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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 a 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 [57, 76] to general Riemannian manifolds. It includes several nonlinear spaces such as the set of positive definite matrices [20, 108], Grassmann manifold of subspaces [5, 17, 38], Stiefel manifold of orthogonal matrices [5, 29, 38], Kendall shape spaces [68, 69, 81], hyperbolic spaces [27, 110, 111], and special Euclidean and orthogonal group [44, 100, 104], 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 [23], learning taxonomy embeddings [87, 88], neural networks [45, 62–64, 86, 92], density estimation [51, 59], optimal transport [9, 31, 54, 84, 101], shape analysis [61, 106], and topological dimension reduction [65], among others.

In addition, privacy preserving machine learning [2, 30, 34–36, 83, 105] has become crucial in real applications, which has been generalized to manifold-constrained problems very recently [52, 94, 112]. Nevertheless, such a feature is absent in existing Riemannian optimization libraries [18, 24, 72, 80, 82, 103, 109].

In this work, we introduce Rieoptax (**Rie**mannian **Opt**imization in **Jax**), an open source Python library for Riemannian optimization in JAX [25, 42]. 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, 22, 43] 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, 22] views it as an unconstrained problem on the manifold space. Riemannian (stochastic) gradient descent [21, 114] 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 [49, 50, 66, 98, 116, 117], adaptive gradient methods [16, 67], accelerated gradient methods [7, 8, 53, 78, 115], quasi-Newton methods [60, 91], zeroth-order methods [77] 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 [34–37]. 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, 11, 33, 39, 85]. Further, it has been shown empirically that DP models resist various kinds of leakage attacks that can cause privacy violations [14, 28, 93, 97, 102, 118].

Recently, there is a surge of interest on differential privacy over Riemannian manifolds, which has been explored in the context of Fréchet mean computation [94, 112] and more generally for empirical risk minimization problems on Riemannian manifolds [52]. [52] proposed differentially private Riemannian (stochastic) gradient descent methods by perturbing the Riemannian gradient with noise from the tangent Gaussian distribution before taking step: $\zeta = \operatorname{grad} f(w) + \epsilon, \epsilon \sim \mathcal{N}_w(0, \sigma^2)$. More recently, [10] has proposed efficient sampling procedures from the tangent Gaussian distribution for large scale and stochastic optimization scenarios.

JAX and its ecosystem. JAX [25, 42] is recently introduced machine learning framework which support automatic differentiation capabilities [15] via `grad()`. Further some of the distinguishing features of JAX are just-in-time (JIT) compilation using the accelerated linear algebra (XLA) compiler [48] 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 many interesting features, its ecosystem has been constantly expanding in the last couple of years. Examples include neural network modules (Flax [56], Haiku [58], Equinox [71], Jraph [46], Equivariant-MLP [40]), reinforcement learning agents (Rlax [13]), Euclidean optimization algorithms (Optax [13]), federated learning (Fedjax [95]), optimal transport toolboxes (Ott [32]), sampling algorithms (Blackjax [73]), differential equation solvers (Diffrax [70]), rigid body simulators (Brax [41]), and differentiable physics (Jax-md [99]), among others.

1.2. Rieoptax

We believe that the proposed framework for Riemannian optimization in JAX is a timely contribution that brings several benefits of JAX and new features (such as privacy support) to the manifold optimization community 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 $\min_{w \in \mathcal{M}} \left\{ \frac{1}{n} \sum_{i=1}^{n} f_i(w) := \frac{1}{n} \sum_{i=1}^{n} \text{dist}^2(w, z_i) \right\}$. Furthermore, vectorization with `vmap()` is usually faster or on par with manual vectorization [25].
- **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 [79], Pytorch [89] 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 [47, 75, 96] or come up with algorithmic modifications [26] 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 [107]. We observe that JAX offer similar benefits for differentially private Riemannian optimization as well.
- **Single Source Multiple Devices (SSMD) paradigm.** JAX follows the SSMD paradigm, and therefore, the code written for CPUs can be run on GPU/TPUs without any additional modification.

Rieoptax is available at https://github.com/SaitejaUtpala/Rieoptax/.

