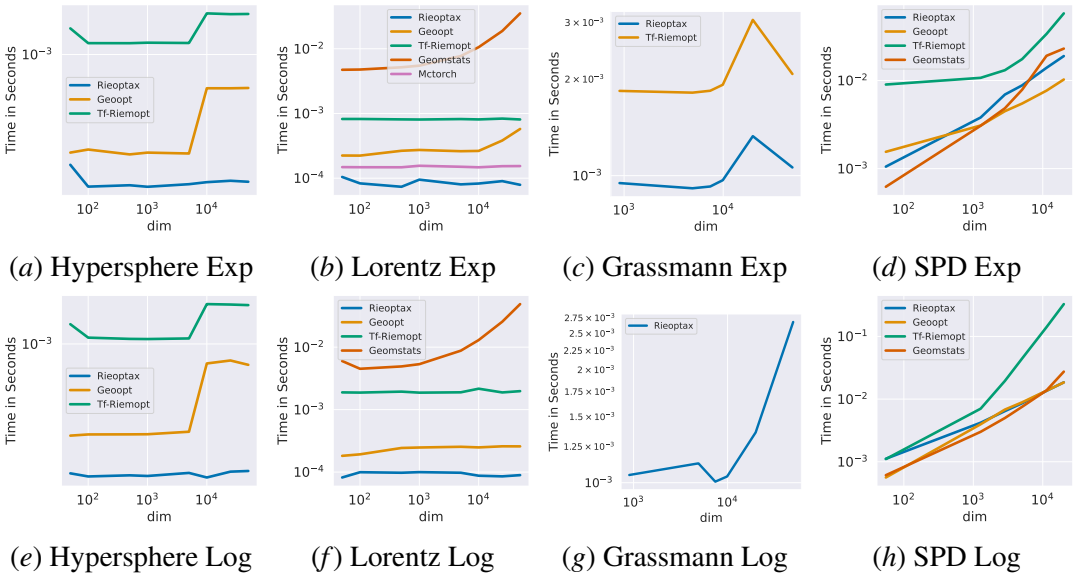
In this work, we present a Python library for (privacy-supported) Riemannian optimization, Rieoptax, and illustrate its efficacy on both CPU and GPU evaluation. Our roadmap includes adding support for more manifold geometries, optimization algorithms, and a collection of example codes showcasing the usage of Rieoptax in various applications.



(*a*) Hypersphere Exp (*b*) Lorentz Exp (*c*) Grassmann Exp (*d*) SPD Exp

(*e*) Hypersphere Log (*f*) Lorentz Log (*g*) Grassmann Log (*h*) SPD Log

Figure 1: Benchmarking of Geometric Primitives on CPU.



(*a*) Hypersphere Exp (*b*) Lorentz Exp (*c*) Grassmann Exp (*d*) SPD Exp

(*e*) Hypersphere Log (*f*) Lorentz Log (*g*) Grassmann Log (*h*) SPD Log

Figure 2: Benchmarking of Geometric Primitives on GPU.

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