2. Design and 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. Core

- `rieoptax.core.ManifoldArray`: lightweight wrapper of the `jax` device array with `manifold` attribute and used to model array constrained to manifold. It is registered as `Pytree` to ensure compatibility jax primitives like `grad()` and `vmap()`.
- `rieoptax.core.rgrad`: Riemannian gradient operator.

2.2. Geometries

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

Manifolds include symmetric positive definite (SPD) matrices $\mathrm{SPD}(m) := \{\mathbf{X} \in \mathbb{R}^{m\times m} : \mathbf{X} = \mathbf{X}^\top, \mathbf{X} \succ 0\}$, 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 $[\mathbf{X}] := \{\mathbf{XO} : O \in O(r)\}$, $O(r)$ 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, 22, 111].

- `rieoptax.geometry.spd.SPDAffineInvariant`: SPD matrices with the affine-invariant metric [90]: $\mathrm{SPD}(m)$ with $\langle \mathbf{U}, \mathbf{V}\rangle_{\mathbf{X}} = \mathrm{tr}(\mathbf{X}^{-1}\mathbf{U}\mathbf{X}^{-1}\mathbf{V})$ for $\mathbf{U}, \mathbf{V} \in T_{\mathbf{X}}\mathrm{SPD}(m)$.
- `rieoptax.geometry.spd.SPDLogEuclidean`: SPD matrices with the Log-Euclidean metric [12]: $\mathrm{SPD}(m)$ with $\langle \mathbf{U}, \mathbf{V}\rangle_{\mathbf{X}} = \mathrm{tr}\big(\mathrm{D}_{\mathbf{U}}\mathrm{logm}(\mathbf{X})\mathrm{D}_{\mathbf{V}}\mathrm{logm}(\mathbf{X})\big)$ where $\mathrm{D}_{\mathbf{U}}\mathrm{logm}(\mathbf{X})$ is the directional derivative of matrix logarithm at $\mathbf{X}$ along $\mathbf{U}$.
- `rieoptax.geometry.hyperbolic.PoincareBall`: the Poincare-ball model of Hyperbolic space with Poincare metric [111], 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`: the Lorentz Hyperboloid model of Hyperbolic space [111], 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 $\langle \mathbf{u}, \mathbf{v}\rangle_{\mathcal{L}} := -u_0v_0 + u_1v_1 + \cdots u_{d-1}v_{d-1}$.
- `rieoptax.geometry.grassmann.GrassmannCanonicalMetric`: the Grassmann manifold with the canonical metric [38], 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`: the hypersphere manifold which canonical metric [5, 22], i.e., $\mathcal{S}(d)$ with $\langle \mathbf{u}, \mathbf{v}\rangle_{\mathbf{x}} = \mathbf{u}^\top\mathbf{v}$ for $\mathbf{u}, \mathbf{v} \in T_{\mathbf{x}}\mathcal{S}(d)$.

2.3. Optimizers

Optimizers module contains Riemannian optimization algorithms. Design of optimizers follows Optax [13], which implements every optimizer by chaining of few common transformations. Where every optimizer

- `riepotax.optimizers.first_order.rsgd`: Riemannian stochastic gradient descent [21].
- `riepotax.optimizers.first_order.rsvrg`: Riemannian stochastic variance reduced gradient descent [116].
- `riepotax.optimizers.first_order.rsrg`: Riemannian stochastic recursive gradient descent [66].

- `riepotax.optimizers.first_order.rasa`: Riemannian adaptive stochastic gradient algorithm [67].
- `riepotax.optimizers.zeroth_order.zo_rgd`: zeroth-order Riemannian gradient descent [77].

2.4. Privacy mechanism

Mechanism module contains differential private mechanisms on Riemannian manifolds.

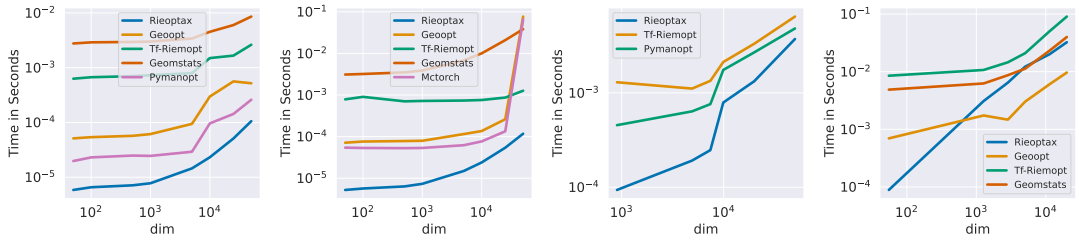
- `rieoptax.mechanism.output_perturbation.RieLaplaceMechanism`: the Riemannian Laplace mechanism [94] which is used for privatizing Fréchet mean computation.
- `rieoptax.mechanism.output_perturbation.LogEuclideanMechanism`: the Log-Euclidean mechanism [112] which is used for differentially private Fréchet mean on SPD matrices with log-Euclidean metric.
- `rieoptax.mechanism.gradient_perturbation.DPRGDMechanism`: noise calibration for differentially private Riemannian gradient descent [52] based on moments accountant [2] in the `autodp` library [113].
- `rieoptax.mechanism.gradient_perturbation.DPRSGDMechanism`: noise calibration for Differentially private Riemannian stochastic gradient descent [52] based on moments accountant [2] in `autodp` library [113].

3. Benchmarking Rieoptax

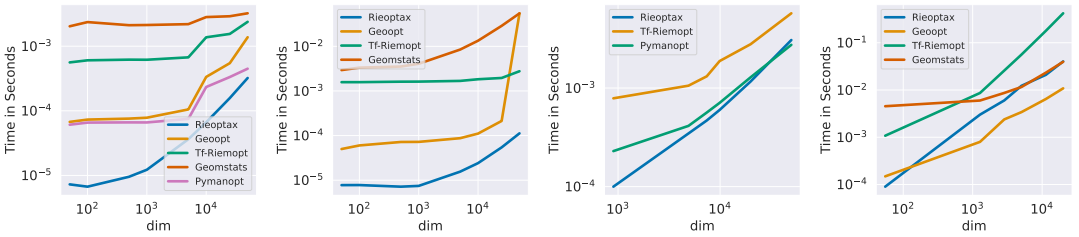
In this section, we benchmark the proposed Rieoptax against existing Riemannian optimization libraries in Python. These include Pytorch [89] based Mctorch [80] and Geoopt [72], Tensorflow [103] based Tensorflow-Riemopt (Tf-Riemopt) [103], Numpy [55] based Pymanopt [109], and Tensorflow based Geomstats [82]. While Geomstats supports Numpy, Pytorch, and Tensorflow as backend, currently only the Tensorflow backend provides support for GPUs. Other non-Python based libraries include Manopt [24] in Matlab and Manopt.jl [18] in Julia [19].

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 the AMD EPYC 7B1 processor with 2 cores and 16GB RAM. For GPU benchmarking, we use CUDA version 11.0 on 16GB Tesla P100.

- **Hypersphere:** hypersphere $\mathcal{S}(d)$ is supported in Geoopt, Tf-Riemopt, Geomstats, McTorch, and Pyamanopt. McTorch does not support the Exp and Log maps. On GPU, Geomstats raises an error. We benchmark all expect McTorch and Geomstats for dimensions $d \in \{50, 100, 500, 1\,000, 5\,000, 10\,000, 25\,000, 50\,000\}$.
- **Lorentz hyperboloid model:** the Lorentz hyperboloid model $\mathbb{H}(d)$ is supported in Geoopt, Tf-Riemopt, Geomstats, and Mctorch. While the Exp map is available in Mctorch, it does not implement the Log map. We benchmark for dimensions $d \in \{50, 100, 500, 1\,000, 5\,000, 10\,000, 25\,000, 50\,000\}$.

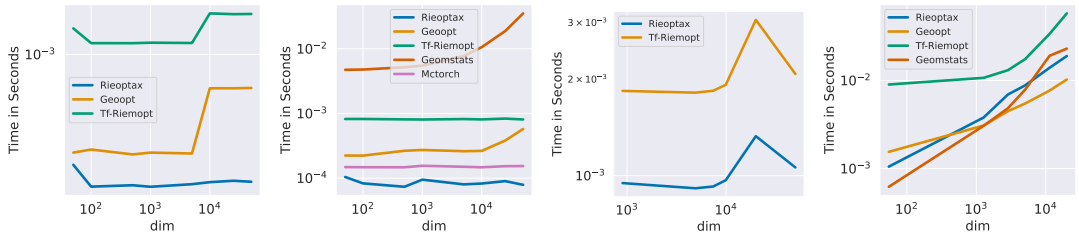


(*a*) Hypersphere Exp (*b*) Lorentz Exp (*c*) Grassmann Exp (*d*) SPD Exp

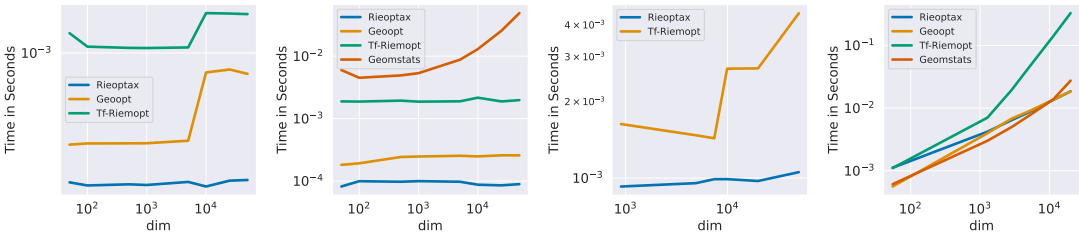


(*e*) Hypersphere Log (*f*) Lorentz Log (*g*) Grassmann Log (*h*) SPD Log

Figure 1: Benchmarking of geometric primitives on CPU.



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



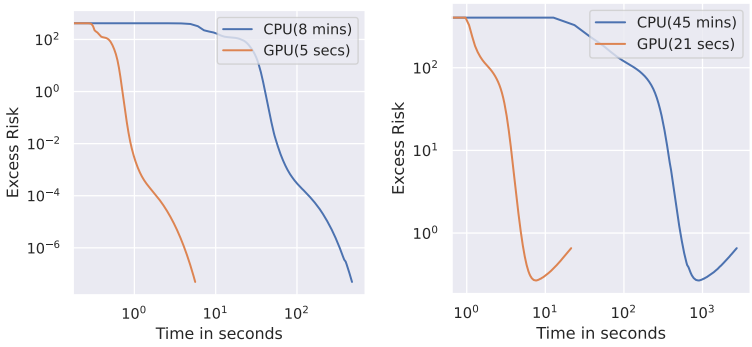
(*e*) Hypersphere Log (*f*) Lorentz Log (*g*) Grassmann Log (*h*) SPD Log

Figure 2: Benchmarking of geometric primitives on GPU.

- **Grassmann:** Grassmann manifold $\mathcal{G}(m, r)$ is supported in Tf-Riemopt, Pymanopt, McTorch, and Geomstats. McTorch does not support the Exp and Log maps. Geomstats represents Grassmann elements in projector matrices form $\mathbf{X}\mathbf{X}^\top \in \mathbb{R}^{m \times m}$ instead of $\mathbf{X} \in \mathbb{R}^{m \times r}$, which is prohibitively expensive. We, therefore, exclude these three libraries from benchmarking. We benchmark for matrix sizes $(m, r) \in \{(100, 10), (500, 10), (750, 10), (1\,000, 10), (2\,000, 10), (5\,000, 10)\}$.

- **SPD with affine-invariant metric:** SPD manifold $\mathrm{SPD}(m)$ with the affine-invariant metric is supported in Geoopt, Tf-Riemopt, Geomstats, and McTorch. McTorch, however, does not support the Exp and Log maps. We benchmark all except McTorch for matrix sizes $m \in \{10, 50, 75, 100, 150, 200\}$.

Figures 1 and 2 present the timing results with CPU- and GPU-based computations, respectively. Overall, we observe that Rieoptax offers significant time improvements, especially on GPUs. For the 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 would be faster even in this case in the near future.



(*a*) Non-private PCA. (*b*) $(0.1, 10^{-6})$-private PCA.

Figure 3: Timing of Rieoptax for PCA on the TinyImagetNet dataset as optimization on Grassmann manifold $\mathcal{G}(12\,288, 5)$ on both CPU and GPU. The GPU implementation achieves a significant speedup than CPU on both non-private and private PCA problems.

4. An example on PCA

In this section, we consider the problem of principal components analysis (PCA) by viewing it as an optimization problem on the Grassmann manifold [5, 22], i.e.,

$$\min_{\mathbf{U} \in \mathcal{G}(m,r)} \frac{1}{n} \sum_{i=1}^{n} \left\| \mathbf{z}_i - \mathbf{U}\mathbf{U}^T \mathbf{z}_i \right\|_2^2, \tag{2}$$

where $\mathbf{z}_i \in \mathbb{R}^n$ denote the data points. The Rieoptax implementation for solving the problem (2) is shown in Listing 3.

We provide timing of Rieoptax on TinyImageNet [74] which has a training set of 10^5 images in dimensions of $3 \times 64 \times 64$ on both CPU and GPU. We take $5\,000$ images and vectorize each image to produce a sample matrix of size $(n, d) = (5\,000, 12\,288)$. We compute the top $r = 5$ principal components, which leads to an optimization problem on $\mathcal{G}(12\,288, 5)$.

For non-private PCA, we run the full Riemannian gradient descent method for 400 epochs. For private PCA, we run the differentially private Riemannian gradient descent method [52] for 200 epochs with a privacy configuration of $\epsilon = 0.1, \delta = 10^{-6}$ and gradient clipping parameter of 0.1.

```python
from functools import partial
from jax import jit, vmap
from jax.numpy.linalg import norm
from rieoptax.core import rgrad, ManifoldArray
from rieoptax.geometry.grassmann import GrassmannCanonical
from rieoptax.optimizer.first_order import rsgd, dp_rsgd
from rieoptax.mechanism.gradient_perturbation import DP_RGD_Mechanism
from rieoptax.optimizer.update import apply_updates

def fit(params, data, optimizer, epochs, private=False):

    @jit
    def step(params, opt_state, data):
        def cost(params, data):
            def _cost(params, data):
                diff = data-params.value @ (params.value.T @ data)
                return norm(diff)**2
            return vmap(_cost, in_axes=(None,0))(params, data).mean()

        rgrad_fn = rgrad(cost)
        if private:
            data = data[:, None]
        #per-example gradient
        rgrad_fn = vmap(rgrad_fn, in_axes=(None, 0))
        #calculates Riemannian gradients
        rgrads = rgrad_fn(params, data)
        updates, opt_state = optimizer.update(rgrads, opt_state, params)
        #update using Riemannian Exp
        params = apply_updates(params, updates)
        return params, opt_state, loss_value

    opt_state = optimizer.init(params)
    for i in range(epochs):
        params, opt_state, loss_value = step(params, opt_state, data)

#initialization
U_init = ManifoldArray(value=init, manifold=GrassmannCanonical())
# non private PCA
lr, epochs = (3e-3, 400)
optimizer = rsgd(lr)
non_private_U = fit(U_init, Z, optimizer, epochs)
#(eps, delta) differentially private PCA
eps, delta, clip_norm, epochs = (1.0, 1e-6, 0.1, 200)
sigma = DP_RGD_Mechanism(eps, delta, clip_norm, n)
private_optimizer = dp_rsgd(lr, sigma, clip_norm)
private_U = fit(U_init, Z, optimizer, epochs, private=True)
```

Listing 1: The Rieoptax code for the private and non-private PCA problem. `dp_rsgd` and `rsgd` are the private and non-private optimizers, respectively.

For both the private and non-private algorithms, we choose the same initialization and a learning rate of 3×10^{-3}. Figures 3(a) and 3(b) show excess risk against runtime (in seconds) for non-private and private PCA, respectively.

5. 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 architectures. 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, especially with differential privacy.

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